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The emergence of time with interactions in quantum and classical mechanics

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Abstract

Physicists are nowadays able to produce and measure light pulses with durations on the inconceivably small scale of attoseconds. While this allows them to probe and explore the dynamics of the most fundamental processes of the physical world on ever shorter time scales, the explicit nature of time itself still remains a mystery even today. This unresolved issue divides the scientific community into two distinct camps. Those in the first camp view time as a fundamental entity of nature, while those in the second camp view it as an effective or emergent quantity derived from more elementary principles. Proponents of the latter view advocate for a static global state as the fundamental entity, in which the whole encompasses a principal "system" and a "clock" as separate subsystems. In this context, the central notion is that of a state of the principal system being conditioned on the physical state of the clock. As a result, time or, more concretely, dynamics emerges from the inherent correlations between both subsystems contained in the global state. Two prominent quantum mechanical approaches for this "timeless" theory have been developed during the last decades. The first relies on a semiclassical treatment in the form of Born-Oppenheimer and Wentzel-Kramers-Brillouin approximations, but allows one to include interactions between system and clock. A second treatment, devised by Page and Wootters, works in abstract Hilbert space instead. Unfortunately, it is as of yet unable to generally deal with interactions and often relies on Hamiltonians of a special form.

The main objective of this thesis is to close the gap between both approaches through construction of an overarching framework in full generality, without relying on specific choices for the underlying subsystems or the Hamiltonians involved. To this end, we single out three central principles on which the previous approaches build, namely a global energy constraint, the existence of subsystems and a definition of the conditional state of the principal system. Based on them, we derive unitary system dynamics and the time-dependent Schrödinger equation with an exact memoryless effective potential from a timeless quantum mechanical formulation, namely the time-independent Schrödinger equation. We find that the traditionally presupposed time is replaced by a scalar path variable parametrizing a global state invariance generated by the energy constraint. Yet, this derivation deals exclusively with pure states and, to widen its scope, we extend the timeless approach to quantum mechanical mixed states and classical probability densities as well. A key concept is the minimization of a unitarity-violating term in the evolution equations, appearing in the presence of an interaction term between system and clock. Useful approximations and analytical and numerical examples complement our results and corroborate our derivations. As a further demonstration of the versatility of our approach, we explain how a long-suspected connection between imaginary-time formulations and inverse temperature in canonical ensembles could be traced to a common physical origin. Finally, we discuss the consequences of our newly developed framework, especially similarities to conventional open systems theory, and conclude with an outlook for future investigations.

Kurzfassung

Heutzutage sind Physiker in der Lage, Lichtimpulse mit einer unvorstellbar kurzen Dauer im Attosekundenbereich zu erzeugen und zu messen. Dies ermöglicht es ihnen, die Dynamik der grundlegendsten Prozesse der physikalischen Welt auf immer kürzeren Zeitskalen zu untersuchen und zu erforschen. Jedoch bleibt die genaue Natur der Zeit selbst bis heute ein Rätsel. Diese ungelöste Frage spaltet die wissenschaftliche Gemeinschaft in zwei unterschiedliche Lager. Die Vertreter des ersten Lagers betrachten Zeit als eine grundlegende Einheit der Natur, während die Vertreter des zweiten Lagers sie als eine effektive oder emergente Größe betrachten, die sich aus elementareren Prinzipien ableiten lässt. Letztere plädieren für einen statischen Gesamtzustand als grundlegende Einheit, wobei das Gesamtsystem ein Primär-„System“ und eine „Uhr“ als getrennte Teilsysteme umfasst. In diesem Zusammenhang ist der zentrale Gedanke ein Zustand des Primärsystems, welcher durch den physikalischen Zustand der Uhr bedingt ist. Infolgedessen ergibt sich Zeit oder, konkreter gesagt, Dynamik aus den inhärenten Korrelationen zwischen den beiden im Gesamtzustand enthaltenen Teilsystemen. In den letzten Jahrzehnten wurden zwei prominente quantenmechanische Ansätze für diese „zeitlose“ Theorie entwickelt. Der erste stützt sich auf eine semiklassische Behandlung in Form von Born-Oppenheimer- und Wentzel-Kramers-Brillouin-Näherungen, erlaubt aber die Einbeziehung von Wechselwirkungen zwischen System und Uhr. Eine zweite Herangehensweise, die von Page und Wootters entwickelt wurde, arbeitet hingegen im abstrakten Hilbertraum. Sie ist jedoch noch nicht in der Lage Wechselwirkungen allgemein zu berücksichtigen und stützt sich häufig auf Hamiltonoperatoren spezieller Form.

Das Hauptziel dieser Arbeit ist es, die Lücke zwischen beiden Herangehensweisen zu schließen, indem ein übergreifender Ansatz in voller Allgemeinheit konstruiert wird, ohne dabei bestimmte Festlegungen für die zugrunde liegenden Teilsysteme oder Hamiltonoperatoren treffen zu müssen. Zu diesem Zweck heben wir drei zentrale Prinzipien hervor, auf denen bisherige Ansätze basieren: eine globale Energiebeschränkung, die Existenz von Teilsystemen und eine Definition des bedingten Zustands des primären Systems. Darauf aufbauend leiten wir die unitäre Systemdynamik und die zeitabhängige Schrödingergleichung mit einem exakten, effektiven Potential ohne Gedächtnis aus einer zeitlosen quantenmechanischen Formulierung, der zeitunabhängigen Schrödingergleichung, her. Wir stellen fest, dass die traditionell vorausgesetzte Zeit durch eine skalare Pfadvariable ersetzt wird, welche eine durch die Energiebeschränkung erzeugte globale Zustandsinvarianz parametrisiert. Diese Herleitung befasst sich jedoch ausschließlich mit reinen Zuständen. Um ihren Anwendungsbereich zu erweitern, dehnen wir den zeitlosen Ansatz auch auf quantenmechanische, gemischte Zustände und klassische Wahrscheinlichkeitsdichten aus. Ein Schlüsselkonzept ist dabei die Minimierung eines die Unitarität verletzenden Terms in den Evolutionsgleichungen, der bei Vorhandensein eines Wechselwirkungsterms zwischen System und Uhr auftritt. Nützliche Näherungen sowie analytische und numerische Beispiele ergänzen unsere Ergebnisse und bestätigen unsere Herleitungen. Als weitere Demonstration der Vielseitigkeit unseres Ansatzes zeigen wir, wie eine lange vermutete Verbindung zwischen Imaginärzeitformulierungen und inverser Temperatur in kanonischen Ensembles auf einen gemeinsamen physikalischen Ursprung zurückgeführt werden kann. Abschließend diskutieren wir die Konsequenzen unseres neu entwickelten Ansatzes, insbesondere die Ähnlichkeiten zur konventionellen Theorie offener Systeme, und geben einen Ausblick auf zukünftige Untersuchungen.

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Chapter 1

Introduction

A clock provides time.

This is undisputed even in the non-scientific community and may in fact seem trivial due to our everyday experience. But what exactly is meant by such a statement? Implicitly, we almost always assume having a universally shared understanding of what constitutes a timepiece or clock, the grammatical subject of said phrase. But in fact, the actual meaning can be much more complex.

The deliberate act of keeping time is probably as old as humanity itself [1] and has played a critical role in technological advances throughout human history [2]. One of the oldest pieces of evidence for man-made structures with calendrical function dates back approximately 10,000 years [3] and represents just one of many historical records demonstrating the need and the ability of human civilization to track the passage of time. Other examples include the famous Stonehenge monument [1, 4], the Nebra Sky Disc [5], the Mayan calendar [1, 6], ancient Egyptian sundials [7], early depictions of hourglasses in the fourteenth century [8], the fifteenth-century Prague astronomical clock [9] and the first marine chronometer by Harrison from the eighteenth century [10, 11], to name but a few. Central to many early timekeeping devices is the reliance on the motion of the Sun across the sky, indicating durations of either days or years due to the Earth's rotation and its orbit around the Sun, respectively. The Sun's influence is even more far-reaching considering the fact that biological life can have a built-in circadian clock [12], which has synchronized with an external stimulus (day-night cycle) through evolutionary development. However, scientific breakthroughs in the twentieth century enabled technological advancements, which have ultimately led to the birth of atomic clocks. Their exceedingly high relative accuracies (Fig. 1.1) finally resulted in the departure from celestial-based clocks as primary sources for standard time durations. This progress in precision manifested itself in the adoption of a new standard definition for the second in 1967, based on the transition between hyperfine-split caesium groundstate levels [10]. Contemporary atomic clocks allow precise timekeeping with fractional uncertainties on the order of 10^{-18} [13–18], which, for comparison, is roughly the equivalent of a deviation of one second or less over the time span of the currently observed age of the universe ($\approx 4.35 \times 10^{17}$ s [19]). Not only does modern quantum physics allow a stable tracking of time over longer and longer durations, but it also facilitates experimental techniques to explore fundamental physical processes at the other extreme end of the scale, namely for extraordinarily short time spans (Fig. 1.1). Nowadays, researchers are capable of producing ultrashort light pulses on the scale of attoseconds (10^{-18} s), providing means to probe electronic motion on an atomic scale [20]. Accordingly, such short pulses also require sophisticated timing mechanisms not only for the determination of their duration [21], but also for the measurement of ultrashort processes [22–30]. In general, the working concept of all these clocks is a combination of

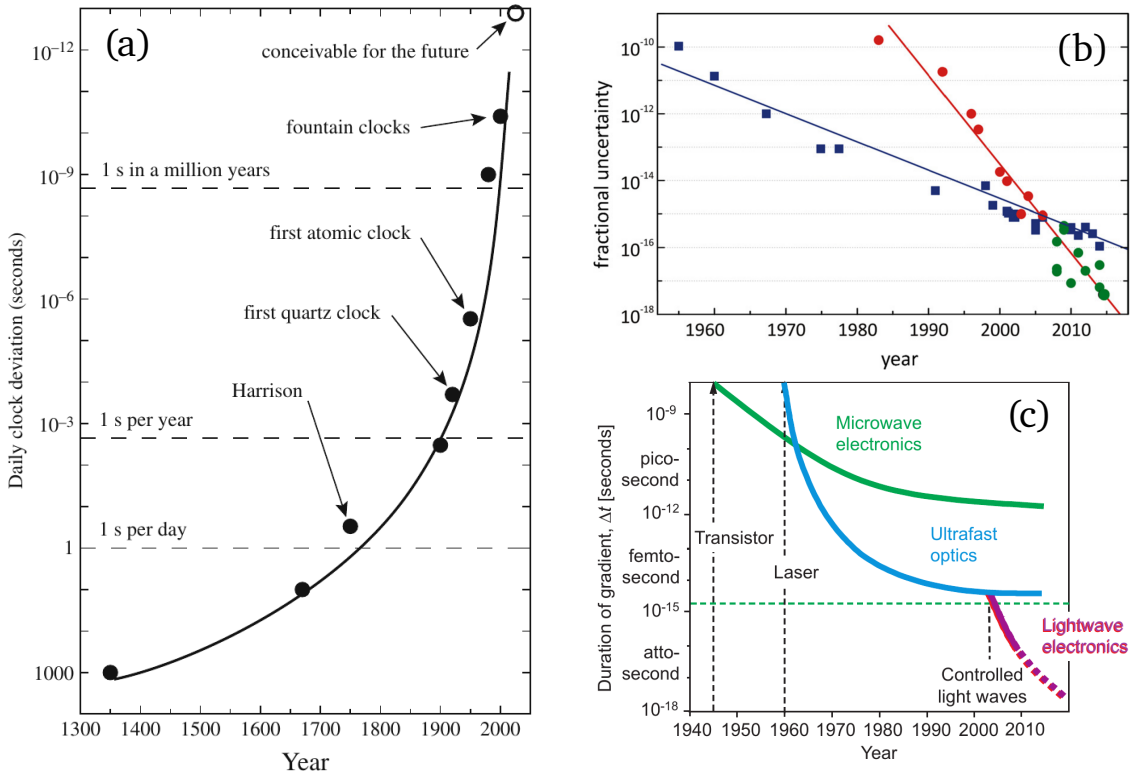

Figure 1.1 – (a) The historical development of timekeeping devices has seen rapid improvements in terms of clock accuracy over the last centuries. (b) Since their inception, atomic clocks have been progressively refined and, as a result, their fractional uncertainties have been reduced exponentially over the last decades. (c) The typical transient time scales for electromagnetic pulses nowadays achievable in ultrafast science have been pushed toward the attosecond regime and are currently at the doorstep of the zeptosecond domain [31, 32]. Reprinted from Refs. [20, 33, 34].

a frequency standard and a counting apparatus [1, 33, 35]. Yet, one easily overlooked, but non-trivial aspect must be mentioned as well, namely the measurement of timekeeping instruments by an observer. What underlies the process of obtaining information about the clock state is the extended interaction over some period of time, due to a generic coupling between clock and observer. The outcome is a correlation among clock and clock-watcher, such that the state of the clock is associated with the state of an observer that has information about the clock state. A continuous buildup of this association can only take place under the premise of temporal evolution and, hence, reveals the fact that *time* must be a presupposed notion in any of these settings. An appropriate portrayal of the situation is described in Ref. [36] as "the passage of time is estimated via the evolution of a reference system—a clock". As a major consequence, these clocks do not constitute a temporal source in the sense of *providing* time as a secondary derived notion, which opposes the meaning of the verb in our opening statement. Although the working principles of such timekeeping devices have been examined from a very fundamental point of view in the literature [36–40], we are instead more concerned with the origin of time itself in this thesis. The necessity to draw this distinction also arises in Ref. [37], in which Erker et al. separate their work on autonomous quantum clocks from ones that rather seek to explore the emergence of time. Due to the operational character, the timekeeping devices mentioned above only *register* time and we accordingly label them "operational clocks". This classification is essential in order to distinguish them from clocks of a complementary class, one which we call "fundamental clocks". Their defining property is a functional existence independent of a concept of time or, in other words, they are a primitive notion

logically prior to time. Such a differentiation is usually not made in the literature, but may help to avoid any confusion about the collective use of the word "clock". The difference between both classes is illustrated by the relations

$$\begin{aligned} \text{time} &\Rightarrow \text{operational clock}, \\ \text{fundamental clock} &\Rightarrow \text{time}. \end{aligned}$$

Certainly, a more precise nomenclature would be useful, but the ambiguous name "clock" has already been established in the field of time emergence as well. Clocks of the second type are the main subject of this thesis and, therefore, we omit the adjective "fundamental" and simply refer to them as "clocks" for the remainder of this thesis. At any rate, clocks and time are always intertwined and it is mandatory to closer examine the concept of time, the grammatical object of our introductory sentence.

The history of time in science is long and convoluted, making it difficult to give a fully comprehensive review and we certainly do not attempt to do so. Yet, several great resources, such as Refs. [41–45], have been published to provide extensive overviews and discussions on the subject. According to historical records, the earliest accounts of time in a mainly non-religious context were given by Greek scholars [44] more than two thousand years ago, by the likes of Plato, Democritus and Aristotle. Subsequently, the view on time took a winding path across multiple cultures in the following centuries [41, 46] and despite some religious influences, which are alien to today's scientists, some ideas have influenced modern thinking about time [45]. A major historical milestone, for science in general, has been the publication of Newton's "Principia" in 1687 [47], in which he famously proclaimed that "absolute, true and mathematical time, of itself, and from its own nature, flows equably without relation to anything external" [41]. This concept of an "absolute time" being an immaterial property of nature [45], which was inspired by Newton's predecessor Barrow [41, 44], has been criticized not only by his contemporary Leibniz, but also by many following scholars [48]. Leibniz's own views, exhibited in the famous Leibniz-Clarke correspondence [45], are nowadays taken as the beginning of "relationism" [45], a doctrine embracing the notion of spatiotemporal relations among physical objects as basic elements and, thus, replacing the concept of absolute space and time [48, 49]. As a characteristic implication follows that "all motion is relative motion" [48], a principle that continues to be relevant in physics to this day. Even the prominent relationist Mach influenced one of the biggest theoretical breakthroughs in physics in the twentieth century [50]. Inspired by him, Einstein discovered general relativity in 1915 [51], in which the classical notions of space and time are inseparably fused to four-dimensional "space-time". Not only did entirely new conceptual questions about time arise with this new theory about gravitation [52], but the very foundation of classical mechanics was challenged by a simultaneously appearing theoretical framework, rivaling most hitherto known physical conceptions.

The advent of quantum mechanics in the early twentieth century has severely changed the landscape of physics and with it came a new scrutiny of the notions of space and time [53–57]. Canonical quantization rules prescribe the promotion of position and momentum variables q and p to operator status, i.e., $\hat{q}$ and $\hat{p}$, respectively. One must be cautious however, as the change from scalars to operators is only applied to position and momentum of point particles and *not* to the static background coordinates [58]. This can cause confusion, because not space itself is quantized, but position, which might have been the origin of a decades-long uncertainty about whether time should be quantized or not [56, 59]. The quantum mechanical operator formalism also gave rise to the now well-known commutation relation $[\hat{q}, \hat{p}] = i\hbar$, indicating the fundamental non-commutativity of position and momentum. On the right-hand side of this relation appears the emblematic

representative of quantum mechanics, Planck's reduced constant $\hbar$ with the dimension of an action. As a consequence, the physical ability to measure position and momentum at the same time is limited by nature and this feature is mathematically expressed by the famous Heisenberg uncertainty $\Delta q \cdot \Delta p \geq \hbar/2$. Right from the beginning of quantum mechanics [56], physicists have been seeking after formally equivalent statements for time, in particular, a genuine operator $\hat{t}$ for time and a corresponding uncertainty relation [60–73], induced by a fundamental commutation relation similar to position and momentum. Yet, time appears only as an external real-valued parameter in the arguments of a Schrödinger wavefunction or Heisenberg operator. Dimensional analysis of action and time implies an energy dimension for the operator being conjugate to a time operator. Since the Hamilton function H obtains an operator status with $\hat{H}$ as well in the transition from classical to quantum mechanics, the relation of interest becomes $[\hat{t}, \hat{H}] = i\hbar$. In hindsight, the goal of finding a time operator seems ill-posed, given that in classical mechanics normally a notion of a time trajectory does not exists. As argued by Hilgevoord, there are only *time-indicating* variables [74], which can be used to track change in time. In contrast, time-energy uncertainties do exist, but they are not rooted in the existence of a fundamental commutation relation with the Hamiltonian. Nonetheless, the apparent contradictions between space and time have sparked a plethora of works about the nature of time. Already Schrödinger noticed the indispensability of clocks to deal with time in quantum theory [54] and performed a preliminary analysis of states of a physical clock. A concise historical review of early day quantum mechanical treatments of time can be found in Ref. [56]. Inspired by the idea that a change in time is associated with the motion of a physical degree of freedom, researchers have attempted to raise the status of coordinate time to that of a physical degree of freedom.

One of the simplest approaches to promote t to a time-indicating physical quantity can be given for a classical non-relativistic particle [75] with the classical action integral

$$S = \int_{t_1}^{t_2} \mathrm{d}t \left[\frac{m}{2} \left(\frac{\mathrm{d}q}{\mathrm{d}t} \right)^2 - V(q,t) \right] = \int_{t_1}^{t_2} \mathrm{d}t \, L\left(q, \frac{\mathrm{d}q}{\mathrm{d}t}, t \right) \tag{1.1}$$

and the non-relativistic Lagrange function $L(q, \mathrm{d}q/\mathrm{d}t\,, t)$. As is standard in classical mechanics, the Legendre transformation

$$H(q,p,t) \equiv p \frac{\mathrm{d}q}{\mathrm{d}t} - L = \frac{p^2}{2m} + V(q,t) \tag{1.2}$$

with momentum $p \equiv \partial L / \partial(\,\mathrm{d}q/\mathrm{d}\lambda\,)$ yields the Hamilton function H in phase space coordinates (q,p). Now, we promote t to a new physical degree of freedom, similar to a position, and introduce a new fictitious time parameter λ, such that the two position degrees of freedom are $q(\lambda)$ and $t(\lambda)$. Then the new action $\tilde{S}$ for the extended system reads

$$\tilde{S} = \int_{\lambda_1}^{\lambda_2} \mathrm{d}\lambda \, \frac{\mathrm{d}t}{\mathrm{d}\lambda} \left[\frac{m}{2} \left(\frac{\mathrm{d}q/\mathrm{d}\lambda}{\mathrm{d}t/\mathrm{d}\lambda} \right)^2 - V(q,t) \right] \equiv \int_{\lambda_1}^{\lambda_2} \mathrm{d}\lambda \, \tilde{L}\left(q, t, \frac{\mathrm{d}q}{\mathrm{d}\lambda}, \frac{\mathrm{d}t}{\mathrm{d}\lambda} \right) \tag{1.3}$$

with the extended Lagrange function $\tilde{L}(q, t, \mathrm{d}q/\mathrm{d}\lambda\,, \mathrm{d}t/\mathrm{d}\lambda\,)$. Consequently, the interaction $V(q,t)$ can now be seen as a coupling between two physical degrees of freedom instead of a time-dependent potential acting only on one degree of freedom. The new extended Lagrange function $\tilde{L}$ has an important property that distinguishes it from the original Lagrange function L, namely its homogeneity in velocity. Any Lagrange function $\tilde{L}$ with this property leads to a vanishing Hamilton function $\tilde{H} = 0$ of the extended system. In addition, the homogeneity implies a form-invariance of $\tilde{L}$ under the reparametrization $s(\lambda)$ with $\mathrm{d}s/\mathrm{d}\lambda > 0$, which is why such systems are called "time-reparametrization invariant".

In this context, “time” refers to the parameter time λ used in the action integral $\tilde{S}$. For the non-relativistic Hamilton function used here, the momentum P_t associated with t gives the constraint

$$C \equiv P_t + \frac{1}{2m}p^2 + V(q,t) = P_t + H = 0\,. \tag{1.4}$$

and the extended Hamilton function reads

$$\tilde{H} = \frac{\mathrm{d}t}{\mathrm{d}\lambda}C = 0\,. \tag{1.5}$$

The constraint C has been used as a starting point for quantization [76, 77]. Already Dirac [78] noted that the function $\mathrm{d}t/\mathrm{d}\lambda$ is arbitrary as long as it is strictly positive and no absolute time exists in such systems. For this reason, $q(\lambda)$ and $t(\lambda)$ have no physical meaning [77]. Choosing a specific (monotonically increasing) parametrization $t(\lambda)$ and "deparametrizing" to $q(t)$ provide the physically relevant relations. In other words, only the relation between two physical degrees of freedom are of physical significance. The known equation of motions for the original system can easily be recovered from $\mathrm{d}q/\mathrm{d}t = (\mathrm{d}q/\mathrm{d}\lambda)/(\mathrm{d}t/\mathrm{d}\lambda) = (\partial\tilde{H}/\partial p)/(\mathrm{d}t/\mathrm{d}\lambda) = p/m$ for example.

Despite the simplistic nature of this example, it suffices to reveal the most important characteristics of the timeless approach in physics. Starting from the global perspective, we find that the state of all physical degrees of freedom must be energy constraint. This is the only requirement of a global character and any further conditions necessitate the pivotal notion of a division of the whole into smaller parts. Although it may seem trivial, due to the ubiquitous usage of subsystems in physics, the existence of at least one partitioning into two separate entities is crucial for the emergence of time. Both parts are typically designated “system” and “clock” (of the fundamental type). Of course, this does not exclude the existence of a further subdivision into multiple smaller subsystems, but we are mainly concerned with the bipartite setting. Due to the global energy constraint, such a division induces correlations between clock and system, which are contained in the state of the whole. Based on these correlations, the final essential of the timeless approach is the notion of a system state depending on the state of the clock and, thus, provides a relational character. An illustrative example of celestial mechanics showing these attributes is displayed in Figure 1.2.

Considerations of this type have not only been applied in classical, but also in quantum mechanics. Perhaps most notable in this regard, at least from a historical perspective, is the book about quantum theory by Born and Jordan [81] from 1930. The authors state that a time-dependent Hamiltonian can only be an approximate calculational tool for a smaller part of a larger *closed* system, for which exact treatments are possible. Furthermore, they assert that any open system can be completed to a closed system by means of appending a second system, which can act as a clock and provide time for the principal system. Although their analysis was only conceptual in nature, it has already anticipated modern approaches appearing decades later. It is rather astounding that Born and Jordan’s view used to be largely ignored [57].

The search for an emergent notion of time appears most prominently in the context of gravity research, where the canonical form of the equations of gravity are not dynamical laws [82], but constraints. In canonical quantum gravity, the central formula is the quantum mechanical Wheeler-deWitt equation [75, 83, 84] of the form $\hat{H}\,|\Psi\rangle = 0$, which can be seen as a quantum version of a constraint similar to Eq. (1.4). Here, $\hat{H}$ is known as the “super-Hamiltonian” [82] and the state Ψ is referred to as the “wavefunction of

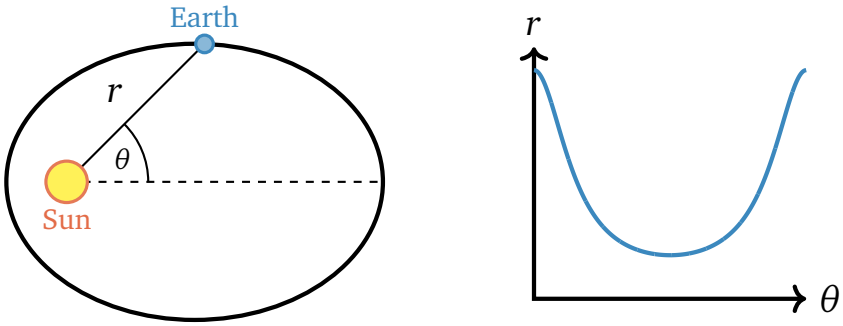

Figure 1.2 – The Earth revolves around the sun on a Kepler orbit with constant energy [79]. Here, the system degree can be seen as the distance r between Earth and sun and depends on the "clock degree" θ. Any correlation between both degrees is encoded in the full orbit, which represents the global state. Fixing the "clock state" to a specific angle θ unequivocally determines the "system state" to be $r(\theta)$ by virtue of the correlations contained in the orbit. For the special case of a circular path, the distance is always constant and, therefore, no correlation exists between distance and angle. This shift in point of view from motion in time (Hamilton's principle) to a path in configuration space (Jacobi's principle) is well-known in classical mechanics [79, 80].

the universe" [75, 84, 85]. In order to yield the dynamical laws known in physics, several strategies have been devised [82] to find a concept of time that is compatible with the static description. Simply put, one tries to find an internally appearing time for a theory in which an external time does not exist. This issue is commonly known as the "problem of time" [86–88] and one widely used attempt for a solution is the semiclassical approach [75, 76, 82, 85, 87, 89–96]. Owing to many mathematical nuances, we only want to mention the simplest method, which is summarized in Ref. [76]. For this approach, the global state is expressed in a configuration space basis which depends on a three-metric and degrees of freedom representing non-gravitational fields. To obtain an intrinsic time from the quantum correlation of three-geometry and matter [96], the global state is chosen as an exact factorization of a Wentzel-Kramers-Brillouin (WKB) wavefunction for the three-metric and a general wavefunction for the non-gravitational degrees conditioned on the three metric [76]. Substitution of this ansatz into the Wheeler-deWitt equation and application of appropriate semiclassical approximations yield a time-dependent Schrödinger equation (TDSE). Crucially, the time derivative originates from a directional derivative along the gradient of the classical action for the gravitational field, which appears in the phase of the WKB-part of the wavefunction. Hence, the three-metric plays the role of the clock degree of freedom and its classical trajectory parametrizes the evolution of the non-gravitational fields. Due to the heavy mathematical machinery of general relativity, we only consider a non-relativistic analog in this thesis, which nevertheless captures key features of the semiclassical timeless approach. A historical precursor of this method, mentioned in a paper authored by Mott in 1931 [97, 98], stems from collision physics. In general, the clock is taken as a heavy-mass non-relativistic particle and the principal system is often represented as a light-mass counterpart, but can be a generic quantum system as well. Similar to the treatment in quantum gravity, a Born-Oppenheimer method and a WKB approximation for the clock are used to derive the TDSE for the system from time-independent Schrödinger equation (TISE) for the global wavefunction [98–102]. The interaction between both particles is typically a function of their positions. Therefore it is not only the system evolution, but also an effective system potential that is parametrized by the classical trajectory of the heavy particle [100, 101].

An alternative timeless approach in quantum mechanics first appeared in 1983 in the paper by Page and Wootters [103] and a subsequent publication by Wootters [104] in 1984. Instead of working in a specific basis representation as in the semiclassical treatment, the Page-Wootters (PW) approach only deals with state vectors in abstract Hilbert space, thus, offering great generality. However, this generalization comes with the trade-off of being able to only deal with non-interacting systems, although Refs. [105, 106] are noteworthy exceptions for specific Hamiltonians. The time-evolved state of the principal system arises from a partial inner product in clock Hilbert space of a unitarily transforming clock state and a global energy eigenstate [107]. This procedure is the quantum analog of the scheme described in Fig. 1.2 and clearly demonstrates the importance of quantum correlations, or entanglement, which are contained in the global state. Consequently, the system TDSE with a time-independent Hamiltonian is straightforwardly found through the application of a derivative with respect to time. Our brief introduction of PW is later supplemented with the corresponding formulas. Experimental tests of this approach have been performed [108–110] from the point of a "super-observer" who has access to the energy eigenstate of a bipartite system, and have confirmed the capability of entanglement to encode the time evolution of a subsystem. Weak points of PW are the presupposition of the clock evolution and the inability to address generally interacting systems. Still, it has the great advantage of applying also to finite-dimensional Hilbert spaces and of not requiring a notion of space [111]. The second aspect is beneficial for isolated investigations of time emergence without any concerns about relativity. Reflecting on the idea that space could be an emergent concept too [112–114], we believe that such a separate treatment is essential. Given the two primary strategies to accomplish the emergence of time and their respective advantages and disadvantages, one naturally seeks to find a common approach combining the individual strengths of the semiclassical and PW approach. In particular, an improved framework should be able to generally deal with coupled systems and should not require a semiclassical approximation, or any approximation for that matter. The attempt to construct such an overarching approach for a timeless formulation without the aforementioned disadvantages is the main objective of this thesis.

We fully accomplish this goal through derivation of a system TDSE with a time-dependent effective potential from a completely generic Hamiltonian, without depending on any approximation. A key element for this achievement constitutes the alternative formulation of the global energy restriction as an invariance principle. The path variable parametrizing the occurring transformations in the invariance appears as a substitute for the traditionally presupposed time t and we elaborate on its metric character in terms of clock properties, which is generally missing in the literature. Our extensive discussions of the features of our theoretical exploration of time are complemented by additional studies on topics, such as semiclassical approximations and time-energy uncertainties. Moreover, we do not only treat pure quantum states, but extend our framework to quantum mixed states and even classical probabilities as a display of the versatile nature of our approach. In contrast to the pure states case, a non-Hermitian term appears as a new element in the evolution equations and is further examined. Since the treatments in quantum and classical mechanics exhibit surprising similarities, we are able to condense our analysis into a unified formulation.

Before outlining the development of our framework, we want to briefly touch on another seemingly unrelated field, namely thermodynamics and the concept of temperature. Physicists have long been puzzled about the apparent mathematical similarities between dynamical and thermodynamical formulations [115], as for example expressed by Zee [116]: "At the arithmetic level this connection comes merely from the fact that the central objects in quantum physics e^{-iHT} and in thermal physics $e^{-\beta H}$ are formally related by analytic continuation. Some physicists, myself included, feel that there may be something pro-

found here that we have not quite understood." Here, time is represented by T and the inverse temperature is denoted by β, while H is the Hamiltonian for the system. The term containing the inverse temperature is proportional to the canonical ensemble, which is exclusively used in this thesis. Although its form is relatively simple, there is no unique physical origin for its derivation. The principal system is presumed to be part of a larger set of degrees of freedom, which have a sharp definite total energy. Usually, the complement part is called a "bath". While traditional quantum mechanical approaches start from a global microcanonical ensemble in the form of a completely mixed state of degenerate energy eigenstates, a more recent formulation called "canonical typicality" only requires a single "typical" global energy eigenstate [117, 118]. Typicality refers to the fact that most random pure states of the whole yield a reduced density operator for a small subsystem that is almost identical to a canonical ensemble. Crucially, the Hilbert space dimension of the bath must be much larger than that of the principal system. Regardless of the specific method (or even specific mechanics) chosen, the general principle for the emergence of temperature is always the same. The global state of a bipartite system is energy constraint and the canonical ensemble can be derived by consideration of only a fraction of the whole, the principal system. Surprisingly, they exactly match those of the timeless approach and deepen the uncanny likeness of temporal and thermal descriptions in physics. That the foundations of theories of time and temperature are the same hints at the possibility for a common origin and strongly suggests to seek for a connection between the two. This closeness has, to our knowledge, first been mentioned by Vedral [119] and later a "peaceful coexistence" of time and temperature within a single global quantum state by virtue of canonical typicality and the PW approach has been declared by Favalli and Smerzi [120]. Incidentally, Mach, whose ideas have been quite influential for investigations of space and time, already drew parallels between time and temperature [121]. Another counterpart is the existence of temperature-energy uncertainties [122–126] as the thermal analog of time-energy uncertainty relations. These inequality relations for temperature and energy do not originate from a temperature operator, as it does not exist, similar to the non-existence of a time-operator. While these insights have either shown a purely mathematical link or a conceptual similarity, a definite arithmetic connection between time and temperature derived from the same physical origin is nevertheless still missing. Employing our adaptable framework in the unified formalism to the realm of imaginary time offers the remarkable opportunity to explore this unusual link. Once the notion of entropy is introduced, we umambiguously identify imaginary time with inverse temperature by virtue of the unique relation between temperature and entropy change for canonical ensembles.

A contemplation on the ideas and challenges presented above has encouraged us to expand the scope of previous approaches by the development of a comprehensive framework that is able to successfully address the issues currently encountered. To this end, we formulate three elementary principles in Chapter 2, which constitute the core concepts of our work and form a minimal set of assumptions for the emergence of time. The main body of this thesis is dedicated to the derivation of time and the characteristic evolution equations in quantum and classical mechanics and is found in Chapter 3. Afterward, we examine the aforementioned connection of imaginary time and inverse temperature in Chapter 4. After having briefly reviewed the canonical ensemble, we analogously derive imaginary time and the differential equations for dynamical changes of the system and determine the necessary conditions for an identification with inverse temperature. Due to the rather mathematical emphasis in the aforementioned two chapters, we reserve discussions of our results and the underlying principles for Chapter 5. Finally, Chapter 6 provides an overview of several interesting directions for future research projects. Whenever necessary, we move extensive calculations into appendices to ensure a fluent reading and to ease comprehension of the main points.

Chapter 2

Concepts

Based on the review of existing research in the previous chapter, our main goal is twofold. On the one hand, we aim at the generalization of the existing approaches of time emergence in order to overcome current shortcomings. On the other hand, we attempt to trace time and temperature back to a common origin, because of the remarkable resemblance of the derivations of dynamical and thermal laws, once time is viewed as an emergent quantity. A necessary step toward this objective is an explicit formulation of the most essential elements of both theories. To this end, a minimal set of two postulates and one proposition is introduced, capturing the core ideas underlying our framework. The global energy constraint in Section 2.1, the existence of subsystems in Section 2.2 and the definition of a subsystem state in Section 2.3 serve as guiding principles throughout this thesis.

2.1 Global energy constraint

A key aspect and central notion of this thesis is the all-encompassing nature of a global state or global system. Hence, no larger systems exist or, in other words, the global state is everything. Naturally, the question arises how such a state is characterized and a reasonable answer is provided by a feature, which is prevalent in many studies investigating time and temperature. One of the crucial properties of time-reparametrization invariant systems is the constancy of the global energy of the extended system (Chapter 1). It also forms the basis for all quantum mechanical treatments of time emergence, for example in Refs. [98, 99, 103–106, 127–132]. As mentioned above, the same principle appears as a fundamental requirement in statistical physics, in which the derivation of the canonical ensemble for a subsystem, quantum or classical, rests on the constraint of constant energy for the global state [117, 133–137]. Considering its importance, the global energy constraint is crucial to our framework. Thus, given that a well-defined notion of energy exists, we formulate our first

> **Postulate (I):** *The global state is energy constraint.*

Not only is the notion of time non-existent for such global states, but also the concept of temperature is entirely absent. As both phenomena are intimately related to a surrounding system, one naturally seeks for their origin through the separation of the whole into parts.

2.2 Existence of subsystems

An omnipresent concept of physics is the existence of individual systems. For this reason, we can routinely make statements like “an electron interacts with an electromagnetic

field". Such classifications are made possible by a clear distinction of different degrees of freedom. Laws governing the independent structure and also the interaction with other distinct systems characterize the nature of each individual system. Even though rarely discussed, the existence and definiteness of such a partitioning are non-trivial and far from obvious [138], which has been brilliantly expressed by Zurek's remark [139] "... without the assumption of a preexisting division of the Universe into individual systems the requirement that they have a right to their own states cannot be even formulated ...". The success of quasi-particle descriptions illustrates how a change in the fragmentation of the whole can lead to more elegant descriptions of physical phenomena. In quantum mechanics, this decomposition is expressed by the tensor product factorization of the whole Hilbert space into smaller Hilbert spaces associated with each subsystem. Crucially, different factorizations can be mathematically realized and even the number of subsystems can vary. To date, it remains unknown if a physical mechanism exists to single out specific fragmentations from the vast set of possible splittings and, if so, how it works. This issue is seldom discussed in the literature, but exceptions such as Ref. [140] do exist.

In this thesis, we do not try to answer the question of preferred decompositions, but instead assume that such a partitioning can be realized at all. In addition, it shall be fixed and singled out by some (unknown) mechanism, which we do not further specify. To quote Zurek [141] again: "However, a compelling explanation of what the systems are—how to define them given, say, the overall Hamiltonian in some suitably large Hilbert space—would undoubtedly be most useful."

The possibility of dividing the global system constitutes our second postulate, namely

> **Postulate (II):** *At least two subsystems must exist.*

Interestingly, it excludes any global system with a prime number dimension. Once a subsystem (S) is specified and fixed, its complementary subsystem (C) is immediately and unambiguously defined as well. In the remainder of this thesis, we denote the principal subsystem (S) by "system" and (C) by "clock" or "complement", depending on the context. As always in physics, we have to separate the notion of a system itself and the physical state this system can be in. Inspired by Page and Wootters [103, 104], we propose a specific definition for the subsystem states in the following section.

2.3 Relational system state

As we have described in the introductory Chapter 1, time can emerge as a parameter characterizing the internal relations in a global timeless energy-constrained state. In order to define the state of the system (S) for which the clock (C) *provides time*, we need to find a procedure, which allows us to relate them both in the correct way. The example in Figure 1.2 reveals the general working mechanism for obtaining a relational system state. One has to harness the internal correlation of the global state by means of associating a specific radius (system state) to a particular angle (clock state). Guided by this insight, we put forth

> **Proposition (III):** *For a given state of the complement (C), the global state provides an internal correlation to the principal system (S), which relates to a unique system state.*

In other words, the state of the system is conditioned on the state of the complement and their relation is encoded in the global state. For this reason, we use "relational state" and "conditional state" for the system state synonymously throughout this thesis. The global state must contain all conditional relations between both subsystem states. That such a view can also be applied to a thermodynamic setting is shown in Chapter 4. In the following chapter, **(I)**–**(III)** are applied to derive *time* in the context of quantum and classical mechanics and, thus, justify the proposition **(III)**.

Chapter 3

Time emergence

This chapter features the application of the three core principles from the preceding chapter in an effort to derive three well-known differential equations governing the evolution of a system, namely the TDSE for pure quantum states, the von Neumann equation for mixed quantum states and the Liouville equation for classical probability densities. The presentation of our results for the emergence of time does not follow the chronological order in which previous publications on the topic appeared. Instead, the aforementioned equations are first derived within our framework and comparisons to previous works in the literature accompany our analysis. Our mathematical treatment commences in Sec. 3.1 with the derivation of the famous TDSE, describing the dynamics of pure states within quantum mechanics. In addition, we provide analytical and numerical examples, as well as possible approximations. The exact results allow us to generalize the derivation to mixed states, i.e., quantum mechanical density operators, and their respective evolution equation in Sec. 3.2. A formulation in the Wigner representation at the end of that section lays the groundwork for Sec. 3.3, in which we try to shed light on the question of the transferability of our results from quantum to classical mechanics. To this end, the focus shifts to classical probability densities in an abstract Hilbert space formulation and connections to the quantum framework are pointed out specifically. At last, motivated by the quantum-classical similarities, this chapter closes with an attempt to combine the results form the preceding sections in a unified, basis-independent formalism in Sec. 3.4.

3.1 Quantum mechanics - Pure states

3.1.1 Subsystems

In the preceding chapter, we have already mentioned that splitting a global system into subsystems is facilitated by a tensor product structure in quantum mechanics. Therefore, postulate **(II)** refers to the ability of expressing the global Hilbert space $\mathscr{H}$ as the tensor product

$$\mathscr{H} = \mathscr{H}_S \otimes \mathscr{H}_C \,. \tag{3.1.1}$$

Here, $\mathscr{H}_S$ and $\mathscr{H}_C$ refer to the system Hilbert space and the complementary clock Hilbert space, respectively. Their corresponding dimensions are denoted by $d_S \equiv \dim \mathscr{H}_S$ and $d_C = \dim \mathscr{H}_C$, such that $\dim \mathscr{H} = d_S \cdot d_C$. In the case of infinite-dimensional Hilbert spaces, we give the dimensions n_S and n_C of the subsystem configuration spaces ($\mathbb{R}^{n_S}$ and $\mathbb{R}^{n_C}$) instead. All parts of our analysis proceed with respect to this decomposition in the following. The rationale to start with postulate **(II)** originates from the intention of expressing the global energy constraint **(I)** in terms of subsystem Hamiltonians and the coupling between them.

3.1.2 Total energy constraint and global invariance

One of the most important equations of the twentieth century, the well-known time-independent Schrödinger equation (TISE)

$$\left(\hat{H} - E\hat{\mathbb{1}}\right)|\Psi\rangle = 0\,, \tag{3.1.2}$$

describes a pure quantum eigenstate $|\Psi\rangle \in \mathscr{H}$[1] of the Hamiltonian $\hat{H}$ with energy eigenvalue E. Put differently, $|\Psi\rangle$ is constrained by the energy operator $\hat{H} - E\hat{\mathbb{1}}$ and, for this reason, Eq. (3.1.2) is ideally suited to express postulate **(I)** in mathematical form. Explicitly, the most general form, in accordance with the product structure (3.1.1), reads

$$\left(\hat{H}_\mathrm{S} \otimes \hat{\mathbb{1}}_\mathrm{C} + \hat{V} + \hat{\mathbb{1}}_\mathrm{S} \otimes \hat{H}_\mathrm{C} - E\hat{\mathbb{1}}\right)|\Psi\rangle = 0\,. \tag{3.1.3}$$

for the global state $|\Psi\rangle$ with fixed energy E. The subsystem Hamiltonians $\hat{H}_\mathrm{S}$ and $\hat{H}_\mathrm{C}$ act only on states in $\mathscr{H}_\mathrm{S}$ and $\mathscr{H}_\mathrm{C}$, respectively, and characterize the nature of the individual subsystems. Any interaction between both subsystems resides in the coupling term $\hat{V}$, which operates in $\mathscr{H}$ and, therefore, acts simultaneously on clock and system. Although being finite, the norm of $|\Psi\rangle$ is arbitrary, because of the absence of any outside agent or observer who would be able to probe this state. In particular, only one single global state $|\Psi\rangle$ physically exists in our framework and embodies the physical entirety. Thus, any probabilistic interpretation becomes meaningless, rendering the numerical value of the norm itself irrelevant. For notational convenience, we choose $\langle\Psi|\Psi\rangle = 1$ and omit identity operators $\hat{\mathbb{1}}_i$ in the following, unless it is useful to point them out explicitly.

Constraint Eq. (3.1.3) can also be expressed in a mathematically equivalent way as the invariance

$$\exp\left[i\lambda(\hat{H}_\mathrm{S} + \hat{V} + \hat{H}_\mathrm{C} - E)\right]|\Psi\rangle = |\Psi\rangle \qquad \forall\lambda \in \mathbb{R} \tag{3.1.4}$$

of the global state $|\Psi\rangle$. Such a view point has generally not been recognized in the literature, but provides a new understanding of the mechanism for time emergence, as explained below. A notable exception is the work by Boette et al. [127, 142], in which the authors establish (3.1.4), but refrain from a further examination. We could, equally well, define another invariance, i.e., $\exp\left[\lambda(\hat{H}_\mathrm{S} + \hat{V} + \hat{H}_\mathrm{C} - E)\right]|\Psi\rangle = |\Psi\rangle$ for all $\lambda \in \mathbb{R}$, which becomes important in Chapter 4. In a strict mathematical sense, another symbol needs to be employed for the parameter in this second invariance, but we slightly abuse our notation and retain the same symbol. Throughout this thesis, the parameter λ is conventionally used as the path variable parametrizing the invariance generated by energy constraints.

As a side note, we want to mention the amusing fact that history has taken a route similar to time emergence approaches [98], when Schrödinger first published the TISE [143] and only later postulated the TDSE [144]. For the derivation of the second equation, a last element is needed, namely the definition of the system state.

[1] A physical global state is actually an element of $\mathscr{H}\backslash\{0\}$, but, as is common, we omit the distinction in this thesis for notational simplicity.

3.1.3 Relational system state

So far, only the global state $|\Psi\rangle$ has been considered and we must put forth a state definition for a fraction of the whole, i.e., the system. According to proposition **(III)**, a state φ of the system ensues from the association to a clock state χ by means of the internal correlations within the global state Ψ. In the present section, all occurring states belong to the class of pure states and, consequently, the normalized vector $|\chi\rangle_C \in \mathscr{H}_C$ with $\langle\chi|\chi\rangle_C = 1$ represents the state of the clock. We define the conditional system state $|\varphi\rangle_S \in \mathscr{H}_S$ as the partial projection of $|\chi\rangle_C$ onto the $\mathscr{H}_C$-part of $|\Psi\rangle$ [103, 104], mathematically expressed as

$$|\varphi\rangle_S \equiv |\varphi[\chi]\rangle_S \equiv \frac{\langle\chi|\Psi\rangle_C}{\sqrt{\langle\Psi|\big(\hat{\mathbb{1}}_S \otimes |\chi\rangle\langle\chi|_C\big)|\Psi\rangle}}\,. \tag{3.1.5}$$

Such a state is always normalized, i.e., $\langle\varphi|\varphi\rangle_S = 1$, and a subscript C for the scalar product signifies a contraction solely in the clock Hilbert space. The conditional dependence on the clock state χ is indicated by the argument in square brackets, but we mostly omit the explicit emphasis in exchange for a clearer notation. In other words, fixing the state in the complement space, the clock sector $\mathscr{H}_C$, unambiguously determines the system state in $\mathscr{H}_S$ via the subsystem relations contained in $|\Psi\rangle$. For illustration, the Bell state $|\Psi_{\text{Bell}}\rangle = \big(|\uparrow_S \otimes \downarrow_C\rangle + |\downarrow_S \otimes \uparrow_C\rangle\big)/\sqrt{2}$ for two spin-1/2 systems [145] can serve as a simple example to demonstrate the definition (3.1.5). If the clock is in the spin-down state $|\chi\rangle_C = |\downarrow_C\rangle_C$, the system is in the spin-up state $|\varphi\rangle_S \propto \langle\chi|\Psi_{\text{Bell}}\rangle_C \propto \langle\downarrow_C|\uparrow_S \otimes \downarrow_C\rangle_C = |\uparrow_S\rangle_S$. Figure 3.1 shows a depiction of the relational statement (3.1.5) and, for later reference, we define the unnormalized system state $|\phi\rangle_S \equiv \langle\chi|\Psi\rangle_C$ as well.

Serving as the starting point for the mixed state treatment and for a comparison with conventional frameworks, we also provide the corresponding pure state density operator

$$|\varphi\rangle\langle\varphi|_S = \frac{\mathrm{tr}_C\big(|\chi\rangle\langle\chi|_C\,|\Psi\rangle\langle\Psi|\big)}{\langle\Psi|\big(\hat{\mathbb{1}}_S \otimes |\chi\rangle\langle\chi|_C\big)|\Psi\rangle} \tag{3.1.6}$$

with the partial trace tr_C over the clock degrees of freedom, which follows from (3.1.5). The system state definition (3.1.5), or Eq. (3.1.6) for that matter, sharply contrasts the one from the standard open systems theory [146], in which the state of the system is described by the reduced density operator

$$\hat{\Upsilon}_{S,\text{red}} \equiv \frac{\mathrm{tr}_C\big(|\Psi\rangle\langle\Psi|\big)}{\langle\Psi|\Psi\rangle}\,. \tag{3.1.7}$$

For an entangled state $|\Psi\rangle$, the reduced density $\hat{\Upsilon}_{S,\text{red}}$ always describes a mixed state. However, the opposite happens for (3.1.5) or (3.1.6), given that the system is always in a pure state for pure $|\chi\rangle_C$ and $|\Psi\rangle$. This difference also appears in terms of mean values, as both system definitions imply

$$\big\langle\hat{A}_S\big\rangle_{\text{red}} = \frac{\langle\Psi|\big(\hat{A}_S \otimes \hat{\mathbb{1}}_C\big)|\Psi\rangle}{\langle\Psi|\big(\hat{\mathbb{1}}_S \otimes \hat{\mathbb{1}}_C\big)|\Psi\rangle} \qquad \text{and} \qquad \big\langle\hat{A}_S\big\rangle = \frac{\langle\Psi|\big(\hat{A}_S \otimes |\chi\rangle\langle\chi|_C\big)|\Psi\rangle}{\langle\Psi|\big(\hat{\mathbb{1}}_S \otimes |\chi\rangle\langle\chi|_C\big)|\Psi\rangle}\,, \tag{3.1.8}$$

respectively, for any system operator $\hat{A}_S$. Comparing both expressions from the relationist perspective shows a conditioning of the system on a clock state with maximal information, i.e., a pure state. In contrast, the open systems theory relates to a fully mixed clock state,

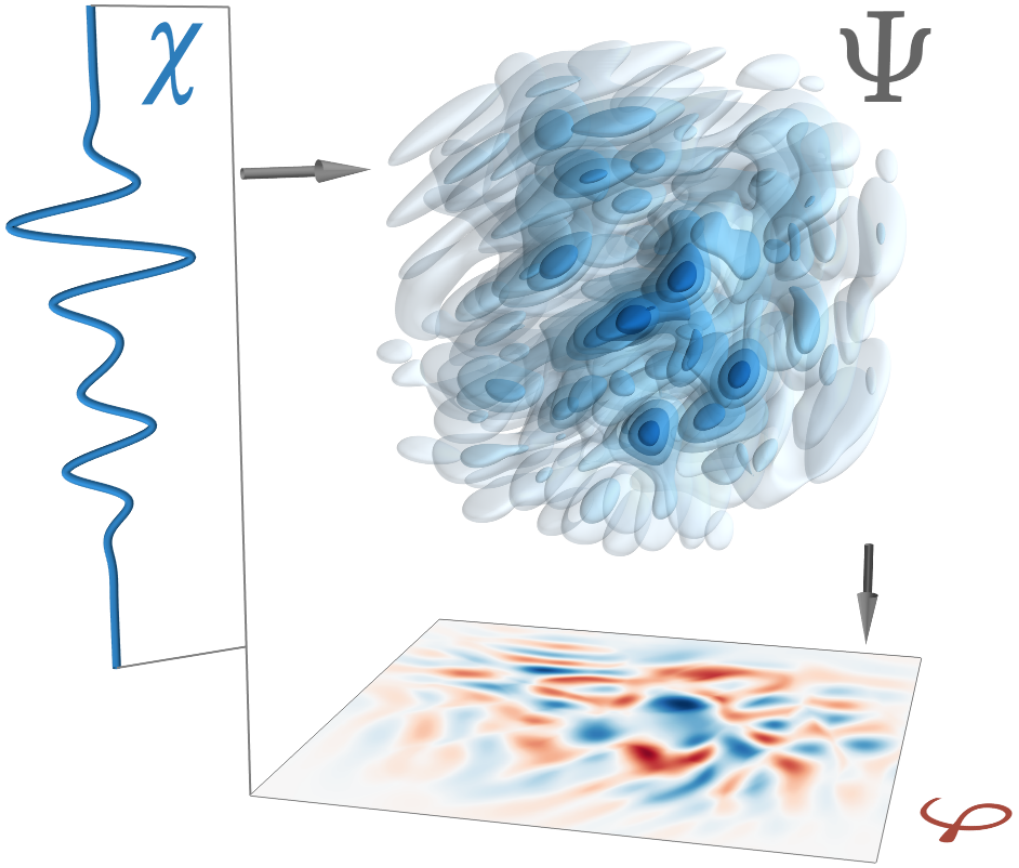

Figure 3.1 – Sketch for the relational system state φ in Equation (3.1.5). The clock state χ, given on a one-dimensional configuration space, is partially projected onto the global state Ψ, which lives on a three-dimensional configuration space. Mathematically, each vertical line segment of Ψ is multiplied with χ and integrated over the clock configuration space. As a result, the system state φ manifests itself on its two-dimensional configuration space. In order to visualize the wavefunctions, only real values are used.

$|\chi\rangle\langle\chi|_C \longrightarrow \hat{\mathbb{1}}_C/n_C$, which has maximal entropy and the lowest information content. In any case, definition (3.1.6) clearly represents a generalization of (3.1.7) once mixed clock states $\hat{\rho}_C$ are allowed and such a perspective lays the foundation for section 3.2. To point out a further difference, we mention that the global state in the theory of open systems [147] is never an energy eigenstate. Otherwise, no global and, therefore, no system dynamics would take place, since time is already presupposed in that framework. In the remainder, we use $\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle \equiv \langle\Psi|(\hat{\mathbb{1}}_S \otimes |\chi\rangle\langle\chi|_C)|\Psi\rangle$ for a more compact notation, unless it causes confusion.

3.1.4 Relational formalism versus measurement process

Here, we must clarify an interpretational issue associated with our system state definition. In quantum mechanics, one usually attaches to Eq. (3.1.5) the notion of a state $|\Psi\rangle$ being *measured* in one of their constituents, the clock degree(s) of freedom. Based on this, the system ends up in the definite state $|\varphi\rangle_S$ after the measurement resulted in the outcome χ. However, we strongly emphasize that our relational state description (3.1.5) does *not* entail an actual *measurement*. Since the topic is vitally important, we systematically explain below how the measurement process unfolds in the description of the nowadays widely accepted theory of decoherence. Scrutinizing the essential elements of this approach

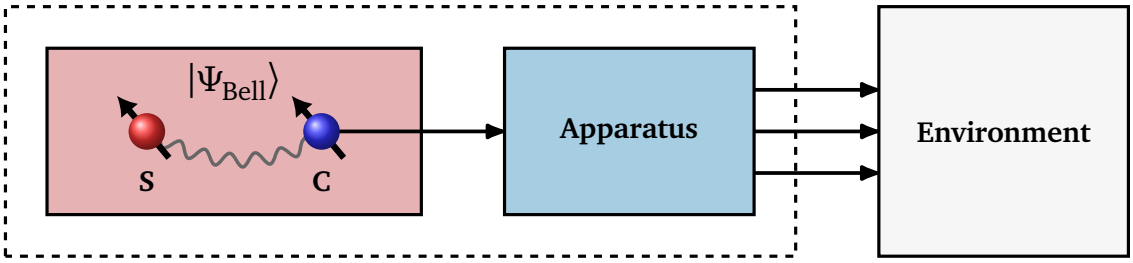

Figure 3.2 – A sketch of the measurement process according to decoherence theory shows the entangling interaction (horizontal arrows) of a measured system (red box) with a measurement apparatus (blue box) and the subsequent coupling to a large environment (gray box). After tracing out the environmental degrees of freedom, the reduced state of measured system and apparatus (dashed lines) exhibits no interference between different measurement outcomes. In particular, the measured system comprises a composite of two spin-1/2 systems (S and C), which are initially in the non-separable Bell state $|\Psi_{\text{Bell}}\rangle$. The gray sinusoidal line represents the internal entanglement between both spins. For the purpose of providing means to compare to the relational formalism, only the clock spin (C) couples to the apparatus, as indicated by the black horizontal arrow. Adapted from Ref. [166].

helps us to work out the underlying assumptions and to clearly distinguish the relational state (3.1.5) formalism from the theory of observations.

The question of how our classical world emanates from within quantum mechanics is broadly known as the "measurement problem" [148]. It originates from the phenomenological fact that we, as classical observers, obtain definite measurement outcomes and do not witness quantum mechanical interference in the macroscopic world. So far, only partial answers have been found, which explains the persistence of the measurement problem in physics even today [138,149–154]. We take the position that such a process must be explained using only concepts native to quantum theory. In this Everettian manner [155], the concepts of "decoherence" [139,149,156,157] and its more sophisticated version, "quantum Darwinism" [158–165], have been pioneered in order to explain the measurement process and the emergence of the classical world [150]. These approaches embrace the pervading idea that any measured quantum system is part of a larger structure, which also constitutes a measuring apparatus and the rest of the world. Without resorting to classical concepts, the fundamental quantum nature of the additional physical degrees of freedom is used to explain how measurement devices record outcomes and how the quantum mechanical interference between measurement results rapidly disappears from the perspective of the observing apparatus. The sketch in Figure 3.2 provides a visual guide for the following exposition, which elucidates this intricate process.

At the core of the aforementioned frameworks lies the entangling interaction of a state $|\Psi\rangle = \sum_i c_i |\Psi_i\rangle \in \mathscr{H}$ with a ready state $|\nu_0\rangle_{\text{app}} \in \mathscr{H}_{\text{app}}$ of the measurement apparatus (Fig. 3.2), which has already been suggested in von Neumann's seminal book about quantum mechanics [147,167]. For a later comparison with the relational formalism, we retain the symbols $|\Psi\rangle$ and $\mathscr{H}$ here, even though they do not have a global nature in the measurement process. Described in a very simplified way [147,168], the entangling interaction with the measurement apparatus evolves the initial state $|\Psi\rangle \otimes |\nu_0\rangle_{\text{app}}$ within finite time T_1

into an entangled state. Schematically, this can be expressed as

$$\left(\sum_i c_i \left|\Psi_i\right\rangle\right) \otimes \left|\nu_0\right\rangle_{\text{app}} \quad \xrightarrow{T_1} \quad \sum_i c_i \left|\Psi_i\right\rangle \otimes \left|\nu_i\right\rangle_{\text{app}} . \tag{3.1.9}$$

The "measured system" should not be confused with the "principal system" (S) associated with $\mathscr{H}_{\text{S}}$. Only a special type of interaction [147, 168, 169] can give rise to the final state in this "quantum nondemolition measurement" (3.1.9), namely one for which $|\Psi_i\rangle$ are eigenstates of the coupling part acting on $\mathscr{H}$ [147, 170, 171]. It ensures that the states $|\Psi_i\rangle$ are not perturbed and this simplification is usually called the "quantum-measurement limit" [147]. As a matter of fact, it is the interaction that determines which states $|\Psi_i\rangle$ are recorded by the apparatus [168]. Anyway, the states $|\nu_i\rangle_{\text{app}}$ are linked (or "entangled") to a specific state $|\Psi_i\rangle$ of the measured system after (3.1.9) and provide the basis for a particular measurement outcome on one of the "branches" $|\Psi_i\rangle \otimes |\nu_i\rangle_{\text{app}}$.

Crucially, the combined system of measurement apparatus and of the measured system couples to another typically large system, called the "environment" (Fig. 3.2). This interaction entangles the individual branches $|\Psi_i\rangle \otimes |\nu_i\rangle_{\text{app}}$ with specific environmental states $|\tau_i\rangle_{\text{env}}$ and we assume once again that these branch states are not disturbed by the coupling term. Hence, the process (3.1.9), called "premeasurement" [168], extends to

$$\left(\sum_i c_i \left|\Psi_i\right\rangle\right) \otimes \left|\nu_0\right\rangle_{\text{app}} \otimes \left|\tau_0\right\rangle_{\text{env}} \quad \xrightarrow{T_2} \quad \sum_i c_i \left|\Psi_i\right\rangle \otimes \left|\nu_i\right\rangle_{\text{app}} \otimes \left|\tau_i\right\rangle_{\text{env}} \tag{3.1.10}$$

with another finite duration T_2. Since the environment consists of a large number of degrees of freedom, the states $|\tau_i\rangle_{\text{env}}$ orthogonalize very rapidly, i.e., $\left\langle \tau_i \middle| \tau_j \right\rangle_{\text{env}} \approx \delta_{ij}$ [138]. In the framework of open system theory, the different branches effectively "decohere", because of the additional contact with the environment. The reduced density operator, without the environmental degrees of freedom, becomes

$$\hat{\rho}_{\text{red}} = \sum_i c_i \left|\Psi_i\right\rangle\!\left\langle\Psi_i\right| \otimes \left|\nu_i\right\rangle\!\left\langle\nu_i\right|_{\text{app}} , \tag{3.1.11}$$

and any coherence between different states $|\nu_i\rangle_{\text{app}}$ of the measurement apparatus vanishes. As a result, a definite outcome or "measurement result" of the apparatus emerges, which is collectively described by the state $|\nu_i\rangle\langle\nu_i|_{\text{app}}$. How observers find themselves in only one of the states $|\nu_i\rangle_{\text{app}}$, a problem called "self-locating uncertainty", is subject of ongoing research [172, 173] and might be closely related to the emergence of Born's rule [174, 175]. At any rate, no quantum mechanical interference with other measurement results can be observed, due to the decohered nature of the branches containing the apparatus and the system of interest.

Once again, we use the Bell state $|\Psi_{\text{Bell}}\rangle \in \mathscr{H} = \mathscr{H}_{\text{S}} \otimes \mathscr{H}_{\text{C}} \simeq \mathbb{C}^2 \otimes \mathbb{C}^2$ as a particular example to illustrate how a term like $\langle\downarrow_{\text{C}}|\Psi_{\text{Bell}}\rangle_{\text{C}}$ is used as a mathematical shortcut to describe a measurement outcome. In our particular case, we assume the measurement device (apparatus) to exclusively couple to the clock spin (Fig. 3.2) and we choose the eigenstates of the interaction as $|\Psi_i\rangle \in \{|\uparrow_{\text{S}} \otimes \downarrow_{\text{C}}\rangle, |\downarrow_{\text{S}} \otimes \uparrow_{\text{C}}\rangle\}$. Individual spin states live in the Hilbert spaces of the clock and the principal system, respectively. After the first entangling interaction, the intermediate state reads $(|\uparrow_{\text{S}} \otimes \downarrow_{\text{C}}\rangle \otimes \left|\nu_{\downarrow_{\text{C}}}\right\rangle_{\text{app}} + |\downarrow_{\text{S}} \otimes \uparrow_{\text{C}}\rangle \otimes \left|\nu_{\uparrow_{\text{C}}}\right\rangle_{\text{app}})/\sqrt{2}$, in which, for example, the apparatus reading $\left|\nu_{\downarrow_{\text{C}}}\right\rangle_{\text{app}}$ coincides with a measurement of the spin-down clock state. The insuppressible contact with the environment ultimately destroys the coherence between both branches in a very short time scale. Ignoring the environmental

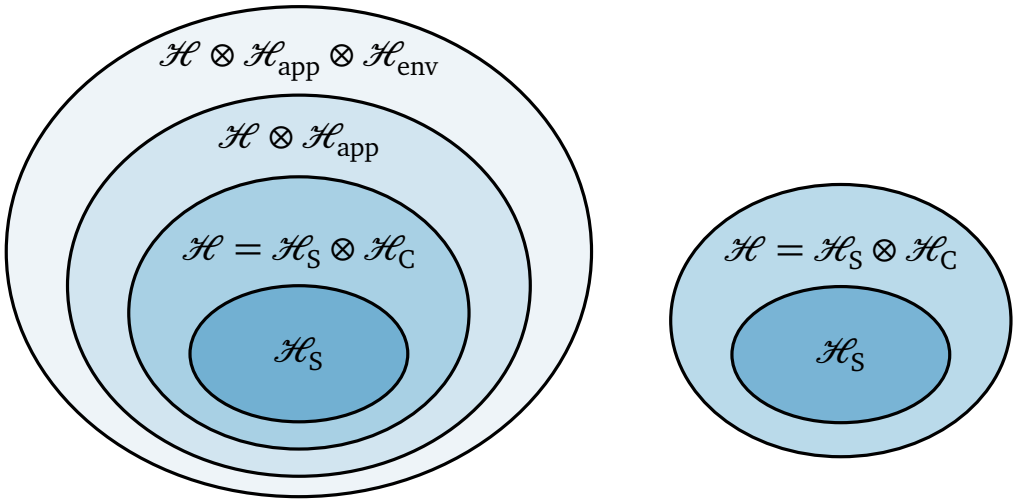

Figure 3.3 – Comparison of the Hilbert space structures involved in a typical measurement process (left) and the quantum mechanical framework for the conditional system states used in this thesis (right). A measurement of a state from Hilbert space $\mathscr{H}$ depends on a larger structure, such as $\mathscr{H} \otimes \mathscr{H}_{\text{app}} \otimes \mathscr{H}_{\text{env}}$, which embeds the measured system and enables decoherence. In contrast, nothing exists outside of $\mathscr{H}$ in our framework.

degrees of freedom leads to the reduced density operator

$$\hat{\rho}_{\text{red}} = \frac{1}{2}\Big(|{\uparrow_{\text{S}}}\rangle\langle{\uparrow_{\text{S}}}|_{\text{S}} \otimes |{\downarrow_{\text{C}}}\rangle\langle{\downarrow_{\text{C}}}|_{\text{C}} \otimes \big|\nu_{\downarrow_{\text{C}}}\big\rangle\big\langle\nu_{\downarrow_{\text{C}}}\big|_{\text{app}} + |{\downarrow_{\text{S}}}\rangle\langle{\downarrow_{\text{S}}}|_{\text{S}} \otimes |{\uparrow_{\text{C}}}\rangle\langle{\uparrow_{\text{C}}}|_{\text{C}} \otimes \big|\nu_{\uparrow_{\text{C}}}\big\rangle\big\langle\nu_{\uparrow_{\text{C}}}\big|_{\text{app}}\Big). \quad (3.1.12)$$

If observers find themselves on the branch with the apparatus indicating a spin-down measurement outcome for the clock, i.e., $\big|\nu_{\downarrow_{\text{C}}}\big\rangle_{\text{app}}$, then they can infer the state of the system to be "spin-up" ($\uparrow_{\text{S}}$), given they have full knowledge about the initial state $|\Psi_{\text{Bell}}\rangle$. Due to its complexity, one uses a simplification to describe this process, which disregards the exact nature of the interactions with the surroundings. In particular, the situation described above is represented by the partial scalar product $\langle{\downarrow_{\text{C}}}|\Psi_{\text{Bell}}\rangle_{\text{C}} \in \mathscr{H}_{\text{S}}$, the general notational shortcut to express a final state after a measurement in quantum mechanics, and is equal in notation to a relation system state in the form (3.1.5).

The actual theory of decoherence and quantum Darwinism is much more subtle and mathematically detailed. Its explanation lies outside the scope of this thesis, but we point out two important and unique properties of this process, already contained in our simplified description. They are implicitly assumed whenever the simple (partial) scalar product is written to describe a state after measurement. First, an evolution in time must exist, no matter how short the actual duration of the interaction. Therefore, time becomes a prerequisite in order for the entanglement between the measured system and the apparatus to change continuously. A subsequent interaction with the environment presumes a temporal evolution as well. Second, a measured system of interest is always embedded in a larger composite system, typically consisting of a vast number of degrees of freedom and allowing for a split into further subsystems, which is elucidated by an illustration on the left side of Fig. 3.3. Both features are *not* present in our framework, because we postulate the global system to encompass all available degrees of freedom [139], such that an extension to a larger system becomes impossible (see Fig. 3.3). Furthermore, time does not exist for $|\Psi\rangle$, but only emerges as an internal relation between subsystems. As such, the entanglement, with respect to the Hilbert space factorization (3.1.1), does not change and remains constant. In fact, we actually derive the subsystem evolution from the constant entanglement between two subsystems, instead of taking the evolution of a global state and its change of

internal entanglement for granted. All aspects considered and given the severe differences, one must unequivocally acknowledge that our definition (3.1.5) of the system state does *not* constitute a measurement, even though the mathematical formulation might indicate differently. This crucial point is either only discussed very briefly or not at all in the literature. Nevertheless, our framework does not exclude the decoherence mechanism, but it must take place in $\mathscr{H}_S$ itself, for which the clock provides time. That process only requires a decomposition of $\mathscr{H}_S$ into further subsystems, for example environment or apparatus. A first attempt to describe a measurement process within a global static state $|\Psi\rangle$ has been given by Deutsch [176]. For now, we content ourselves with the provisional interpretation of Eq. (3.1.5) as a relational statement and return to a discussion on the subject in Chapter 5.

Interestingly, Gisin already used such a relational state definition in 1982 to derive a dissipative Schrödinger equation [177] and, thus, his publication pre-dates the seminal paper of Page and Wootters [103] by one year, even though it was not presented in the context of time emergence. In the subsequent section, we formulate the influential findings from Refs. [103, 104] in the language of our framework.

3.1.5 Time emergence without interaction

The arguably simplest setup occurs for a vanishing interaction in the energy constraint (3.1.3), i.e., $\hat{V} = 0$, and underlies PW [103, 104]. Despite its widespread use in the literature, the absence of any coupling severely limits the applicability to generic physical situations and requires additional restrictions on the global Hamiltonian and on the global state. Any emergent, non-trivial system dynamics relies on the internal entanglement of the global state (Chapter 1) and, therefore, necessitates the global Hamiltonian to possess degenerate energy subspaces. Otherwise, only separable $|\Psi\rangle$ fulfill the TISE (3.1.2). Not only does the degeneracy become an essential prerequisite, but also the presumption that the global state actually exhibits entanglement, as separable states still solve the TISE. In contrast, generic coupling terms $\hat{V}$ in the global Hamiltonian imply entangled energy eigenstates and do not impose any additional preconditions, which makes our approach for interacting subsystems all the more vital. Nevertheless, neglecting the interaction allows us to demonstrate and to discuss our framework in a comprehensible way, without mathematical intricacies. To this end, the unitary transformation in the invariance (3.1.4) becomes separable, namely

$$e^{i\lambda\hat{H}_S} \otimes e^{i\lambda(\hat{H}_C - E)}\,|\Psi\rangle = |\Psi\rangle\ . \tag{3.1.13}$$

We seek an equation for a system state defined by (3.1.5), which must involve a contraction in the $\mathscr{H}_C$-part. To this end, we partially project a fixed clock state $|\chi_0\rangle_C \in \mathscr{H}_C$ onto Eq. (3.1.13). The clock subscript is associated with $\lambda = 0$ and indicates the initial clock state, which becomes clear in the following.

Applying also the inverse transformation $\exp\left(-i\lambda\hat{H}_S\right)$ after the partial projection yields

$$\langle\chi_0|e^{i\lambda(\hat{H}_C - E)}|\Psi\rangle_C = e^{-i\hat{H}_S\lambda}\,\langle\chi_0|\Psi\rangle_C\ . \tag{3.1.14}$$

Through the definition of

$$|\chi(\lambda)\rangle \equiv e^{-i\lambda(\hat{H}_C - E)}\,|\chi_0\rangle \tag{3.1.15}$$

and a normalization on both sides, we obtain the result

$$\frac{\langle\chi(\lambda)|\Psi\rangle_C}{\sqrt{\langle\Psi|\chi(\lambda)\rangle\langle\chi(\lambda)|\Psi\rangle}} = e^{-i\hat{H}_S\lambda}\,\frac{\langle\chi(0)|\Psi\rangle_C}{\sqrt{\langle\Psi|\chi(0)\rangle\langle\chi(0)|\Psi\rangle}}\ . \tag{3.1.16}$$

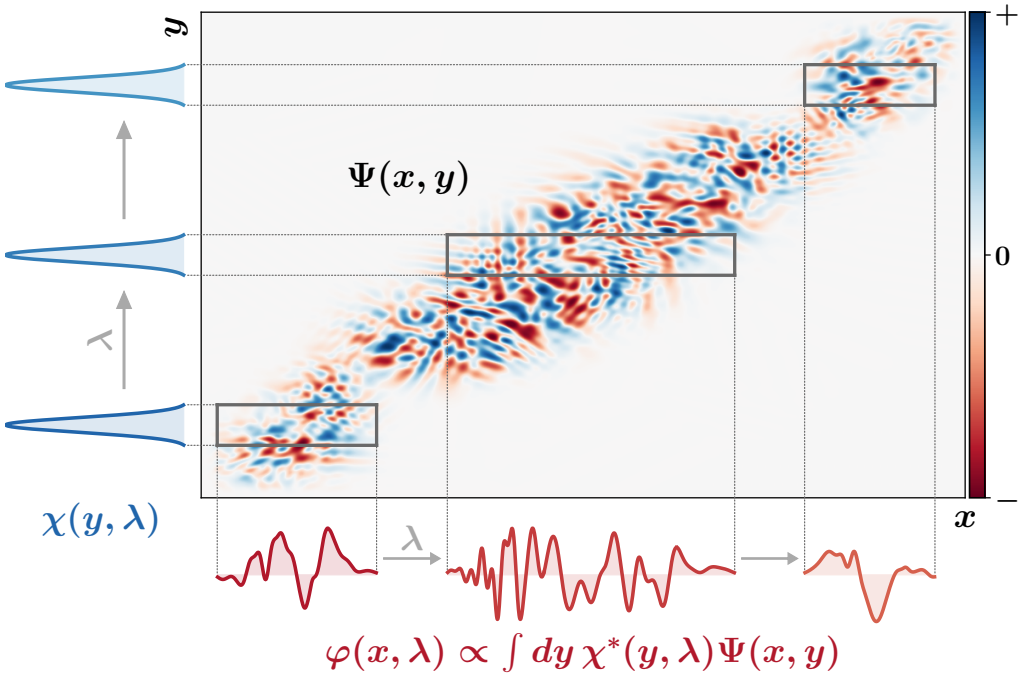

Figure 3.4 – Conditional system state $|\varphi(\lambda)\rangle_S$ in position representation. Any change of the clock state (blue wavefunctions on the left) induces a change in the relational system state (red wavefunctions on the bottom). The TDSEs for both subsystems emerge from the invariance (3.1.4) of the global state Ψ (middle). Gray dotted lines indicate the partial projection of each clock state and their corresponding system states. Moreover, the quantum correlations contained in $|\Psi\rangle$ make it even possible for simple clock wavefunctions to yield intricate system wavefunctions. Only real-valued wavefunctions are used for an easy visualization.

Both denominators are equal, because of invariance (3.1.3). The left hand side corresponds to the conditional system state $|\varphi(\lambda)\rangle_S = \langle\chi(\lambda)|\Psi\rangle_C / \sqrt{\langle\Psi|\chi(\lambda)\rangle\langle\chi(\lambda)|\Psi\rangle}$ of Eq. (3.1.5) and, as a result, the change of the system state is described by

$$|\varphi(\lambda)\rangle_S = e^{-i\lambda\hat{H}_S}\,|\varphi(0)\rangle_S\,. \tag{3.1.17}$$

Fig. 3.4 shows a pictorial representation of Eqs. (3.1.5), (3.1.15), (3.1.16) and (3.1.17). Simple differentiation with respect to the parameter λ yields the TDSE

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\,|\varphi(\lambda)\rangle_S = \hat{H}_S\,|\varphi(\lambda)\rangle_S\,, \tag{3.1.18}$$

in which λ takes the place of the usual time t. Similarly, one finds $i\,\mathrm{d}|\chi\rangle_C/\mathrm{d}\lambda = (\hat{H}_C - E)|\chi\rangle_C$ for the clock. In its core, our derivation entails the concept devised by Page and Wootters [103, 104], but several remarks are added in order to point out previously unnoticed aspects and to gain a deepened understanding of our formalism.

3.1.5.1 Remarks

First, the evolution equations for clock and system emerge simultaneously. In contrast, the form of the clock evolution has previously been assumed in advance, for example in Refs. [103–105, 128, 178, 179]. Their derivation proceeds in a symmetrical fashion, such that starting with the reversed relational state $|\chi[\varphi]\rangle_C \equiv \langle\varphi|\Psi\rangle_S / \sqrt{\langle\Psi|\varphi\rangle\langle\varphi|\Psi\rangle}$ gives the same differential equations as a result. However, the initial clock state would not be the same, because $|\chi[\varphi(0)]\rangle_C = |\chi[\varphi[\chi(0)]]\rangle_C \neq |\chi(0)\rangle_C$ in general. The class of global maximally entangled states (MES) is an exception to this discrepancy, as explained in Appendix G. Furthermore, time or motion reversal simply refers to the parity transformation $\lambda \to -\lambda$, in which the motion of clock and system are synchronously reversed.

Second, the clock can be more complex than just a single degree of freedom, such as a quantum particle on a one-dimensional configuration space $\mathbb{R}$. It may constitute a complex composite system itself or can have a finite-dimensional Hilbert space. In the case of a finite dimension d_C and the assumption of commensurate clock energy differences, a natural periodicity $\mathcal{T}_C$ exists for the clock, after which any initial state $|\chi_0\rangle_C$ must return to itself (if not earlier). As a consequence, the system must respect this periodicity as well, i.e., $|\chi(\mathcal{T}_C)\rangle_C = |\chi(0)\rangle_C$ implies $|\varphi(\mathcal{T}_C)\rangle_S = |\varphi(0)\rangle_S$.

Third, the derivation does not depend on the dimensionality of the global system. Even though the Hilbert space basis may be discrete and finite, the state space itself always has a continuous structure. A specific example is a two-level system, with a continuous state space, the Bloch sphere, allowing for infinitely many different states. Due to this property, changes in clock or system appear continuous and give rise to a continuous notion of time.

Fourth, dynamics emerges via the entanglement contained in $|\Psi\rangle$. As already indicated by the notation used in definition (3.1.5), the system depends explicitly on the state $|\chi(\lambda)\rangle_C$ of the clock and only implicitly on the parameter λ. Hence, time or dynamics must physically be seen as the relation to the motion of another subsystem and can only mathematically be expressed by a physically meaningless quantity λ, which parametrizes this motion. Simply put, we could change the parametrization with $\lambda \to s(\lambda)$ via a smooth monotonically increasing function $s(\lambda)$ with $\mathrm{d}s/\mathrm{d}\lambda > 0$ and no physical change in the theory would occur, because $|\varphi[\chi(s)]\rangle_S$ relates to a specific state $|\chi(s)\rangle_C$ and not the actual value of s. Thus, λ only has topological meaning for the order of different states [121, 180], but no metric property [181]. In the elementary classical point particle model of Chapter 1, we consider the simple clock mapping $t(\lambda) : \mathbb{R} \to \mathbb{R}$ and the corresponding "system state" $q(\lambda)$, which has lead to the deparametrization $q(t)$ via the inverse $\lambda(t)$, independent of the actual parametrization λ or $s(\lambda)$. The quantum world features the more complex mapping $|\chi(\lambda)\rangle_C : \mathbb{R} \to \mathscr{H}_C$ and, even though the system state (3.1.5) is already parametrized by the clock state vector, it is not a function of a single scalar clock quantity. Despite this obstacle, it is possible to condense the necessary clock information into the mapping $\mathsf{A}_C(\lambda) \equiv \langle\chi(\lambda)|\hat{A}_C|\chi(\lambda)\rangle_C : \mathbb{R} \to \mathbb{R}$ with a suitable Hermitian clock operator $\hat{A}_C$. If the chosen operator allows for a smooth monotonically increasing function $\mathsf{A}_C(\lambda)$ and its associated inverse $\lambda(\mathsf{A}_C)$ (at least on a finite interval), then we can deparametrize (3.1.18) to

$$i\frac{\mathrm{d}}{\mathrm{d}\mathsf{A}_C}|\varphi(\mathsf{A}_C)\rangle_S = \frac{\mathrm{d}\lambda(\mathsf{A}_C)}{\mathrm{d}\mathsf{A}_C}\hat{H}_S|\varphi(\mathsf{A}_C)\rangle_S\,. \tag{3.1.19}$$

The system state

$$|\varphi(\mathsf{A}_C)\rangle_S = e^{-i\hat{H}_S\lambda(\mathsf{A}_C))}|\varphi(0)\rangle_S \tag{3.1.20}$$

is now given in terms of a scalar clock property, which we can call "quantum ephemeris time" and which has the property of a metric time [121, 180]. For that reason, λ merely obtains the status of an ordering label for the relations between clock and system. As long as the order of these labels is preserved, their actual value does not matter. To illustrate, we take the example of the clock Hamiltonian $\hat{H}_C = \hat{K}^2/2$ for a free particle with momentum operator $\hat{K}$. The Ehrenfest theorem [182, 183] yields

$$Q(\lambda) = \lambda K + Q(0) \tag{3.1.21}$$

as a classical motion for mean clock position $Q \equiv \langle\chi(\lambda)|\hat{Q}|\chi(\lambda)\rangle_C$ and constant mean momentum $K \equiv \langle\chi(0)|\hat{K}|\chi(0)\rangle_C$. In this case, the system Hamiltonian in the TDSE

$$i\frac{d}{dQ}|\varphi(Q)\rangle_S = \frac{1}{K}\hat{H}_S|\varphi(Q)\rangle_S \tag{3.1.22}$$

is simply rescaled by the constant factor $1/K$ and the clock mean position Q parametrizes the system motion. So far, the reparametrization invariance has never been recognized in the literature before and, thus, represents an important result of this thesis. Of course, such an operator choice depends explicitly on the clock state, owing to the fact that certain mean values may not change. For example, a clock without mean momentum ($K = 0$) must be tracked by another choice. Higher-order operators, such as $\hat{Q}^2$ in $\langle\hat{Q}^2\rangle - \langle\hat{Q}\rangle^2$, do represent valid choices as well and, in this particular case, would track the dispersing nature of a wavepacket. It is not necessary either to find a suitable operator for all values of λ, because it suffices to find a set of clock operators such that the whole range of λ can be adequately covered. In a way, this procedure resembles the covering of a differentiable manifold with different charts providing coordinate systems for different parametrizations of the manifold [184]. A simple circle represents such a manifold, for which at least two charts are necessary to cover it completely and this example provides an analogy for cyclic clocks. The periodicity entails the requirement to have at least two different clock mean values to fully parametrize the system motion. Another important example is a spin system $\hat{H}_C = \Omega\hat{S}_z$ with $2S+1$ energy levels, for which the evolution can be tracked with $\langle\hat{S}_x\rangle_C(\lambda) = S_0\cos(\Omega\lambda + \theta_0)$, yielding $\lambda = (\arccos[\langle\hat{S}_x\rangle_C(\lambda)/S_0] - \theta_0)/\Omega$. The spin operators $\hat{S}_i$ for $i \in \{x, y, z\}$ fulfill the usual commutation relation $[\hat{S}_j, \hat{S}_k] = i\varepsilon_{jkl}\hat{S}_l$ [185] and the constants S_0 and θ_0 are determined by the initial state $|\chi_0\rangle_C$. If $\langle\hat{S}_x\rangle_C(\lambda)$ approaches the positive turning point and ceases to provide a monotonically increasing function, then switching to $\langle\hat{S}_y\rangle_C(\lambda)$ provides another suitable tracking function. For the ranges of λ-values for which both the sine and the cosine function are decreasing, one can simply use $\langle-\hat{S}_x\rangle_C(\lambda)$ or $\langle-\hat{S}_y\rangle_C(\lambda)$. One can even use functions of mean values, such as $f(\langle\hat{S}_x\rangle_C, \langle\hat{S}_y\rangle_C) = [\arctan(\langle\hat{S}_y\rangle_C/\langle\hat{S}_x\rangle_C) - \theta_0]/\Omega$ with $df/d\lambda = 1$. This spin treatment holds broad applicability, because any state with a finite number of populated energy states and commensurate energy differences can be mapped to a spin system. The frequency Ω represents the smallest energy unit, such that all energy differences are integer multiples of Ω.

Fifth, a key aspect is the non-classicality of the clock state. Classical characteristics can only occur by means of the time parametrization $\langle\hat{A}_C\rangle$ and the use of Ehrenfest's theorem in its general form without any approximation. If the resulting system of coupled first-order linear equations is finite or cyclic [186], such as for a free particle or a harmonic oscillator, then a single (possibly higher-order) differential equation for $\langle\hat{A}_C\rangle$ appears and can resemble known classical equations for single trajectories of point particles. However, this set of differential equations is in general infinite [186]. To emphasize this important distinction again, the classical behavior of mean values does *not* imply classical behavior of the wave function [187]. For notational simplicity, we still use the parameter λ for the remainder of this thesis, but with the implicit understanding of always being able to find

a reparametrization in terms of a clock property. Although the arbitrariness of choosing a specific clock parametrization seems adverse, it is the search for simplicity of the fundamental equations in physics that distinguishes linear relations with λ, such as Eq. (3.1.21), from more complicated ones. The demand for a time definition leading to the most simple mechanical equations goes back to Poincaré [121].

Sixth, if no entanglement is present in $|\Psi\rangle$ with respect to the tensor product structure Eq. (3.1.1), then it is a product state $|\Psi\rangle = |\tilde{\varphi}\rangle_S \otimes |\tilde{\chi}\rangle_C$ with $\langle\tilde{\chi}|\tilde{\chi}\rangle_C = 1$ and $\langle\tilde{\varphi}|\tilde{\varphi}\rangle_S = 1$. This separability leads to the simple system evolution

$$|\varphi(\lambda)\rangle = \underbrace{\frac{\langle\chi_0|e^{i\lambda(\hat{H}_C-E)}|\tilde{\chi}\rangle_C}{\left|\langle\chi_0|e^{i\lambda(\hat{H}_C-E)}|\tilde{\chi}\rangle_C\right|}}_{\in\exp(i\mathbb{R})}|\tilde{\varphi}\rangle_S\,. \tag{3.1.23}$$

Regardless of the initial clock state $|\chi_0\rangle_C$, the system state changes only by a complex phase, which does not entail any physical change. Hence, entanglement ("quantum correlation") is essential for any non-trivial unitary changes in the physical state of the system. Without a coupling $\hat{V}$, the energy eigenstate can only exhibit internal correlations if its eigenenergy E has a degenerate associated eigenspace.

Seventh, any non-trivial dynamical change in the system requires a non-vanishing $\hat{H}_C \neq 0$, otherwise the clock changes only by a complex factor $|\chi(\lambda)\rangle_C = \exp(iE\lambda)\,|\chi_0\rangle_C$ and induces an irrelevant phase in the system, i.e., $|\varphi(\lambda)\rangle_S = \exp(-iE\lambda)\,|\varphi(0)\rangle_S$. In other words, if no physical change occurs for the clock, then the system does not change either. Interestingly, this characteristic remains even for non-vanishing couplings $\hat{V} \neq 0$ between system and clock. We note that $\hat{H}_C = 0$ does not preclude an entangled global state $|\Psi\rangle$.

Eighth, in light of invariance (3.1.4), the emergence of the system dynamics can be understood from a new point of view. To elaborate, any phase changes in the clock state must be compensated by complementary phase changes in the system in order to preserve the global invariance generated by the total Hamiltonian (minus energy E).

Ninth, the absence of a coupling term $\hat{V}$ allows us to split the unitary transformation $\exp\left(i\lambda\hat{G}\right) = \exp\left(i\lambda\hat{H}_S\right) \otimes \exp\left(i\lambda(\hat{H}_C - E)\right)$, and the part operating on the system Hilbert space $\mathscr{H}_S$ simply commutes with the clock projection. Such a straightforward derivation is not possible if $\hat{H}$ features an interaction between clock and system, and the need for a more sophisticated derivation arises. The more general case with $\hat{V} \neq 0$ is treated in the next section, after we clarify two remaining technical aspects and briefly discuss previous studies of PW.

Although we regard the full clock Hilbert space spanned by the eigenstates of $\hat{H}_C$, only the energy eigenstates that are contained in the global state $|\Psi\rangle$ are relevant. Any part $|\delta\chi\rangle_C$ of a generic clock state $|\chi\rangle_C$ that has no overlap with $|\Psi\rangle$, e.g. $\langle\delta\chi|\Psi\rangle_C = 0$, is irrelevant. More precisely, any state $|\delta\chi\rangle_C$ that fulfills

$$\langle\delta\chi|e^{i\lambda(\hat{H}_C-E)}|\Psi\rangle_C = 0 \qquad \forall\lambda\in\mathbb{R} \tag{3.1.24}$$

cannot be part of the correlation contained in $|\Psi\rangle$. Alternatively stated, we cannot partially project a clock state (or part of it) for which no specific relation of a system state to this clock state is encoded in the global state. We can illustrate this fact with a wall clock having, for simplicity, only the positions 1 to 12 for the hand of the clock. It is pointless to

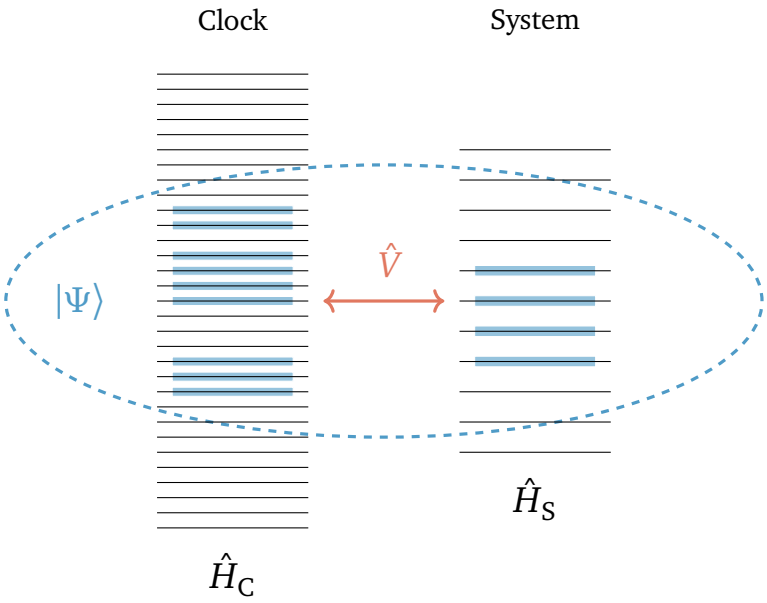

Figure 3.5 – Illustration of the energy level structure of clock and system, in which the black lines indicate the energies of $\hat{H}_C$ and $\hat{H}_S$, respectively. The blue colored levels are elements of the subsets $\pi_{C,\Psi}$ and $\pi_{S,\Psi}$. These are the only relevant states in the process and depend explicitly on the global state $|\Psi\rangle$. A possible interaction $\hat{V}$ between both subsystems is indicated by the red symbols.

ask which system state we measure at a clock position 13, because it is not contained in our description of the global system, i.e., $|\Psi\rangle$. If the clock state is decomposed into

$$|\chi_0\rangle_C \propto |\bar{\chi}_0\rangle_C + |\delta\chi\rangle_C \tag{3.1.25}$$

for which Eq. (3.1.24) holds, then the partial projection onto Eq. (3.1.4) simply reduces to

$$\langle\bar{\chi}(\lambda)|\Psi\rangle_C = e^{-i\lambda\hat{H}_S}\,\langle\bar{\chi}_0|\Psi\rangle_C \tag{3.1.26}$$

with $|\bar{\chi}(\lambda)\rangle_C \equiv e^{-i\lambda(\hat{H}_C - E)}\,|\bar{\chi}_0\rangle_C$. The clock vector $|\delta\chi\rangle_C$ has no influence on the system state.

For a further clarification, which also holds for $\hat{V} \neq 0$, we use the energy eigenstates $|\chi_m\rangle_C \in \mathscr{H}_C$ and $|\varphi_n\rangle_S \in \mathscr{H}_S$ of clock Hamiltonian $\hat{H}_C$ and system Hamiltonian $\hat{H}_S$ as a specific basis. Expressed in this basis, the global state reads

$$|\Psi\rangle = \sum_{mn} c_{mn}\,|\chi_m \otimes \varphi_n\rangle \tag{3.1.27}$$

and we define the subsets of participating energy levels by

$$\pi_{C,\Psi} \equiv \left\{ |\chi_m\rangle_C \,\middle|\, \exists\, n : c_{mn} \neq 0 \right\} \tag{3.1.28}$$

and

$$\pi_{S,\Psi} \equiv \left\{ |\varphi_n\rangle_S \,\middle|\, \exists\, m : c_{mn} \neq 0 \right\} \tag{3.1.29}$$

for clock and system, illustrated in Fig. 3.5. These sets describe the physically accessible states [188] in system and clock Hilbert space. Alternatively, we use the reduced density matrices of the subsystems to define the same sets via

$$\pi_{C,\Psi} \equiv \left\{ |\chi_m\rangle_C \,\middle|\, \langle\chi_m|\big(\mathrm{tr}_S\,|\Psi\rangle\langle\Psi|\big)|\chi_m\rangle_C \neq 0 \right\}, \tag{3.1.30}$$

$$\pi_{S,\Psi} \equiv \left\{ |\varphi_n\rangle_S \;\middle|\; \langle\varphi_n|\big(\operatorname{tr}_C |\Psi\rangle\langle\Psi|\big)|\varphi_n\rangle_S \neq 0 \right\} . \tag{3.1.31}$$

These sets span the effective subsystem Hilbert spaces in which the dynamics can take place and we define the projectors $\hat{\Pi}_{S,\Psi} = \sum_{|\varphi_n\rangle_S \in \pi_{S,\Psi}} |\varphi_n\rangle\langle\varphi_n|_S$ and $\hat{\Pi}_{C,\Psi} = \sum_{|\chi_m\rangle_C \in \pi_{C,\Psi}} |\chi_m\rangle\langle\chi_m|_C$. From here on, we only take into account the effective subspaces and clock states $|\chi\rangle_C$, which are at most a superposition of the states contained in $\Pi_{C,\Psi}$. In particular, we use the following redefinitions

$$\begin{aligned}
\hat{\Pi}_{C,\Psi}\, \hat{H}_C\, \hat{\Pi}_{C,\Psi} &\to \hat{H}_C\,, \\
\hat{\Pi}_{S,\Psi}\, \hat{H}_S\, \hat{\Pi}_{S,\Psi} &\to \hat{H}_S\,, \\
\left(\hat{\Pi}_{S,\Psi} \otimes \hat{\Pi}_{C,\Psi}\right) \hat{V} \left(\hat{\Pi}_{S,\Psi} \otimes \hat{\Pi}_{C,\Psi}\right) &\to \hat{V}\,, \\
\operatorname{tr}_C \hat{\Pi}_{C,\Psi} &\to d_C\,, \\
\operatorname{tr}_S \hat{\Pi}_{S,\Psi} &\to d_S\,, \\
\hat{\Pi}_{C,\Psi} &\to \hat{\mathbb{1}}_C\,, \\
\hat{\Pi}_{S,\Psi} &\to \hat{\mathbb{1}}_S\,,
\end{aligned} \tag{3.1.32}$$

instead of introducing a new set of variables and considerably simplify all treatments in the remainder of this thesis.

The very last remark touches upon the boundedness of the Hamiltonian. A traditional wisdom in physics states that any Hamiltonian must be bounded from below, otherwise the system would decay infinitely long and would continuously reach lower and lower energy states. Although such a process is conceivable, it relies on two essential assumptions. First, one assumes an additional system, the environment, into which energy is released, such as the electromagnetic field for an excited atom for instance. Second, only the presence of a coupling with these environmental degrees allows for an energy exchange. In our setup, neither of the two does exist for the global state and, for this reason, unbounded Hamiltonians are allowed. Similar arguments are conveyed in Ref. [189].

In the tradition of PW [103, 104], we do not assume a particular physical system for the clock or specify any clock Hamiltonian $\hat{H}_C$. While references such as [190] employ generic clock Hamiltonians as well, the authors of many newer studies [105, 107, 128, 129] choose the clock Hamiltonian to equal the one-dimensional momentum operator $\hat{K}$ of a particle, i.e., $\hat{H}_C = \hat{K}$. The rationale behind this choice is twofold. First, the clock position operator $\hat{Q}$ can supposedly take the role of a "time operator" by virtue of the commutation relation $[\hat{Q}, \hat{H}_C] = i$. Second, the position eigenstates $|Q\rangle_C$ form a distinct class of clock states, because of their simple evolution in form of $|\chi(\lambda)\rangle_C = |Q + \lambda\rangle_C$ and the property of being an eigenstate of a "time operator".

3.1.6 Time emergence with interaction

The majority of scientific works about time emergence (outside the quantum gravity community) considers setups without an interaction between clock and system. Yet, such a setting is very special and, in general, a generic Hamiltonian $\hat{H}$ does not allow for a bipartite tensor structure exhibiting two non-interacting systems. In light of this fact, it becomes imperative to have a general treatment for coupled subsystems readily available. We extend an existing collection of publications [98–100, 102, 105, 106, 191, 192] that consider this sophisticated configuration, with a thorough analysis within the quantum mechanical framework administered by the postulates **(I)** and **(II)** and proposition **(III)**. A decisive element of these previous works is the appearance of an effective potential acting on the

system and depending on the state of the clock, or simply put, a time-dependent system Hamiltonian. As demonstrated in the preceding section, the occurrence of such a term is tied to the presence of a coupling term $\hat{V}$. The following derivation of the TDSE with interactions is of great generality, because of its model-independence and the appearance of an effective system potential $\hat{V}_S$ in its most general form. Furthermore, the existence of an interaction almost always ensures a non-separable energy eigenstate $|\Psi\rangle$ possessing non-vanishing entanglement, unless the coupling commutes with the self-Hamiltonians, i.e., $[\hat{H}_S + \hat{H}_C, \hat{V}] = 0$. An example for this special case is $\hat{V} = \hat{H}_S \otimes \hat{H}_C$ from Ref. [193].

3.1.6.1 Invariance and infinitesimal transformations

As before, the invariance Eq. (3.1.4) provides a starting point, but the clock projection cannot easily be resolved into a unitary evolution for the system, as already stated in the preceding section. The key to determining the correct unitary system dynamics is the splitting of λ into many infinitesimal segments $\kappa \equiv \lambda/N \ll 1$ with $N \gg 1$ and the associated division of $\exp\big(i\lambda(\hat{H}_C + \hat{H}_S + \hat{V} - E)\big)$ into many infinitesimal transformations $\exp\big(i\kappa(\hat{H}_C + \hat{H}_S + \hat{V} - E)\big)$. After initially treating only one small transformation, the form of the system evolution for finite λ becomes apparent.

Since κ is a small quantity, we can Taylor expand Eq. (3.1.4) up to first order in κ and partially project an initial clock state $|\chi_0\rangle_C$ onto it, yielding

$$\langle\chi_0|e^{i\kappa(\hat{H}_C+\hat{H}_S+\hat{V}-E)}|\Psi\rangle_C = \langle\chi_0|\Psi\rangle_C + i\kappa\,\langle\chi_0|\big(\hat{H}_C + \hat{H}_S + \hat{V} - E\big)|\Psi\rangle_C + \mathcal{O}(\kappa^2)\,. \tag{3.1.33}$$

3.1.6.2 Optimization of effective potential and non-Hermitian remainder

Clearly, the term $\langle\chi_0|\hat{V}|\Psi\rangle_C$ in (3.1.33) needs further evaluation. We wish to obtain an effective operator $\hat{V}_S$ acting only on the relation system state. To this end, we introduce

$$\hat{V}_S(0)\,\langle\chi_0|\Psi\rangle_C \equiv \langle\chi_0|\hat{V}|\Psi\rangle_C - |\Delta(0)\rangle_S \tag{3.1.34}$$

with the remainder vector $|\Delta(0)\rangle_S \equiv \langle\chi_0|\big(\hat{V} - \hat{V}_S(0)\big)|\Psi\rangle_C$. So far, the effective potential $\hat{V}_S(0)$, which operates solely in the system Hilbert space $\mathscr{H}_S$, is undetermined. In order to capture with $\hat{V}_S$ the unitary part of the system evolution to the fullest extent, we minimize the contribution from the potentially unitarity-violating term $|\Delta\rangle_S$. In other words, we seek an effective potential generating (together with $\hat{H}_S$) a unitary evolution that is as close as possible to the exact relational dynamics. For an ease in notation, we introduce the projectors

$$\hat{P}_\chi(\lambda) \equiv e^{-i\lambda(\hat{H}_C - E)}\,|\chi_0\rangle\langle\chi_0|_C\,e^{i\lambda(\hat{H}_C-E)}\,, \tag{3.1.35}$$

$$\hat{P}_\Psi \equiv |\Psi\rangle\langle\Psi|\,, \tag{3.1.36}$$

$$\hat{P}_\varphi(\lambda) \equiv |\varphi(\lambda)\rangle\langle\varphi(\lambda)|_S = \frac{|\phi(\lambda)\rangle\langle\phi(\lambda)|_S}{\langle\phi(\lambda)|\phi(\lambda)\rangle_S} \tag{3.1.37}$$

and omit the argument λ in the following, which is implicitly taken as $\lambda = 0$ for now. Expressing the norm of the remainder vector in a trace form yields

$$\langle\Delta|\Delta\rangle_S = \mathrm{tr}\Big[\hat{P}_\Psi(\hat{V} - \hat{V}_S)\hat{P}_\chi(\hat{V} - \hat{V}_S)\Big] \geq 0\,. \tag{3.1.38}$$

This term is bounded from below and must posses at least one minimum. On the contrary, it has no upper bound, because $\hat{V}_S$ can always be rescaled by a scalar factor and can increase the norm by an arbitrary factor. In order to find a $\hat{V}_S$ minimizing the remainder norm, we use a variational approach in which the effective system potential varies by a small, but

arbitrary Hermitian term $\widehat{\delta V}_S$, namely $\hat{V}_S \longrightarrow \hat{V}_S + \widehat{\delta V}_S$. This ensures a variation within the space of Hermitian operators and the subsequent variation of the norm reads

$$\delta\langle\Delta|\Delta\rangle_S = \mathrm{tr}\Big[\hat{P}_\Psi \widehat{\delta V}_S \hat{P}_\chi (\hat{V}_S - \hat{V}) + \hat{P}_\Psi (\hat{V}_S - \hat{V}) \hat{P}_\chi \widehat{\delta V}_S\Big] \tag{3.1.39}$$

$$= \mathrm{tr}\Big[\widehat{\delta V}_S \Big\{\hat{P}_\chi (\hat{V}_S - \hat{V}) \hat{P}_\Psi + \hat{P}_\Psi (\hat{V}_S - \hat{V}) \hat{P}_\chi\Big\}\Big] \tag{3.1.40}$$

$$= \mathrm{tr}_S\Big[\widehat{\delta V}_S \langle\chi_0|\Big\{(\hat{V}_S - \hat{V})\hat{P}_\Psi + \hat{P}_\Psi(\hat{V}_S - \hat{V})\Big\}|\chi_0\rangle_C\Big] \stackrel{!}{=} 0\,, \tag{3.1.41}$$

where we used the cyclic property of the trace. As stated above, the variation $\widehat{\delta V}_S$ is arbitrary and, therefore, the norm variation can only equal zero if the operator-valued mean value with respect to $|\chi_0\rangle_C$ vanishes. It leads to

$$\langle\chi_0|\big(\hat{P}_\Psi \hat{V} + \hat{V}\hat{P}_\Psi\big)|\chi_0\rangle_C = \langle\chi_0|\hat{P}_\Psi|\chi_0\rangle_C \hat{V}_S(0) + \hat{V}_S(0)\langle\chi_0|\hat{P}_\Psi|\chi_0\rangle_C \tag{3.1.42}$$

$$= \langle\phi(0)|\phi(0)\rangle_S \Big(\hat{P}_\varphi \hat{V}_S(0) + \hat{V}_S(0)\hat{P}_\varphi\Big) \tag{3.1.43}$$

for $\hat{V}_S$ and cannot be further simplified. Despite that, an additional property aids in the extraction of all relevant parts. Before doing so, it is useful the define the complementary projector $\hat{\bar{P}}_\varphi \equiv \hat{\mathbb{1}}_S - \hat{P}_\varphi$. With a Feshbach-Fano-like partitioning [194, 195], we can bring the effective system potential to the block form

$$\hat{V}_S = \hat{P}_\varphi \hat{V}_S \hat{P}_\varphi + \hat{\bar{P}}_\varphi \hat{V}_S \hat{P}_\varphi + \hat{P}_\varphi \hat{V}_S \hat{\bar{P}}_\varphi + \hat{\bar{P}}_\varphi \hat{V}_S \hat{\bar{P}}_\varphi = \left(\begin{array}{c|c} \hat{P}_\varphi \hat{V}_S \hat{P}_\varphi & \hat{P}_\varphi \hat{V}_S \hat{\bar{P}}_\varphi \\ \hline \hat{\bar{P}}_\varphi \hat{V}_S \hat{P}_\varphi & \hat{\bar{P}}_\varphi \hat{V}_S \hat{\bar{P}}_\varphi \end{array}\right). \tag{3.1.44}$$

Since $\hat{V}_S$ never appears stand-alone in the equation of motions, but always in conjunction with $|\phi\rangle_S$ as $\hat{V}_S|\phi\rangle_S$, it is clear that the last term in Eq. (3.1.44) has no influence on the system dynamics. Additionally, Eq. (3.1.43) gives no constraint for this term and, without loss of generality, it can be defined in the most convenient way. The third term gives also zero when applied to $|\phi\rangle_S$, but it is kept in order to ensure the Hermiticity of $\hat{V}_S$. Solving Eq. (3.1.44) yields the optimal effective system potential

$$\hat{V}_S = \frac{\langle\chi|\big(\hat{V}\hat{P}_\Psi + \hat{P}_\Psi\hat{V}\big)|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - \mathrm{Re}(a)\hat{P}_\varphi \tag{3.1.45}$$

and, furthermore, an evaluation of the remainder vector leads to

$$|\Delta\rangle_{S,\min} = -i\,\mathrm{Im}(a)\,|\phi\rangle_S\,. \tag{3.1.46}$$

The complex scalar $a(\lambda)$ is defined as $a \equiv \langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle \,/\, \langle\Psi|\hat{P}_\chi|\Psi\rangle \in \mathbb{C}$ and further details of the calculations can be found in Appendix A.1. An alternative form for a follows from the global energy constraint (3.1.3) and reads

$$a = E - \langle\varphi|\hat{H}_S|\varphi\rangle_S - \frac{\langle\Psi|\hat{H}_C\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}\,. \tag{3.1.47}$$

Using the aforementioned freedom, we can add $-\mathrm{Re}(a)\hat{\bar{P}}_\varphi$ to the effective potential $\hat{V}_S$ without any change in the system dynamics, yielding the simpler expression

$$\hat{V}_S = \frac{\langle\chi|\big(\hat{V}\hat{P}_\Psi + \hat{P}_\Psi\hat{V}\big)|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - \mathrm{Re}(a)\,. \tag{3.1.48}$$

This is a surprising result, because the term we suspected to spoil the linearity and hermiticity of the first order term in Eq. (3.1.33) is actually linear in the system state $|\phi\rangle_S$, regardless of the choice for $|\chi\rangle_C$. Therefore, only a purely imaginary scalar violates the Hermiticity. Although the norm of $|\phi\rangle_S$ is not conserved, the dynamics remains unaffected upon renormalization. Put differently, only the hermitian term $\hat{H}_S + \hat{V}_S$ governs the evolution in projective system Hilbert space[2]. We also note that the contributions to the imaginary part $\mathrm{Im}(a) = \mathrm{Im}\,\langle\Psi|\hat{\bar{P}}_\chi \hat{V} \hat{P}_\chi|\Psi\rangle_C / \langle\Psi|\hat{P}_\chi|\Psi\rangle$ represent only transitions from the clock state to its complement through $\hat{V}$. An alternative form, which does not rely on the interaction $\hat{V}$, is presented in Appendix A.2.

In hindsight, another way to attain the same result exists. Rewriting the important term as

$$\langle\chi|\hat{V}|\Psi\rangle_C = \langle\chi|\hat{V}|\Psi\rangle_C \frac{\langle\phi|\phi\rangle_S}{\langle\phi|\phi\rangle_S} = \frac{\langle\chi|\hat{V}\hat{P}_\Psi|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}|\phi\rangle_S \tag{3.1.49}$$

resembles an operator acting linearly on the unnormalized system state $|\phi\rangle_S$. It is not Hermitian, but we can add zero in a clever way to obtain a Hermitian operator and an additional scalar term, namely

$$\langle\chi|\hat{V}|\Psi\rangle_C = \frac{\langle\chi|\hat{V}\hat{P}_\Psi|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}|\phi\rangle_S + \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}|\phi\rangle_S - \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}|\phi\rangle_S \tag{3.1.50}$$

$$= \frac{\langle\chi|\big(\hat{V}\hat{P}_\Psi + \hat{P}_\Psi\hat{V}\big)|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}|\phi\rangle_S - \underbrace{\frac{\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}}_{\equiv a\in\mathbb{C}}|\phi\rangle_S\,. \tag{3.1.51}$$

Again, we find the same Hermitian effective system potential $\hat{V}_S$ acting on the system and a purely imaginary term spoiling the norm conservation of $|\phi\rangle_S$, i.e.,

$$\boxed{\langle\chi|\hat{V}|\Psi\rangle_C = \big[\hat{V}_S - i\,\mathrm{Im}\,a\big]|\phi\rangle_S} \tag{3.1.52}$$

With this new insight, Eq. (3.1.33) can be expressed as

$$\begin{aligned}\langle\chi_0|e^{i(\hat{H}_C+\hat{H}_S+\hat{V}-E)\kappa}|\Psi\rangle_C &= \langle\chi_0|\Psi\rangle_C + i\kappa\Big(\hat{H}_S + \hat{V}_S(0) - i\,\mathrm{Im}\,a(0)\Big)\langle\chi_0|\Psi\rangle_C \\ &\quad + i\kappa\,\langle\chi_0|(\hat{H}_C - E)|\Psi\rangle_C + \mathcal{O}(\kappa^2) && (3.1.53)\\ &= e^{i\kappa\left(\hat{H}_S+\hat{V}_S(0)\right)}e^{\kappa\,\mathrm{Im}\,a(0)}\,\langle\chi_0|e^{i\kappa(\hat{H}_C-E)}|\Psi\rangle_C + \mathcal{O}(\kappa^2) && (3.1.54)\\ &\overset{!}{=} \langle\chi_0|\Psi\rangle_C && (3.1.55)\end{aligned}$$

and, subsequently, we find

$$e^{-i\kappa\left(\hat{H}_S+\hat{V}_S(0)\right)}\,\langle\chi_0|\Psi\rangle_C = e^{\kappa\,\mathrm{Im}\,a(0)}\,\langle\chi_0|e^{i\kappa(\hat{H}_C-E)}|\Psi\rangle_C + \mathcal{O}(\kappa^2) \tag{3.1.56}$$

for a small step size κ. To understand the meaning of the exponential prefactor on the right-hand side, we note that

$$\mathrm{Im}(a) = \mathrm{Im}\,\frac{\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} = \mathrm{Im}\,\frac{\langle\Psi|\big(E - \hat{H}_C - \hat{H}_S\big)\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} \tag{3.1.57}$$

[2] This is the space ("ray space") in which $\gamma|\varphi\rangle_S$ and $|\varphi\rangle_S$ are identified for $\gamma \in \mathbb{C}\backslash\{0\}$ and belong to the same equivalence class.

$$= -\operatorname{Im}\frac{\langle\Psi|\hat{H}_C\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} = -\frac{1}{2}\frac{\langle\Psi|\left[-i\hat{H}_C,\hat{P}_\chi\right]|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} \tag{3.1.58}$$

$$= -\frac{1}{2}\frac{\langle\Psi|\left(\mathrm{d}\hat{P}_\chi/\mathrm{d}\lambda\right)|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\langle\Psi|\hat{P}_\chi|\Psi\rangle\,. \tag{3.1.59}$$

Hence,

$$e^{\int_0^\lambda \mathrm{d}\lambda'\,\mathrm{Im}\,a(\lambda')} = \sqrt{\frac{\langle\Psi|\hat{P}_\chi(0)|\Psi\rangle}{\langle\Psi|\hat{P}_\chi(\lambda)|\Psi\rangle}} \tag{3.1.60}$$

and a small $\lambda = \kappa \ll 1$ allows for the approximation

$$\sqrt{\frac{\langle\Psi|\hat{P}_\chi(0)|\Psi\rangle}{\langle\Psi|\hat{P}_\chi(\kappa)|\Psi\rangle}} = e^{\int_0^\kappa \mathrm{d}\lambda'\,\mathrm{Im}\,a(\lambda')} = e^{\kappa\,\mathrm{Im}\,a(0)} + \mathcal{O}(\kappa^2)\,. \tag{3.1.61}$$

Clearly, the prefactor normalizes the system state. Dividing both sides of Eq. (3.1.56) by $\sqrt{\langle\Psi|\chi_0\rangle\langle\chi_0|\Psi\rangle}$ provides us with the final version for the "infinitesimal" step for the normalized system state

$$e^{-i\kappa\left(\hat{H}_S+\hat{V}_S(0)\right)}|\varphi(0)\rangle_S = \frac{\langle\chi(\kappa)|\Psi\rangle_C}{\sqrt{\langle\Psi|\chi(\kappa)\rangle\langle\chi(\kappa)|\Psi\rangle}} + \mathcal{O}(\kappa^2) = |\varphi(\kappa)\rangle_S + \mathcal{O}(\kappa^2) \tag{3.1.62}$$

with the same clock state $|\chi(\lambda)\rangle_C = \exp\left[-i\lambda(\hat{H}_C - E)\right]|\chi_0\rangle_C$ as in Eq. (3.1.15) of the preceding section.

3.1.6.3 Consecutive transformations

For illustration, we perform two infinitesimal steps, i.e.,

$$\langle\chi_0|\Psi\rangle_C = \langle\chi_0|e^{2i\kappa(\hat{H}_C+\hat{H}_S+\hat{V}-E)}|\Psi\rangle_C \tag{3.1.63}$$

$$= e^{i\kappa\left(\hat{H}_S+\hat{V}_S(0)-i\,\mathrm{Im}\,a(0)\right)}\langle\chi(\kappa)|e^{i\kappa(\hat{H}_C+\hat{H}_S+\hat{V}-E)}|\Psi\rangle_C + \mathcal{O}(\kappa^2) \tag{3.1.64}$$

$$= e^{i\kappa\left(\hat{H}_S+\hat{V}_S(0)-i\,\mathrm{Im}\,a(0)\right)}e^{i\kappa\left(\hat{H}_S+\hat{V}_S(\kappa)-i\,\mathrm{Im}\,a(\kappa)\right)}\langle\chi(2\kappa)|\Psi\rangle_C + \mathcal{O}(\kappa^2)\,. \tag{3.1.65}$$

Using the same operations as above, the system state transforms as

$$|\varphi(2\kappa)\rangle_S = e^{i\kappa\left(\hat{H}_S+\hat{V}_S(\kappa)\right)}e^{i\delta\left(\hat{H}_S+\hat{V}_S(0)\right)}|\varphi(0)\rangle_S + \mathcal{O}(\kappa^2) \tag{3.1.66}$$

and progressive use of this form for finite λ yields

$$\langle\chi_0|e^{i\lambda(\hat{H}_C+\hat{H}_S+\hat{V}-E)}|\Psi\rangle_C = \left(\overline{\mathcal{T}}e^{i\int_0^\lambda \mathrm{d}\lambda'\left[\hat{H}_S+\hat{V}_S(\lambda')\right]}\right)\langle\chi_0|e^{i\lambda(\hat{H}_C-E)+\int_0^\lambda \mathrm{d}\lambda'\,\mathrm{Im}\,a(\lambda')}|\Psi\rangle_C \tag{3.1.67}$$

in the limit $N \to \infty$ and with anti-λ-ordering operator $\overline{\mathcal{T}}$. The exponential term involving $\mathrm{Im}\,a(\lambda)$ ensures the system state's normalization for all λ. With the definitions from above, we get

$$|\varphi(\lambda)\rangle_S = \mathcal{T}e^{-i\int_0^\lambda \mathrm{d}\lambda'\left[\hat{H}_S+\hat{V}_S(\lambda')\right]}|\varphi(0)\rangle_S \tag{3.1.68}$$

with λ-ordering operator $\mathscr{T}$ and, after applying a simple derivative with respect to λ, also the system TDSE

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\varphi(\lambda)\rangle_\mathrm{S} = \left[\hat{H}_\mathrm{S} + \hat{V}_\mathrm{S}(\lambda)\right]|\varphi(\lambda)\rangle_\mathrm{S}\,. \tag{3.1.69}$$

Once again, the parameter λ appears in place of the traditional time t, even under the presence of an interaction between clock and system. Equation (3.1.69) represents one of the main results of this thesis. Despite the presence of a system-clock coupling, the form of the clock evolution (3.1.15) remains unchanged. Subsequently, a notable property from Sec. 3.1.5 holds, namely that only non-vanishing clock Hamiltonians $\hat{H}_\mathrm{C} \neq 0$ can induce physical changes in the system, regardless of the initial state $|\chi_0\rangle_\mathrm{C}$. Otherwise, only the global phase of the system state changes by $\exp(-i\lambda E)$ for $\hat{H}_\mathrm{C} = 0$. A major feature of the effective system TDSE is the inextricable link between the effective system potential and the initial system state. Any change of the initial clock state results in a simultaneous change of the potential and the initial system state in general.

To the best of our knowledge, the only other works treating the PW approach with an interaction term [105,106] are solely able to derive a system TDSE with a time-convoluted effective potential, which reduces to a time-local expression only for special interactions. In addition, the authors rely on $\hat{H}_\mathrm{C} = \hat{K}$, the existence of a time operator with $[\hat{H}_\mathrm{C}, \hat{T}_\mathrm{C}] = i$ and the eigenstates of $\hat{T}_\mathrm{C}$ as clock states. As we have demonstrated successfully, neither the time-convolution nor a very special clock is necessary to obtain unitary dynamics with an exact effective potential. Interestingly, this situation resembles a historical development in open systems theory. In 1977, Hashitsume et al. [196] published a derivation of a time-convolutionless formulation of master equations and, thus, their approach succeeded the Nakajima-Zwanzig formalism [197,198] from around 1960, which contains memory effects.

3.1.6.4 Second order contributions

We omitted the remaining term scaling with $\mathscr{O}(\kappa^2)$ in Eq. (3.1.69). However, a careful researcher could argue that a summation of all small transformations can lead to a scaling $\mathscr{O}(N\kappa^2) = \mathscr{O}(\lambda\kappa)$ which is linear in κ. In that case, the remainder term could be as important as the effective system Hamiltonian. To rule out this possibility, we perform a simple check by assuming the clock evolution to be *a priori* given by $|\chi(\lambda)\rangle_\mathrm{C} = \exp\left[-i\lambda(\hat{H}_\mathrm{C} - E)\right]|\chi_0\rangle_\mathrm{C}$. Our previous treatment provides this form of the evolution and it suffices now to show that the conditional system state is governed by Eq. (3.1.69). The important terms are

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\chi|\Psi\rangle_\mathrm{C} = -\langle\Psi|(\hat{H}_\mathrm{C} - E)|\chi\rangle_\mathrm{C} = \langle\Psi|(\hat{H}_\mathrm{S} + \hat{V})|\chi\rangle_\mathrm{C}\,, \tag{3.1.70}$$

$$i\frac{\mathrm{d}\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}{\mathrm{d}\lambda} = \langle\Psi|\left[\hat{H}_\mathrm{C}, |\chi\rangle\langle\chi|_\mathrm{C}\right]|\Psi\rangle = -\langle\Psi|\left[\hat{V}, |\chi\rangle\langle\chi|_\mathrm{C}\right]|\Psi\rangle \tag{3.1.71}$$

and the change of the conditional system state reads

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\varphi\rangle_\mathrm{S} = i\frac{\mathrm{d}}{\mathrm{d}\lambda}\frac{\langle\chi|\Psi\rangle_\mathrm{C}}{\sqrt{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}} \tag{3.1.72}$$

$$= \frac{\langle\chi|\left(\hat{H}_\mathrm{S} + \hat{V}\right)|\Psi\rangle_\mathrm{C}}{\sqrt{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}} + |\varphi\rangle_\mathrm{S}\underbrace{\frac{\langle\Psi|\left[\hat{V}, |\chi\rangle\langle\chi|_\mathrm{C}\right]|\Psi\rangle}{2\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}}_{=i\,\mathrm{Im}\,a} \tag{3.1.73}$$

$$\overset{(3.1.52)}{=} \left[\hat{H}_C + \hat{V}_S\right]|\varphi\rangle_S \underbrace{-i\,\mathrm{Im}\,a\,|\varphi\rangle_S + i\,\mathrm{Im}\,a\,|\varphi\rangle_S}_{=0}\,. \tag{3.1.74}$$

Clearly, no additional term appears and, indeed, we verify our treatment of neglecting the $\mathcal{O}(\kappa^2)$ contributions to be correct. The analytical exactness of the final result is worth mentioning, because the derivation does not require any approximation. However, the possibility for a simplification of the effective system potential exists under specific circumstances. Before we present those, we showcase our formalism with a specific example. Not only can we point out certain important features of our framework, but we demonstrate how fully analytical solutions to time-dependent problems can be obtained.

3.1.7 Illustration for coupled harmonic oscillators

For any application, we need to calculate an energy eigenstate $|\Psi\rangle$ as an essential element of our framework, either analytically or numerically. Such a formidable task is difficult in general, but the mathematical freedom to change the tensor product structure of the Hilbert space may provide means for its realization. Specifically, we assume a partitioning $\mathscr{H} = \mathscr{H}'_S \otimes \mathscr{H}'_C$ to exist, in which the global Hamiltonian $\hat{H}'$ allows for an easy computation of the energy eigenstate $|\Psi\rangle$. One example is an interaction-free global system with well-known subsystem Hamiltonians. A change in the tensor product structure induces a new factorization $\mathscr{H} = \mathscr{H}_S \otimes \mathscr{H}_C$ and, simultaneously, transforms the Hamiltonian to a new form $\hat{H}$. Such an operation effectively corresponds to a basis transformation and leaves the global state $|\Psi\rangle$ unaltered. This procedure shifts the main task from solving a complicated TISE to finding the correct transformation from a simple Hamiltonian $\hat{H}'$ to a desired Hamiltonian $\hat{H}$. For illustration, we present one example in this section, namely two coupled oscillators obtained from a single harmonic oscillator and a free particle, which are not coupled.

The combination of a harmonic oscillator and a non-interacting free particle can be described by the separable Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2} + \frac{1}{2}\hat{x}^2\,. \tag{3.1.75}$$

For simplicity, the frequency ω of the oscillator and the two masses M_x and M_y are set to one. Both systems are well known and allow for an easy determination of the energy spectrum [199]

$$E(n,k) = \frac{1}{2}k^2 + \left(n + \frac{1}{2}\right) \geq 0 \qquad\qquad n \in \mathbb{N}_0, k \in \mathbb{R}\,. \tag{3.1.76}$$

Their associated eigenstates

$$\Psi_{n,k}(x,y) = \frac{1}{\sqrt{2\pi}} e^{-iky} \cdot \eta_n(x)\,. \tag{3.1.77}$$

include the energy eigenstates

$$\eta_n(x) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(x)\, e^{-x^2/2}\,. \tag{3.1.78}$$

of the harmonic oscillator $\hat{H}_{\mathrm{osc}} = (\hat{p}_x^2 + \hat{x}^2)/2$ [183]. The physicist's version of the Hermite polynomials is $H_n(x) = (-1)^n e^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}y^n}\left(e^{-x^2}\right)$ and some of their properties are detailed in Appendix B. Hence, the global energy eigenstate reads

$$\Psi_{n,k}(x,y) = \frac{1}{\pi^{1/4}\sqrt{2^{n+1}\pi n!}}\, e^{-iky}\, H_n(x)\, e^{-x^2/2}\,. \tag{3.1.79}$$

Interestingly, most eigenenergies E possess a degenerate subspace and the set $\{n_i\}_{0\leq n\leq E-1/2}$ labels the corresponding momenta

$$k_i = k(E,n_i) = \pm\sqrt{2(E-n_i)-1}\,, \tag{3.1.80}$$

which provide different orthogonal states for fixed energy E. The most general energy eigenstate can be expressed as

$$\Psi(x,y) = \sum_i c_i\,\Psi_{n_i,k_i}(x,y) \tag{3.1.81}$$

with complex coefficients c_i.

In order to introduce an interaction, we modify the tensor product structure of $\mathscr{H}$. Such a change is facilitated by a variable transformation $(x,y)\to(r,s)$ and we define the new variables

$$x = r\cos\theta - s\sin\theta \tag{3.1.82}$$
$$y = s\cos\theta + r\sin\theta \tag{3.1.83}$$

with a fixed rotation angle θ. For simplicity, we assume θ to only take the values

$$0<\cos\theta<1 \qquad \text{and} \qquad 0<\sin\theta<1 \tag{3.1.84}$$

or $0<\theta<\pi/2$ and note that $\mathrm{d}x\,\mathrm{d}y = \mathrm{d}r\,\mathrm{d}s$. Applying this basis transformation yields the transformed Hamiltonian

$$\hat{H} = \underbrace{\frac{\hat{p}_r^2}{2}+\frac{\cos^2\theta}{2}\hat{r}^2}_{=\hat{H}_\mathrm{C}} + \underbrace{\frac{\hat{p}_s^2}{2}+\frac{\sin^2\theta}{2}\hat{s}^2}_{=\hat{H}_\mathrm{S}} + \underbrace{\sin(2\theta)\cdot\hat{s}\otimes\hat{r}}_{=\hat{V}}, \tag{3.1.85}$$

which describes two coupled harmonic oscillators with natural frequencies $\omega_r\equiv\cos\theta$ and $\omega_s\equiv\sin\theta$, respectively. As a side note, it is also possible to start from two position-coupled harmonic oscillators with different masses and frequencies and, subsequently, find an inverse coordinate transformation to obtained two uncoupled system [200]. Expressed in the new variables, the global energy eigenstates read

$$\Psi_{n,k}(r,s) = \frac{1}{\pi^{1/4}\sqrt{2^{n+1}\pi n!}}e^{-ik(s\cos\theta+r\sin\theta)}\,H_n(r\cos\theta-s\sin\theta)\,e^{-(r\cos\theta-s\sin\theta)^2/2}\,. \tag{3.1.86}$$

and clearly reveal the entanglement between the two degrees of freedom, r and s, respectively, due to a loss of separability.

We employ well-known wavefunctions for the clock states, namely the coherent states [183, 201]

$$\begin{aligned}\alpha(r,\lambda,\omega,r_0) = \left(\frac{\omega}{\pi}\right)^{\frac{1}{4}}&\exp\left[-\frac{i}{2}\big(\omega\lambda + r_\mathrm{cl}(\lambda)\cdot p_\mathrm{cl}(\lambda)\big)\right]\\ &\cdot\exp\left[-\frac{\omega}{2}\big(x-r_\mathrm{cl}(\lambda)\big)^2\right]\exp\big[ir\cdot p_\mathrm{cl}(\lambda)\big]\end{aligned} \tag{3.1.87}$$

evolving under the Hamiltonian $\hat{H}_\mathrm{osc} = (\hat{p}_r^2+\omega^2\hat{r}^2)/2$ with the classical trajectories

$$r_\mathrm{cl}(\lambda) = r_0\cos(\omega\lambda) \tag{3.1.88}$$
$$p_\mathrm{cl}(\lambda) = -\omega r_0\sin(\omega\lambda)\,. \tag{3.1.89}$$

This particularly simple form is linked to special initial conditions $r_{\mathrm{cl}}(0) = r_0$ and $p_{\mathrm{cl}}(0) = 0$. Complex conjugation of the coherent state yields

$$\alpha^*(r,\lambda,\omega,r_0) = \left(\frac{\omega}{\pi}\right)^{1/4} e^{i\left(\omega\lambda + r_{\mathrm{cl}}(\lambda)\cdot p_{\mathrm{cl}}(\lambda)\right)/2}\, e^{-ir\cdot p_{\mathrm{cl}}(\lambda)}\, e^{-\omega\left(r - r_{\mathrm{cl}}(\lambda)\right)^2/2} \tag{3.1.90}$$

and, therefore, the density in position space reads

$$|\alpha(r,\lambda,\omega,r_0)|^2 = \sqrt{\frac{\omega}{\pi}}\,\exp\left[-\omega\left(r - r_{\mathrm{cl}}(\lambda)\right)^2\right]. \tag{3.1.91}$$

The prefactor ensures the normalization $\int \mathrm{d}x\, |\alpha(r,\lambda,\omega,r_0)|^2 = 1$. Using these special states, we define the clock state to be

$$\langle\chi(\lambda)|r\rangle_{\mathrm{C}} \equiv \alpha^*(r,\lambda,\omega_r,r_0)\cdot\exp\left[-i\lambda E\right] \tag{3.1.92}$$

with the clock frequency $\omega_r = \cos\theta$. In essence, all clock states considered are characterized by their initial mean position r_0. Obviously, other clock states can be used, but coherent states allow to analytically calculate some of the occurring integrals, because of to their Gaussian nature.

The unnormalized conditional system state is

$$|\phi(\lambda)\rangle_{\mathrm{S}} = \langle\chi(\lambda)|\Psi\rangle_{\mathrm{C}} = \sum_i c_i \left\langle\chi(\lambda)\middle|\Psi_{n_i,k_i}\right\rangle_{\mathrm{C}}. \tag{3.1.93}$$

For the sake of simplicity, we only take the simple form $|\Psi\rangle = \left|\Psi_{n,k}\right\rangle$ in the following for a fixed pair of n and k. Individual conditional system states in s-basis are

$$\phi_{n,k}(s,\lambda) = \left\langle s\otimes\chi(\lambda)\middle|\Psi_{n,k}\right\rangle \tag{3.1.94}$$

and have the exact form

$$\begin{aligned}\phi_{n,k}(s,\lambda) = \mathcal{N}_{n,k}(\lambda)\, e^{-i\zeta(\lambda)}\,\exp\left[-is\left(k + \frac{p_{\mathrm{cl}}(\lambda)\sin\theta}{1+\cos\theta}\right)\right]\exp\left[-\frac{\left(s - r_{\mathrm{cl}}(\lambda)\cot\theta\right)^2}{2(1-\cos\theta)}\right]\\ \cdot H_n\left[s - r_{\mathrm{cl}}(\lambda)\cot\theta + i\mathsf{L}(\lambda)\right].\end{aligned} \tag{3.1.95}$$

The details of the calculation and the definitions of the prefactor $\mathcal{N}_{n,k}$, the phase ζ and the modified momentum L can be found in Appendix C. Parts of expression (3.1.95) resemble a coherent state, namely the second and third exponential terms with a slightly adjusted classical momentum. However, the λ-dependent Hermite polynomial modulates the shape of the system wavefunction and is a remnant of the harmonic oscillator energy eigenfunction η in Ψ. Such a composite expression promises interesting system dynamics and an illustration for $n = 1$ is shown in Fig. 3.6, together with the free evolution ($\hat{V}_{\mathrm{S}} = 0$) for comparison. Equation (3.1.95) exhibits an important feature of our formalism, namely the cyclic structure. All λ-dependencies in the system state are linked to the classical phase space trajectory $\left(r_{\mathrm{cl}}(\lambda), p_{\mathrm{cl}}(\lambda)\right)$ of the clock and must follow the periodicity of the clock. In other words, once the clock state returns to its initial state $|\chi_0\rangle_{\mathrm{C}}$, the system must inevitably return to its initial state as well. Any natural periodicity of the system (here $2\pi/\omega_s$) can loose its meaning. If system and clock freely evolve on very different time scales and the interaction is weak, then the dynamics can still display both scales. However, our example does not allow for this possibility. A further display of the cyclic property occurs through the mean position

$$\frac{\left\langle\phi_{n,k}\middle|\hat{s}\middle|\phi_{n,k}\right\rangle_{\mathrm{S}}}{\left\langle\phi_{n,k}\middle|\phi_{n,k}\right\rangle_{\mathrm{S}}} = r_{\mathrm{cl}}\cot\theta \tag{3.1.96}$$

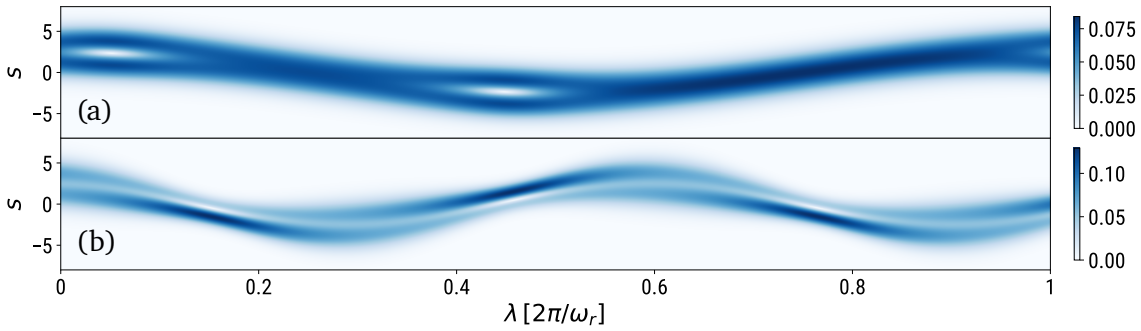

Figure 3.6 – The evolution of the system wavefunctions for an uncoupled and coupled harmonic oscillator, due to (3.1.85), is compared by means of their absolute values. Panel (a) shows the exact system evolution of the relational system state $|\varphi(s,\lambda)|$, whereas the free evolution of the harmonic oscillator, due to $\hat{H}_S$ and with the same initial state as in (a), is presented in (b) for comparison. The shown dynamics corresponds to total energy $E = 1.8$, basis rotation angle $\theta = 0.325\pi$ and momentum $k \approx 0.775$ in atomic units (see App. D). Clearly, the coupled harmonic oscillator (principal system) does not display its natural periodicity any longer.

of the system (App. C), which, in addition, does not depend on n or k.

The squared norm of these states is

$$\left\langle \phi_{n,k} \middle| \phi_{n,k} \right\rangle_S = \frac{\mathcal{N}_{n,k}^2}{\sqrt{1-\cos\theta}} \sum_{\substack{l,m=0 \\ l+m \text{ even}}}^{n} \binom{n}{m}\binom{n}{l} (2\mathsf{L})^{2n-(l+m)}\, i^{l-m}\, 2^{m+l}\, \Gamma\left(\frac{m+l+1}{2}\right) \cdot \sqrt{\frac{\cos\theta}{1-\cos\theta}}^{\,l+m} {}_2F_1\left(-m,-l;\frac{1-l-m}{2};\frac{\cos\theta-1}{2\cos\theta}\right) \tag{3.1.97}$$

with the hypergeometric functions ${}_2F_1(a,b;c;z)$ and allows us to express the normalized system state $\left|\varphi_{n,k}\right\rangle_S$ in an analytically exact fashion. Specifically for the $n = 1$ example, the normalized system state in position basis reads

$$\varphi_{1,k} = -\left(\frac{1-\cos\theta}{\pi}\right)^{1/4} \sqrt{\frac{1-\cos\theta}{2\mathsf{L}^2(1-\cos\theta)+1}}\,(s - r_{\mathrm{cl}}\cot\theta + i\mathsf{L})\, e^{-i\zeta} \cdot \exp\left[-is\left(k + \frac{p_{\mathrm{cl}}\sin\theta}{1+\cos\theta}\right)\right] \exp\left[-\frac{\left(s - r_{\mathrm{cl}}\cot\theta\right)^2}{2(1-\cos\theta)}\right]. \tag{3.1.98}$$

In general, the states (3.1.95) evolve under the influence of the effective system potential

$$\hat{V}_S = r_{\mathrm{cl}}\sin(2\theta)\left(\hat{P}_\varphi\,\hat{s} + \hat{s}\,\hat{P}_\varphi\right) - (2r_{\mathrm{cl}}^2\cos^2\theta + \cos\theta) + 2i\left[\hat{P}_\varphi\left(\cos\theta\,\hat{p}_s + k + p_{\mathrm{cl}}\sin\theta\right)\hat{s} - \hat{s}\left(\cos\theta\,\hat{p}_s + k + p_{\mathrm{cl}}\sin\theta\right)\hat{P}_\varphi\right], \tag{3.1.99}$$

which is also calculated in Appendix C. A slight simplification follows from the operation on the system state $|\varphi\rangle_S$, because of the cancellation of two terms. The resulting expression is

$$\hat{V}_S\left|\varphi_{n,k}\right\rangle_S = \Big\{\underbrace{r_{\mathrm{cl}}\sin(2\theta)\hat{s}}_{=\langle\chi|\hat{V}|\chi\rangle_C} + \cos\theta + 2i\,(k + p_{\mathrm{cl}}\sin\theta)\left[\hat{P}_\varphi,\hat{s}\right] + i\cos\theta\left[\hat{P}_\varphi,\hat{s}\,\hat{p}_s + \hat{p}_s\,\hat{s}\right]\Big\}\left|\varphi_{n,k}\right\rangle_S \tag{3.1.100}$$

and features the operator-valued mean value $\langle\chi|\hat{V}|\chi\rangle_C$. Such a term modifies the minimum position of the harmonic system potential and oscillates with the natural frequency ω_r of the clock. Unfortunately, the other terms do not allow for an easy interpretation, except for the trivial energy shift from the constant term. For a validity check of our results, we numerically compared the relational framework with the sequential time evolution and found perfect agreement. A representation of $\hat{V}_S$ in position basis can be straightforwardly calculated. However, instead of presenting the results for $n = 1$ in the main text, we provide these more complex expressions in Appendix C.

In summary, we have derived an analytical solution to a time-dependent problem, which features a complicated time-dependent potential. Although special, such exact solutions are very rare in physics. The change of the tensor product structure of the global Hilbert space proves essential in our derivation and might be useful for other problems too. As a significant consequence of our approach, the obtained system dynamics clearly exhibits the cyclic structure of the clock.

3.1.8 Approximations for effective potential

The evaluation of the effective system potential can be complicated, because it depends on $|\Psi\rangle$, $\hat{V}$ and $|\chi\rangle_C$. In this section, we show two approximations, which simplify the expression for $\hat{V}_S$. Additionally, we point out a relation between both approximations and provide connections to previous works, as well as another numerical example.

3.1.8.1 Clock quasi-eigenstate of interaction

A straightforward approximation concerns the action of the coupling $\hat{V}$ on the clock state $|\chi\rangle_C$. If $|\chi\rangle_C$ is almost an eigenstate, a "quasi-eigenstate", of the $\mathscr{H}_C$-part of the interaction $\hat{V}$, then one can neglect the components of $\hat{V}|\chi\rangle_C$ that are orthogonal to $|\chi\rangle_C$. In mathematical notation, this statement translates to

$$\hat{V}|\chi\rangle_C = \big(\hat{P}_\chi + \underbrace{\hat{\bar{P}}_\chi}_{\approx 0}\big)\hat{V}|\chi\rangle_C \approx \langle\chi|\hat{V}|\chi\rangle_C\,|\chi\rangle_C \tag{3.1.101}$$

with the complementary clock state projector $\hat{\bar{P}}_\chi \equiv \hat{\mathbb{1}}_C - \hat{P}_\chi$. The term $\langle\chi|\hat{V}|\chi\rangle_C$ is an effective operator acting in the system Hilbert space $\mathscr{H}_S$, because the scalar product is only taken in $\mathscr{H}_C$. Ideally, this approximation should hold true for all λ, but for numerical purposes it may suffice to hold only for a certain range of interest.

Surprisingly, an element of decoherence theory mentioned in Section 3.1.4 has an intriguing reappearance here, namely the "pointer state". These states are characterized by their robustness against entanglement buildup with an environment under the evolution of a total Hamiltonian, which includes the self-Hamiltonians and an interaction with the environment [147]. In the "quantum-measurement limit", which neglects the self-Hamiltonian (here $\hat{H}_C$), the pointer states are simply the eigenstates of the interaction and are absolutely stable [202]. Yet, the aforementioned situation might be too idealized in most applications and it is necessary to include the self-Hamiltonian. In this case, the pointer states are determined by their ability to become the least entangled with the environment (on the time scale of interest). This procedure, known as "predictability sieve" [139, 159], has been employed to find coherent states as the most robust pointer states for a harmonic oscillator coupled linearly via its position to a heat bath [202], even though the eigenstates of the interaction are position eigenstates. These ideas seem to be in close analogy to Eq. (3.1.101) and, for this reason, we suspect that the predictability sieve might be a useful

procedure to find clock states well-suited for the quasi-eigenstate approximation.

Since our framework does not require the stand-alone term (3.1.101), but only the partial scalar product $\langle\chi|\hat{V}|\Psi\rangle_C$, the slightly weaker condition

$$\langle\chi(\lambda)|\hat{V}\hat{\bar{P}}_\chi|\Psi\rangle_C \approx 0 \tag{3.1.102}$$

can be used. It allows for non-vanishing orthogonal parts $\hat{\bar{P}}_\chi\hat{V}\,|\chi(\lambda)\rangle_C$ as long as they are not contained in $|\Psi\rangle$. For simplicity, we keep the name "quasi-eigenstate approximation", even though the weaker form does not necessitate an approximate eigenstate in principle. However, it is much easier in practice to find genuine quasi-eigenstates and, as is shown below, we can connect our approach to prior works with Eq. (3.1.101). If this approximation is sufficiently accurate, then the effective system potential reduces to

$$\hat{V}_S(\lambda)\,|\varphi\rangle_S \approx \langle\chi(\lambda)|\hat{V}|\chi(\lambda)\rangle_C\,|\varphi\rangle_S \tag{3.1.103}$$

for all relevant λ applied to the system state and $\hat{V}_S$ does no longer depend on $|\Psi\rangle$. In case approximation (3.1.102) holds exactly true, the norm of $|\phi\rangle_S = \langle\chi|\Psi\rangle_C$ is preserved, as can be easily proven with

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\langle\phi|\phi\rangle_S = \mathrm{Im}\,\frac{\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} \overset{(3.1.102)}{=} \mathrm{Im}\underbrace{\frac{\langle\phi\otimes\chi|\hat{V}|\phi\otimes\chi\rangle}{\langle\phi|\phi\rangle_S}}_{\in\mathbb{R}} = 0 \tag{3.1.104}$$

from Eq. (3.1.59). As a result, the norm change of $|\phi\rangle$ provides a quantifier for the error induced by the quasi-eigenstate approximation (3.1.102). A more rigorous error analysis can be facilitated by the difference vector

$$|\Xi\rangle_S \equiv \left(\hat{V}_S - \langle\chi|\hat{V}|\chi\rangle_C\right)|\varphi\rangle_S \tag{3.1.105}$$

$$= \left(\langle\chi|\hat{V}|\chi\rangle_C\hat{P}_\varphi + \hat{P}_\varphi\langle\chi|\hat{V}|\chi\rangle_C\right)|\varphi\rangle_S - \left(\mathrm{Re}\,a + \langle\chi|\hat{V}|\chi\rangle_C\right)|\varphi\rangle_S + \frac{\langle\chi|\left(\hat{V}\hat{\bar{P}}_\chi\hat{P}_\Psi + \hat{P}_\Psi\hat{\bar{P}}_\chi\hat{V}\right)|\chi\rangle_C}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}|\varphi\rangle_S \tag{3.1.106}$$

$$= \frac{\langle\chi|\left(\hat{V}\hat{\bar{P}}_\chi\hat{P}_\Psi + \hat{P}_\Psi\hat{\bar{P}}_\chi\hat{V}\right)|\chi\rangle_C}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}|\varphi\rangle_S - \left(\mathrm{Re}\,\frac{\langle\Psi|\hat{\bar{P}}_\chi\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}\right)|\varphi\rangle_S \tag{3.1.107}$$

$$= \frac{\langle\chi|\hat{V}\hat{\bar{P}}_\chi|\Psi\rangle_C}{\sqrt{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}} + |\varphi\rangle_S\cdot i\underbrace{\mathrm{Im}\,\frac{\langle\Psi|\hat{\bar{P}}_\chi\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}}_{=\mathrm{Im}\,a}, \tag{3.1.108}$$

because its norm

$$Z^2 \equiv \langle\Xi|\Xi\rangle_S \tag{3.1.109}$$

$$= (\mathrm{Im}\,a)^2 + \frac{\langle\Psi|\hat{\bar{P}}_\chi\hat{V}\hat{P}_\chi\hat{V}\hat{\bar{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} + i\,\mathrm{Im}\,a\underbrace{\left[\frac{\langle\Psi|\left(\hat{\bar{P}}_\chi\hat{V}\hat{P}_\chi - \hat{P}_\chi\hat{V}\hat{\bar{P}}_\chi\right)|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}\right]}_{=2i\,\mathrm{Im}\,a} \tag{3.1.110}$$

$$= \frac{\langle\Psi|\hat{\bar{P}}_\chi \hat{V} \hat{P}_\chi \hat{V} \hat{\bar{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} - (\mathrm{Im}\, a)^2 \tag{3.1.111}$$

quantifies the instantaneous error due to the approximation. It is used in Sec. 3.1.8.4 to numerically assess the deviation from the exact evolution.

Considering that $|\Psi\rangle$ appears in Eq. (3.1.111), one might prefer an error measure for the stronger form (3.1.101) of the quasi-eigenstate approximation, because it does not depend on $|\Psi\rangle$. In a fashion similar to the analysis above, the definition of a difference operator

$$\hat{\Xi}_\mathrm{S} \equiv \langle\chi|\hat{V}\hat{\bar{P}}_\chi\hat{V}|\chi\rangle_\mathrm{C}\,, \tag{3.1.112}$$

acting in $\mathscr{H}_\mathrm{S}$, can shed light on the issue of finding a suitable quantifier. Yet, we must find a contracted form to yield a single real number. To this end, we could either use a matrix norm, such as the Hilbert-Schmidt norm $\left\|\hat{A}_\mathrm{S}\right\|_\mathrm{S}^2 \equiv \mathrm{tr}_\mathrm{S}(\hat{A}_\mathrm{S}^\dagger \hat{A}_\mathrm{S})$ [203], or use the mean value with respect to a certain normalized system state $|\tau\rangle_\mathrm{S} \in \mathscr{H}_\mathrm{S}$. Unfortunately, both options can yield infinity for unbounded operators, unless we restrict to the effective system Hilbert space spanned by the states in $\Pi_{\mathrm{S},\Psi}$ from the end of Sec. 3.1.5. However, determining $\Pi_{\mathrm{S},\Psi}$ requires once again knowledge of the global state $|\Psi\rangle$. Being aware of this issue, we nevertheless define

$$Z^2_\mathrm{strong} \equiv \max_{\substack{|\tau\rangle_\mathrm{S}\in\mathscr{H}_\mathrm{S}\\ \langle\tau|\tau\rangle_\mathrm{S}=1}} \langle\tau|\hat{\Xi}_\mathrm{S}|\tau\rangle_\mathrm{S} = \max_{\substack{|\tau\rangle_\mathrm{S}\in\mathscr{H}_\mathrm{S}\\ \langle\tau|\tau\rangle_\mathrm{S}=1}} \langle\tau\otimes\chi|\hat{V}\hat{\bar{P}}_\chi\hat{V}|\tau\otimes\chi\rangle \tag{3.1.113}$$

and acknowledge its inadequacy for unbounded $\hat{V}$. In practice, most interactions are of the simple form

$$\hat{V} = \hat{W}_\mathrm{S} \otimes \hat{W}_\mathrm{C} \tag{3.1.114}$$

for $\hat{W}_\mathrm{S}$ and $\hat{W}_\mathrm{C}$ acting only in $\mathscr{H}_\mathrm{S}$ and $\mathscr{H}_\mathrm{C}$, respectively. For instance, position-position coupling $\hat{V} \propto \hat{q}_1 \otimes \hat{q}_2$ [204, 205] and spin-spin interaction $\hat{V} \propto \hat{\sigma}_{1,i} \otimes \hat{\sigma}_{2,j}$ [206] represent just two of many examples. Here, $\hat{\sigma}_{n,i}$ represent the Pauli matrices [145] for $n \in \{1,2\}$ and $i \in \{x,y,z\}$. For the separable interaction (3.1.114), the error (3.1.113) factorizes to

$$Z^2_\mathrm{strong,sep} = \underbrace{\langle\chi|\hat{W}_\mathrm{C}\hat{\bar{P}}_\chi\hat{W}_\mathrm{C}|\chi\rangle_\mathrm{C}}_{=\mathrm{Var}_\chi[\hat{W}_\mathrm{C}]} \cdot \max_{\substack{|\tau\rangle_\mathrm{S}\in\mathscr{H}_\mathrm{S}\\ \langle\tau|\tau\rangle_\mathrm{S}=1}} \langle\tau|\hat{W}_\mathrm{S}^2|\tau\rangle_\mathrm{S} \tag{3.1.115}$$

and the second factor is independent of the clock state. Hence, the variance of $\hat{W}_\mathrm{C}$ with respect to the clock state $|\chi\rangle_\mathrm{C}$ quantifies the deviation from being in an exact eigenstate of $\hat{W}_\mathrm{S}$, as was to be expected. In addition, by focusing only on the first factor, a possible unboundedness of the second factor can be tolerated. For example, the variance $\mathrm{Var}_\chi[\hat{W}_\mathrm{C}]$ is used in Section 3.1.8.4. If the variance cannot give a conclusive answer as in Section 3.1.8.3, we can use the relative error

$$Z^2_\mathrm{rel} \equiv \frac{\mathrm{Var}_\chi[\hat{W}_\mathrm{C}]}{\langle\chi|\hat{W}_\mathrm{C}|\chi\rangle^2_\mathrm{C}} \tag{3.1.116}$$

as a dimensionless alternative. In this form, the variance is compared to the strength of the interaction.

3.1.8.2 Connection to quantization of constrained system

As mentioned in Chapter 1, the classical constraint (1.4) has been used as the starting point for a quantization procedure in order to derive the TDSE [76, 77]. The quantized version of constraint (1.4) is the TISE

$$\hat{H}\,|\Psi\rangle = \left(\hat{P}_t + \frac{1}{2m}\hat{p}^2 + V(\hat{q},\hat{t})\right)|\Psi\rangle = 0 \tag{3.1.117}$$

with the position operator $\hat{t}$ and its associated momentum operator $\hat{P}_t$. A representation of the TISE in a global position basis reads

$$\left(-i\hbar\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + V(q,t)\right)\Psi(x,t) = 0 \tag{3.1.118}$$

and its form equivalence to the TDSE is then used as a claim for a successful emergence of time. However, this derivation depends explicitly on a special basis and does not explain any relation to a physical clock state. Effectively, the resulting TDSE is just a TISE in disguise. Nonetheless, we can use the quasi-eigenstate approximation to derive a genuine TDSE of the same form. The special nature of the clock Hamiltonian $\hat{H}_\mathrm{C} = \hat{P}_t$ allows for a straightforward relation, because any wavepacket in the t-position basis is non-dispersing. If the initial clock state is chosen as a position eigenstates (or a very narrow wavepacket), i.e.,

$$|\chi_0\rangle_\mathrm{C} = |t_0\rangle_\mathrm{C}\,, \tag{3.1.119}$$

then its associated λ-evolution has the simple form

$$|\chi(\lambda)\rangle_\mathrm{C} = |t_0+\lambda\rangle_\mathrm{C}\,. \tag{3.1.120}$$

In this case, the clock states are actual eigenstates of the interaction, because

$$V(\hat{q},\hat{t})\,|\chi(\lambda)\rangle_\mathrm{C} = V(\hat{q},t_0+\lambda)\,|\chi(\lambda)\rangle_\mathrm{C}\,. \tag{3.1.121}$$

The system TDSE becomes

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\,|\varphi(\lambda)\rangle_\mathrm{S} = \left(\frac{1}{2m}\hat{p}^2 + V(\hat{q},t_0+\lambda)\right)|\varphi(\lambda)\rangle_\mathrm{S} \tag{3.1.122}$$

with the effective potential $\langle\chi(\lambda)|V(\hat{q},\hat{t})|\chi(\lambda)\rangle_\mathrm{C} = V(\hat{q},t_0+\lambda)$ as a result. Obviously, the mean clock position $\mathrm{t} \equiv \langle\chi(\lambda)|\hat{t}|\chi(\lambda)\rangle_\mathrm{C} = t_0+\lambda$ represents an adequate quantity to track the clock evolution and the deparametrization yields

$$i\frac{\mathrm{d}}{\mathrm{dt}}\,|\varphi(\mathrm{t})\rangle_\mathrm{S} = \left(\frac{1}{2m}\hat{p}^2 + V(\hat{q},\mathrm{t})\right)|\varphi(\mathrm{t})\rangle_\mathrm{S}\,. \tag{3.1.123}$$

Finally, this genuine TDSE makes reference to a specific clock property via t and not to a static configuration space coordinate.

There is another important difference between the approach described at the beginning of this section and our relational framework, namely the fixing of the initial system state. While the basis-dependent form (3.1.118) may resemble the TDSE, it does not describe how an initial state is extracted from the global state. In contrast, our procedure yields the definite state $|\varphi(0)\rangle_\mathrm{S} = \langle\chi_0|\Psi\rangle_\mathrm{C}/\sqrt{\langle\Psi|\chi_0\rangle\langle\chi_0|\Psi\rangle}$ in addition to the TDSE. The same issue occurs in semiclassical treatments and is shown later.

3.1.8.3 Monochromatic mode interacting with atomic system

In reference [191], Braun et al. consider time emergence for a generic atomic system interacting with a monochromatic field mode. For the sake of consistency, their results are presented in a notation consistent with this thesis in the following. Upon quantization of the classical electromagnetic fields [207], their Hamiltonian describes a sum of many uncoupled harmonic oscillator. By picking just a single field mode for the clock, the corresponding clock Hamiltonian

$$\hat{H}_\mathrm{C} = \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{3.1.124}$$

describes a single harmonic oscillator with creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$, respectively. Here, ω denotes the angular frequency. The generic system Hamiltonian for an atom is

$$\hat{H}_\mathrm{S} = \sum_i \varepsilon_i \hat{c}_i^\dagger \hat{c}_i \tag{3.1.125}$$

and the interaction reads

$$\hat{V} = \sum_{ij} g_{ij}\hat{c}_i^\dagger\hat{c}_j \otimes (\hat{a} + \hat{a}^\dagger) \equiv \hat{S} \otimes (\hat{a} + \hat{a}^\dagger)\,. \tag{3.1.126}$$

Choosing the ground state $|\varphi_0\rangle_\mathrm{S}$ as a reference state allows the authors of Ref. [191] to express the atomic operators as $\hat{c}_i^\dagger \equiv |\varphi_i\rangle\langle\varphi_0|_\mathrm{S}$, such that $\hat{c}_i^\dagger\hat{c}_j = \left|\varphi_i\right\rangle\!\left\langle\varphi_j\right|_\mathrm{S}$. The sum $\hat{a} + \hat{a}^\dagger$ of annihilation and creation operator corresponds to the electric field of the mode (or position for a mechanical harmonic oscillator). Quite similar to our example in Sec. 3.1.7, the clock state is effectively chosen as a coherent state $|\chi(\lambda)\rangle_\mathrm{C} = |\alpha(\lambda)\rangle_\mathrm{C}$ with $\hat{a}\,|\alpha(\lambda)\rangle_\mathrm{C} = \alpha_0 e^{-i\omega\lambda}\,|\alpha(\lambda)\rangle_\mathrm{C}$ and, after applying semiclassical approximations, Braun et al. yield the TDSE

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\,|\varphi(\lambda)\rangle_\mathrm{S} = \left[\hat{H}_\mathrm{S} + \hat{S}\left(\alpha_0 e^{-i\omega\lambda} + \alpha_0^* e^{i\omega\lambda}\right)\right]|\varphi(\lambda)\rangle_\mathrm{S}\,. \tag{3.1.127}$$

In essence, this result is the quasi-eigenstate approximation, because

$$\langle\chi(\lambda)|\hat{V}|\chi(\lambda)\rangle_\mathrm{C} = \langle\alpha(\lambda)|\hat{S}\otimes(\hat{a}+\hat{a}^\dagger)|\alpha(\lambda)\rangle_\mathrm{C} \tag{3.1.128}$$

$$= \hat{S}\left(\alpha_0 e^{-i\omega\lambda} + \alpha_0^* e^{i\omega\lambda}\right). \tag{3.1.129}$$

Equipped with the error estimates from Sec. 3.1.8.1, it is now even possible to quantify the deviation from the exact dynamics. After a simple calculation, one realizes that the clock variance

$$\mathrm{Var}_\chi[\hat{a} + \hat{a}^\dagger] = 1 \tag{3.1.130}$$

is constant, regardless of α_0, and cannot provide a convincing error estimate. For this reason, we prefer the use of the relative error

$$Z_\mathrm{rel}^2 = \frac{1}{4|\alpha|^2}\cdot\frac{1}{\cos^2(\omega\lambda+\vartheta_0)} \tag{3.1.131}$$

with mean interacting strength $\langle\chi(\lambda)|(\hat{a}+\hat{a}^\dagger)|\chi(\lambda)\rangle_\mathrm{C} = 2|\alpha_0|\cdot\cos(\omega\lambda+\vartheta_0)$ for $\alpha_0 \equiv |\alpha_0|\cdot\exp(i\vartheta_0)$. Clearly, the clock must have a large mean energy $\omega|\alpha|^2$ for a small error. However, the relative error becomes infinite at the turning points $\omega\lambda+\vartheta_0 = (n+1/2)\pi$ ($n\in\mathbb{Z}$) and the approximation becomes the least exact. While the variance is still finite at

these points, the mean interaction strength vanishes and causes the singular behavior.

This is an interesting example in view of our hypothesis in Sec. 3.1.8.1 about the use of pointer states as clock states. The setup in Ref. [202] corresponds directly to the analysis considered here. Even though, the interaction features the harmonic oscillator position of the clock in a linear form, coherent states are used instead of position (quasi-)eigenstates. For very short time scales, position (quasi-)eigenstates are useful, but on longer time scales the coherent states provide a much better approximation, in agreement with the findings in Ref. [202].

While the analysis of Braun et al. [191] provided more insight into time emergence, the authors did not mention that the cyclic property of the clock is also imprinted on the system. In other words, only system dynamics within a single clock cycle can be probed in this case, which is inadequate for the description of the interaction with an electromagnetic field over typically many cycles. A better description of this scenario can be given with a more realistic finite laser pulse and is provided in the next section.

3.1.8.4 Atomic system interacting with a laser pulse

Instead of using a monochromatic field for the clock, we study an atomic system interacting with the electric field of a finite laser pulse. To this end, we consider a free heavy non-relativistic particle with mass M in one dimension as a clock with $\hat{H}_C = \hat{K}^2/(2M)$ and use the interaction

$$\hat{V} = \hat{S} \otimes F(\hat{Q}) \tag{3.1.132}$$

for the clock position operator $\hat{Q}$ and momentum operator $\hat{K}$. As in the preceding section, we use a generic system operator $\hat{S}$. The central idea of this section is to employ the quasi-eigenstate approximation to emulate a classical electric field $F(\lambda)$. To be specific, we choose the form of the electric field as

$$F(Q) = \exp\left(-4(\ln 2)\frac{Q^2}{\bar{T}^2}\right) \cdot \cos(\omega Q)\,, \tag{3.1.133}$$

representing a short pulse centered at $Q = 0$ with central frequency ω and full width half maximum $\bar{T}$. For an easier notation, we define the rescaled variable $T \equiv \bar{T}/(2\sqrt{\ln 2})$. Initially, the clock state is taken to be a Gaussian wave packet

$$\chi(K,0) \propto \exp\left[-\sigma_0^2(K-K_0)^2\right] \exp[iQ_0K] \tag{3.1.134}$$

in momentum space centered at initial momentum $K_0 > 0$, with mean position $Q_0 < 0$ and initial width σ_0. In position space, the λ-evolved clock state reads [183]

$$\chi(Q,\lambda) \propto e^{iK_0(Q-Q_0)} e^{-iK_0^2\lambda/(2M)} \exp\left[-\frac{(Q-Q_0-K_0\lambda/M)^2}{4(\sigma_0^2 + i\lambda/(2M))}\right] \tag{3.1.135}$$

with normalization constant $N(\lambda) = \sqrt{2\pi\left(\sigma_0^2 + (\lambda/(2M\sigma_0))^2\right)} \equiv \sqrt{2\pi\sigma^2(\lambda)}$ and has the density

$$|\chi|^2(Q,\lambda) = \frac{1}{N(\lambda)} \exp\left[-\frac{(Q-Q_0-K_0\lambda/M)^2}{2(\sigma_0^2 + (\lambda/2M\sigma_0)^2)}\right]. \tag{3.1.136}$$

The time-dependent width $\sigma(\lambda) \equiv \sqrt{\sigma_0^2 + (\lambda/2M\sigma_0)^2}$ shows the dispersing character and the center of the wavepacket $Q(\lambda) \equiv Q_0 - K_0\lambda/M = \langle\chi|\hat{Q}|\chi\rangle_C$ advances linearly in λ. For

the approximate effective system potential, the mean value of $F(\hat{Q})$ with respect to $|\chi\rangle_C$ is essential and evaluates to

$$\langle\chi(\lambda)|F(\hat{Q})|\chi(\lambda)\rangle_C = \frac{1}{N(\lambda)}\int_{-\infty}^{\infty} \mathrm{d}Q\; e^{-Q^2/T^2}\cos(\omega Q)\exp\left[-\frac{(Q-Q(\lambda))^2}{2\sigma^2(\lambda)}\right] \tag{3.1.137}$$

$$= \frac{1}{\sqrt{1+2\sigma^2(\lambda)/T^2}}\exp\left[-\frac{\omega^2\sigma^2(\lambda)}{2(1+2\sigma^2(\lambda)/T^2)}\right] \cdot \exp\left[-\frac{Q^2(\lambda)}{T^2}\cdot\frac{1}{1+2\sigma^2(\lambda)/T^2}\right]\cos\left[\frac{\omega Q(\lambda)}{1+2\sigma^2(\lambda)/T^2}\right] \tag{3.1.138}$$

$$\neq F\big(\langle\chi|\hat{Q}|\chi\rangle_C\big) = F\big(Q(\lambda)\big). \tag{3.1.139}$$

At this point, it becomes already apparent that, in order to match the original electric field, the width $\sigma(\lambda)$ must be small for λ at which $F(Q(\lambda))$ differs significantly from zero. In this limit, we obtain $\langle\chi|F(\hat{Q})|\chi\rangle_C \approx F(Q(\lambda))$. A simplification of the expression above is certainly wanted and the equation above suggests the first condition

$$2\cdot\frac{2\sigma^2(\lambda)}{T^2} \ll 1 \qquad \text{for} \qquad \frac{Q^2(\lambda)}{T^2} < 1\,, \tag{3.1.140}$$

which yields

$$\langle\chi(\lambda)|F(\hat{Q})|\chi(\lambda)\rangle_C \approx e^{-\frac{\omega^2\sigma^2(\lambda)}{2}} e^{-\frac{Q^2(\lambda)}{T^2}}\cos\left[\omega Q(\lambda)\right] \tag{3.1.141}$$

in zeroth order. The inclusion of an additional factor of two becomes intelligible with the mean value

$$\langle\chi(\lambda)|F(\hat{Q})^2|\chi(\lambda)\rangle_C = \frac{1}{N(\lambda)}\int_{-\infty}^{\infty} \mathrm{d}Q\; e^{-2Q^2/T^2}\cos^2(\omega Q)\exp\left[-\frac{(Q-Q(\lambda))^2}{2\sigma^2(\lambda)}\right] \tag{3.1.142}$$

$$= \frac{1}{\sqrt{1+4\sigma^2(\lambda)/T^2}}\, e^{-2Q^2(\lambda)/\left[T^2\cdot(1+4\sigma^2(\lambda)/T^2)\right]} \cdot\frac{1}{2}\left\{1+e^{-2\omega^2\sigma^2(\lambda)/\left[1+4\sigma^2(\lambda)/T^2\right]}\cos\left(\frac{2\omega Q(\lambda)}{1+4\sigma^2(\lambda)/T^2}\right)\right\} \tag{3.1.143}$$

$$\approx \frac{1}{2}\, e^{-2Q^2(\lambda)/T^2}\cdot\left\{1+e^{-2\omega^2\sigma^2(\lambda)}\cos\left[2\omega Q(\lambda)\right]\right\} \tag{3.1.144}$$

of the squared clock operator $F(\hat{Q})^2$, in which the last line was obtained with the zeroth order expansion in $4\sigma^2(\lambda)/T^2$. Subsequently, the clock variance reads

$$\mathrm{Var}_{\chi(\lambda)}[F(\hat{Q})] \approx e^{-2Q^2(\lambda)/T^2}\left[\frac{1}{2}\left(1+e^{-2\omega^2\sigma^2(\lambda)}\cos(2\omega Q)\right) - e^{-\omega^2\sigma^2(\lambda)}\cos^2(\omega Q)\right] \tag{3.1.145}$$

for $Q^2(\lambda) < T^2$ and suggests the second condition

$$2\omega^2\sigma^2(\lambda) \ll 1 \qquad \text{for} \qquad \frac{Q^2(\lambda)}{T^2} < 1\,. \tag{3.1.146}$$

Typically, the inverse frequency $1/\omega$ of a pulse is smaller than the extension T and, in this case, condition (3.1.146) also supersedes the previous requirement (3.1.140). With the help of the trigonometric relation $\cos^2(y) = (1+\cos(2y))/2$, we find

$$\mathrm{Var}_{\chi(\lambda)}[F(\hat{Q})] \approx \omega^2\sigma^2(\lambda)\, e^{-2Q^2(\lambda)/T^2}\sin^2(\omega Q) \qquad \text{for} \qquad Q^2(\lambda) < T^2 \tag{3.1.147}$$

for the first order expansion in $2\omega^2\sigma^2(\lambda)$. Clearly, demanding inequality (3.1.146) leads to a vanishing clock variance for $F(\hat{Q})$, which also permits an easy interpretation. For a wavepacket to be able to sample the form of the function $F(\hat{Q})$ requires wavepacket widths smaller than the extension T and the inverse frequency $1/\omega$ of the laser pulse.

So far only the situation $Q^2 < T^2$ has been considered and we briefly show the vanishing of $\mathrm{Var}_{\chi(\lambda)}[F(\hat{Q})]$ in the limit of large λ. More specifically, we start with an analysis of the case $\sigma^2(\lambda) \gg T^2$ for which the mean values yield

$$\langle\chi(\lambda)|F(\hat{Q})|\chi(\lambda)\rangle_C^2 \approx \frac{T^2}{2\sigma^2(\lambda)} e^{-\frac{\omega^2\sigma^2(\lambda)}{2}} e^{-\frac{Q^2(\lambda)}{\sigma^2(\lambda)}} \cos\left[\frac{\omega Q(\lambda) T^2}{2\sigma^2(\lambda)}\right] \leq \frac{T^2}{2\sigma^2(\lambda)}, \tag{3.1.148}$$

$$\langle\chi(\lambda)|F(\hat{Q})^2|\chi(\lambda)\rangle_C \approx \frac{T}{4\sigma(\lambda)} e^{-\frac{Q^2(\lambda)}{2\sigma^2(\lambda)}} \left(1 + e^{-\frac{\omega^2\sigma^2(\lambda)}{2}} \cos\left[\frac{\omega Q(\lambda) T^2}{2\sigma^2(\lambda)}\right]\right) \leq \frac{T}{2\sigma(\lambda)}. \tag{3.1.149}$$

Given the always increasing width $\sigma(\lambda \to \infty) \propto \lambda$, both terms converge toward zero and, consequently, the variance as well.

A very narrow wavepacket requires a broad distribution in momentum space and, therefore, a large spread in energy distribution. However, if the initial width is too small and the momentum distribution very broad, then the wavepacket expands very fast on the time scale of traversing the potential. We infer this behavior from the width formula

$$\sigma(\lambda) \equiv \sqrt{\sigma_0^2 + (\lambda/2M\sigma_0)^2}, \tag{3.1.150}$$

and its two asymptotic regions

$$\sigma(\lambda) \approx \sigma_0 \qquad \text{for} \quad \frac{\lambda^2}{4M^2\sigma_0^4} \ll 1, \tag{3.1.151}$$

$$\sigma(\lambda) \approx \frac{1}{2M\sigma_0^2} \cdot \lambda \qquad \text{for} \quad \frac{\lambda^2}{4M^2\sigma_0^4} \gg 1. \tag{3.1.152}$$

The second asymptote leads to a fast increase of the clock variance for very small initial widths $\sigma_0 \ll \lambda^2/M^2$. In turn, choosing a large initial width leads to a constant width, but at the expanse of having a large error. Therefore, the condition for an appropriate clock state is a small width of the wavepacket for the typical scale $\lambda_{\text{traversal}} \equiv T/(K_0/M)$ of traversing the central part of $F(Q)$. Hence, an optimal initial width and a corresponding initial energy distribution exist for a given $F(Q)$. Having an even broader energy distribution does not decrease the error, but actually increases it. However, another possible way to reduce the error is to use a more massive particle and a slower spreading of the wavepacket. From a relativistic viewpoint, the low momentum approximation of the relativistic energy

$$E_{\text{relativistic}} = \sqrt{(M c_{\text{light}}^2)^2 + (K c_{\text{light}})^2} = M c_{\text{light}}^2 \sqrt{1 + \left(\frac{K c_{\text{light}}}{M c_{\text{light}}^2}\right)^2} \tag{3.1.153}$$

$$\approx M c_{\text{light}}^2 \left(1 + \frac{1}{2}\frac{K^2}{M^2 c_{\text{light}}^2}\right) = M c_{\text{light}}^2 + \frac{K^2}{2M} \tag{3.1.154}$$

shows an energy increase for an increase in mass. Despite the usual omission in the Hamiltonian, the rest mass energy term $M c_{\text{light}}^2$ naturally contributes to the energy distribution. For this reason, the clock must have a large mean energy for very slow wavepacket spreading and a broad energy distribution for a small wavepacket width, in order to allow us

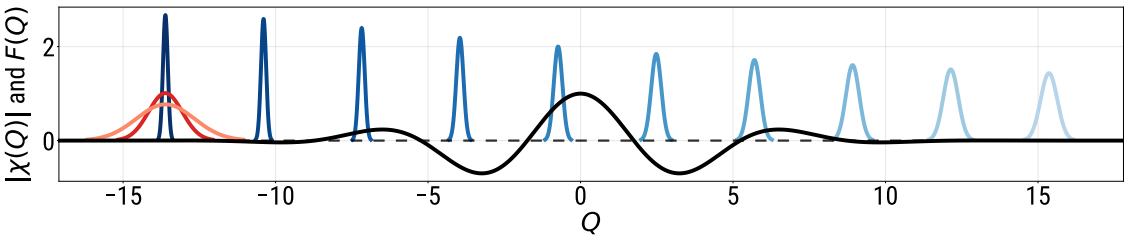

Figure 3.7 – The evolving clock state (blue lines) and the electric field function $F(Q)$ (black line) used in the numerical example are displayed. Two additional initial widths, shown in red and orange color and employed in the numerical calculations, provide means for a comparison and assessment of the accuracy of the quasi-eigenstate approximation.

to make use of the quasi-eigenstate approximation. In addition, if the clock variance is indeed small, then the Taylor expansion of the mean value

$$\langle\chi|F(\hat{Q})|\chi\rangle_C = F(Q) + F'(Q)\underbrace{\langle\chi|(\hat{Q}-Q)|\chi\rangle_C}_{=0} + \frac{1}{2}F''(Q)\underbrace{\langle\chi|(\hat{Q}-Q)^2|\chi\rangle_C}_{=\mathrm{Var}_\chi[\hat{Q}]=\sigma^2(\lambda)} + \dots \tag{3.1.155}$$

can be used to simplify the expression of the effective system potential.

We corroborate our findings and demonstrate the usefulness of the error quantifier Z from Sec. 3.1.8.1 by a numerical example in which we take a simple two-level atom as the system. The system Hamiltonian is chosen as $\hat{H}_S = \varepsilon\hat{\sigma}_z/2$ with the energy scale ε and we use the energy eigenstates of a large box for the clock in order to have a finite-dimensional clock Hilbert space $\mathscr{H}_C$. We choose the coupling to the electric field as

$$\hat{V} = g\,\hat{\sigma}_x \otimes F(\hat{Q}) \tag{3.1.156}$$

with the coupling constant g and we use the parameters $\varepsilon = 0.84$, $\omega = 0.90$, $T = 5.60$, $g = 1$, $M = 1400$, $K_0 = 1400$ and $Q_0 = -13.61$, given in atomic units (Appendix D). The dynamics of the corresponding clock wavepacket is illustrated in Fig. 3.7. After numerically diagonalizing the Hamiltonian, we pick an energy level that contains significant population on clock energy levels for which the clock state has a large population as well. In general, many different energy eigenstates can serve the same purpose, but our choice ensures numerical stability. For each time step, we calculate the normalized system state $|\varphi(\lambda)\rangle_S$ from the partial clock state projection (3.1.5) onto the global state $|\Psi\rangle$ and the approximate evolution, due to the Schrödinger equation $i\,\mathrm{d}\left|\varphi_{\mathrm{approx}}(\lambda)\right\rangle/\mathrm{d}\lambda = \left(\hat{H}_S + \langle\chi(\lambda)|\hat{V}|\chi(\lambda)\rangle\right)\left|\varphi_{\mathrm{approx}}(\lambda)\right\rangle$ with the initial state $\left|\varphi_{\mathrm{approx}}(0)\right\rangle_S = |\varphi(0)\rangle_S \propto \langle\chi(0)|\Psi\rangle_C$. We denote them by "projected" and "sequential", because the propagation with the TDSE has to be performed in a sequential manner. In addition, we compute the norm deviations $\sqrt{\left|1 - \langle\phi(\lambda)|\phi(\lambda)\rangle_S / \langle\phi(0)|\phi(0)\rangle_S\right|}$, the standard deviation $\sqrt{\mathrm{Var}_{\chi(\lambda)}[F(\hat{Q})]}$ and the error $Z(\lambda)$. Figure 3.8 contains the time-dependent coefficients of the ground and excited state, as well as the error quantifiers for three different initial clock wavepacket widths (Fig. 3.7). The smallest width fulfills the derived inequalities and demonstrates excellent agreement between both procedures. Before concluding with this example, we mention another way of modeling the finite pulse through an extension of the model in Ref. [191], considered in the previous section. It is possible to keep the harmonic oscillator degree and instead promote the envelope to a function of an additional clock degree of freedom. In such a

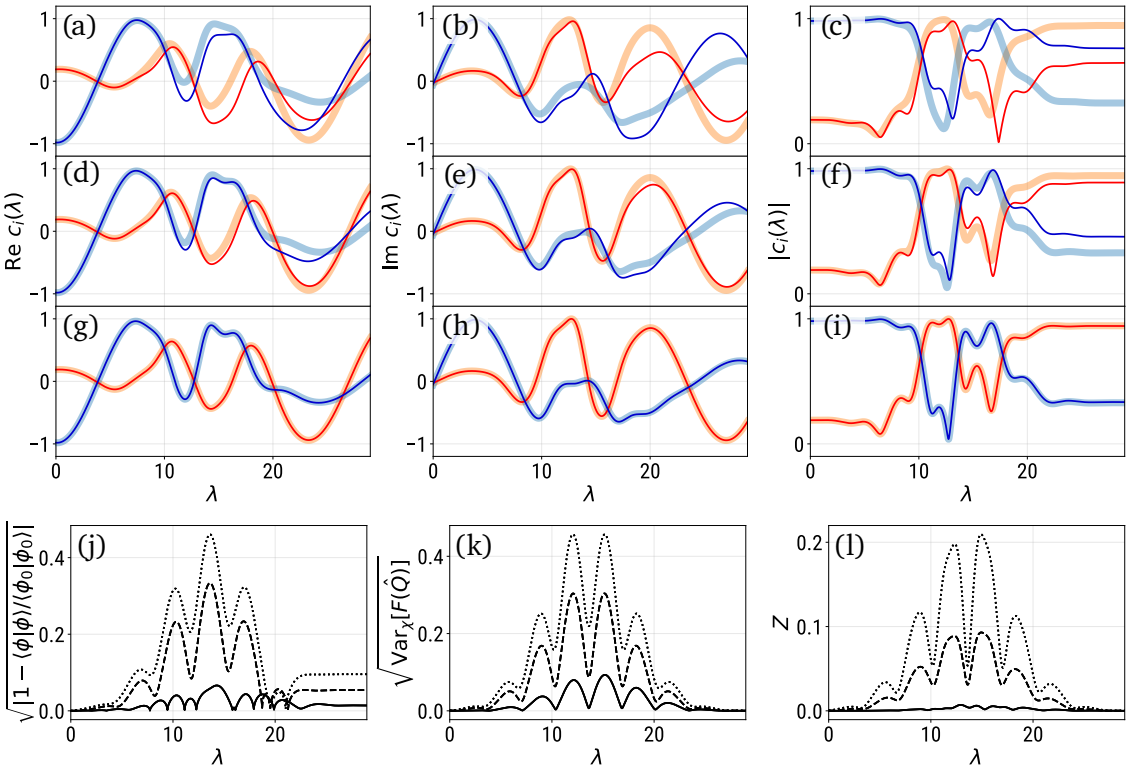

Figure 3.8 – The coefficients $c_i(\lambda)$ for the ground ($i = 0$, orange/red) and excited state ($i = 1$, blue) of a two-level system interacting with the electric field of a laser pulse are shown in panels (a) to (i). They emphasize a direct comparison between the relational system state $|\varphi(\lambda)\rangle_S$ (thicker transparent lines) and the sequential evolution (thin solid lines), due to the TDSE with the effective system Hamiltonian $\hat{H}_S + \langle\chi(\lambda)|\hat{V}|\chi(\lambda)\rangle$. The presentation of the complex coefficients separates into real parts (a), (d), (g), imaginary parts (b), (e), (h) and absolute values (c), (f), (i). In decreasing order, each of the first three rows represents a different initial width from the set $\{0.112, 0.781, 1.340\}$, which appears in Fig. 3.7 as well. We note that the coefficients differ slightly across rows because the effective system potential is slightly different for each initial width. Additionally, the deviation from the exact dynamics of $|\varphi(\lambda)\rangle_S$, due to the quasi-eigenstate approximation, are quantified in the last row. Panel (j) corresponds to the relative norm change of $|\phi(\lambda)\rangle_S$ and panel (k) shows the standard deviation of $F(\hat{Q})$ with respect to the clock state $|\chi(\lambda)\rangle_C$. Lastly, the full error (3.1.111) in panel (l) designates the most accurate measure for the deviation. Solid, dashed and dotted lines represent the different initial widths in increasing order. As expected, $Z(\lambda)$ is smaller for a narrow initial clock wavepacket and indicates a remarkable agreement between both methods. The case of an even smaller initial width is not shown here, but would correspond to a rapidly increasing error, potentially even exceeding the largest error in (l).

case, the interaction would read $\hat{V} = g\,\hat{\sigma}_x \otimes (\hat{a} + \hat{a}^\dagger) \otimes f(\hat{Q})$.

Not only do these results prove the correctness of our analytical results, but also show the potential computational advantage of finding a single energy eigenstate of an enlarged system and obtaining at once the time evolution of a system at all (relevant) times instead of sequentially computing each small time step.

3.1.8.5 Semiclassical clock state

The influential works of Briggs and Rost [98, 99] showed how the TDSE can be derived from a static global state when an interaction between clock and system exists. This task was accomplished by the use of a semiclassical treatment. In this section, we connect our results to such a formulation and reveal its relation to the quasi-eigenstate approximation.

Since semiclassical formulations are typically derived in orders of $\hbar$, we reinstate $\hbar$ in this section. Following reference [100], the TISE (3.1.3) is solved in the form

$$\Psi(q,Q) = \sum_m \varphi_m(q)\,\bar{\chi}_m(Q) \tag{3.1.157}$$

in position representation, for which we assume a one-dimensional position space for system and clock, respectively. The set $\{|\varphi_m\rangle_S\}$ describes an orthonormal basis for the system, which are chosen as the eigenstates of $\hat{H}_S$, i.e., $\hat{H}_S\,|\varphi_m\rangle_S = \varepsilon_m\,|\varphi_m\rangle_S$. We note that $\langle\bar{\chi}_m|\bar{\chi}_n\rangle_C \neq \delta_{mn}$. Furthermore, the clock Hamiltonian

$$\hat{H}_C = \frac{1}{2M}\hat{K}^2 + V_C(\hat{Q}) \tag{3.1.158}$$

describes a non-relativistic particle in the potential $V_C(Q)$. According to reference [100], the clock states in Eq. (3.1.157) can be expressed as

$$\bar{\chi}_m(Q) \equiv c_m(Q)\,e^{iW_m(Q)/\hbar}\,, \tag{3.1.159}$$

in the position basis, for which the $W_m(Q)$ are chosen as real-valued functions. After projecting $\langle\varphi_n|_S$ from the left onto the TISE (3.1.3) [100], we choose for the zeroth-order in $\hbar$, that W_n fulfills

$$\frac{1}{2M}\left(\frac{\partial W_n(Q)}{\partial Q}\right)^2 + V_C(Q) - (E-\varepsilon_n) = 0\,. \tag{3.1.160}$$

This is the classical Hamilton-Jacobi equation for the clock Hamiltonian and W_n are classical reduced actions. The action functions have the form

$$W_n(Q) = W(Q, E-\varepsilon_n)\,, \tag{3.1.161}$$

because of the structure of Eq. (3.1.160). Since these are classical equations, we also define the classical momentum

$$K_{cl}(Q,E) \equiv \frac{\partial W(Q,E)}{\partial Q}\,. \tag{3.1.162}$$

Still exact, the global state reads

$$|\Psi\rangle = \int \mathrm{d}Q \sum_m c_m(Q)\,e^{iW(Q,E-\varepsilon_m)/\hbar}\,|\varphi_m\rangle_S \otimes |Q\rangle_C \tag{3.1.163}$$

in bra-ket notation. A central element in the derivation of the TDSE is the λ-evolved clock state

$$|\chi(\lambda)\rangle_C = e^{-i\lambda(\hat{H}_C - E)/\hbar}\,|\chi_0\rangle_C \tag{3.1.164}$$

$$= \int \mathrm{d}\mathscr{E}\,e^{-i\lambda(\mathscr{E}-E)/\hbar} g(\mathscr{E})\,|\mathscr{E}\rangle_C \tag{3.1.165}$$

with $|\chi_0\rangle_C = \int \mathrm{d}\mathscr{E}\, g(\mathscr{E})\,|\mathscr{E}\rangle_C$. Energy eigenstates $|\mathscr{E}\rangle_C$ of $\hat{H}_C$ with clock energy $\mathscr{E}$ can be approximated by a WKB-solution

$$\langle Q|\mathscr{E}\rangle_C \approx h(Q,\mathscr{E})\, e^{iW(Q,\mathscr{E})/\hbar}, \tag{3.1.166}$$

in which the reduced action $W(Q,\mathscr{E})$ is the same as in Eq. (3.1.160), the classical Hamilton-Jacobi equation for the same clock Hamiltonian $\hat{H}_C$. The clock state

$$\chi(Q,\lambda) = \int \mathrm{d}\mathscr{E}\, e^{-i\lambda(\mathscr{E}-E)/\hbar} g(\mathscr{E})\, h(Q,\mathscr{E})\, e^{iW(Q,\mathscr{E})/\hbar} \tag{3.1.167}$$

further simplifies with the use of the stationary phase approximation (SPA) [208]

$$\int \mathrm{d}x\, e^{if(x)/\delta} g(x) \overset{\delta\to 0}{=} \sqrt{\frac{2\pi i\delta}{f''(x_{\mathrm{SPA}})}}\, e^{if(x_{\mathrm{SPA}})/\delta}\, g(x_{\mathrm{SPA}}) \qquad \text{for} \quad f'(x_{\mathrm{SPA}}) = 0\,. \tag{3.1.168}$$

For simplicity, we assume only a single stationary point x_{SPA}, which proves sufficient in the following. Such an approximation becomes particularly well-suited, when the classical reduced action is much larger than $\hbar$. The stationarity condition

$$\frac{\partial}{\partial\mathscr{E}}\left[\frac{W(Q,\mathscr{E})}{\hbar} - \frac{\lambda(\mathscr{E}-E)}{\hbar}\right]_{\mathscr{E}=\mathscr{E}_{\mathrm{SPA}}} = \frac{1}{\hbar}\left[\frac{\partial W(Q,\mathscr{E})}{\partial\mathscr{E}} - \lambda\right]_{\mathscr{E}=\mathscr{E}_{\mathrm{SPA}}} \overset{!}{=} 0 \tag{3.1.169}$$

must be solved for $\mathscr{E}_{\mathrm{SPA}}$ and, therefore, depends on the knowledge of $\partial W(Q,\mathscr{E})/\partial\mathscr{E}$. As a result, the stationary point $\mathscr{E}_{\mathrm{SPA}}(Q,\lambda)$ becomes a function of Q and λ. For the one-dimensional case, the reduced action reads

$$W(Q,\mathscr{E}) = \int^{Q} \mathrm{d}Q'\, K_{\mathrm{cl}}(Q',\mathscr{E}) = \int^{Q} \mathrm{d}Q'\, \sqrt{2\mathsf{M}(\mathscr{E}-V_C(Q'))} \tag{3.1.170}$$

which gives

$$\frac{\partial W(Q,\mathscr{E})}{\partial\mathscr{E}} = \int^{Q} \mathrm{d}Q'\, \frac{\mathsf{M}}{K_{\mathrm{cl}}(Q',\mathscr{E})}\,. \tag{3.1.171}$$

The last equation depends implicitly on the clock potential $V_C(Q)$ and in order to simplify the treatment, we assume a free particle with $V_C(Q) = 0$, as in Refs. [98, 99, 102, 192, 209]. In this instance, analytical results are possible, namely

$$W(Q,\mathscr{E}) = K_{\mathrm{cl}}(Q,\mathscr{E})\,Q = \sqrt{2\mathsf{M}\mathscr{E}}\,Q\,, \tag{3.1.172}$$

$$\frac{\partial W(Q,\mathscr{E})}{\partial\mathscr{E}} = \frac{\mathsf{M}Q}{K_{\mathrm{cl}}(Q,\mathscr{E})} = \frac{\mathsf{M}Q}{\sqrt{2\mathsf{M}\mathscr{E}}} = \sqrt{\frac{\mathsf{M}}{2\mathscr{E}}}\,Q\,. \tag{3.1.173}$$

Without loss of generality, we set the additional integration constant to zero. A dependence on the position Q is no longer present in the classical momentum $K_{\mathrm{cl}}(Q,\mathscr{E}) = \sqrt{2\mathsf{M}\mathscr{E}}$ and the stationary energy becomes

$$\mathscr{E}_{\mathrm{SPA}}(Q,\lambda) = \frac{\mathsf{M}}{2}\left(\frac{Q}{\lambda}\right)^2, \tag{3.1.174}$$

which resembles the kinetic energy for a classical point particle with velocity Q/λ. Without emphasis on the prefactors, which we describe collectively in a new coefficient g_1, the semiclassical clock state reads

$$\chi(Q,\lambda) \approx g_1(Q,\lambda)\, \exp\left[\frac{i}{\hbar}W\big(Q,\mathscr{E}_{\mathrm{SPA}}(Q,\lambda)\big) - \frac{i}{\hbar}\lambda\big(\mathscr{E}_{\mathrm{SPA}}(Q,\lambda) - E\big)\right] \tag{3.1.175}$$

$$= g_1(Q,\lambda)\exp\left[\frac{i}{\hbar}\left(\frac{MQ^2}{2\lambda}+\lambda E\right)\right]. \tag{3.1.176}$$

The unnormalized system state $|\phi(\lambda)\rangle_S = \langle\chi(\lambda)|\Psi\rangle_C$, conditioned on the clock state $|\chi(\lambda)\rangle_C$, yields

$$|\phi(\lambda)\rangle_S = e^{-i\lambda E/\hbar}\int \mathrm{d}Q\, g_1^*(Q,\lambda)\, e^{-iMQ^2/(2\lambda\hbar)}\sum_m c_m(Q)\, e^{i\sqrt{2M(E-\varepsilon_m)}Q/\hbar}\,|\varphi_m\rangle_S\,, \tag{3.1.177}$$

with the use of the result from above. At this point, another SPA can be employed. However, the phase information of the coefficients g_1 and c_m remains unknown, but we assume the clock to be semiclassical and highly energetic. In particular, its classical reduced action changes rapidly with Q and dominates any other phase change. Accordingly, the stationary point Q_{SPA} can be approximated from

$$\frac{\partial}{\partial Q}\left[\frac{\sqrt{2M(E-\varepsilon_m)}Q}{\hbar}-\frac{MQ^2}{2\lambda\hbar}\right]_{Q=Q_{\mathrm{SPA}}} = \frac{1}{\hbar}\left[\sqrt{2M(E-\varepsilon_m)}-\frac{MQ}{\lambda}\right]_{Q=Q_{\mathrm{SPA}}} \overset{!}{=} 0\,, \tag{3.1.178}$$

and its solution

$$Q_{\mathrm{SPA}}(\lambda, E-\varepsilon_m) = \frac{\lambda}{M}\sqrt{2M(E-\varepsilon_m)} \tag{3.1.179}$$

represents a classical linear motion. As a result, we find

$$|\phi(\lambda)\rangle_S \approx e^{-i\lambda E/\hbar}\sum_m f_m(\lambda, E-\varepsilon_m)\, e^{-i\lambda(E-\varepsilon_m)/\hbar}\, e^{i2\lambda(E-\varepsilon_m)/\hbar}\,|\varphi_m\rangle_S \tag{3.1.180}$$

$$= \sum_m f_m(\lambda, E-\varepsilon_m)\, e^{-i\lambda\varepsilon_m/\hbar}\,|\varphi_m\rangle_S \tag{3.1.181}$$

with the new complex-valued coefficients $f_m(\lambda, E-\varepsilon_m)$. In the spirit of semiclassics, we assume the system energies ε_m to be small compared to the typical energy scale of the clock and, for this reason, the influence of ε_m on the change of the coefficients is rendered minuscule. Consequently, the unnormalized system state becomes

$$|\phi(\lambda)\rangle_S \approx \sum_m f_m(\lambda)\, e^{-i\lambda\varepsilon_m/\hbar}\,|\varphi_m\rangle_S\,, \tag{3.1.182}$$

in which we omit the dependence of the coefficients on the total energy E.

The TDSE for the system in the semiclassical context can be derived from a partial projection with $\langle\chi(\lambda)|_C$ onto the TISE (3.1.3). It yields

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\phi(\lambda)\rangle_S = \hat{H}_S\,|\phi(\lambda)\rangle_S + \langle\chi(\lambda)|\hat{V}|\Psi\rangle_C\,, \tag{3.1.183}$$

but the semiclassical form of the last term is not immediately clear. We start with the assumption that the interaction is solely a function of position operators, namely

$$\hat{V} = V(\hat{x},\hat{Q})\,. \tag{3.1.184}$$

This allows us to use the clock position representation for this term in order to derive

$$\langle\chi(\lambda)|\hat{V}|\Psi\rangle_C \approx e^{-i\lambda E/\hbar}\int \mathrm{d}Q\, g_1^*(Q,\lambda)\, e^{-iMQ^2/(2\lambda\hbar)}$$

$$\cdot \sum_m c_m(Q)\, e^{i\sqrt{2\mathsf{M}(E-\varepsilon_m)}Q/\hbar}\, V(\hat{x},Q)\,|\varphi_m\rangle_{\mathrm{S}}\,. \tag{3.1.185}$$

Similarly to before, we assume the phase change in dependence of Q to be dominated by the classical reduced action. In this case, the SPA yields

$$\langle\chi(\lambda)|\hat{V}|\Psi\rangle_{\mathrm{C}} \approx \sum_m f_m(\lambda, E-\varepsilon_m)\, V\Big(\hat{x}, Q_{\mathrm{SPA}}(\lambda, E-\varepsilon_m)\Big)\, e^{-i\lambda\varepsilon_m/\hbar}\,|\varphi_m\rangle_{\mathrm{S}}\,. \tag{3.1.186}$$

As before, the neglect of the system energies ε_m, due to their weak influence in the arguments of the coefficients f_m and the interaction V, implies

$$\begin{aligned}\langle\chi(\lambda)|\hat{V}|\Psi\rangle_{\mathrm{C}} &\approx \sum_m f_m(\lambda)\, V\big(\hat{x}, Q_{\mathrm{SPA}}(\lambda)\big)\, e^{-i\lambda\varepsilon_m/\hbar}\,|\varphi_m\rangle_{\mathrm{S}} &(3.1.187)\\ &= V\big(\hat{x}, Q_{\mathrm{SPA}}(\lambda)\big) \sum_m f_m(\lambda)\, e^{-i\lambda\varepsilon_m/\hbar}\,|\varphi_m\rangle_{\mathrm{S}} &(3.1.188)\\ &\equiv V_{\mathrm{S}}(\hat{x},\lambda)\,|\phi(\lambda)\rangle_{\mathrm{S}}\,. &(3.1.189)\end{aligned}$$

Evidently, Eq. (3.1.183) describes a unitary evolution of the unnormalized system state within the semiclassical approximation and, accordingly, its norm stays constant. Therefore, the TDSE

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}\lambda}\,|\varphi(\lambda)\rangle_{\mathrm{S}} = \big[\hat{H}_{\mathrm{S}} + V_{\mathrm{S}}(\hat{x},\lambda)\big]\,|\varphi(\lambda)\rangle_{\mathrm{S}} \tag{3.1.190}$$

for the normalized system state $|\varphi(\lambda)\rangle_{\mathrm{S}}$ emerges in the semiclassical context, in which the effective system potential is λ-dependent via the classical path $Q_{\mathrm{SPA}}(\lambda,E)$ of the clock. In light of the discussion in Sec. 3.1.5.1, we point out that $Q_{\mathrm{SPA}}(\lambda,E)$ is enough to relate a property of the clock to λ, but does not represent the full information about the clock state. Though derived differently, our final results match those of Briggs and Rost [98,99] for a one-dimensional clock, without the necessity to invoke a Born-Oppenheimer approximation.

A further difference originates from a small overlooked detail in the previous semiclassical derivations, namely from the way the clock path enters the formulas and closely relates to the issue discussed in Sec. 3.1.8.2. In the above treatment, it is unambiguously clear how the λ-dependence enters the system change by means of stationary phases. This dependence ought to hold also in the case of a multi-dimensional clock configuration space, even if it requires multiple stationary points for the SPA in general. In contrast, the classical momentum (3.1.162) is used in Refs. [100,101,191,192] in order to find a mapping $\mathbb{R}\to\mathbb{R}$ from the one-dimensional Q-position space to t-space. We must note that the classical momentum (3.1.162) is a real-valued function over the whole position space and *not* a classical trajectory. The definition $\partial Q(t,E)/\partial t \equiv K_{\mathrm{cl}}(Q,E)/\mathsf{M}$, or equivalently $t(Q,E)\equiv \partial W(Q,E)/\partial E$, is used in these references to transform the space derivative into a t-derivative [100], i.e.,

$$i\hbar\frac{K_{\mathrm{cl}}(Q,E)}{\mathsf{M}}\frac{\partial}{\partial Q} = i\hbar\frac{\partial}{\partial t}\,. \tag{3.1.191}$$

Such a mapping is certainly valid, but effectively represent just a reparametrization of the one-dimensional position space. As a result, the derived TDSE in Refs. [100,101,191,192] is

actually a TISE in disguise, just as in Section 3.1.8.2, and also does not determine an initial system state. Although conceptually unsatisfactory, this methodology is mathematically consistent for one-dimensional position space. The issue becomes even more pronounced for a multi-dimensional clock position space $\mathbb{R}^{n_C}$, which is considered in Refs. [98,99,102]. In this case, the classical real-valued momentum vector field $\mathbf{K}_{cl}(\mathbf{Q},E)$ is now a function of the coordinate vector $\mathbf{Q}$. A real-valued "time field" defined on position space can be introduced by $\partial/\partial t(\mathbf{Q},E) \equiv (1/M)\,\mathbf{K}_{cl}(\mathbf{Q},E)\cdot\nabla_{\mathbf{Q}}$ or $t(\mathbf{Q},E) \equiv \partial W(\mathbf{Q},E)/\partial E$. In contrast to the one-dimensional clock case, it is *not* possible to define $\partial\mathbf{Q}(t,E)/\partial t \equiv \mathbf{K}_{cl}(\mathbf{Q},E)$, because it would require a one-dimensional parametrization $\mathbb{R}\to\mathbb{R}^{n_C}$ of a vector quantity, in other words a trajectory through position space. Such a trajectory is not part of the fully quantum Born-Oppenheimer treatment and, therefore, is not available for a parametrization of the system dynamics. A static multi-dimensional configuration space cannot be reduced to a simple one-dimensional trajectory. On the same footing, it is not possible to define an inverse relation like $\mathbf{Q}^{-1}(t,E)$ and this poses a conceptual problem in the derivations of Refs. [98,99,102]. All authors place emphasis on the appearance of the first-order time derivative, but do not explicitly consider how t enters the coefficients or the effective system potential for multi-dimensional position spaces. For instance, after starting from the TISE and employing the relevant approximations [98,99,102], the cited authors end up with

$$i\hbar\frac{\partial}{\partial t(\mathbf{Q})}f_m(\mathbf{Q}) = \sum_k \langle\varphi_m|V(\hat{x},\mathbf{Q})|\varphi_k\rangle_S\, f_k(\mathbf{Q})\,\exp\left[-\frac{i}{\hbar}(\varepsilon_k-\varepsilon_m)\,t(\mathbf{Q})\right], \tag{3.1.192}$$

where we neglect arguments of the constant total energy E. This equation for the (interaction picture-like) coefficients $f_m(\mathbf{Q}) : \mathbb{R}^{n_C}\to\mathbb{C}$ is still defined on the full multi-dimensional position space $\mathbb{R}^{n_C}$. The same holds true for the transition elements $\langle\varphi_m|V(\hat{x},\mathbf{Q})|\varphi_k\rangle_S : \mathbb{R}^{n_C}\to\mathbb{C}$. Without a more refined analysis, Eq. (3.1.192) is then simply transformed to

$$i\hbar\frac{\partial}{\partial t}f_m(t) = \sum_k \langle\varphi_m|V(\hat{x},t)|\varphi_k\rangle_S\, f_k(t)\,\exp\left[-\frac{i}{\hbar}(\varepsilon_k-\varepsilon_m)\,t\right] \tag{3.1.193}$$

in Refs. [98,99,102] under the false premise of having a genuine classical trajectory available. Despite all this, an additional assumption about the global state could save the former semiclassical treatments from mathematical inconsistencies. If the particular form of the global state $|\Psi\rangle$ allows for the coefficients to approximate $f_m(\mathbf{Q}) \propto \int \mathrm{d}s\,\delta[\mathbf{Q}-\mathbf{Q}_{cl}(s)]$ with the classical clock trajectory $\mathbf{Q}_{cl}(s)$, then one has a way to facilitate the dimensional reduction necessary to derive (3.1.193). However, assuming such a form for $|\Psi\rangle$ is either a very crude approximation or severely limits the set of admissible global states.

For a further illustration without additional global restrictions, let us consider the very simple example of a two-dimensional clock position space, but with the clock Hamiltonian $\hat{H}_C = \hat{K}_x^2/(2M)$ depending only on the momentum in Q_x-direction. Eq. (3.1.192) becomes

$$i\hbar\sqrt{\frac{2E}{M}}\frac{\partial}{\partial Q_x}f_m(Q_x,Q_y) = \sum_k \langle\varphi_m|V(\hat{x},Q_x,Q_y)|\varphi_k\rangle_S\, f_k(Q_x,Q_y)\,e^{-i(\varepsilon_k-\varepsilon_m)\,t(Q_x,Q_y)/\hbar}, \tag{3.1.194}$$

which can be transformed to

$$i\hbar\frac{\partial}{\partial t}f_m(t,Q_y) = \sum_k \langle\varphi_m|V(\hat{x},t,Q_y)|\varphi_k\rangle_S\, f_k(t,Q_y)\,\exp\left[-\frac{i}{\hbar}(\varepsilon_k-\varepsilon_m)\,t\right] \tag{3.1.195}$$

with $t = t(Q_x) = Q_x\sqrt{M/2E}$. Surely, we got an equation that features a first order derivative in t, but what about the remaining clock position variable Q_y? It cannot be eliminated from the equation, because the effective potential depends explicitly on it and the coefficients can vary for different Q_y too. This contradiction confirms our arguments and shows that the framework of this thesis, in which a specific clock state is chosen, should be preferred for time emergence with interactions.

One last example for this general misconception is Ref. [191], already encountered in Sec. 3.1.8.3. The authors express the clock part of the TISE in the over-complete coherent state basis $\{|\alpha\rangle_C\}_{\alpha\in\mathbb{C}}$, which corresponds to a representation in two-dimensional space $(\mathrm{Re}\,\alpha, \mathrm{Im}\,\alpha)$. Thus, the global state $|\Psi\rangle$ is given as a complex-valued function on the system basis and the two-dimensional complex plane. Without any further explanation, the authors reduce the two-dimensional complex plane to the trajectory $\alpha(t) = \alpha_0 \exp(-i\omega t)$, a one-dimensional object. No mathematical justification is given for this reduction in their approach. A more consistent treatment has been presented in Sec. 3.1.8.3, where the use of such a trajectory originates from the choice of the clock state in our framework and, in addition, does not depend on the coherent state basis.

Finally, it is interesting to compare the semiclassical results with the Taylor expanded form of the quasi-eigenstate approximation. As already mentioned in Section 3.1.8.4 and presented by Eq. (3.1.155), the effective potential can be Taylor expanded around the clock mean position as

$$\langle\chi|V(\hat{x},\hat{Q})|\chi\rangle_C = V\big(\hat{x},\,\langle\chi|\hat{Q}|\chi\rangle_C\big) + \frac{1}{2}\mathrm{Var}_\chi[\hat{Q}]\cdot V''\big(\hat{x},\,\langle\chi|\hat{Q}|\chi\rangle_C\big) + \dots\,. \tag{3.1.196}$$

The partial derivative of the potential function V is taken with respect to the second argument, the clock position and the same procedure can be applied to the Ehrenfest theorem for the clock, namely

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\chi|\hat{K}|\chi\rangle_C = -\langle\chi|V_C'(\hat{Q})|\chi\rangle_C \tag{3.1.197}$$

$$= -V_C'\big(\langle\chi|\hat{Q}|\chi\rangle_C\big) + \frac{1}{2}\mathrm{Var}_\chi[\hat{Q}]\cdot V_C'''\big(\langle\chi|\hat{Q}|\chi\rangle_C\big) + \dots\,. \tag{3.1.198}$$

Neglecting all orders higher than zero in both expressions yields an effective system potential $\hat{V}_S$ which becomes λ-dependent by virtue of a classical trajectory, similar to the semiclassical approximation. In detail, the mean clock position $\langle\chi|\hat{Q}|\chi\rangle_C$ follows the classical trajectory given by Newton's classical equation of motion

$$\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\langle\chi|\hat{Q}|\chi\rangle_C(\lambda) = -\frac{1}{M}V_C'\big(\langle\chi|\hat{Q}|\chi\rangle_C(\lambda)\big)\,. \tag{3.1.199}$$

3.1.9 Time-energy uncertainty

An important topic, whenever the issue of time is raised, concerns uncertainty relations. Their examination has a long history, dating back to the beginning years of quantum mechanics [56] in the early twentieth century and is still relevant in today's research [131, 210–212]. Due to its characteristic appearance and for dimensional reasoning, $\hbar$ is used explicitly within this section. Initially made famous by Heisenberg's inequality $\Delta q\cdot\Delta p \geq \hbar/2$ [213, 214], the more general uncertainty relation

$$\mathrm{Var}(\hat{A})\cdot\mathrm{Var}(\hat{B}) \geq \frac{1}{4}\Big|\big\langle\big[\hat{A},\hat{B}\big]\big\rangle\Big|^2 + \frac{1}{4}\Big[\big\langle\big\{\hat{A},\hat{B}\big\}_+\big\rangle - 2\big\langle\hat{A}\big\rangle\cdot\big\langle\hat{B}\big\rangle\Big]^2 \tag{3.1.200}$$

for two Hermitian operators $\hat{A}$ and $\hat{B}$ has been provided by Schrödinger [215, 216]. This relation holds for pure, as well as for mixed states and relies, in general, on the non-commutability of two observables. The anti-commutator is denoted by $\{\hat{A},\hat{B}\}_+ \equiv \hat{A}\hat{B}+\hat{B}\hat{A}$. A modern formulation borrows from the language of mathematics, specifically probability theory, and expresses the inequality in terms of a generalized covariance matrix [216]. In particular, the generalized covariance

$$\mathrm{Cov}(\hat{A},\hat{B}) \equiv \left\langle \{\hat{A}-\langle\hat{A}\rangle, \hat{B}-\langle\hat{B}\rangle\}_+ \right\rangle /2 = \left\langle \{\hat{A},\hat{B}\}_+ \right\rangle /2 - \langle\hat{A}\rangle\cdot\langle\hat{B}\rangle = \mathrm{Cov}(\hat{B},\hat{A}) \tag{3.1.201}$$

applies also to non-commutating observables and is still real-valued. Consequently, the uncertainty principle reads

$$\det\sigma[\hat{A},\hat{B}] \geq \frac{1}{4}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|^2 \tag{3.1.202}$$

with the determinant of the generalized covariance matrix

$$\sigma[\hat{A},\hat{B}] \equiv \begin{pmatrix} \mathrm{Var}(\hat{A}) & \mathrm{Cov}(\hat{A},\hat{B}) \\ \mathrm{Cov}(\hat{A},\hat{B}) & \mathrm{Var}(\hat{B}) \end{pmatrix}. \tag{3.1.203}$$

For simple scalars X and Y, the inequality reduces to the standard result $\mathrm{Var}(X)\cdot\mathrm{Var}(Y) \geq \mathrm{Cov}(X,Y)$ in probability theory [217]. Neglecting the covariance, the second term in Eq. (3.1.200), yields the more well-known Robertson uncertainty relation [218] $\mathrm{Var}(\hat{A})\cdot\mathrm{Var}(\hat{B}) \geq \left|\langle[\hat{A},\hat{B}]\rangle\right|^2/4$, from which the Heisenberg inequality can be derived by means of $[\hat{q},\hat{p}] = i\hbar$. The inequality (3.1.200) does hold for mixed states as well[3]. Since many decades (Chapter 1), a strong motivation exists to find similar uncertainty principles for time and energy [73], in the form of

$$\Delta t\Delta E \gtrsim \hbar, \tag{3.1.204}$$

based on the same dimensionality as the product of position and momentum. In view of the fact that a universal time operator does not exist, it has been argued that Δt in Eq. (3.1.204) must describe an actual time interval and not an uncertainty due to quantum fluctuations [131]. Also the Mandelstam-Tamm uncertainty [73]

$$\Delta E\cdot\tau_A \geq \hbar/2, \tag{3.1.205}$$

which relies on $(\Delta E)^2 = \mathrm{Var}(\hat{H})$ and the variance $(\Delta A)^2 = \mathrm{Var}(\hat{A})$ of another observable $\hat{A}$, includes a time interval $\tau_A \equiv \Delta A/\left|\mathrm{d}\langle\hat{A}\rangle/\mathrm{d}t\right|$ describing the time needed to change the mean value $\langle\hat{A}\rangle$ by one standard deviation ΔA. Relations of type (3.1.204) are generally called "speed limits" [219, 220] and they exist for quantum, as well as for classical mechanics [220, 221]. In essence, they describe the limits of the dynamical evolution between an initial and a final state. Concise surveys and reviews of all the different kinds of speed limits in the literature can be found in Refs. [219, 220]. For our purpose, it is only relevant that such quantum speed limits depend on parameter time and not a time operator. As a result, they apply independently to the system and the clock in our framework. At the same time, it raises the question if an uncertainty relation or quantum speed limit can be found, which relates both subsystems.

[3] The proof relies on the general inequality $\mathrm{tr}\left(\hat{\rho}\hat{F}\hat{F}^\dagger\right) \geq 0$ with $\hat{F} = \hat{A} + z\hat{B}$ for a complex number $z \in \mathbb{C}$. A variation of z and z^* yields the minimum value for the left-hand side of the inequality and implies $\mathrm{tr}\left(\hat{\rho}\hat{A}\hat{A}^\dagger\right)\mathrm{tr}\left(\hat{\rho}\hat{B}\hat{B}^\dagger\right) \geq \left|\mathrm{tr}\left(\hat{\rho}\hat{A}\hat{B}^\dagger\right)\right|^2$.

3.1.9.1 Approach by Briggs et al.

Briggs et al. [98, 222] approach this idea through a consideration of the energy constraint $E = E_S + E_C$ and the equality of the energy variances $\Delta E_S^2 = \Delta E_C^2$. Using the Mandelstam-Tamm relation (3.1.205) for a heavy particle $\hat{H}_C = \hat{K}^2/(2M)$, they derive

$$\Delta E_C \cdot \tau_Q = \Delta E_S \cdot \tau_Q \geq \frac{\hbar}{2}, \tag{3.1.206}$$

where the time interval is determined from the change of the mean clock position $\langle \hat{Q} \rangle$. Unfortunately, it is neither explicitly mentioned how the mean energies or the energy variances are obtained in this formulation, nor how the coupling between system and clock enters the spectral analysis. In Ref. [222], Briggs provides an additional assumption for the energy considerations, namely that one determines the energy distributions only when the interaction vanishes. This would imply that (3.1.206) only holds true asymptotically or in certain regions in clock position space.

3.1.9.2 Approach by Fadel and Maccone

Alternatively, Fadel and Maccone [131] formulate a time-energy uncertainty in the context of PW, based on the Robertson inequality for two non-commutating variables. They consider the specific setting of two non-interacting systems, in which the clock Hamiltonian is the momentum operator, $\hat{H}_C = \hat{K}$, and the position operator effectively functions as a "time operator" $\hat{T}_C = \hat{Q}$, such that $[\hat{T}_C, \hat{H}_C] = [\hat{Q}, \hat{K}] = i\hbar$. Furthermore, a projector $\hat{\Theta}_S = \hat{\Theta}_S^2$ is introduced, corresponding to some "event happening" [131] in the system, and it shall commute with the generic system Hamiltonian $\hat{H}_S$, i.e., $[\hat{\Theta}_S, \hat{H}_S] = 0$. Comprehending mean values as a conditional statement connected to the occurrence of an event Θ_S is the central idea of their analysis. For instance, the mean clock position

$$\left\langle \hat{Q} \right\rangle_{\Theta_S} \equiv \int \mathrm{d}Q\, Q\, p(Q|\Theta_S) = \int \mathrm{d}Q\, Q\, \frac{\langle \Psi | \left(\hat{\Theta}_S \otimes |Q\rangle\langle Q|_C \right) | \Psi \rangle_C}{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C}, \tag{3.1.207}$$

stems from the conditional probability $p(x|y) = p(x,y)/\int \mathrm{d}x\, p(x,y)$ [217]. More generally, the conditional mean value can be expressed as

$$\left\langle \hat{A}_S \otimes \hat{B}_C \right\rangle_{\Psi,\Theta_S} \equiv \frac{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) \left(\hat{A}_S \otimes \hat{B}_C \right) \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C}{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C} \tag{3.1.208}$$

for any operator $\hat{A}_S \otimes \hat{B}_C$. For the mean energy follows the relation

$$\left\langle \hat{\mathbb{1}}_S \otimes \hat{H}_C \right\rangle_{\Psi,\Theta_S} = -\left\langle \hat{H}_S \otimes \hat{\mathbb{1}}_C \right\rangle_{\Psi,\Theta_S} \tag{3.1.209}$$

and the conditional energy variance reads

$$\mathrm{Var}_{\Psi,\Theta_S}(\hat{\mathbb{1}}_S \otimes \hat{H}_C) = \frac{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{H}_C^2 \right) | \Psi \rangle_C}{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C} - \left[\frac{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{H}_C \right) | \Psi \rangle_C}{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C} \right]^2 \tag{3.1.210}$$

$$= \frac{\langle \Psi | \left(\hat{\Theta}_S \hat{H}_S^2 \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C}{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C} - \left[\frac{\langle \Psi | \left(\hat{\Theta}_S \hat{H}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C}{\langle \Psi | \left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C \right) | \Psi \rangle_C} \right]^2 \tag{3.1.211}$$

$$= \mathrm{Var}_{\Psi,\Theta_S}(\hat{H}_S \otimes \hat{\mathbb{1}}_C). \tag{3.1.212}$$

Using the Robertson inequality yields

$$\mathrm{Var}_{\Psi,\Theta_S}(\hat{H}_S \otimes \hat{\mathbb{1}}_C) \cdot \mathrm{Var}_{\Psi,\Theta_S}(\hat{\mathbb{1}}_S \otimes \hat{T}_C) \geq \frac{1}{4}\left| \frac{\langle\Psi|\left[\hat{\Theta}_S \otimes \hat{T}_C, \hat{\Theta}_S \otimes \hat{H}_C\right]|\Psi\rangle}{\langle\Psi|\left(\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C\right)|\Psi\rangle_C} \right|^2 = \frac{\hbar^2}{4} \tag{3.1.213}$$

with $[\hat{\Theta}_S \otimes \hat{T}_C, \hat{\Theta}_S \otimes \hat{H}_C] = \hat{\Theta}_S \otimes [\hat{T}_C, \hat{H}_C] = i\hbar\hat{\Theta}_S \otimes \hat{\mathbb{1}}_C$. Additionally, it is claimed in Ref. [131] that the same relations hold for $[\hat{\Theta}_S, \hat{H}_S] \neq 0$. Yet, we could not find this statement to be true. Obviously, from $\hat{\Theta}_S = \hat{\mathbb{1}}_S$ follows the standard uncertainty relation

$$\mathrm{Var}_{\Psi}(\hat{H}_S \otimes \hat{\mathbb{1}}_C) \cdot \mathrm{Var}_{\Psi}(\hat{\mathbb{1}}_S \otimes \hat{T}_C) \geq \frac{1}{4}\left| \langle\Psi|\left(\hat{\mathbb{1}}_S \otimes \left[\hat{T}_C, \hat{H}_C\right]\right)|\Psi\rangle \right|^2 = \frac{\hbar^2}{4} \tag{3.1.214}$$

with an unconditional character. This inequality also holds, except for the last equal sign, for any clock operator other than $\hat{T}_C$. Unfortunately, the authors of Ref. [131] abstain from discussing system-clock uncertainty relations without a conditional characteristic. Instead, they state that the event Θ_S can be associated with a photon detection on a screen for example, but, as we have already argued in Section 3.1.4, there is no additional environment surrounding the composite of clock and principal system. Furthermore, any detection or actual measurement presupposes time, a problem we already alluded to in Chapter 1. If one accepts the special nature of the clock in this treatment, then inequality (3.1.214) is a valid statement connecting the uncertainty in the position of the clock with the uncertainty in the system through the energy constraint of the global state $|\Psi\rangle$. Using Schrödinger's original inequality, we can provide an even tighter bound than (3.1.214), by addition of the covariance term $\mathrm{Cov}(\hat{H}_C, \hat{T}_C) = \langle\Psi|(\hat{H}_S - \langle\hat{H}_S\rangle) \otimes \hat{T}_C|\Psi\rangle^2$ on the right-hand side.

The statement (3.1.214) can be generalized to arbitrary clock Hamiltonians $\hat{H}_C$ by the use of Pegg's age operator, which is explained in Appendix E. Such a generalization becomes useful for finite dimensional Hilbert spaces, for which commutator relations like $[\hat{q}, \hat{p}] = i\hbar\hat{\mathbb{1}}$ do not exist. This can be easily seen from the cyclic property of the trace, namely $\mathrm{tr}\left[\hat{A}, \hat{B}\right] = 0 \neq i\hbar\,\mathrm{tr}\,\hat{\mathbb{1}} = i\hbar d$, in which the finite dimension d of $\mathscr{H}$ appears[4]. Introduced by Pegg [188] in 1998, the operator $\hat{\alpha}_C(\alpha_0)$ is used to track the elapsed time, or "age", for a generic clock state evolving under a time-independent Hamiltonian. Its form depends explicitly on the initial clock state itself by virtue of the populated energy levels and on the unnormalized ket vectors $|\overline{\alpha}\rangle$. They describe a state which is initially in an equally weighted superposition of all relevant energy levels and, subsequently, evolves until $\lambda = \alpha$ (App. E). The free parameter α_0, characteristic to each age operator, designates a specific choice for the zero point. In our case, all relevant energy levels are the associated eigenvalues of the elements in the set (3.1.28), which encompasses all clock energy eigenstates contained in $|\Psi\rangle$. With an explicit reference to the redefinitions (3.1.32), the appropriate age operator for our case has the commutation relation

$$\left[\hat{\alpha}_C(\alpha_0), \hat{H}_C\right] = \hat{\mathbb{1}}_C - |\overline{\alpha}_0\rangle\langle\overline{\alpha}_0|_C\,, \tag{3.1.215}$$

which correctly yields zero on both sides under the trace operation, due to the norm $\langle\overline{\alpha}_0|\overline{\alpha}_0\rangle_C = d_C$ (App. E). As a side note, Pegg's operator also appears in the context of PW in Ref. [190]. By replacing the clock operator $\hat{T}_C$ with the age operator $\hat{\alpha}_C(\alpha_0)$, the inequality (3.1.214) becomes

$$\mathrm{Var}_{\Psi}(\hat{H}_S \otimes \hat{\mathbb{1}}_C) \cdot \mathrm{Var}_{\Psi}\left(\hat{\mathbb{1}}_S \otimes \hat{\alpha}_C(\alpha_0)\right) \geq \frac{1}{4}\left| \langle\Psi|\left(\hat{\mathbb{1}}_S \otimes \left[\hat{\alpha}_C(\alpha_0), \hat{H}_C\right]\right)|\Psi\rangle \right|^2 \tag{3.1.216}$$

[4] The same analysis does not apply in infinite-dimensional Hilbert spaces, because the trace of the identity operator does not exist in these spaces [223].

$$= \frac{\hbar^2}{4}\left|\langle\Psi|\Big(\hat{\mathbb{1}}_S \otimes \Big(\hat{\mathbb{1}}_C - |\overline{\alpha}_0\rangle\langle\overline{\alpha}_0|_C\Big)\Big)|\Psi\rangle\right|^2 \tag{3.1.217}$$

$$= \frac{\hbar^2}{4}\left|1 - \langle\overline{\alpha}_0|\hat{\Upsilon}_C|\overline{\alpha}_0\rangle_C\Big)\right|^2 \tag{3.1.218}$$

with the reduced density operator $\hat{\Upsilon}_C = \mathrm{tr}_S(|\Psi\rangle\langle\Psi|)$. Inequality (3.1.218) represents a static relation and choosing an α_0 that minimizes $\langle\overline{\alpha}_0|\hat{\Upsilon}_C|\overline{\alpha}_0\rangle_C$ brings the right-hand side close to $\hbar^2/4$. However, the more general Schrödinger uncertainty (3.1.200) should be used for a tighter bound.

3.1.9.3 Alternative approach

Even though (3.1.218) is already encouraging, it does not make reference to a clock state $|\chi(\lambda)\rangle_C$. One could argue that the approach by Fadel and Maccone [131] presumes the use of $|\chi(\lambda)\rangle_C = |Q+\lambda\rangle_C$, which represents an eigenstate of the position operator $\hat{Q}$. In this case, the position operator, disguised as "time operator" $\hat{T}_C$, contains all possible positions and is in some way a reference to the specific clock states, which advance through all possible positions for $\lambda \in (-\infty, \infty)$. Anyway, as we have already stated, their work relies on a special setting and more general expressions are still missing. To this end, we consider an uncertainty relation, which depends explicitly on the state of the clock. However, the age operator must differ from the one used in the previous section, because the energy levels populated by $|\chi\rangle_C$ can differ from the ones contained in $\hat{\Upsilon}_C$. To remedy the situation, we use the modified age operator $\hat{\alpha}_\chi(\alpha_0)$ given in Appendix E, for which the uncertainty relation reads

$$\mathrm{Var}_{\chi(\lambda)}(\hat{H}_C)\cdot\mathrm{Var}_{\chi(\lambda)}\Big(\hat{\alpha}_\chi(\alpha_0)\Big) \geq \frac{\hbar^2}{4}\left|1 - \frac{1}{D_\chi}\left|\langle\chi(\lambda)|\chi(\alpha_0)\rangle_C\right|^2\right|^2. \tag{3.1.219}$$

Here, D_χ is the cycle-averaged absolute squared autocorrelation function of $|\chi(\lambda)\rangle_C$. Importantly, relation (3.1.219) does not make any reference to $|\Psi\rangle$ so far, in contrast to the aforementioned approaches. By following the idea of connecting the clock energy variance with the system energy variance, the global state $|\Psi\rangle$ enters the picture via the system state. For simplicity, we consider only $\hat{V} = 0$ here and express the mean system energy

$$\langle\varphi|\hat{H}_S|\varphi\rangle_S = E - \frac{\langle\Psi|\hat{P}_\chi\hat{H}_C|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} = E - \langle\chi|\hat{H}_C|\chi\rangle_C - \frac{\langle\Psi|\hat{P}_\chi\hat{H}_C\hat{\overline{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} \tag{3.1.220}$$

in terms of the clock state. The last term is real-valued and indicates a deviation from the energy relation $E = \langle\hat{H}_S\rangle_\varphi + \langle\hat{H}_C\rangle_\chi$ in general. For arbitrary clock states, this correction term does only vanish for global MES $|\Psi\rangle$, even in the case of $\hat{V} \neq 0$ (Appendix G). Similarly, the system energy variance

$$\mathrm{Var}_\varphi(\hat{H}_S) = \mathrm{Var}_\varphi(E - \hat{H}_S) \tag{3.1.221}$$

$$= \langle\varphi|\Big(E - \hat{H}_S\Big)^2|\varphi\rangle_S - \langle\varphi|\Big(E - \hat{H}_S\Big)|\varphi\rangle_S^2 \tag{3.1.222}$$

$$= \frac{\langle\Psi|\hat{P}_\chi\hat{H}_C^2|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} - \left[\langle\hat{H}_C\rangle_\chi + \frac{\langle\Psi|\hat{P}_\chi\hat{H}_C\hat{\overline{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}\right]^2 \tag{3.1.223}$$

$$= \mathrm{Var}_\chi(\hat{H}_C) + \frac{\langle\Psi|\hat{P}_\chi\hat{H}_C\hat{\overline{P}}_\chi\hat{H}_C\hat{\overline{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} - \left[\frac{\langle\Psi|\hat{P}_\chi\hat{H}_C\hat{\overline{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}\right]^2$$

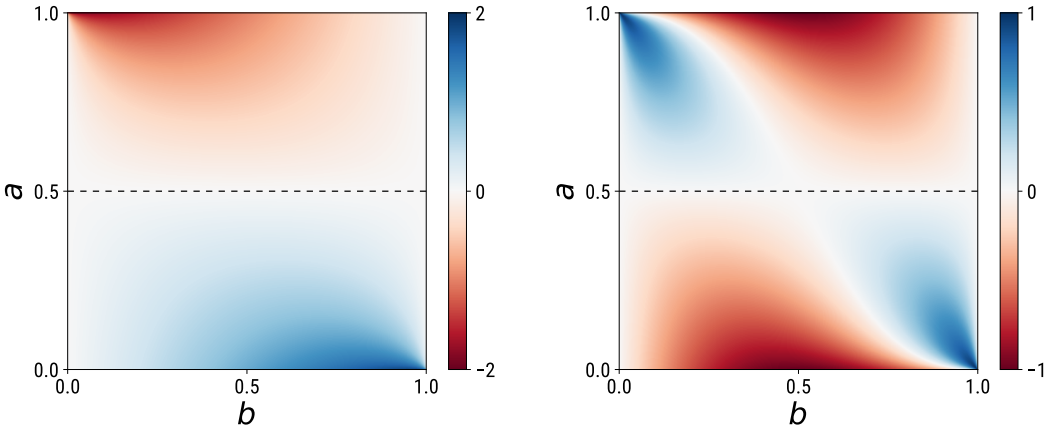

Figure 3.9 – Two non-interacting two-level systems with equal energy splitting $\varepsilon = 2$ are described by the Hamiltonian $\hat{H} = \hat{\sigma}_{S,z} + \hat{\sigma}_{C,z}$ and possess the global energy eigenstates $|\Psi\rangle = \sqrt{a}\,|\uparrow_S\downarrow_C\rangle + \sqrt{1-a}\,|\downarrow_S\uparrow_C\rangle$ with energy $E = 0$. All numerical values are given in atomic units (Appendix D) and the chosen clock state has the simple form $|\chi\rangle_C = \sqrt{1-b}\,|\uparrow\rangle_C + \sqrt{b}\,|\downarrow\rangle_C$ with the non-negative coefficients $a, b \in [0,1]$. The left panel shows the energy correction $E - \langle\hat{H}_S\rangle_\varphi - \langle\hat{H}_C\rangle_\chi$ and the right panel the difference $\mathrm{Var}_\varphi(\hat{H}_S) - \mathrm{Var}_\chi(\hat{H}_C)$ between the energy variances. Clearly, no strict inequality can be found and the signs of the correction terms depend on the specific global state and the chosen clock state. An exception is indicated by the dashed horizontal line, which describes the MES. All corrections simultaneously vanish for this special state (Appendix G).

$$-\frac{\langle\Psi|\hat{P}_\chi\hat{H}_C\hat{P}_\chi\hat{H}_C\hat{\bar{P}}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} \tag{3.1.224}$$

features a deviation from the exact equality of the energy variances too. As before, maximally entangled states $|\Psi\rangle$ with $\mathrm{tr}_S\,|\Psi\rangle\langle\Psi| = \hat{\mathbb{1}}_C/d_C$ lead to a vanishing of all correction terms (Appendix G). We must investigate the sign of the variance correction for a further assessment of the uncertainty relation. Instead of continuing an analytic treatment, we provide a simple, but illustrative numerical example in Figure 3.9. It shows that the correction terms are neither non-negative nor non-positive and, hence, our attempt to derive a general uncertainty relation with variances depending on $|\varphi[\chi]\rangle_S$ and $|\chi\rangle_C$ fails. Only the inequality $\mathrm{Var}_\varphi(\hat{H}_S) \geq \mathrm{Var}_\chi(\hat{H}_C)$ would allow us to derive $\mathrm{Var}_{\varphi(\lambda)}(\hat{H}_S)\cdot\mathrm{Var}_{\chi(\lambda)}\big(\hat{\alpha}_\chi(\alpha_0)\big) \geq \hbar^2\big|1 - |\langle\chi(\lambda)|\chi(\alpha_0)\rangle|^2/D_\chi\big|^2/4$. Unfortunately, such a relation does not hold in general.

3.2 Quantum mechanics - Mixed states

After the successful treatment of pure states in the previous section, we attempt a generalization to mixed states. Such an investigation is considered in this section, where the guiding core principles **(I)**-**(III)** are translated to the framework of mixed state at the beginning. Subsequently, the change of the system state is derived for $\hat{V} = 0$ and $\hat{V} \neq 0$, respectively, and we examine a newly appearing non-Hermitian term. All results derived in this section become essential for a comparison with the associated classical framework and, to this end, we give a formulation of Wigner functions at the end.

3.2.1 Energy constraint

For pure global states $|\Psi\rangle$, only one global constraint exists, but nonetheless generates two different kinds of transformations, namely $\exp\big[i\lambda(\hat{H}-E)\big]$ and $\exp\big[\lambda(\hat{H}-E)\big]$. The first can be understood as changing the complex phase of the coefficients in the energy eigenbasis, while the second changes the magnitude. A change in the absolute value corresponds to imaginary time evolution, a concept treated in the subsequent Chapter 4. Different from the pure state treatment, we need two constraints to achieve two similar transformations for mixed states. They can be derived from the known transformations on the pure state vector $|\Psi\rangle$ and their counterparts for the global pure state density $|\Psi\rangle\langle\Psi|$. First, we convert (3.1.4) to

$$e^{i\lambda(\hat{H}-E)}\,|\Psi\rangle\langle\Psi|\,e^{-i\lambda(\hat{H}-E)} = e^{i\lambda[\hat{H}-E,\bullet]}\,|\Psi\rangle\langle\Psi| = e^{i\lambda[\hat{H},\bullet]}\,|\Psi\rangle\langle\Psi| \tag{3.2.1}$$

and, after requiring the invariance $\exp\big(i\lambda[\hat{H},\bullet]\big)\hat{\rho}_\Psi \overset{!}{=} \hat{\rho}_\Psi$ for a general density operator $\hat{\rho}_\Psi$, the constraint becomes

$$0 = \big[\hat{H},\hat{\rho}_\Psi\big]. \tag{3.2.2}$$

For a valid representation of a quantum state, the density operator $\hat{\rho}_\Psi$ must be a Hermitian operator with non-negative eigenvalues. Even though we do not attach a probabilistic interpretation to the global state (Sec. 3.1.2), $\hat{\rho}_\Psi$ is normalized, such that its trace equals unity ($\mathrm{tr}\,\hat{\rho}_\Psi = 1$). Second, the non-unitary, but Hermitian transformation $\exp\big[\lambda(\hat{H}-E)\big]|\Psi\rangle = |\Psi\rangle$ yields

$$e^{\lambda(\hat{H}-E)}\,|\Psi\rangle\langle\Psi|\,e^{\lambda(\hat{H}-E)} = e^{\lambda\{\hat{H}-E,\bullet\}_+}\,|\Psi\rangle\langle\Psi| \tag{3.2.3}$$

and we find

$$0 = \big\{\hat{H}-E,\hat{\rho}_\Psi\big\}_+ = \big\{\hat{H},\hat{\rho}_\Psi\big\}_+ - 2E\hat{\rho}_\Psi \tag{3.2.4}$$

for general invariant global states. For the sake of being able to compare our results for subsystem density operators with the pure states result, we keep $\hat{\rho}_\Psi = |\Psi\rangle\langle\Psi| = \hat{P}_\Psi$ for postulate **(I)** with $(\hat{H}-E)|\Psi\rangle = 0$. The mixed state nature enters our treatment through the use of mixed clock density operators instead, which subsequently induce mixed system states, as we show in the following. Constraints (3.2.2) and (3.2.2) are then automatically fulfilled. Notwithstanding our choice, we explore the space of possible mixed state solutions for completeness. To this end, Eq. (3.2.2) yields

$$0 = \sum_{m,n}\sum_{\alpha_m,\alpha_n} c_{mn,\alpha_m\alpha_n}\,\big|E_{m,\alpha_m}\big\rangle\big\langle E_{n,\alpha_n}\big|\,(E_m - E_n) \tag{3.2.5}$$

for a general state $\hat{\rho}_\Psi = \sum_{m,n}\sum_{\alpha_m,\alpha_n} c_{mn,\alpha_m\alpha_n}\,\big|E_{m,\alpha_m}\big\rangle\big\langle E_{n,\alpha_n}\big|$, where α_i labels possible energy degeneracies. We find that

$$c_{mn,\alpha_m\alpha_n} = 0 \qquad \text{for} \quad E_m \neq E_n \tag{3.2.6}$$

and the matrix form in energy basis reduces to block form, where each block corresponds to a degenerate energy subspace. The other constraint (3.2.4) gives

$$0 = \sum_{m,n} \sum_{\alpha_m,\alpha_n} c_{mn,\alpha_m\alpha_n} \left|E_{m,\alpha_m}\right\rangle\!\left\langle E_{n,\alpha_n}\right| (E_m + E_n - 2E) \tag{3.2.7}$$

and, in combination with (3.2.6), further limits the coefficients to

$$c_{mn\alpha_m\alpha_n} = 0 \qquad \text{for} \quad E_m \neq E\,. \tag{3.2.8}$$

Hence, only a single block of the density operator can be non-zero in the energy eigenbasis, namely the one associated with energy E. If this energy level possesses a degeneracy, then a mixed state is possible for postulate **(I)** in general, i.e.,

$$\hat{\rho}_\Psi = \sum_{\alpha_m\alpha_n} \tilde{c}_{\alpha_m\alpha_m} \left|E_{\alpha_m}\right\rangle\!\left\langle E_{\alpha_n}\right| . \tag{3.2.9}$$

At any rate, we do not pursue this line of thought here in order to directly compare our mixed state results to the pure state vector formalism. Nevertheless, we compare this expression with the classical equivalent in Section 3.3.

In this chapter, we focus on the unitary changes and use only the invariance generated by Eq. (3.2.2), namely

$$e^{i\lambda[\hat{H},\bullet]}\,|\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi|\,. \tag{3.2.10}$$

To provide a different perspective on the energy constraints, we mention that the Hermiticity $\hat{\rho}_\Psi^\dagger = \hat{\rho}_\Psi$ and $(\hat{H}-E)\hat{\rho}_\Psi = 0$ imply constraints (3.2.2) and (3.2.4), respectively, which corresponds to the vanishing of the Hermitian and anti-Hermitian part of $(\hat{H}-E)\hat{\rho}_\Psi = \{\hat{H}-E,\hat{\rho}_\Psi\}_+/2 + [\hat{H},\hat{\rho}_\Psi]/2$. The anti-Hermitian part is responsible for the generation of real-time dynamics, whereas the Hermitian counterpart is later used for imaginary time evolution (Sec. 4.2).

3.2.2 Conditional system state

The relational system state from proposition **(III)** can be deduced from the density operator form (3.1.6) of the pure state case. Upon substitution of the general mixed clock state $\hat{\rho}_\mathrm{C}$ for $|\chi\rangle\langle\chi|_\mathrm{C}$, the system density operator becomes

$$\hat{\rho}_\mathrm{S} \equiv \frac{\mathrm{tr}_\mathrm{C}\left(\hat{\rho}_\mathrm{C}\hat{P}_\Psi\right)}{\langle\Psi|\left(\hat{\mathbb{1}}_\mathrm{S}\otimes\hat{\rho}_\mathrm{C}\right)|\Psi\rangle} \tag{3.2.11}$$

and constitutes a mixed state in general. Regardless of the exact form of the clock state, the system state is always normalized to $\mathrm{tr}_\mathrm{S}\,\hat{\rho}_\mathrm{S} = 1$ with the partial trace tr_S over the system degree of freedom. As before, we omit the identity operator in the denominator in the following treatment.

3.2.3 Time emergence

Straightforwardly, the interaction-free case $\hat{V} = 0$ is resolved by application of $\mathrm{tr}_\mathrm{C}\big(\hat{\rho}_\mathrm{C}(0)\,\bullet\big)$ to Eq. (3.2.10), yielding

$$e^{-i\lambda\hat{H}_\mathrm{S}}\,\mathrm{tr}_\mathrm{C}\Big(\hat{\rho}_\mathrm{C}(0)\,\hat{P}_\Psi\Big)\,e^{i\lambda\hat{H}_\mathrm{S}} = \mathrm{tr}_\mathrm{C}\Big(e^{-i\lambda\hat{H}_\mathrm{C}}\,\hat{\rho}_\mathrm{C}(0)\,e^{i\lambda\hat{H}_\mathrm{C}}\hat{P}_\Psi\Big), \tag{3.2.12}$$

in close analogy to the pure state case. Here, $\hat{\rho}_\mathrm{C}(0)$ denotes a fixed initial state associated with $\lambda = 0$. Since no norm changes occur for $\mathrm{tr}_\mathrm{C}\big(\hat{\rho}_\mathrm{C}(0)\,\hat{P}_\Psi\big)$ under transformations generated by $\hat{H}_\mathrm{S}$, the von Neumann equation

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_\mathrm{S}(\lambda) = \Big[\hat{H}_\mathrm{S}, \hat{\rho}_\mathrm{S}(\lambda)\Big] \tag{3.2.13}$$

follows immediately with the λ-evolved mixed clock state

$$\hat{\rho}_\mathrm{C}(\lambda) = e^{-i\lambda\hat{H}_\mathrm{C}}\,\hat{\rho}_\mathrm{C}(0)\,e^{i\lambda\hat{H}_\mathrm{C}}\,. \tag{3.2.14}$$

All remarks for the pure state setting from Sec. 3.1.5.1 directly carry over to mixed states. In particular, the ability to deparametrize the system evolution in terms of a clock property $\mathrm{A}_\mathrm{C}(\lambda) \equiv \mathrm{tr}_\mathrm{C}[\hat{A}_\mathrm{C}\hat{\rho}_\mathrm{C}(\lambda)]$ with a suitable Hermitian clock operator $\hat{A}_\mathrm{C}$ is unaltered by the use of mixed clock states. One notable difference does however exist. Previously, the use of a pure clock state implied a strictly pure system state, but utilizing mixed clock states does not inevitably lead to mixed system states. To demonstrate this fact, we assume the existence of a Hermitian clock operator $\hat{M}_\mathrm{C}$, which commutes with the clock Hamiltonian ($[\hat{H}_\mathrm{C}, \hat{M}_\mathrm{C}] = 0$) and connects two pure initial clock states through the unitary transformation $|\chi_2(0)\rangle_\mathrm{C} = \exp\big(i\hat{M}_\mathrm{C}\big)\,|\chi_1(0)\rangle_\mathrm{C}$. This additional (continuous or discrete) symmetry of the clock implies that both clock states can be related at all times λ, i.e., $|\chi_2(\lambda)\rangle_\mathrm{C} = \exp\big(i\hat{M}_\mathrm{C}\big)\,|\chi_1(\lambda)\rangle_\mathrm{C}$. If the global state is simultaneously invariant under $\hat{\mathbb{1}}_\mathrm{S} \otimes \exp\big(i\hat{M}_\mathrm{C}\big)$, then the relational system states conditioned on $|\chi_1\rangle_\mathrm{C}$ and $|\chi_2\rangle_\mathrm{C}$ are the same, because $\langle\chi_2(\lambda)|\Psi\rangle_\mathrm{C} = \langle\chi_1(\lambda)|\Psi\rangle_\mathrm{C}$. Thus, any mixed clock state $\hat{\rho}_\mathrm{C} = a\,|\chi_1\rangle\langle\chi_1|_\mathrm{C} + (1-a)\,|\chi_2\rangle\langle\chi_2|_\mathrm{C}$ for $a \in (0,1)$ induces a pure system state for all λ. The presence of an interaction term $\hat{V}$ does not change this fact, as can be seen from $\langle\chi_2|\hat{V}|\Psi\rangle_\mathrm{C}$ $= \langle\chi_1|\hat{V}|\Psi\rangle_\mathrm{C} + \langle\chi_2|[\hat{H}_\mathrm{C}, \hat{M}_\mathrm{C}]|\Psi\rangle_\mathrm{C} = \langle\chi_1|\hat{V}|\Psi\rangle_\mathrm{C}$. We treat generally interacting subsystems in the analysis below.

As shown in Section 3.1, the λ-dependent change of the clock did not transform with the introduction of an interaction $\hat{V}$ and, for this reason, we assume this property to hold also for mixed states. It can be rigorously shown using infinitesimal transformation steps in a fashion similar to the pure state case, but this tedious derivation does not provide any additional insight. Instead, we start with the λ-evolved clock state and derive the equation of motion for the system from it. Whenever appropriate, we omit the λ-argument in the following. Taking the derivative of the system state with respect to λ and using the TISE (3.1.3) yields

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_\mathrm{S} = \frac{\mathrm{tr}_\mathrm{C}\Big(\big[\hat{H}_\mathrm{C}, \hat{\rho}_\mathrm{C}\big]\hat{P}_\Psi\Big)}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} - \frac{\mathrm{tr}\Big(\big[\hat{H}_\mathrm{C}, \hat{\rho}_\mathrm{C}\big]\hat{P}_\Psi\Big)}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle}\,\hat{\rho}_\mathrm{S} \tag{3.2.15}$$

$$\overset{\text{TISE}}{=} \Big[\hat{H}_\mathrm{S}, \hat{\rho}_\mathrm{S}\Big] + \frac{\mathrm{tr}_\mathrm{C}\Big(\hat{\rho}_\mathrm{C}\big[\hat{V}, \hat{P}_\Psi\big]\Big)}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} + \frac{\langle\Psi|\big[\hat{V}, \hat{\rho}_\mathrm{C}\big]|\Psi\rangle}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle}\,\hat{\rho}_\mathrm{S}\,. \tag{3.2.16}$$

The numerator of the last term was transformed with $\langle\Psi|\big[\hat{H}_\mathrm{C},\hat{\rho}_\mathrm{C}\big]|\Psi\rangle = \langle\Psi|\big[E-\hat{V}-\hat{H}_\mathrm{S},\hat{\rho}_\mathrm{C}\big]|\Psi\rangle = -\langle\Psi|\big[\hat{V},\hat{\rho}_\mathrm{C}\big]|\Psi\rangle$. In the current form, it remains unclear if Eq. (3.2.16) describes a unitary evolution of the system state. Encouraged by the successful application for pure states, we seek an effective potential $\hat{V}_\mathrm{S}$ that captures as much of the unitary contribution to the system evolution as possible. To this end, we define

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_\mathrm{S} = \big[\hat{H}_\mathrm{S}+\hat{V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big] + \hat{\Delta} + 2i\,\mathrm{Im}(a)\,\hat{\rho}_\mathrm{S} \tag{3.2.17}$$

with the remainder term

$$\hat{\Delta} \equiv \frac{\mathrm{tr}_\mathrm{C}\big(\hat{\rho}_\mathrm{C}\big[\hat{V}-\hat{V}_\mathrm{S},\hat{P}_\Psi\big]\big)}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} = \frac{\mathrm{tr}_\mathrm{C}\big(\hat{\rho}_\mathrm{C}\big[\hat{V},\hat{P}_\Psi\big]\big)}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} - \big[\hat{V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big] \equiv \hat{M} - \big[\hat{V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big]. \tag{3.2.18}$$

and the complex scalar $a \equiv \langle\Psi|\hat{V}\hat{\rho}_\mathrm{C}|\Psi\rangle\,/\,\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle$. As is shown later, the last term in Eq. (3.2.17) must not be included in $\hat{\Delta}$. The trace of the newly defined operator $\hat{M} \equiv \mathrm{tr}_\mathrm{C}\big(\hat{\rho}_\mathrm{C}\big[\hat{V},\hat{P}_\Psi\big]\big)/\,\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle$ compensates the purely imaginary term, namely

$$\mathrm{tr}_\mathrm{S}\,\hat{M} = \frac{\langle\Psi|\big[\hat{\rho}_\mathrm{C},\hat{V}\big]|\Psi\rangle}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} = -2i\,\mathrm{Im}(a) \tag{3.2.19}$$

and preserves the norm of $\hat{\rho}_\mathrm{S}$. A Hermitian conjugation of the remainder term leads to

$$\hat{\Delta}^\dagger = \frac{\mathrm{tr}_\mathrm{C}\big(\hat{\rho}_\mathrm{C}\big[\hat{V}_\mathrm{S}-\hat{V},\hat{P}_\Psi\big]\big)}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} = -\hat{\Delta}\,, \tag{3.2.20}$$

which renders $\hat{\Delta}$ anti-Hermitian.

To find the optimal $\hat{V}_\mathrm{S}$, we use a variational approach to identify a minimum in the norm of the remainder term, equivalent to the pure state case. We define the aforementioned norm as

$$\big\|\hat{\Delta}\big\|_\mathrm{S}^2 \equiv \mathrm{tr}_\mathrm{S}\big(\Delta^\dagger\hat{\Delta}\big) = -\,\mathrm{tr}_\mathrm{S}\big(\hat{\Delta}^2\big) \geq 0\,. \tag{3.2.21}$$

The variation of the effective system potential is facilitated by a small, but arbitrary hermitian term $\widehat{\delta V}_\mathrm{S}$, i.e., $\hat{V}_\mathrm{S} \longrightarrow \hat{V}_\mathrm{S} + \widehat{\delta V}_\mathrm{S}$, and the variationally induced change of $\hat{\Delta}$ reads

$$\delta\hat{\Delta} = -\big[\widehat{\delta V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big]. \tag{3.2.22}$$

Using the last relation and exploiting the cyclic property of the trace, we can express the variational change of the norm as

$$\delta\big\|\hat{\Delta}\big\|_\mathrm{S}^2 = -\delta\,\mathrm{tr}_\mathrm{S}\big(\Delta^2\big) = -2\,\mathrm{tr}_\mathrm{S}\big(\hat{\Delta}\cdot\delta\Delta\big) = 2\,\mathrm{tr}_\mathrm{S}\Big(\hat{\Delta}\big[\widehat{\delta V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big]\Big) \tag{3.2.23}$$

$$= 2\,\mathrm{tr}_\mathrm{S}\Big(\widehat{\delta V}_\mathrm{S}\big[\hat{\rho}_\mathrm{S},\hat{\Delta}\big]\Big) \stackrel{!}{=} 0\,. \tag{3.2.24}$$

As stated above, the variation $\widehat{\delta V}_\mathrm{S}$ is arbitrary and therefore the norm change can only be zero if the commutator in the last expression vanishes. This leads to

$$0 \stackrel{!}{=} \big[\hat{\rho}_\mathrm{S},\hat{\Delta}\big] = \big[\hat{\rho}_\mathrm{S},\hat{M}\big] - \Big[\hat{\rho}_\mathrm{S},\big[\hat{V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big]\Big] \tag{3.2.25}$$

or

$$\Big[\big[\hat{V}_\mathrm{S},\hat{\rho}_\mathrm{S}\big],\hat{\rho}_\mathrm{S}\Big] = \hat{\rho}_\mathrm{S}^2\hat{V}_\mathrm{S} + \hat{V}_\mathrm{S}\hat{\rho}_\mathrm{S}^2 - 2\hat{\rho}_\mathrm{S}\hat{V}_\mathrm{S}\hat{\rho}_\mathrm{S} \stackrel{!}{=} \big[\hat{M},\hat{\rho}_\mathrm{S}\big] = \hat{M}\hat{\rho}_\mathrm{S} - \hat{\rho}_\mathrm{S}\hat{M} \tag{3.2.26}$$

as the constraint for $\hat{V}_\mathrm{S}$. Evidently, the term $2i\,\mathrm{Im}\,a\hat{\rho}_\mathrm{S}$ in Eq. (3.2.17) has no relevance for the system potential, because $[2i\,\mathrm{Im}\,a\hat{\rho}_\mathrm{S}, \hat{\rho}_\mathrm{S}] = 0$. Unfortunately, no general solution exists for this equation and we must revert to a basis-dependent form for $\hat{V}_\mathrm{S}$.

For later reference, we give the constraint in terms of quantum Liouville operators

$$\hat{L}_A^{(\mathrm{qm})} \equiv \big[\hat{A}, \bullet\big], \tag{3.2.27}$$

also called "superoperators" [224,225] in order to distinguish them from the usual operators in quantum mechanics. To give an example, the energy anticommutator equation (3.2.2) becomes $\hat{L}_H^{(\mathrm{qm})}\hat{\rho}_\Psi = 0$ in this notation. For an operator $\hat{A} = \sum_n a_n |n\rangle\langle n|$, we can express the eigenoperators of such a quantum Liouville operator as $|n\rangle\langle m|$ with eigenvalues $a_n - a_m$. Constraint (3.2.26) becomes

$$\Big(\hat{L}_{\rho_\mathrm{S}}^{(\mathrm{qm})}\Big)^2 \hat{V}_\mathrm{S} \stackrel{!}{=} -\hat{L}_{\rho_\mathrm{S}}^{(\mathrm{qm})}\hat{M}\,. \tag{3.2.28}$$

Furthermore, we can expand the effective system potential in terms of the eigenoperators $|\varphi_m\rangle\langle\varphi_n|_\mathrm{S}$ by virtue of

$$\hat{V}_\mathrm{S} = \sum_{m,n} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\ \mathrm{tr}_\mathrm{S}\Big(|\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\,\hat{V}_\mathrm{S}\Big) = \sum_{m,n} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\ \langle\varphi_n|\hat{V}_\mathrm{S}|\varphi_m\rangle_\mathrm{S}\,. \tag{3.2.29}$$

3.2.3.1 Eigenbasis of system state

In order to solve Eq. (3.2.26) for $\hat{V}_\mathrm{S}$, one needs a suitable basis. Since the system state

$$\hat{\rho}_\mathrm{S} = \sum_{m=1}^{K_\mathrm{S}} q_m\,|\varphi_m\rangle\langle\varphi_m|_\mathrm{S} \tag{3.2.30}$$

appears on both sides of the equation, we use the eigenbasis $\{|\varphi_m\rangle_\mathrm{S}\}_{0\le m\le d_\mathrm{S}}$ to find a solution for the effective potential. Here, the rank $K_\mathrm{S} \le d_\mathrm{S}$ of $\hat{\rho}_\mathrm{S}$ is lower or equal to the Hilbert space dimension d_S of the system space, which implies $q_m = 0$ for $m > K_\mathrm{S}$. The eigenvalues are probabilities with $\sum_m q_m = 1$ and the associated basis vectors are orthonormal, i.e., $\langle\varphi_m|\varphi_n\rangle_\mathrm{S} = \delta_{mn}$. Even though not explicitly stated, it is important to remember that K_S, q_m and $|\phi_m\rangle_\mathrm{S}$ depend on λ. Projecting $\langle\varphi_m|_\mathrm{S}$ from the left and $|\varphi_n\rangle_\mathrm{S}$ from the right onto Eq. (3.2.26) yields

$$\underbrace{\big(q_m^2 + q_n^2 - 2q_m q_n\big)}_{=(q_n-q_m)^2=|q_n-q_m|^2}\langle\varphi_m|\hat{V}_\mathrm{S}|\varphi_n\rangle_\mathrm{S} = \big(q_n - q_m\big)\langle\varphi_m|\hat{M}|\varphi_n\rangle_\mathrm{S}\,, \tag{3.2.31}$$

$$\Rightarrow \quad \langle\varphi_m|\hat{V}_\mathrm{S}|\varphi_n\rangle_\mathrm{S} = \mathrm{sgn}(q_n - q_m)\frac{|q_n - q_m|}{|q_n - q_m|^2}\langle\varphi_m|\hat{M}|\varphi_n\rangle_\mathrm{S} \qquad \forall q_n \neq q_m \tag{3.2.32}$$

$$= \frac{1}{q_n - q_m}\langle\varphi_m|\hat{M}|\varphi_n\rangle_\mathrm{S} \qquad \forall q_n \neq q_m\,. \tag{3.2.33}$$

For $q_n = q_m$, the matrix elements of the effective system potential are undetermined and can be arbitrarily chosen, similar to the pure state case in Sec. 3.1.6.2. Although we set them to zero in the following, this freedom provides means to choose a convenient form for the effective system potential. Ultimately, we find the effective system potential

$$\hat{V}_S = \sum_{\substack{m=1 \\ n=1 \\ q_m \neq q_n}}^{d_S} \frac{|\varphi_m\rangle\langle\varphi_m|_S \hat{M} |\varphi_n\rangle\langle\varphi_n|_S}{q_n - q_m} \tag{3.2.34}$$

in the eigenbasis of the system density operator $\hat{\rho}_S$.

3.2.3.2 System potential for pure state case

As a useful consistency check, we evaluate the effective system potential (3.2.34) for pure states and compare the result to Eq. (3.1.48). In this case, only one system eigenstate $|\varphi_1\rangle_S = \langle\chi|\Psi\rangle_C / \sqrt{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}$ with $q_1 = 1$ exists, while all other coefficients vanish, i.e., $q_{m\neq 1} = 0$. Furthermore, the clock density operator reads $\hat{\rho}_C = |\chi\rangle\langle\chi|_C$, giving

$$\hat{M}_{\text{pure}} = \frac{\langle\chi|\hat{V}|\Psi\rangle_C \langle\Psi|\chi\rangle_C - \langle\chi|\Psi\rangle_C \langle\Psi|\hat{V}|\chi\rangle_C}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} = \frac{\langle\chi|\hat{V}|\Psi\rangle_C \langle\varphi_1|_S - |\varphi_1\rangle_S \langle\Psi|\hat{V}|\chi\rangle_C}{\sqrt{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}} . \tag{3.2.35}$$

Therefore, we get

$$\hat{V}_S = -\sum_{n=2}^{d_S} |\varphi_1\rangle\langle\varphi_1|_S \hat{M}_{\text{pure}} |\varphi_n\rangle\langle\varphi_n|_S + \sum_{m=2}^{d_S} |\varphi_m\rangle\langle\varphi_m|_S \hat{M}_{\text{pure}} |\varphi_1\rangle\langle\varphi_1|_S \tag{3.2.36}$$

$$= -|\varphi_1\rangle\langle\varphi_1|_S \hat{M}_{\text{pure}} \left[\hat{\mathbb{1}}_S - |\varphi_1\rangle\langle\varphi_1|_S\right] + \left[\hat{\mathbb{1}}_S - |\varphi_1\rangle\langle\varphi_1|_S\right] \hat{M}_{\text{pure}} |\varphi_1\rangle\langle\varphi_1|_S \tag{3.2.37}$$

$$= \hat{M}_{\text{pure}} |\varphi_1\rangle\langle\varphi_1|_S - |\varphi_1\rangle\langle\varphi_1|_S \hat{M}_{\text{pure}} \tag{3.2.38}$$

$$= \frac{\langle\chi|\left(\hat{V}\hat{P}_\Psi + \hat{P}_\Psi\hat{V}\right)|\chi\rangle_C}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} - \underbrace{(a + a^*)}_{=2\,\mathrm{Re}\,a} |\varphi_1\rangle\langle\varphi_1|_S , \tag{3.2.39}$$

which matches the result from the pure state case, up to a scalar shift. The second term has no influence on the dynamics of the system and, in fact, any additional part $\hat{O}$ of the interaction which commutes with the system ($[\hat{O}, \hat{\rho}_S] = 0$) is irrelevant. In our case, $\hat{O}$ is proportional to the system state, which obviously commutes with itself.

3.2.3.3 Remainder term for optimal system potential

After finding the effective potential (3.2.34) in terms of the system eigenbasis, we need to determine the remainder

$$\hat{\Delta} = \hat{M} - \left[\hat{V}_S, \hat{\rho}_S\right] = \sum_{\substack{m=1 \\ n=1}}^{d_S} |\varphi_m\rangle\langle\varphi_n|_S M_{mn} - \left[\hat{V}_S, \hat{\rho}_S\right] \tag{3.2.40}$$

with the components $M_{mn} = \langle\varphi_m|\hat{M}|\varphi_n\rangle_S$. The individual terms

$$\hat{V}_S\hat{\rho}_S = \sum_{\substack{m=1 \\ n=1 \\ q_m \neq q_n}}^{K_S} |\varphi_m\rangle\langle\varphi_n|_S \frac{M_{mn} q_n}{q_n - q_m} + \sum_{m=K_S+1}^{d_S} \sum_{n=1}^{K_S} M_{mn} |\varphi_m\rangle\langle\varphi_n|_S \tag{3.2.41}$$

and

$$\hat{\rho}_\mathrm{S}\hat{V}_\mathrm{S} = \left(\hat{V}_\mathrm{S}\hat{\rho}_\mathrm{S}\right)^\dagger = \sum_{\substack{m=1\\n=1\\q_m\neq q_n}}^{K_\mathrm{S}} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\, \frac{q_m M_{mn}}{q_n - q_m} - \sum_{m=1}^{K_\mathrm{S}}\sum_{n=K_\mathrm{S}+1}^{d_\mathrm{S}} M_{mn}\,|\varphi_m\rangle\langle\varphi_n|_\mathrm{S} \tag{3.2.42}$$

yield the commutator

$$[\hat{V}_\mathrm{S}, \hat{\rho}_\mathrm{S}] = \sum_{\substack{m=1\\n=1\\q_m\neq q_n}}^{K_\mathrm{S}} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\, M_{mn} + \left(\sum_{m=K_\mathrm{S}+1}^{d_\mathrm{S}}\sum_{n=1}^{K_\mathrm{S}} + \sum_{m=1}^{K_\mathrm{S}}\sum_{n=K_\mathrm{S}+1}^{d_\mathrm{S}}\right) M_{mn}\,|\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\,, \tag{3.2.43}$$

which we use to express the remainder term as

$$\hat{\Delta} = \sum_{\substack{m=1\\n=1\\q_m=q_n}}^{K_\mathrm{S}} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\, M_{mn} + \sum_{\substack{m=K_\mathrm{S}+1\\n=K_\mathrm{S}+1}}^{d_\mathrm{S}} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\, M_{mn} \tag{3.2.44}$$

$$= \sum_{\substack{m=1\\n=1\\q_m=q_n}}^{K_\mathrm{S}} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S}\, M_{mn} + \hat{\overline{P}}_\mathrm{S}\hat{M}\hat{\overline{P}}_\mathrm{S} \tag{3.2.45}$$

with the projectors $\hat{P}_\mathrm{S} \equiv \sum_{m=1}^{K_\mathrm{S}} |\varphi_m\rangle\langle\varphi_m|_\mathrm{S}$ and $\hat{\overline{P}}_\mathrm{S} \equiv \hat{\mathbb{1}}_\mathrm{S} - \hat{P}_\mathrm{S} = \sum_{m=K_\mathrm{S}+1}^{d_\mathrm{S}} |\varphi_m\rangle\langle\varphi_m|_\mathrm{S}$. In the following, we show that the second term vanishes. It is helpful to express the clock state in its unnormalized eigenbasis, i.e., $\hat{\rho}_\mathrm{C} = \sum_{m=1}^{K_\mathrm{C}} |\chi_m\rangle\langle\chi_m|_\mathrm{C}$, which remains normalized with $\mathrm{tr}_\mathrm{C}\,\hat{\rho}_\mathrm{C} = \sum_m \langle\chi_m|\chi_m\rangle_\mathrm{C} = 1$. Similar to before, we denote the rank of $\hat{\rho}_\mathrm{C}$ by K_C, which fulfills the relation $K_\mathrm{C} \geq K_\mathrm{S}$. The system state reads

$$\hat{\rho}_\mathrm{S} = \frac{1}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle}\sum_{m=1}^{K_\mathrm{C}} \langle\chi_m|\hat{P}_\Psi|\chi_m\rangle_\mathrm{C} = \frac{1}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle}\sum_{m=1}^{K_\mathrm{C}} \langle\chi_m|\Psi\rangle_\mathrm{C}\,\langle\Psi|\chi_m\rangle_\mathrm{C} \tag{3.2.46}$$

and the individual system vectors in the sum can be expressed in the system eigenbasis, namely

$$\frac{\langle\chi_m|\Psi\rangle_\mathrm{C}}{\sqrt{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle}} = \sum_{a=1}^{d_\mathrm{S}} f_{ma}\,|\varphi_a\rangle_\mathrm{S} \tag{3.2.47}$$

with complex coefficients f_{ma}. We find

$$\hat{\rho}_\mathrm{S} = \sum_{\substack{a=1\\b=1}}^{d_\mathrm{S}}\sum_{m=1}^{K_\mathrm{C}} f_{ma} f_{mb}^*\,|\varphi_a\rangle\langle\varphi_b|_\mathrm{S} = \sum_{\substack{a=1\\b=1}}^{d_\mathrm{S}} |\varphi_a\rangle\langle\varphi_b|_\mathrm{S} \sum_{m=1}^{K_\mathrm{C}} f_{ma} f_{mb}^* \tag{3.2.48}$$

$$\stackrel{!}{=} \sum_{a=1}^{K_\mathrm{S}} q_a\,|\varphi_a\rangle\langle\varphi_a|_\mathrm{S} \tag{3.2.49}$$

and the constraints on the coefficients f_{ma} become

$$\sum_{m=1}^{K_\mathrm{C}} f_{ma} f_{mb}^* \stackrel{!}{=} \delta_{ab}\begin{cases} q_a & \text{for} \quad a \leq K_\mathrm{S} \\ 0 & \text{for} \quad a > K_\mathrm{S} \end{cases}. \tag{3.2.50}$$

One of them is

$$\sum_{m=1}^{K_\mathrm{C}} |f_{ma}|^2 \stackrel{!}{=} 0 \qquad \forall a > K_\mathrm{S} \tag{3.2.51}$$

and can only be fulfilled if

$$f_{ma} = 0 \qquad \forall m, \forall a > K_S\,, \tag{3.2.52}$$

because Eq. (3.2.51) is a sum of positive semi-definite real numbers. The immediate consequence

$$\hat{\bar{P}}_S \frac{\langle \chi_m|\Psi\rangle_C}{\sqrt{\langle\Psi|\hat{\rho}_C|\Psi\rangle}} = 0 \tag{3.2.53}$$

follows, because of $\langle\chi_m|\Psi\rangle_C = \sum_{a=1}^{K_S} f_{ma}\,|\varphi_a\rangle_S$ for all m. This result is anticipated, because $\hat{\rho}_S$ is an incoherent sum of mutually non-orthogonal projectors $\langle\chi_m|\hat{P}_\Psi|\chi_m\rangle_C\,/\,\langle\Psi|\chi_m\rangle\langle\chi_m|\Psi\rangle$. Such a state must live in the subspace associated with projector $\hat{P}_S$ and, hence, cannot have contributions in the complement space. As a consequence, the block

$$\hat{\bar{P}}_S \hat{M} \hat{\bar{P}}_S = \frac{1}{\langle\Psi|\hat{\rho}_C|\Psi\rangle} \hat{\bar{P}}_S \,\mathrm{tr}_C\Big(\hat{\rho}_C\big[\hat{V}, \hat{P}_\Psi\big]\Big)\hat{\bar{P}}_S \tag{3.2.54}$$

$$= \frac{1}{\langle\Psi|\hat{\rho}_C|\Psi\rangle} \sum_m^{K_C} \hat{\bar{P}}_S\, \langle\chi_m|\Big(\hat{V}\hat{P}_\Psi - \hat{P}_\Psi\hat{V}\Big)|\chi_m\rangle_C\, \hat{\bar{P}}_S \tag{3.2.55}$$

$$= 0 \tag{3.2.56}$$

of $\hat{M}$ vanishes and, furthermore, the trace of $\hat{M}$ reduces to

$$\mathrm{tr}_S\,\hat{M} = \mathrm{tr}_S\Big[\hat{M}(\hat{P}_S + \hat{\bar{P}}_S)\Big] = \mathrm{tr}_S\big(\hat{M}\hat{P}_S\big) = \sum_{m=1}^{K_S} M_{mm}\,. \tag{3.2.57}$$

Overall, the remainder becomes

$$\hat{\Delta} = \sum_{\substack{m=1\\n=1\\q_m=q_n}}^{K_S} |\varphi_m\rangle\langle\varphi_n|_S\, M_{mn} = \sum_{m=1}^{K_S} |\varphi_m\rangle\langle\varphi_m|_S\, M_{mm} + \sum_{\substack{m=1\\n=1\\n\neq m\\q_m=q_n}}^{K_S} |\varphi_m\rangle\langle\varphi_n|_S\, M_{mn} \tag{3.2.58}$$

and its trace reads

$$\mathrm{tr}_S\,\hat{\Delta} = \mathrm{tr}_S\,\hat{M}\,. \tag{3.2.59}$$

For a verification of (3.2.58) as a solution of Eq. (3.2.25), we evaluate the commutator

$$\big[\hat{\rho}_S, \hat{\Delta}\big] = \sum_{\substack{m=1\\n=1\\q_m=q_n}}^{K_S} M_{mn} \sum_{k=1}^{K_S} q_k \Big[|\varphi_k\rangle\langle\varphi_k|_S\,, |\varphi_m\rangle\langle\varphi_n|_S\Big] \tag{3.2.60}$$

$$= \sum_{\substack{m=1\\n=1\\q_m=q_n}}^{K_S} M_{mn}\,|\varphi_m\rangle\langle\varphi_n|_S\,\big(q_m - q_n\big) = 0 \tag{3.2.61}$$

and its vanishing confirms our result. The differential equation for the system state becomes

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_S = \big[\hat{H}_S + \hat{V}_S, \hat{\rho}_S\big] + \underbrace{\hat{\Delta} - \mathrm{tr}_S(\hat{\Delta})\,\hat{\rho}_S}_{\equiv\hat{\bar{\Delta}}} \tag{3.2.62}$$

with the modified remainder

$$\hat{\tilde{\Delta}} \equiv \sum_{m=1}^{K_S} |\varphi_m\rangle\langle\varphi_m|_S \left(M_{mm} - \mathrm{tr}_S(\hat{\Delta})\, q_m\right) + \sum_{\substack{m=1 \\ n=1 \\ n\neq m \\ q_m=q_n}}^{K_S} |\varphi_m\rangle\langle\varphi_n|_S\, M_{mn}\,. \tag{3.2.63}$$

Before a further analysis of this operator, we use the pure state limit once again in order to check our results for consistency. If correct, the modified remainder is expected to vanish.

3.2.3.4 Remainder term for pure states

As in Sec. 3.2.3.2, a pure system state reads $|\varphi_1\rangle_S = \langle\chi|\Psi\rangle_C / \sqrt{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}$ with $q_1 = 1$ and its density operator has the rank $K_S = 1$. In this case, only a single component of $\hat{M}$ contributes to (3.2.63), namely

$$M_{11} = \langle\varphi_1|\hat{M}|\varphi_1\rangle_S = \frac{\langle\Psi|\left[\hat{\rho}_C, \hat{V}\right]|\Psi\rangle}{\langle\Psi|\hat{\rho}_C|\Psi\rangle} = -2i\,\mathrm{Im}(a) = \mathrm{tr}_S\,\hat{M}\,. \tag{3.2.64}$$

Additionally, the number of summands in the second term in Eq. (3.2.63) equals zero, because of $K_S = 1$, which results in the absence of any off-diagonal elements M_{mn}. We find the new remainder term to vanish, i.e.,

$$\hat{\tilde{\Delta}} = |\varphi_1\rangle\langle\varphi_1|_S \left(M_{11} - \mathrm{tr}_S\,\hat{M}\right) = |\varphi_1\rangle\langle\varphi_1|_S \left(\mathrm{tr}_S\,\hat{M} - \mathrm{tr}_S\,\hat{M}\right) = 0\,, \tag{3.2.65}$$

and confirm its correctness for pure system states.

3.2.3.5 Anti-Hermitian part of a Hamiltonian

Although Eq. (3.2.62) is already in a general form, we aim to gain a better understanding of the modified remainder $\hat{\tilde{\Delta}}$. Its form in terms of $\hat{\Delta}$ indicates the structure of an anti-Hermitian Hamiltonian and the general influence of such an operator on the state dynamics requires a brief review. To this end, we present the evolution equation for a density operator governed by a Hamiltonian featuring a Hermitian term $\hat{H} = \hat{H}^\dagger$ and an anti-Hermitian term $-i\hat{B}/2$ with $\hat{B}^\dagger = \hat{B}$. Such a Hamiltonian changes an initial state $\hat{\rho}_0$ to

$$\hat{\tilde{\rho}}(\lambda) \equiv \left(\mathscr{T} e^{-i\int^\lambda \mathrm{d}\lambda' \left[\hat{H}(\lambda') - i\hat{B}(\lambda')/2\right]}\right) \hat{\rho}_0 \left(\overline{\mathscr{T}} e^{i\int^\lambda \mathrm{d}\lambda' \left[\hat{H}(\lambda') + i\hat{B}(\lambda')/2\right]}\right) \tag{3.2.66}$$

and has the associated differential equation

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\tilde{\rho}}(\lambda) = \left[\hat{H}(\lambda), \hat{\tilde{\rho}}(\lambda)\right] - \frac{i}{2}\left\{\hat{B}(\lambda), \hat{\tilde{\rho}}(\lambda)\right\}_+\,. \tag{3.2.67}$$

Clearly, the norm $\mathrm{tr}\left(\hat{\tilde{\rho}}(\lambda)\right)$ is not conserved, because

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\,\mathrm{tr}\,\hat{\tilde{\rho}}(\lambda) = -\mathrm{tr}\left[\hat{B}(\lambda)\,\hat{\tilde{\rho}}(\lambda)\right] \tag{3.2.68}$$

is non-vanishing in general. To remedy the situation, we define the normalized state

$$\hat{\rho}(\lambda) \equiv \frac{\hat{\tilde{\rho}}(\lambda)}{\mathrm{tr}\,\hat{\tilde{\rho}}(\lambda)} \tag{3.2.69}$$

and obtain the corresponding differential equation

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}(\lambda) = \left[\hat{H}(\lambda), \hat{\rho}(\lambda)\right] - \frac{i}{2}\left\{\hat{B}(\lambda) - \left\langle\hat{B}\right\rangle_{\hat{\rho}}(\lambda), \hat{\rho}(\lambda)\right\}_+ \tag{3.2.70}$$

with mean value $\left\langle\hat{B}\right\rangle_{\hat{\rho}} \equiv \mathrm{tr}\left(\hat{\rho}\hat{B}\right)$. In the following, we show that the modified remainder $\hat{\tilde{\Delta}}$ can take the form of such an anti-Hermitian Hamiltonian part in the evolution equation.

3.2.3.6 Derivation of anti-Hermitian term

Despite the existence of a constructive way to derive the anti-Hermitian part, we first present the final outcome explicitly in the system eigenbasis in order to understand its general working. Afterward, the same result is derived in a basis-independent way. Accordingly, we define the conjectured Hermitian term appearing in the anti-Hermitian part as the operator

$$\hat{B}_\mathrm{S} \equiv i \sum_{\substack{m=1 \\ n=1 \\ q_m=q_n}}^{K_\mathrm{S}} |\varphi_m\rangle\langle\varphi_n|_\mathrm{S} \, \frac{M_{mn}}{q_n}\,, \tag{3.2.71}$$

which acts on the system state $\hat{\rho}_\mathrm{S}$ as $\hat{B}_\mathrm{S}\hat{\rho}_\mathrm{S} = \hat{\rho}_\mathrm{S}\hat{B}_\mathrm{S} = i\hat{\Delta}$ and has the mean value $\langle\hat{B}_\mathrm{S}\rangle_{\hat{\rho}_\mathrm{S}} = i\,\mathrm{tr}_\mathrm{S}\,\hat{\Delta} = i\,\mathrm{tr}_\mathrm{S}\,\hat{M}$. Using these properties yields

$$-\frac{i}{2}\Big\{\hat{B}_\mathrm{S} - \big\langle\hat{B}_\mathrm{S}\big\rangle_{\hat{\rho}_\mathrm{S}}, \hat{\rho}_\mathrm{S}\Big\}_+ = -i\Big(\hat{B}_\mathrm{S} - \big\langle\hat{B}_\mathrm{S}\big\rangle_{\hat{\rho}_\mathrm{S}}\Big)\hat{\rho}_\mathrm{S} = \hat{\Delta} - \mathrm{tr}_\mathrm{S}(\hat{M})\,\hat{\rho}_\mathrm{S} = \hat{\bar{\Delta}} \tag{3.2.72}$$

and confirms the status of $\hat{B}_\mathrm{S}$ as the correct operator in the anti-Hermitian term of the system Hamiltonian. Its direct derivation uses the orthogonality of $\hat{\Delta}$ to $\hat{\bar{P}}_\mathrm{S}$ and the Moore-Penrose inverse [226, 227] $\hat{\rho}_\mathrm{S}^\ominus$ (or "pseudoinverse") of the system density $\hat{\rho}_\mathrm{S}$ with the property $\hat{\rho}_\mathrm{S}^\ominus\hat{\rho}_\mathrm{S} = \hat{\rho}_\mathrm{S}\hat{\rho}_\mathrm{S}^\ominus = \hat{P}_\mathrm{S}$. Specifically, the modified remainder can be expressed as

$$\begin{aligned}
\hat{\bar{\Delta}} &= \hat{\Delta} - \mathrm{tr}_\mathrm{S}(\hat{M})\,\hat{\rho}_\mathrm{S} && (3.2.73)\\
&= \hat{\Delta}\left(\hat{P}_\mathrm{S} + \hat{\bar{P}}_\mathrm{S}\right) - \mathrm{tr}_\mathrm{S}(\hat{M})\,\hat{\rho}_\mathrm{S} && (3.2.74)\\
&= \hat{\Delta}\hat{P}_\mathrm{S} - \mathrm{tr}_\mathrm{S}(\hat{M})\,\hat{\rho}_\mathrm{S} && (3.2.75)\\
&= \hat{\Delta}\hat{\rho}_\mathrm{S}^\ominus\hat{\rho}_\mathrm{S} - \mathrm{tr}_\mathrm{S}(\hat{M})\,\hat{\rho}_\mathrm{S} && (3.2.76)\\
&= \left(\hat{\Delta}\hat{\rho}_\mathrm{S}^\ominus - \mathrm{tr}_\mathrm{S}(\hat{M})\right)\hat{\rho}_\mathrm{S} && (3.2.77)\\
&\overset{\text{Eq. (3.2.25)}}{=} (-i)\frac{i}{2}\left\{\hat{\Delta}\hat{\rho}_\mathrm{S}^\ominus - \mathrm{tr}_\mathrm{S}(\hat{M}), \hat{\rho}_\mathrm{S}\right\}_+, && (3.2.78)
\end{aligned}$$

which implies the Hermitian operator $\hat{B}_\mathrm{S} \equiv i\hat{\Delta}\hat{\rho}_\mathrm{S}^\ominus$ by way of comparison with Eq. (3.2.70). This basis-independent form of Eq. (3.2.71) has the same mean value

$$\big\langle\hat{B}_\mathrm{S}\big\rangle_{\hat{\rho}_\mathrm{S}} = \mathrm{tr}_\mathrm{S}(\hat{B}_\mathrm{S}\hat{\rho}_\mathrm{S}) = i\,\mathrm{tr}_\mathrm{S}\left(\hat{\Delta}\hat{P}_\mathrm{S}\right) \overset{(3.2.58)}{=} i\,\mathrm{tr}_\mathrm{S}\,\hat{\Delta} \overset{\text{Eq. (3.2.59)}}{=} i\,\mathrm{tr}_\mathrm{S}\,\hat{M} \tag{3.2.79}$$

with respect to the system state $\hat{\rho}_\mathrm{S}$. We emphasize that $\hat{B}_\mathrm{S}$ always commutes with the system state, which finally leads to the von Neumann equation

$$\begin{aligned}
i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_\mathrm{S} &= \Big[\hat{H}_\mathrm{S} + \hat{V}_\mathrm{S}, \hat{\rho}_\mathrm{S}\Big] - \frac{i}{2}\Big\{\hat{B}_\mathrm{S} - \big\langle\hat{B}_\mathrm{S}\big\rangle_{\hat{\rho}_\mathrm{S}}, \hat{\rho}_\mathrm{S}\Big\}_+ && (3.2.80)\\
&= \Big[\hat{H}_\mathrm{S} + \hat{V}_\mathrm{S}, \hat{\rho}_\mathrm{S}\Big] - i\Big(\hat{B}_\mathrm{S} - \big\langle\hat{B}_\mathrm{S}\big\rangle_{\hat{\rho}_\mathrm{S}}\Big)\hat{\rho}_\mathrm{S}\,. && (3.2.81)
\end{aligned}$$

Even though the additional non-Hermitian term would technically promote this equation to the status of a "master equation", we still call it a "von Neumann equation" for two reasons. First, we obtain unitary dynamics for pure states, which is untypical for master equations and, second, the non-Hermitian term is of a special form, which almost never occurs in open system dynamics.

3.2.4 Quasi-eigenstate approximation

An equivalent of the quasi-eigenstate approximation of the pure case can be thought of as

$$\hat{V}\hat{\rho}_{\mathrm{C}} = \hat{\overline{V}}_{\mathrm{S}}\hat{\rho}_{\mathrm{C}} \qquad \forall\lambda \tag{3.2.82}$$

with the system-operator-valued eigenvalue $\hat{\overline{V}}_{\mathrm{S}}$. In this case, the clock state commutes with the full interaction, namely

$$\left[\hat{V}, \hat{\rho}_{\mathrm{C}}\right] = 0 \tag{3.2.83}$$

and, in addition, we get

$$\hat{M} = \left[\hat{\overline{V}}_{\mathrm{S}}, \hat{\rho}_{\mathrm{S}}\right]. \tag{3.2.84}$$

The imaginary part of a vanishes, i.e,

$$2i\,\mathrm{Im}\,a = \frac{\langle\Psi|\left[\hat{V}, \hat{\rho}_{\mathrm{C}}\right]|\Psi\rangle}{\langle\Psi|\hat{\rho}_{\mathrm{C}}|\Psi\rangle} = 0 \tag{3.2.85}$$

and the remainder $\hat{\Delta}$ as well. It is immediately clear, that the system evolution is described by the von Neumann equation

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_{\mathrm{S}} = \left[\hat{H}_{\mathrm{S}} + \hat{\overline{V}}_{\mathrm{S}}, \hat{\rho}_{\mathrm{S}}\right], \tag{3.2.86}$$

which induces strictly unitary system motion.

3.2.5 Wigner function formalism

Before closing the section about time emergence in the quantum density operator framework and commencing the same analysis in the realm of classical mechanics, we seek to emphasize a connection between both theories [225]. "Quasi-probability distribution functions" on classical phase space have been proven to provide a strong link and many formal similarities between quantum and classical mechanics [228]. Though not the only transform to phase space, we use the Wigner representation [185, 229] to express our framework in terms of phase space coordinates $(\mathbf{q}, \mathbf{p})$ and $(\mathbf{Q}, \mathbf{K})$ for system and clock, respectively. The dimension of each continuous configuration space is denoted by n_i for $i \in \{\mathrm{S}, \mathrm{C}\}$. Discrete versions of the Wigner function do exist for finite-dimensional Hilbert spaces [230–232], but, for simplicity, only the continuous case is considered here. Quantum-classical transitions are intimately related to the smallness of Planck's reduced constant $\hbar$ and, therefore, we reinstate it in this section.

Any quantum mechanical state $\hat{\rho}$ can be transformed to the Wigner function

$$W_\rho(q,p) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}x\,\left\langle q - \frac{x}{2}\middle|\hat{\rho}\middle|q + \frac{x}{2}\right\rangle e^{ipx/\hbar} \tag{3.2.87}$$

for a simple two-dimensional phase space (q,p). Its generalization to higher dimensions is straightforward and requires, besides the transition to vectors, only a change of the denominator to $(2\pi\hbar)^{n_i}$. The marginal distributions $\int \mathrm{d}p\, W_\rho(q,p) = \langle q|\hat{\rho}|q\rangle$ and $\int \mathrm{d}q\, W_\rho(q,p) = \langle p|\hat{\rho}|p\rangle$ provide genuine probability densities, even though $W_\rho(q,p)$ itself does not constitute one, because $W_\rho(q,p) < 0$ is possible [185]. Nevertheless, it provides a

direct comparison with classical probability distributions. For any operators $\hat{A}$ other than a state density, the representation is defined as

$$\overline{W}_A(q,p) \equiv \int_{-\infty}^{\infty} \mathrm{d}x \left\langle q - \frac{x}{2}\middle|\hat{A}\middle|q + \frac{x}{2}\right\rangle e^{ipx/\hbar} \tag{3.2.88}$$

with a different prefactor. We use a bar over the same symbol to indicate the difference of this so-called "Weyl transform" [233] to (3.2.87). The prefactors are chosen such that

$$\left\langle \hat{A}\right\rangle_{\hat{\rho}} = \mathrm{tr}\left(\hat{\rho}\hat{A}\right) = \int_{-\infty}^{\infty} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p \; W_\rho(q,p)\, \overline{W}_A(q,p) \tag{3.2.89}$$

and

$$\mathrm{tr}(\hat{\rho}) = \mathrm{tr}\left(\hat{\rho}\,\hat{\mathbb{1}}\right) = \int_{-\infty}^{\infty} \mathrm{d}q \int_{-\infty}^{\infty} \mathrm{d}p \; W_\rho(q,p) = 1 \tag{3.2.90}$$

with $\overline{W}_{\mathbb{1}}(q,p) = 1$. These transformations from operators to phase space representations are also called "Weyl-Wigner correspondences" and always yield real-valued functions for Hermitian operators. In addition, the Wigner representations take simple forms for operators diagonal in either momentum or position space. For example, the potential $\left\langle q\middle|\hat{V}\middle|q'\right\rangle = V(q)\,\delta(q-q')$ has the Wigner representation $\overline{W}_V(q,p) = V(q)$.
Equipped with the appropriate algebraic tools, we translate the essential equations of our framework to their representations on a classical phase space. The relational system state is

$$W_{\rho_\mathrm{S}}(\mathbf{q},\mathbf{p}) = \frac{1}{\langle\Psi|\hat{\rho}_\mathrm{C}|\Psi\rangle} \int \mathrm{d}^{n_\mathrm{C}}\mathbf{Q}\,\mathrm{d}^{n_\mathrm{C}}\mathbf{K}\, W_{\rho_\mathrm{C}}(\mathbf{Q},\mathbf{K})\, W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) \tag{3.2.91}$$

and details of the calculation are given in appendix F. We note that $\hbar$ does not appear and, hence, we expect this form to hold equivalently in the classical framework. Moreover, the energy anticommutator constraint (3.2.4) for the global state $|\Psi\rangle\langle\Psi|$ reads

$$\overline{W}_H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) \cos\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right) W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) = E\, W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) \tag{3.2.92}$$

and contains $\hbar$ explicitly in the cosine function. Here, the derivatives in the Poisson bracket operator

$$\overleftrightarrow{\Lambda} \equiv \overleftarrow{\partial}_{(\mathbf{q},\mathbf{Q})}\overrightarrow{\partial}_{(\mathbf{p},\mathbf{K})} - \overleftarrow{\partial}_{(\mathbf{p},\mathbf{K})}\overrightarrow{\partial}_{(\mathbf{q},\mathbf{Q})} \tag{3.2.93}$$

act on functions to the left and to the right, indicated by the arrows above (App. F). We point out that $\overline{W}_H$ and $W_{|\Psi\rangle\langle\Psi|}$ are real-valued functions on phase space. In the limit $\hbar \to 0$, we would naively expect to obtain

$$\left(\overline{W}_H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) - E\right) W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) = 0\,, \tag{3.2.94}$$

but this only holds true if the derivatives of $\overline{W}_H$ and of $W_{|\Psi\rangle\langle\Psi|}$ do not become singular in this limit [185, 234]. Transforming the second energy constraint (3.2.2) to Wigner form corresponds to

$$\overline{W}_H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) \sin\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right) W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) = 0\,. \tag{3.2.95}$$

To lowest order in $\hbar$, we approximate

$$\sin\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right) \approx \frac{\hbar}{2}\overleftrightarrow{\Lambda} \tag{3.2.96}$$

and guess the classical equivalent to have a form identical to

$$\overline{W}_H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) \overleftrightarrow{\Lambda} W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) = \left\{\overline{W}_H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}), W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})\right\} = 0\,. \quad (3.2.97)$$

As before, this only holds if no derivative term scales with positive orders of $1/\hbar$. Even though the lowest order expansion is linear in $\hbar$, the final equation does not contain $\hbar$. In other words, Eqs. (3.2.94) and (3.2.97) do not contain Planck's reduced constant and, thus, their forms are available in the realm of classical mechanics.

For completeness, we also present the Weyl-Wigner correspondence for the von Neumann equation $i\hbar\partial_\lambda\hat{\rho} = [\hat{H},\hat{\rho}\,]$, which yields

$$\frac{\partial}{\partial\lambda}W_\rho = \frac{2}{\hbar}\overline{W}_H \sin\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right) W_\rho \equiv -i\overline{L}_H^{(\mathrm{qm})} W_\rho \quad (3.2.98)$$

with the quantum Liouville operator [235]

$$\overline{L}_H^{(\mathrm{qm})} \equiv \frac{2i}{\hbar}\overline{W}_H \sin\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right) \quad (3.2.99)$$

in Wigner representation. Its lowest order expansion in $\hbar$ reads $\overline{L}_H^{(\mathrm{qm})} \approx i\overline{W}_H \overleftrightarrow{\Lambda}$ and is a precursor of the classical version. Further discussions about the classical equations are given in the following section.

3.3 Classical mechanics

The emergence of time in quantum mechanics relies fundamentally on the linearity of the theory. Since classical mechanics is a limiting case of quantum mechanics, one strongly suspects a similar emergence in a purely classical setting. But how can we transfer results from a linear theory to one which is famously known for nonlinear dynamics? The answer lies in the way in which the dynamics is represented. Even though classical trajectories in configuration space are archetypal objects in classical mechanics, they only constitute one class of admissible states. In particular, they represent classical probability distributions which, for a fixed point in time, are proportional to a single delta-function on classical phase space, while the most general class of states is actually one containing arbitrary phase space probability densities. For the latter, the classical theory becomes inherently linear and, as a remarkable consequence, allows for convex combinations. For example, the fundamental dynamical equation for probability densities, the "Liouville equation", features a linear operator containing only first order derivatives. The reason for this linearity originates from the different character of the dynamical objects. For probability densities, the Hamilton function and the states depend only on the static background coordinates, while for classical trajectories the arguments of the Hamilton function are taken as the dynamical objects themselves, i.e., the position and momentum of the point particle. The importance of such a distinction has also been highlighted by Hilgevoord [189]. As a consequence, the classical treatment in this section is based on classical probability densities instead of classical trajectories. In addition, it has been pointed out that the classical limit of quantum states is not a single classical trajectory, but an ensemble of classical orbits [187]. We note in passing that the quantum mechanical evolution equation (3.2.81) for mixed states does indeed feature a non-linear term, however, it simply ensures normalization and does not induce physical change. Remarkably, the idea to map nonlinear dynamics to linear ones has matured into a full-fledged framework, called "Koopman theory", and is utilized even outside traditional fields of physics [236].

The general treatment of the classical case is formulated in a Hilbert space formulation of classical mechanics, which is introduced in Section 3.3.1. In this regard, the main idea is to treat classical probability densities on phase space as basis-independent objects, similar to a state vector $|\Psi\rangle$ with its representation $\Psi(x)$ on configuration space. In Section 3.3.2, we translate the three guiding principles from Chapter 2 into the Hilbert space formalism and, subsequently, show time emergence without and with an interaction term in Sections 3.3.3 and 3.3.4, respectively. The classical analysis concludes with the examination of a pure state counterpart for the system in Sec. 3.3.5, a brief consideration of the quasi-eigenstate approximation in Sec. 3.3.6 and an explicit example for unitary dynamics in Section 3.3.7. As it is turns out, the classical and the quantum formalism are strongly related, which is brought forth by comparison with basis-dependent Wigner representations and basis-independent quantum mechanical expressions in "Liouville space" [237].

3.3.1 Hilbert space formulation of classical mechanics

The beginning of a Hilbert space formulation for classical mechanics reaches back to the 1930s with the pioneering works by Koopman and von Neumann [238,239] and the utilization by Hopf [240]. Since then the formalism has been further developed and extensively used [235,241–255], for example in the description of non-equilibrium statistical mechanics [256]. Its close connection to quantum mechanics did not go unnoticed [198,246,257] and is present even in modern research. For instance, Bondar et al. [258] formulate an operational dynamical modeling in a Hilbert space formulation applying to quantum and classical mechanics and Okuyama and Ohzeki [221] use the classical Hilbert space language for the formulation of classical speed limits as the analog of quantum speed limits (Sec. 3.1.9). Knowing of this close association, it is not surprising that diagrammatic perturbation techniques, more well-known from quantum mechanics, have been applied in classical mechanics as well [259–261].

Even though not strictly necessary, we present our framework for classical mechanics in terms of abstract vectors by following the ideas of Refs. [243,244,246,262]. This provides us with the advantage of having elegant and basis-independent formulas at our disposal, without the need for long and bulky integral expression. Nevertheless, basis-dependent formulas in phase space coordinates (q,p) can be obtained at any time when necessary and we specifically use them to connect to the Wigner function representation from Sec. 3.2.5. Thus, as promised in the beginning, the general point of view shifts from single trajectories to the evolution of distributions and allows for a representation in more useful basis sets. One such example is the set of eigenfunctions of the Liouville operator [235,241,246,256,262], for which the time evolution of an initial distribution can be easily expressed by use of the associated eigenvectors. For instance, regions in phase space that can be accessed at later times by an initial distribution can be read off from the expansion into the Liouville eigenfunctions (for a time-independent Hamilton function) for which the overlap does not vanish [246]. An excellent resource for further technical details is Ref. [262].

For simplicity, only a two-dimensional phase space is used for now, but the generalization to higher dimensions is almost effortless. We define the inner product of two complex-valued functions f,g on phase space (q,p) as

$$\langle f\,|g\rangle \equiv \int \mathrm{d}q\,\mathrm{d}p\, f^*(q,p)\, g(q,p) = \langle g|f\rangle^* \,. \tag{3.3.1}$$

Furthermore, a basis $\{|q,p\rangle\}$ on Hilbert space with $\langle q',p'|q,p\rangle = \delta(q-q')\,\delta(p-p')$, representing single points in phase space, is defined. With the use of this basis, any function

$f(q,p)$ on phase space (q,p) can be represented as an element of the Hilbert space as

$$|f\rangle = \left(\int \mathrm{d}q\,\mathrm{d}p\,|q,p\rangle\langle q,p|\right)|f\rangle \equiv \int \mathrm{d}q\,\mathrm{d}p\,f(q,p)\,|q,p\rangle\ . \tag{3.3.2}$$

The representation

$$|\rho\rangle = \int \mathrm{d}q\,\mathrm{d}p\,\rho(q,p)\,|q,p\rangle \tag{3.3.3}$$

of a classical probability density $\rho(q,p) \geq 0$ needs to be supplemented by the normalization condition

$$\langle \mathbb{1}|\rho\rangle = \int \mathrm{d}q\,\mathrm{d}p\,\rho(q,p) = 1. \tag{3.3.4}$$

Here, we used the constant unit function[5] with $\langle q,p|\mathbb{1}\rangle = 1$. We note that such a formulation for the probability density is not the only possible mapping to vectors in a Hilbert space. Some modern investigations, for example [248–250, 252–254, 258], use the probability amplitude $r(q,p)$ with $\rho(q,p) = |r(q,p)|^2$ instead to define $|r\rangle$ with $\langle r|r\rangle = 1$. The motivation for this formulation stems from the aspiration to show a formal equivalence to complex-valued pure state quantum mechanics and the fact that $r(q,p,\lambda)$ and $\rho(q,p,\lambda)$ fulfill the same Liouville equation, due to the linearity of the classical Liouville operator in first-order derivatives [249, 250, 254]. In any case, the formulation in terms of the probability density ρ is favored in this thesis, because it is less mathematically involved and closely matches the quantum mechanical formulation for mixed states, if we were to define the inner product $\langle \hat{A}|\hat{B}\rangle \equiv \mathrm{tr}(\hat{A}^\dagger \hat{B})$ on the space of operators. Likewise, the correspondence due to Wigner functions is given in terms of the probability density and not its amplitude. Especially, the definition of the relational system state, defined below, would not match the Wigner representation (3.2.91).

In the Hilbert space formulation, two kinds of operators are needed, which both derive from an arbitrary function $A(q,p)$ on phase space. First, we define "multiplicative operators" $\hat{A}$ as

$$\langle f|\hat{A}g\rangle \equiv \int \mathrm{d}q\,\mathrm{d}p\ f^*(q,p)A(q,p)\,g(q,p) = \langle \hat{A}^* f|g\rangle\ , \tag{3.3.5}$$

indicated by a caret above the function variable. They are diagonal in the $\{|q,p\rangle\}$-basis and may, alternatively, be expressed as $A(\hat{q},\hat{p})$. Hence, the phase space average of a real-valued $A(q,p)$ with respect to a state ρ reads

$$\langle A\rangle_\rho = \langle A|\rho\rangle = \int \mathrm{d}q\,\mathrm{d}p\ A(q,p)\,\rho(q,p) \tag{3.3.6}$$

and is the classical equivalent of the quantum mechanical mean value in terms of Wigner functions, namely $\langle \hat{A}\rangle_\rho = \mathrm{tr}(\hat{A}\hat{\rho}_\Psi) = \int \mathrm{d}q\,\mathrm{d}p\ \overline{W}_A(q,p)\,W_\rho(q,p)$. The second kind of operator is responsible for canonical transformations on phase space [245], namely

$$\langle q,p|\hat{L}_A f\rangle \equiv iA(q,p)\overleftrightarrow{\Lambda} f(q,p) = i\left(\frac{\partial A(q,p)}{\partial q}\frac{\partial f(q,p)}{\partial p} - \frac{\partial A(q,p)}{\partial p}\frac{\partial f(q,p)}{\partial q}\right) \tag{3.3.7}$$

[5] $|\mathbb{1}\rangle$ is not strictly an element of Hilbert space, but an "improper state". These are also encountered in quantum mechanics, for example as momentum eigenstates and require an extension to "rigged Hilbert spaces" [185, 262, 263], as is routinely done in quantum mechanics. This issue is however of a mathematical nature and shall not be of any concern for the physical considerations here.

These operators are of the "Liouville type" and, accordingly, we denote them by $\hat{L}_A$ for generating functions $A(q,p)$. It holds that

$$\left\langle f \middle| \hat{L}_A g \right\rangle = -\left\langle \hat{L}_A g \middle| f \right\rangle \tag{3.3.8}$$

for real-valued f, g, A and

$$\left\langle f \middle| \hat{L}_A g \right\rangle = \left\langle \hat{L}_{A^*} f \middle| g \right\rangle \tag{3.3.9}$$

for generation functions A with commuting second partial derivatives. Furthermore, the application of the Liouville type operators on a ket vector has the property

$$\hat{L}_A |f\rangle = -\hat{L}_f |A\rangle \,, \tag{3.3.10}$$

which is the equivalent of $[\hat{A},\hat{f}] = -[\hat{f},\hat{A}]$ for quantum mechanical operators. Using that

$$\left\langle q,p \middle| \hat{L}_p f \right\rangle = -i\frac{\partial}{\partial q} f(q,p)\,, \tag{3.3.11}$$

$$\left\langle q,p \middle| \hat{L}_q f \right\rangle = i\frac{\partial}{\partial p} f(q,p) \tag{3.3.12}$$

holds, any Liouville type operator can also be written as

$$\hat{L}_A = \widehat{\frac{\partial A}{\partial q}}\,\hat{L}_q + \widehat{\frac{\partial A}{\partial p}}\,\hat{L}_p\,. \tag{3.3.13}$$

Any canonical transformation on phase corresponds [244] to $\exp\left(-i\lambda\hat{L}_A\right)|f\rangle$ or, in phase space coordinates,

$$e^{\lambda\{A(q,p),\bullet\}} f(q,p) = f(q,p) + \lambda\Big\{A(q,p), f(q,p)\Big\} + \frac{\lambda^2}{2!}\Big\{A(q,p), \Big\{A(q,p), f(q,p)\Big\}\Big\} + \dots \tag{3.3.14}$$

for $\lambda \in \mathbb{R}$. The classical Liouville equation $\partial\rho/\partial\lambda = \{\hat{H},\rho\}$ is now readily available in the basis-independent form

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho\rangle = -i\hat{L}_H|\rho\rangle \tag{3.3.15}$$

with the formal solution

$$|\rho(\lambda)\rangle = e^{-i\lambda\hat{L}_H}|\rho(0)\rangle \tag{3.3.16}$$

for λ-independent Hamilton functions H. For later use, we list some properties of both types of operators for Liouville type operators, namely

$$\hat{L}_{\gamma A} = \gamma\hat{L}_A \qquad \text{for} \quad \gamma \in \mathbb{C}\,, \tag{3.3.17}$$

$$\hat{L}_{A+\gamma\mathbb{1}} = \hat{L}_A \qquad \text{for} \quad \gamma \in \mathbb{C}\,, \tag{3.3.18}$$

$$\hat{L}_{A+B} = \hat{L}_A + \hat{L}_B\,. \tag{3.3.19}$$

3.3.2 Subsystems, energy constraints and relational system state

Postulate **(II)** corresponds to splitting the phase space coordinates into system and clock coordinates, i.e., the pairs $(\mathbf{q},\mathbf{p})$ and $(\mathbf{Q},\mathbf{K})$. As in Section 3.2.5, we denote the number of continuous degrees of freedom by n_S and n_C for system and clock, respectively, and the dimension of the global phase space is $2(n_\mathrm{S}+n_\mathrm{C})$.

We have already established in Section 3.2 that two independent equations are necessary to express the desired global energy constraint for postulate **(I)**. From Section 3.2.5 we take the classical limits of the quantum mechanical constraints as the corresponding classical equivalents. To this end, we require

$$\Big(H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})-E\Big)\rho_\Psi(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})=0 \tag{3.3.20}$$

with the Hamilton function $H(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})=H_S(\mathbf{q},\mathbf{p})+H_C(\mathbf{Q},\mathbf{K})+V(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})$ or

$$\big(\hat{H}-E\big)\,|\rho_\Psi\rangle=0 \tag{3.3.21}$$

for the global state ρ_Ψ, as the equivalent of (3.2.94). This equation is fulfilled for densities ρ_Ψ that can only be non-zero at points where the Hamilton function is equal to E or must vanish otherwise. Simultaneously, one quickly realizes that $\hat{H}-E$ generates the Hermitian transformations $\exp\big(\lambda(\hat{H}-E)\big)$, which results in the invariance $\exp\big[\lambda(\hat{H}-E)\big]\,|\rho_\Psi\rangle=|\rho_\Psi\rangle$ for all λ.[6] The consequences of this type of invariance are examined in Chapter 4, but it should be clear that it does not provide a pathway to the sought-after Liouville equation (3.3.15) for the system. Thus, we need the second classical equation (3.2.97) from section 3.2.5 to propose a classical counterpart, namely

$$\hat{L}_H\,|\rho_\Psi\rangle=0\,. \tag{3.3.22}$$

It generates the invariance

$$\exp\big(i\lambda\hat{L}_H\big)\,|\rho_\Psi\rangle=|\rho_\Psi\rangle\qquad\qquad\forall\lambda\in\mathbb{R} \tag{3.3.23}$$

and is indeed the correct starting point, as is shown in the next section. The total energy E does not appear, because the shift $\hat{H}\to\hat{H}-E\hat{\mathbb{1}}$ leaves $\hat{L}_H$ invariant, due to Eq. 3.3.18. Interestingly, the only eigenfunctions of $\hat{L}_{\hat{H}}$ satisfying the probability requirements are the ones with eigenvalue zero [246]. An open question is how the quantum mechanical demand for a global pure energy eigenstate translates to classical mechanics.

For the purpose of gaining intuition about the global states fulfilling both energy constraints, namely Eqs. (3.3.21) and (3.3.22), we present a simple, but illustrative example [246]. To this end, the Hamilton function

$$H(q,p)=\frac{1}{2}(p^2+q^2) \tag{3.3.24}$$

[6] The transformation $\big|\rho'\big\rangle=\exp\big[i\lambda(\hat{H}-E)\big]|\rho\rangle$ would not preserve the reality of a state in phase space. In particular, $\big(\rho'(q,p)\big)^*=\exp\big[-i\lambda(H(q,p)-E)\big]\rho(q,p)\neq\rho'(q,p)$. While it may be true that the invariance $|\rho_\Psi\rangle=\exp\big[i\lambda(\hat{H}-E)\big]|\rho_\Psi\rangle$ still holds for states fulfilling Eq. (3.3.21), it does not yield valid transformations for the subsystem states. Specifically, the real-valuedness of their phase space representations would be violated. For $V=0$, $\langle\rho_C|e^{i\lambda(\hat{H}-E)}|\rho_\Psi\rangle_C=\langle\rho_C|\rho_\Psi\rangle_C$ becomes $|\rho_S(\lambda)\rangle_S=\exp\big(-i\lambda\hat{H}_S\big)|\rho_S(0)\rangle_S$ after proper normalization. Clearly, $\rho_S(\mathbf{q},\mathbf{p},\lambda)=\exp\big(-i\lambda H_S(\mathbf{q},\mathbf{p})\big)\rho_S(\mathbf{q},\mathbf{p},0)$ takes on complex values and only modifies the complex phase at each phase space point.

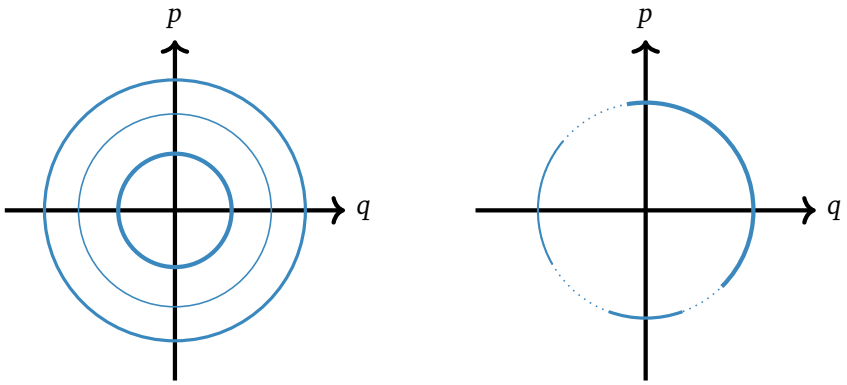

Figure 3.10 – Phase space representation of the type of solutions allowed under the constraint $\hat{L}_H|\rho\rangle = 0$ are shown on the left. Each of the concentric circles lies on an energy hypersurface with constant probability density along each circle. These constant values can however differ between different energy shells, as indicated by the different line widths. The right plot constitutes a depiction of a typical element of the class of states fulfilling $(\hat{H}-E)|\rho\rangle = 0$. Their support is restricted to one energy shell (dotted line) with energy E, but the distribution on this shell is arbitrary. This fact is illustrated by lines of different widths and the absence of lines on parts of the dotted circle.

of the harmonic oscillator is used. The associated Liouville operator

$$\left\langle q,p\middle|\hat{L}_H f\right\rangle = i\left(q\frac{\partial}{\partial p} - p\frac{\partial}{\partial q}\right)f(q,p) \tag{3.3.25}$$

is the generator of rotations in the (q,p) plane and it is useful to express everything in polar coordinates (r,φ) with $q = r\cos\varphi$ and $p = r\sin\varphi$. The Hamilton function becomes $H(r,\varphi) = r^2/2$ and the phase space representation of $\hat{L}_H$ is $i\,\partial/\partial\varphi$. Clearly, the eigenfunctions $\rho_{n,\alpha}$ are of the form

$$\rho_{n,\alpha} = \frac{1}{2\pi}e^{-in\varphi}f_\alpha(r) \qquad n\in\mathbb{Z} \tag{3.3.26}$$

for some radial function $f_\alpha(r)$, which is undetermined and indicates the degeneracy α of the eigenspace [246]. Here, we can use $f_E(r) \propto \delta\left(E - r^2/2\right)$ for simplicity, which corresponds to a classification of the degeneracies according to $(\hat{H}-E)\left|\rho_{0,\alpha=E}\right\rangle = 0$. Hence, the constraint $\hat{L}_H|\rho_\Psi\rangle = 0$ corresponds to a superposition of concentric circles in (q,p), i.e., $\rho_\Psi \propto \int_0^\infty \mathrm{d}E\, c(E)\,\delta\left(E - r^2/2\right)$, a radial distribution with rotational symmetry. On the other hand, $(\hat{H}-E)|\rho_\Psi\rangle = 0$ corresponds to an arbitrary angular density $g(\varphi)$ on the energy shell with constant energy E. Both behaviors are illustrated in Fig. 3.10. The combination of both constraints yields a single circle in phase space (q,p), which is, at the same time, the microcanonical ensemble for this simple system. In general, such ensembles always fulfill both constraints, but do not exhaust the set of all possible solutions. Guided by these results, it is apparent that, in general, the energy constraint (3.3.21) dictates on which energy surface ρ_Ψ lives and the Liouville constraint (3.3.22) governs the functional form on these energy surfaces. Ref. [246] provides with the one-dimensional pendulum another example for a full spectral analysis of the Liouville operator $\hat{L}_H$. General evaluations of the spectral content regarding integrable and fully chaotic systems have been treated in [235, 262]. In the special case of pure quantum energy eigenstates of ergodic systems, which are solutions to Eq. 3.2.2, the classical limit converges to microcanonical ensembles [264] and further supports our arguments above.

Lastly, the relational system state from proposition **(III)** is straightforwardly defined as

$$|\rho_S\rangle_S \equiv |\rho_S[\rho_C]\rangle_S \equiv \frac{\langle\rho_C|\rho_\Psi\rangle_C}{\langle \mathbb{1}_S \otimes \rho_C|\rho_\Psi\rangle}\,, \tag{3.3.27}$$

where ρ_Ψ, ρ_S and ρ_C denote the probability density of the global state, the system and the clock, respectively. The additional argument $[\rho_C]$ shows the conditional dependence on the specific clock state ρ_C. Expressed in terms of the phase space coordinates $(\mathbf{q},\mathbf{p})$, the system state reads

$$\langle \mathbf{q},\mathbf{p}|\rho_S\rangle_S = \rho_S(\mathbf{q},\mathbf{p}) = \frac{1}{\langle \mathbb{1}_S \otimes \rho_C|\Psi\rangle}\int \mathrm{d}^{n_C}\mathbf{Q}\,\mathrm{d}^{n_C}\mathbf{K}\,\rho_C(\mathbf{Q},\mathbf{K})\,\rho_\Psi(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})\,, \tag{3.3.28}$$

and the nature of a conditional probability for the system is evident. The denominator, which ensures the normalization of $|\rho_S\rangle_S$, can also be expressed as an integral over the global phase space, but was taken in its abstract form for better readability. This classical system state is formally equivalent to the quantum mechanical system state Eq. (3.2.91) in terms of Wigner functions for pure and mixed states. As in Sec. 3.1.5.1, we have to assume $\langle\rho_C|\rho_\Psi\rangle_C \neq 0$ for a non-trivial behavior. The completed translation of the postulates into the mathematical language for classical mechanics enables us to show in the next two sections how time can emerge within this framework.

3.3.3 Time emergence without interaction

In view of the structure of the quantum mechanical treatments, the first derivation proceeds without an interaction between both subsystems, i.e., $V = 0$. Hence, for a given global state $|\rho_\Psi\rangle$, the invariance equation (3.3.23) reads

$$e^{i\hat{L}_H\lambda}\,|\rho_\Psi\rangle = e^{-i\hat{L}_{H_S}\lambda}e^{-i\hat{L}_{H_C}\lambda}\,|\rho_\Psi\rangle = e^{-i\hat{L}_{H_C}\lambda}e^{-i\hat{L}_{H_S}\lambda}\,|\rho_\Psi\rangle \tag{3.3.29}$$

for all $\lambda \in \mathbb{R}$ and follows from $[\hat{L}_{H_S}, \hat{L}_{H_C}] = 0$. Straightforwardly, we calculate the partial projection of the clock state $\left|\rho_{\chi_0}\right\rangle_C$ onto invariance (3.3.23) to be

$$\begin{aligned}
\left\langle\rho_{\chi_0}\middle|\rho_\Psi\right\rangle_C &= \left\langle\rho_{\chi_0}\middle|e^{i\hat{L}_H\lambda}\rho_\Psi\right\rangle_C && (3.3.30)\\
&= e^{i\hat{L}_{H_S}\lambda}\left\langle\rho_{\chi_0}\middle|e^{i\hat{L}_{H_C}\lambda}\,\rho_\Psi\right\rangle_C && (3.3.31)\\
&= e^{i\hat{L}_{H_S}\lambda}\left\langle e^{-i\hat{L}_{H_C}\lambda}\rho_{\chi_0}\middle|\rho_\Psi\right\rangle_C && (3.3.32)\\
&\equiv e^{i\hat{L}_{H_S}\lambda}\,\langle\rho_C(\lambda)|\rho_\Psi\rangle_C\,. && (3.3.33)
\end{aligned}$$

Here, we define the λ-evolved clock state $|\rho_C(\lambda)\rangle_C \equiv e^{-i\hat{L}_{H_C}\lambda}\left|\rho_{\chi_0}\right\rangle_C$ and note the relation $\hat{L}_{H_S}\left|\rho_{\chi_0}\right\rangle_C = 0$. Applying the inverse operator $e^{-i\hat{L}_{H_S}\lambda}$ and dividing by the constant $\langle\mathbb{1}_S\otimes\rho_C(\lambda)|\rho_\Psi\rangle = \langle\mathbb{1}_S\otimes\rho_C(0)|\rho_\Psi\rangle$ on both sides yields the λ-evolved system state

$$|\rho_S(\lambda)\rangle_S = e^{-i\hat{L}_{H_S}\lambda}\left|\rho_{\varphi_0}\right\rangle_S = \frac{\langle\rho_C(\lambda)|\rho_\Psi\rangle_C}{\langle\mathbb{1}_S\otimes\rho_C(\lambda)|\rho_\Psi\rangle}\,. \tag{3.3.34}$$

That $\langle \mathbb{1}_S \otimes \rho_C(\lambda)|\rho_\Psi\rangle$ is constant follows from $\hat{L}_{H_S}|\mathbb{1}_S\rangle_S = 0$ and $\exp\left(-i\lambda\hat{L}_{H_S}\right)|\mathbb{1}_S\rangle_S = |\mathbb{1}_S\rangle_S$. The classical Liouville equation is obtained by means of a differentiation with respect to λ and gives

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_S(\lambda)\rangle_S = -i\hat{L}_{H_S}|\rho_S(\lambda)\rangle_S \,. \tag{3.3.35}$$

It shows that the emergent time evolution in classical mechanics originates from the *classical* correlations between system and clock, contained in the global state $|\rho_\Psi\rangle$. Astonishingly, all remarks from Sec. 3.1.5.1 regarding the properties of this derivation do also hold for the classical setting. Moreover, the special circumstance of a one-dimensional point particle being a clock and its position trajectory being a "time-indicating variable" [74] is readily included by using the state $\langle Q,K|\rho_C(\lambda)\rangle_C = \delta[Q-\mathsf{Q}(\lambda)]\cdot\delta[K-\mathsf{K}(\lambda)]$ and the mean value $\mathsf{Q}_C(\lambda) \equiv \langle \mathbb{1}_C|\hat{Q}|\rho_C(\lambda)\rangle_C = \mathsf{Q}(\lambda)$. As before, we continue with the treatment of interacting subsystems.

3.3.4 Time emergence with interaction

For the time emergence with interaction, we follow the route taken in Sec. 3.2.3. Namely, we take the λ-evolution of the clock from the previous section as given and derive the differential equation for the system state with an optimal effective system potential. The derivative of system state (3.3.27) with respect to λ reads

$$\begin{aligned}
i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_S\rangle_S &= \frac{i\,\mathrm{d}\langle\rho_C|\rho_\Psi\rangle_C/\mathrm{d}\lambda}{\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle} - |\rho_S\rangle_S\frac{i\,\mathrm{d}\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle/\mathrm{d}\lambda}{\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle} && (3.3.36)\\
&= -\frac{\left\langle\rho_C\middle|\hat{L}_{H_C}\rho_\Psi\right\rangle_C}{\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle} + |\rho_S\rangle_S\frac{\left\langle\mathbb{1}_S\otimes\rho_C\middle|\hat{L}_{H_C}\rho_\Psi\right\rangle}{\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle} && (3.3.37)\\
&\overset{(3.3.22)}{=} \hat{L}_{H_S}|\rho_S\rangle_S + \frac{\left\langle\rho_C\middle|\hat{L}_V\rho_\Psi\right\rangle_C}{\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle} - |\rho_S\rangle_S\underbrace{\frac{\left\langle\mathbb{1}_S\otimes\rho_C\middle|\hat{L}_V\rho_\Psi\right\rangle}{\langle\mathbb{1}_S\otimes\rho_C|\rho_\Psi\rangle}}_{\in i\mathbb{R}} && (3.3.38)
\end{aligned}$$

for $\hat{L}_H = \hat{L}_{H_S} + \hat{L}_{H_C} + \hat{L}_V$, where we use $\left\langle\mathbb{1}_S,\rho_C\middle|\hat{L}_{H_S}\rho_\Psi\right\rangle = 0$ and $-i\,\mathrm{d}\langle\rho_C|_C/\mathrm{d}\lambda = \left\langle\hat{L}_{H_C}\rho_C\right|_C$. Following our notation from the quantum framework, we introduce

$$|M\rangle_S \equiv \frac{\left\langle\rho_C\middle|\hat{L}_V\rho_\Psi\right\rangle_C}{\langle\mathbb{1}_S,\rho_C|\rho_\Psi\rangle} \tag{3.3.39}$$

and rewrite the differential equation as

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_S\rangle_S = \hat{L}_{H_S}|\rho_S\rangle_S + |M\rangle_S - |\rho_S\rangle_S\langle\mathbb{1}_S|M\rangle_S \,. \tag{3.3.40}$$

The system norm changes as

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\mathbb{1}_S|\rho_S(\lambda)\rangle_S = \left[1-\langle\mathbb{1}_S|\rho_S(\lambda)\rangle_S\right]\langle\mathbb{1}_S|M(\lambda)\rangle_S \tag{3.3.41}$$

and is conserved, because $\langle\mathbb{1}_S|\rho_S(0)\rangle_S = 1$.

As before, we employ a variational approach to obtain an optimal system potential V_S by minimizing the norm of the remainder vector

$$|\Delta\rangle_S \equiv \frac{\langle\rho_C|\left(\hat{L}_V - \hat{L}_{V_S}\right)\rho_\Psi\rangle_C}{\langle\mathbb{1}_S, \rho_C|\rho_\Psi\rangle} = \frac{\langle\rho_C|\hat{L}_V\rho_\Psi\rangle_C}{\langle\mathbb{1}_S, \rho_C|\rho_\Psi\rangle} - \hat{L}_{V_S}|\rho_S\rangle_S = |M\rangle_S - \hat{L}_{V_S}|\rho_S\rangle_S \tag{3.3.42}$$

for arbitrary λ. The variation $V_S \to V_S + \delta V_S$ with a real-valued function δV_S induces the vector change

$$|\delta\Delta\rangle_S = -\hat{L}_{\delta V_S}|\rho_S\rangle_S = \hat{L}_{\rho_S}|\delta V_S\rangle_S \tag{3.3.43}$$

and norm change

$$\delta\langle\Delta|\Delta\rangle_S = 2\,\mathrm{Re}\,\langle\delta\Delta|\Delta\rangle_S \stackrel{!}{=} 0\,. \tag{3.3.44}$$

Setting this norm change to zero yields an equation for the effective system potential V_S that minimizes the term which induces non-unitary evolution in the system. Specifically, we find

$$\langle\delta\Delta|\Delta\rangle_S = \left\langle\hat{L}_{\rho_S}\delta V_S\right|_S \cdot \frac{\langle\rho_C|\left(\hat{L}_V - \hat{L}_{V_S}\right)\rho_\Psi\rangle_C}{\langle\mathbb{1}_S \otimes \rho_C|\rho_\Psi\rangle} \tag{3.3.45}$$

$$= \langle\delta V_S|_S \cdot \hat{L}_{\rho_S}\left(|M\rangle_S - \hat{L}_{V_S}|\rho_S\rangle_S\right) \tag{3.3.46}$$

$$= \langle\delta V_S|_S \cdot \hat{L}_{\rho_S}\left(|M\rangle_S + \hat{L}_{\rho_S}|V_S\rangle_S\right), \tag{3.3.47}$$

which is purely real, since all involved functions are real-valued and imaginary units are squared, yielding a minus sign. The function δV_S is arbitrary and, hence, the defining equation for the system potential is

$$\hat{L}^2_{\rho_S}|V_S\rangle_S \stackrel{!}{=} -\hat{L}_{\rho_S}|M\rangle_S\,, \tag{3.3.48}$$

which is the classical analog of the quantum mechanical Eq. (3.2.28). Unfortunately, the correspondence between quantum and classical mechanics does also extend to the unability to find a general, basis-independent solution for equation (3.3.48). In the same manner as in the quantum setting, we proceed with the use of a set of basis vectors, which derives from the system state by virtue of the eigenvectors of $\hat{L}_{\rho_S}$. Refs. [235, 265] provide us with the correct treatment of eigenfunctions of Liouville type operators and, therefore, we do not dwell on the mathematical details. The spectrum of these Liouville type operators is degenerate and we classify them further by their eigenvalue with respect to $\hat{\rho}_S$, because this operator commutes with $\hat{L}_{\rho_S}$, and we recognize that further degeneracies can occur if a larger set of commuting operators exist [235]. The eigenfunctions form a complete basis and we denote them by $|\rho_{\nu\mu\zeta}\rangle_S$, such that

$$\hat{L}_{\rho_S}|\rho_{\nu\mu\zeta}\rangle_S = \nu|\rho_{\nu\mu\zeta}\rangle_S\,, \tag{3.3.49}$$

$$\hat{\rho}_S|\rho_{\nu\mu\zeta}\rangle_S = \mu|\rho_{\nu\mu\zeta}\rangle_S \tag{3.3.50}$$

and the index ζ denotes additional degeneracies. In the following, we suppress a possibly occurring unilateral dependence of these indices in the notation, but keep the order of summations or integration fixed. Such a notation is well-known from the bound hydrogen wavefunctions, in which the three quantum numbers n, l and m are often appearing without the explicit dependence on themselves, such as $l = l(n)$ or $m = m(l)$. All eigenstates with non-vanishing eigenvalue $\nu \neq 0$ have the curious property $\langle\mathbb{1}_S|\rho_{\nu\mu\zeta}\rangle_S = 0$ [246]. Furthermore, we find that the system state ρ_S has no overlap with $\mu = 0$ eigenstates,

i.e., $\langle \rho_S | \rho_{\nu 0 \zeta} \rangle_S = 0$ and, through the previous relation, that $\langle \rho_S | \rho_{\nu\mu\zeta} \rangle_S = 0$ for $\nu \neq 0$. Expressing Eq. (3.3.50) in system phase space coordinates $(\mathbf{q}, \mathbf{p})$ reveals the non-negativity of $\mu \geq 0$ and that $\rho_{\nu\mu\zeta}(\mathbf{q}, \mathbf{p})$ is only non-vanishing on the support of $\rho_S(\mathbf{q}, \mathbf{p})$ for $\mu > 0$. In other words, the conditions $\mu > 0$ and $\mu = 0$ split the phase space into two regions, the support of ρ_S and its complement, respectively. Thus, the expansion of the system state in this eigenbasis reads

$$|\rho_S\rangle_S = \sum\!\!\!\!\!\!\int_{\mu>0} \sum\!\!\!\!\!\!\int_{\zeta} |\rho_{0\mu\zeta}\rangle_S \langle \rho_{0\mu\zeta} | \rho_S \rangle_S \,. \tag{3.3.51}$$

For quantum mixed state, the analogs of the classical eigenfunctions are the eigenoperators of $\hat{L}^{(\mathrm{qm})}_{\rho_S} = [\hat{\rho}_S, \bullet]$ and of $\{\hat{\rho}_S, \bullet\}_+/2$, which are $|\varphi_m\rangle\langle\varphi_n|_S$ [247, 265] with eigenvalues $q_m - q_n$ and $(q_m + q_n)/2$, respectively (Sec. 3.2.3). In the system eigenbasis, we find

$$\langle \rho_{\nu\mu\zeta} | V_S \rangle_S = -\frac{1}{\nu} \langle \rho_{\nu\mu\zeta} | M \rangle \qquad \text{for} \quad \nu \neq 0 \tag{3.3.52}$$

or

$$|V_S\rangle_S = -\sum\!\!\!\!\!\!\int_{\nu\neq 0} \frac{1}{\nu} \sum\!\!\!\!\!\!\int_{\mu} \sum\!\!\!\!\!\!\int_{\zeta} |\rho_{\nu\mu\zeta}\rangle_S \langle \rho_{\nu\mu\zeta} | M \rangle_S \,. \tag{3.3.53}$$

The associated remainder vector is

$$\begin{aligned}
|\Delta\rangle_S &= |M\rangle_S - \hat{L}_{V_S} |\rho_S\rangle_S && (3.3.54)\\
&= |M\rangle_S + \hat{L}_{\rho_S} |V_S\rangle_S && (3.3.55)\\
&= |M\rangle_S - \left(\sum\!\!\!\!\!\!\int_{\nu\neq 0} \sum\!\!\!\!\!\!\int_{\mu} \sum\!\!\!\!\!\!\int_{\zeta} |\rho_{\nu\mu\zeta}\rangle\!\rangle\langle\!\langle \rho_{\nu\mu\zeta}|_S \right) |M\rangle_S && (3.3.56)\\
&= \left(\hat{\mathbb{1}}_S - \sum\!\!\!\!\!\!\int_{\nu\neq 0} \sum\!\!\!\!\!\!\int_{\mu} \sum\!\!\!\!\!\!\int_{\zeta} |\rho_{\nu\mu\zeta}\rangle\!\rangle\langle\!\langle \rho_{\nu\mu\zeta}|_S \right) |M\rangle_S && (3.3.57)\\
&= \sum\!\!\!\!\!\!\int_{\mu} \sum\!\!\!\!\!\!\int_{\zeta} |\rho_{0\mu\zeta}\rangle_S \langle \rho_{0\mu\zeta} | M \rangle_S && (3.3.58)
\end{aligned}$$

and can immediately be associated with the quantum remainder (3.2.58). In contrast, the sum over quantum eigenstates in Eq. (3.2.58) extends only to terms with non-vanishing eigenvalues due to $\hat{\bar{P}}_S \hat{M} \hat{\bar{P}}_S = 0$. This gives the important clue to seek the classically equivalent relation

$$\begin{aligned}
0 &= \langle \rho_{\nu 0 \zeta} | M \rangle && (3.3.59)\\
&\propto \langle \rho_{\nu 0 \zeta} \otimes \rho_C | \hat{L}_V \rho_\Psi \rangle && (3.3.60)\\
&= i \int \mathrm{d}^{n_S}\mathbf{q}\, \mathrm{d}^{n_S}\mathbf{p}\, \rho_{\nu 0\zeta}(\mathbf{q}, \mathbf{p}) \int \mathrm{d}^{n_C}\mathbf{Q}\, \mathrm{d}^{n_C}\mathbf{K}\, \rho_C(\mathbf{Q}, \mathbf{K}) \big\{ \rho_\Psi(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K}), V(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K}) \big\} \,. && (3.3.61)
\end{aligned}$$

for $\nu \neq 0$, which is proven in the following. We start with a closer examination of the relation

$$0 = \langle \rho_{\nu 0 \zeta} | \rho_S \rangle \propto \langle \rho_{\nu 0 \zeta} \otimes \rho_C | \rho_\Psi \rangle \,. \tag{3.3.62}$$

This inner product equals zero because the support of ρ_S and $\rho_{\nu 0 \zeta}$ do not overlap in system phase space. The phase space representation

$$\rho_S(\mathbf{q}, \mathbf{p}) \propto \int \mathrm{d}^{n_C}\mathbf{Q}\, \mathrm{d}^{n_C}\mathbf{K}\, \rho_C(\mathbf{Q}, \mathbf{K})\, \rho_\Psi(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K}) \tag{3.3.63}$$

of the system state depends explicitly on the support of the product $\rho_C(\mathbf{Q}, \mathbf{K}) \cdot \rho_\Psi(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K})$. Since both functions are probability densities, it becomes clear that any product involving ρ_C and any first-order derivatives of ρ_Ψ cannot have a larger support, because

$$\mathrm{supp}\left(\frac{\partial \rho_\Psi}{\partial x}\right) \subseteq \mathrm{supp}\,(\rho_\Psi) \qquad \text{for} \quad x \in \{q_i, p_i, Q_i, K_i\}\,. \tag{3.3.64}$$

Specifically, any points $(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K}) \in \overline{\mathrm{supp}\,(\rho_\Psi)}$, where $\rho_\Psi(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K}) = 0$, are automatically local minima and it follows that $\partial \rho_\Psi(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K})/\partial x = 0$ at these points for any $x \in \{q_i, p_i, Q_i, K_i\}$. In addition, multiplying two functions f and g can only make the support smaller than that of any of the original ones, namely

$$\mathrm{supp}\,(f \cdot g) = \mathrm{supp}\,(f) \cap \mathrm{supp}\,(g) \subseteq \mathrm{supp}\,(f)\,. \tag{3.3.65}$$

All things considered, we state

$$\mathrm{supp}\left(\int \mathrm{d}^{n_C}\mathbf{Q}\, \mathrm{d}^{n_C}\mathbf{K}\, \rho_C(\mathbf{Q}, \mathbf{K})\, \frac{\partial \rho_\Psi(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K})}{\partial x} f(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K})\right) \subseteq \mathrm{supp}\big(\rho_S(\mathbf{q}, \mathbf{p})\big) \tag{3.3.66}$$

for any function $f(\mathbf{q}, \mathbf{p}, \mathbf{Q}, \mathbf{K})$ and any $x \in \{q_i, p_i, Q_i, K_i\}$. A quick comparison of this relation with Eq. (3.3.61) shows a sum of terms with a support lying within $\mathrm{supp}\big(\rho_S(\mathbf{q}, \mathbf{p})\big)$ and implies

$$\mathrm{supp}\big(M(\mathbf{q}, \mathbf{p})\big) \subseteq \mathrm{supp}\big(\rho_S(\mathbf{q}, \mathbf{p})\big)\,. \tag{3.3.67}$$

As a result, the last relation proves the sought-after equation (3.3.59), because of $\langle \rho_{\nu 0 \zeta} | \rho_S \rangle = 0$, which is facilitated by $\mathrm{supp}\big(\rho_{\nu 0 \zeta}(\mathbf{q}, \mathbf{p})\big) \cap \mathrm{supp}\big(\rho_S(\mathbf{q}, \mathbf{p})\big) = \emptyset$. The close similarities between classical and quantum mechanics have proven very useful and the associated remainder vector in its final form reads

$$|\Delta\rangle_S = \sum_{\mu>0}\!\!\!\!\!\!\int \sum_{\zeta}\!\!\!\!\!\!\int |\rho_{0\mu\zeta}\rangle_S \langle \rho_{0\mu\zeta} | M\rangle_S \,. \tag{3.3.68}$$

Additionally, its support in $(\mathbf{q}, \mathbf{p})$ fulfills

$$\mathrm{supp}\big(\Delta(\mathbf{q}, \mathbf{p})\big) \subseteq \mathrm{supp}\big(\rho_S(\mathbf{q}, \mathbf{p})\big) \tag{3.3.69}$$

and we note that the full expansion of M reads

$$|M\rangle_S = \sum_{\nu}\!\!\!\!\!\!\int \sum_{\mu>0}\!\!\!\!\!\!\int \sum_{\zeta}\!\!\!\!\!\!\int |\rho_{\nu\mu\zeta}\rangle_S \langle \rho_{\nu\mu\zeta} | M\rangle_S \,. \tag{3.3.70}$$

With these insights, the system evolution equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_S\rangle_S = -i\hat{L}_{H_S+V_S}|\rho_S\rangle_S - i\left(\sum_{\mu>0}\!\!\!\!\!\!\int \sum_{\zeta}\!\!\!\!\!\!\int |\rho_{0\mu\zeta}\rangle\!\rangle\langle\!\langle \rho_{0\mu\zeta}|_S - |\rho_S\rangle\langle\!\langle \mathbb{1}_S|_S\right)|M\rangle_S \,. \tag{3.3.71}$$

and is the classical analog of the quantum mechanical Eq. (3.2.62). Since a further investigation of the term in brackets has proven useful in the quantum case, we attempt the same in the following.

3.3.4.1 Anti-Hermitian part of the Hamilton function

The determination of the term generating non-unitary dynamics can be addressed in two different representations, namely the phase space representation and the system state eigenbasis. In particular, the first method proceeds with the introduction of the system projector

$$\hat{P}_S \equiv \int\limits_{\mathrm{supp}(\rho_S)} \mathrm{d}^{n_S}\mathbf{q}\,\mathrm{d}^{n_S}\mathbf{p}\;|\mathbf{q},\mathbf{p}\rangle\langle\mathbf{q},\mathbf{p}|_S \tag{3.3.72}$$

$$= \int\limits_{\mathrm{supp}(\rho_S)} \mathrm{d}^{n_S}\mathbf{q}\,\mathrm{d}^{n_S}\mathbf{p}\;\frac{\rho_S(\mathbf{q},\mathbf{p})}{\rho_S(\mathbf{q},\mathbf{p})}\;|\mathbf{q},\mathbf{p}\rangle\langle\mathbf{q},\mathbf{p}|_S \tag{3.3.73}$$

$$\equiv \int \mathrm{d}^{n_S}\mathbf{q}\,\mathrm{d}^{n_S}\mathbf{p}\;\rho_S(\mathbf{q},\mathbf{p})\,\rho_S^{\ominus}(\mathbf{q},\mathbf{p})\;|\mathbf{q},\mathbf{p}\rangle\langle\mathbf{q},\mathbf{p}|_S \tag{3.3.74}$$

$$= \hat{\rho}_S^{\ominus}\,\hat{\rho}_S \tag{3.3.75}$$

with the scalar pseudo-inverse

$$f^{\ominus}(x) \equiv \begin{cases} \frac{1}{f(x)} & \text{for} \quad f(x) \neq 0 \\ 0 & \text{otherwise} \end{cases} . \tag{3.3.76}$$

Subsequently, we can derive

$$i\,|\Delta\rangle_S = i\hat{P}_S\,|\Delta\rangle_S = i\hat{\rho}_S^{\ominus}\,\hat{\rho}_S\,|\Delta\rangle_S = i\hat{\rho}_S^{\ominus}\hat{\Delta}\,|\rho_S\rangle_S = i\hat{\Delta}\hat{\rho}_S^{\ominus}\,|\rho_S\rangle_S \equiv \hat{B}_S\,|\rho_S\rangle_S \tag{3.3.77}$$

with $[\hat{\Delta},\hat{\rho}_S^{\ominus}] = 0$ and a newly defined operator

$$\hat{B}_S \equiv i\hat{\Delta}\hat{\rho}_S^{\ominus} . \tag{3.3.78}$$

The similarity with the quantum mechanical version (3.2.71) is striking and, in addition, we find

$$\left\langle \hat{B}_S \right\rangle_{\rho_S} = \langle\rho_S|B_S\rangle_S = i\,\langle\mathbb{1}_S|\Delta\rangle_S = \langle\mathbb{1}_S|M\rangle_S + \underbrace{\left\langle \mathbb{1}_S\middle|\hat{L}_{V_S}\rho_S\right\rangle_S}_{=0} = \langle\mathbb{1}_S|M\rangle_S . \tag{3.3.79}$$

Inspired by the quantum mechanical result in Section 3.2.3.6, an alternative form in terms of system eigenfunctions can be found as well, namely

$$|B_S\rangle_S = i\sum_{\mu>0}\frac{1}{\mu}\sum_{\zeta}\left|\rho_{0\mu\zeta}\right\rangle_S\left\langle\rho_{0\mu\zeta}\middle|M\right\rangle_S . \tag{3.3.80}$$

A simple calculation yields

$$\hat{\rho}_S\,|B_S\rangle_S = i\sum_{\mu>0}\frac{1}{\mu}\sum_{\zeta}\underbrace{\hat{\rho}_S\left|\rho_{0\mu\zeta}\right\rangle_S}_{=\mu\left|\rho_{0\mu\zeta}\right\rangle_S}\left\langle\rho_{0\mu\zeta}\middle|M\right\rangle_S = i\sum_{\mu>0}\sum_{\zeta}\left|\rho_{0\mu\zeta}\right\rangle_S\left\langle\rho_{0\mu\zeta}\middle|M\right\rangle_S , \tag{3.3.81}$$

$$\left\langle \hat{B}_S \right\rangle_{\rho_S} = \langle\mathbb{1}_S|\hat{\rho}_S|B_S\rangle \tag{3.3.82}$$

$$= i\sum_{\mu>0}\sum_{\zeta}\left\langle\mathbb{1}_S\middle|\rho_{0\mu\zeta}\right\rangle_S\left\langle\rho_{0\mu\zeta}\middle|M\right\rangle_S \tag{3.3.83}$$

$$= i\sum_{\nu}\sum_{\mu}\sum_{\zeta}\left\langle\mathbb{1}_S\middle|\rho_{0\mu\zeta}\right\rangle_S\left\langle\rho_{0\mu\zeta}\middle|M\right\rangle_S \tag{3.3.84}$$

$$= i \langle \mathbb{1}_S | M \rangle_S \tag{3.3.85}$$

and shows the validity of this form in the specific basis derived from the system state. Thus, the final form for the differential equation governing the change in the classical system state is

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} |\rho_S\rangle_S = -i\hat{L}_{H_S+V_S} |\rho_S\rangle_S - \left(\hat{B}_S - \langle \hat{B}_S \rangle_{\rho_S}\right) |\rho_S\rangle_S \,. \tag{3.3.86}$$

At this point, it should come as no surprise that this equation is completely analogous to the quantum version (3.2.81) for mixed state, given the many parallels pointed out in the derivation above. It is worth mentioning that the appearance of a non-Hermitian term is not inherent to quantum mechanics, but a common element in both theories. In the following, we consider three situations in which the second term on the right-hand side vanishes and purely unitary evolution takes place.

3.3.5 Pure state equivalent

The pure state studies in Sections 3.1.6, 3.2.3.2 and 3.2.3.4 have remarkably shown the exact unitarity of the effective system evolution in quantum mechanics. As we have already mentioned above, the equivalent conditions for a classical state being pure are not entirely clear. Nevertheless, since we established that $|\varphi_m\rangle\langle\varphi_n|_S$ are the eigenoperators of $\hat{L}^{(\mathrm{qm})}_{\rho_S}$ and only one eigenstate $|\varphi_1\rangle_S$ with $q_1 = 1$ exists for a pure state density operator $\hat{\rho}_S = |\varphi_1\rangle\langle\varphi_1|_S$, our guess for a classical equivalent is

$$|\rho_S\rangle_S = \left|\rho_{0\bar{\mu}0}\right\rangle_S \tag{3.3.87}$$

for a fixed value $\bar{\mu}$. We assume that no degeneracy $\zeta(\nu = 0, \mu = \bar{\mu}) = 0$ exists. While a further investigation including possible degeneracies is interesting, it is not pursued in the following for simplicity. As a consequence of this assumption, it follows that

$$|\Delta\rangle_S = \left|\rho_{0\bar{\mu}0}\right\rangle_S \left\langle\rho_{0\bar{\mu}0}\middle|M\right\rangle_S \tag{3.3.88}$$

and

$$|\rho_S\rangle_S \langle \mathbb{1}_S | M \rangle_S = \left|\rho_{0\bar{\mu}0}\right\rangle_S \langle \mathbb{1}_S | M \rangle_S \tag{3.3.89}$$

$$= \left|\rho_{0\bar{\mu}0}\right\rangle_S \sum_{\nu} \sum_{\zeta} \underbrace{\left\langle \mathbb{1}_S \middle| \rho_{\nu\bar{\mu}\zeta} \right\rangle_S}_{\propto \delta_{0\nu}} \left\langle \rho_{\nu\bar{\mu}\zeta} \middle| M \right\rangle_S \tag{3.3.90}$$

$$= \left|\rho_{0\bar{\mu}0}\right\rangle_S \left\langle\rho_{0\bar{\mu}0}\middle|M\right\rangle_S \tag{3.3.91}$$

$$= |\Delta\rangle_S \,, \tag{3.3.92}$$

because $\zeta(\nu = 0, \mu = \bar{\mu}) = 0$. Therefore, the term leading to a non-unitary system evolution vanishes and the effective system change follows

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} |\rho_S\rangle_S = -i\hat{L}_{H_S+V_S} |\rho_S\rangle_S \tag{3.3.93}$$

with

$$V_S = -\sum_{\nu\neq 0} \frac{1}{\nu} \sum_{\zeta} \left|\rho_{\nu\bar{\mu}\zeta}\right\rangle_S \left\langle\rho_{\nu\bar{\mu}\zeta}\middle|M\right\rangle_S \tag{3.3.94}$$

as the analog of Eq. (3.2.39). This is a surprising result and certainly demands closer examination in future work. It should be noted that a full treatment should start with pure global state and a pure clock state, from which a pure system state can potentially be derived. In any case, here we content ourselves with the conceptual verification of pure state unitary evolution at some λ, even though a comprehensive proof for unitarity and ρ_S-purity for all λ is missing. Later, we surmise in Sec. 3.4.3 how a general classical condition for purity might be established.

3.3.6 Quasi-eigenstate approximation

Analogous to Sec. 3.2.4, we briefly touch upon the quasi-eigenstate approximation. If the clock is approximately an eigenstate of the interaction, in the sense of

$$\frac{\left\langle \rho_C \middle| \hat{L}_V \rho_\Psi \right\rangle_C}{\langle \mathbb{1}_S, \rho_C | \rho_\Psi \rangle} \approx \hat{L}_{\overline{V}_S} \frac{\langle \rho_C | \rho_\Psi \rangle_C}{\langle \mathbb{1}_S, \rho_C | \rho_\Psi \rangle} = \hat{L}_{\overline{V}_S} |\rho_S\rangle_S \,, \tag{3.3.95}$$

then the last term of Eq. (3.3.38) vanishes, i.e.,

$$\frac{\left\langle \mathbb{1}_S, \rho_C \middle| \hat{L}_V \rho_\Psi \right\rangle}{\langle \mathbb{1}_S, \rho_C | \rho_\Psi \rangle} = \left\langle \hat{L}_{\overline{V}_S} \mathbb{1}_S \middle| \rho_S \right\rangle_S = 0 \,. \tag{3.3.96}$$

Straightforwardly, Eq. (3.3.38) becomes

$$i \frac{\mathrm{d}}{\mathrm{d}\lambda} |\rho_S\rangle_S = \hat{L}_{H_S + \overline{V}_S} |\rho_S\rangle_S \tag{3.3.97}$$

and, again, induces only unitary dynamics in the system. A specific example of this situation is considered in the following section, in which Eq. (3.3.95) is even exact.

3.3.7 Example for unitary dynamics

In this section, we present a classical model exhibiting unitary system dynamics. To this end, we consider the global Hamilton function

$$H = H_S(q,p) + H_C(Q,K) + V(q,Q) \tag{3.3.98}$$

representing two subsystems which are coupled via their positions. The clock shall be a harmonic oscillator

$$H_C(Q,K) = \frac{1}{2}\Big(K^2 + Q^2\Big) \tag{3.3.99}$$

and its state is that of a point particle with clock density

$$\rho_C(Q,K,\lambda) = \delta\Big(Q - \mathsf{Q}(\lambda)\Big)\,\delta\Big(K - \mathsf{K}(\lambda)\Big) \,. \tag{3.3.100}$$

A simple form of the phase space trajectories is chosen, namely

$$\mathsf{Q}(\lambda) = \mathsf{Q}_0 \cos\lambda = -\frac{\mathrm{d}\mathsf{K}(\lambda)}{\mathrm{d}\lambda} \tag{3.3.101}$$

$$\mathsf{K}(\lambda) = -\mathsf{Q}_0 \sin\lambda = \frac{\mathrm{d}\mathsf{Q}(\lambda)}{\mathrm{d}\lambda} \tag{3.3.102}$$

with the initial values $\mathsf{Q}(0) = \mathsf{Q}_0$ and $\mathsf{K}(0) = 0$. Consequently, the potential term in the evolution reads

$$\frac{\left\langle q, p, \rho_\chi \middle| \hat{L}_V \rho_\Psi \right\rangle}{\langle \mathbb{1}_S, \rho_C | \rho_\Psi \rangle} = \frac{i}{\langle \mathbb{1}_S, \rho_C | \rho_\Psi \rangle} \frac{\partial V(q,\mathsf{Q})}{\partial q} \cdot \frac{\partial \rho_\Psi(q,p,\mathsf{Q},\mathsf{K})}{\partial p}$$

$$+\frac{i}{\langle \mathbb{1}_S, \rho_C|\rho_\Psi\rangle}\frac{\partial V(q,Q)}{\partial Q}\bigg|_Q \cdot \frac{\partial \rho_\Psi(q,p,\mathsf{Q},K)}{\partial K}\bigg|_K . \tag{3.3.103}$$

A definition of an effective system potential is hindered by the last term, which is not composed of system variable derivatives of the relational system state $\rho_S \propto \rho_\Psi(q,p,\mathsf{Q},\mathsf{K})$. We try to use Eq. (3.3.21) in order to find an alternative expression for the clock momentum derivative of the global state. Specifically, the equation

$$0 = \frac{\partial}{\partial K}\langle q,p,Q,K|(\hat{H}-E)|\rho_\Psi\rangle \tag{3.3.104}$$

$$= \Big(H(q,p,Q,K)-E\Big)\frac{\partial \rho_\Psi(q,p,Q,K)}{\partial K} + \underbrace{\frac{\partial H(q,p,Q,K)}{\partial K}}_{=\partial H_C(Q,K)/\partial K}\rho_\Psi(q,p,Q,K) \tag{3.3.105}$$

provides an expression for the clock momentum derivative of the global state, namely

$$\frac{\partial \rho_\Psi(q,p,Q,K)}{\partial K} = \underbrace{\frac{\partial H_C(Q,K)}{\partial K}}_{=K}\frac{\rho_\Psi(q,p,Q,K)}{E-H(q,p,Q,K)} . \tag{3.3.106}$$

The same energy equation can also be used to find

$$\frac{1}{\partial H_S(q,p)/\partial p}\frac{\partial \rho_\Psi(q,p,Q,K)}{\partial p} = \frac{\rho_\Psi(q,p,Q,K)}{E-H(q,p,Q,K)} \tag{3.3.107}$$

and, thus, the problematic term can be written as

$$\frac{\partial \rho_\Psi(q,p,Q,K)}{\partial K} = \frac{K}{\partial H_S(q,p)/\partial p}\frac{\partial \rho_\Psi(q,p,Q,K)}{\partial p} . \tag{3.3.108}$$

As a result, the potential term becomes

$$\frac{\langle q,p,\rho_\chi|\hat{L}_V\rho_\Psi\rangle}{\langle \mathbb{1}_S,\rho_C|\rho_\Psi\rangle} = i\frac{\partial V(q,\mathsf{Q})}{\partial q}\cdot\frac{\partial \rho_S(q,p,\lambda)}{\partial p} + i\frac{\partial V(q,Q)}{\partial Q}\bigg|_Q \cdot \frac{\mathsf{K}}{\partial H_S(q,p)/\partial p}\frac{\partial \rho_S(q,p,\lambda)}{\partial p} \tag{3.3.109}$$

$$= i\left[\left(\frac{\partial V(q,\mathsf{Q})}{\partial q}+\frac{\partial V(q,Q)}{\partial Q}\bigg|_Q\cdot\frac{\mathsf{K}}{\partial H_S(q,p)/\partial p}\right)\frac{\partial}{\partial p}\right]\rho_S(q,p,\lambda) \tag{3.3.110}$$

and we can define

$$\frac{\partial V_S(q,p,\lambda)}{\partial q} \equiv \frac{\partial V(q,\mathsf{Q})}{\partial q}+\frac{\partial V(q,Q)}{\partial Q}\bigg|_Q\cdot\frac{\mathsf{K}}{\partial H_S(q,p)/\partial p} \tag{3.3.111}$$

with the solution

$$V_S(q,p,\lambda) = V(q,\mathsf{Q})-V(q_0,\mathsf{Q})+\mathsf{K}\int_{q_0}^{q}\mathrm{d}q'\,\frac{\partial V(q',Q)}{\partial Q}\bigg|_Q\cdot\frac{1}{\partial H_S(q',p)/\partial p} . \tag{3.3.112}$$

The integration point q_0 can be chosen arbitrarily, because it does not change the equations of motion. However, the additional momentum-dependence of the second term poses a problem. Given that Eq. (3.3.110) does not feature a derivative of the system state with respect to q, we require $\partial V_S/\partial p = 0$. It induces the constraint

$$0 \overset{!}{=} \frac{\partial V_S(q,p,\lambda)}{\partial p} \tag{3.3.113}$$

$$= -\mathsf{K}\int_{q_0}^{q} \mathrm{d}q' \left.\frac{\partial V(q',Q)}{\partial Q}\right|_{\mathsf{Q}} \cdot \frac{1}{\left[\partial H_{\mathrm{S}}(q',p)/\partial p\right]^2} \cdot \frac{\partial^2 H_{\mathrm{S}}(q',p)}{\partial p^2}\,, \tag{3.3.114}$$

which is only non-trivially fulfilled for system Hamilton functions linear in p. This represents a very restricted class with $\partial H_{\mathrm{S}}(q,p)/\partial p = \alpha$ for some $\alpha \in \mathbb{R}$. In this case, the effective potential becomes

$$V_{\mathrm{S}}(q,p,\lambda) = V(q,\mathsf{Q}) - V(q_0,\mathsf{Q}) + \frac{\mathsf{K}}{\alpha}\int_{q_0}^{q} \mathrm{d}q' \left.\frac{\partial V(q',Q)}{\partial Q}\right|_{\mathsf{Q}} \tag{3.3.115}$$

and it is clear at this point, that we are specifically searching for a combination of clock states and interactions, such that the quasi-eigenstate approximation (3.3.95) becomes an exact relation. To make it explicit, we choose the system Hamilton function

$$H_{\mathrm{S}}(q,p) = p + \frac{q^2}{2} \tag{3.3.116}$$

and the simple coupling

$$V_{\mathrm{S}}(q,Q) = q\,Q\,. \tag{3.3.117}$$

This is arguably a rather special case due to the linear kinetic term, but it suffices to demonstrate the possibility for exact unitary evolution. For the specific aforementioned Hamilton functions, the effective potential (3.3.115) reads

$$V_{\mathrm{S}}(q,p,\lambda) = q\mathsf{Q}(\lambda) + \frac{1}{2}\mathsf{K}(\lambda)q^2 \tag{3.3.118}$$

with the integration limit $q_0 = 0$. The last missing element for displaying the system dynamics corresponding to (3.3.116) and the effective potential (3.3.118) is a suitable global state, which we take to be the microcanonical ensemble

$$\rho_{\Psi} \propto \delta\Big[E - H(q,p,Q,K)\Big]. \tag{3.3.119}$$

Consequently, the system state

$$\rho_{\mathrm{S}}(q,p,\lambda) \propto \rho_{\Psi}(q,p,\mathsf{Q},\mathsf{K}) \tag{3.3.120}$$

$$\equiv \delta\left[E_{\mathrm{S}} - \left(p + \frac{q^2}{2} + q\mathsf{Q}_0\cos\lambda\right)\right] \tag{3.3.121}$$

also represents a microcanonical ensemble for fixed energy $E_{\mathrm{S}} \equiv E - \mathsf{Q}_0^2/2$ and λ-varying Hamilton function $p + q^2/2 + q\mathsf{Q}_0\cos\lambda$. In contrast, we derive the system Hamilton function

$$H_{\mathrm{S}}(q,p) + V_{\mathrm{S}}(q,p,\lambda) = p + \frac{1}{2}q^2 + q\mathsf{Q}_0\cos\lambda - \frac{1}{2}q^2\mathsf{Q}_0\sin\lambda\,, \tag{3.3.122}$$

which features the additional term $-q^2\mathsf{Q}_0\sin(\lambda)/2$ not showing up in Eq. (3.3.121). This is a curious characteristic of our model and, even though the goal of achieving unitary system dynamics is reached, we investigate the dynamics a bit further. To this end, single point particle trajectories $\big(\mathsf{q}(\lambda),\mathsf{p}(\lambda)\big)$ are examined and their evolution is determined from Hamilton's equations of motion, i.e., $\mathrm{d}\mathsf{q}/\mathrm{d}\lambda = \mathrm{d}(H_{\mathrm{S}} + V_{\mathrm{S}})/\mathrm{d}\mathsf{p} = 1$ and $\mathrm{d}\mathsf{p}/\mathrm{d}\lambda = -\mathrm{d}(H_{\mathrm{S}} + V_{\mathrm{S}})/\mathrm{d}\mathsf{q} = -\mathsf{q}(1+\mathsf{K}) - \mathsf{Q} = \mathrm{d}\mathsf{K}/\mathrm{d}\lambda - \mathsf{q}(1 + \mathrm{d}\mathsf{Q}/\mathrm{d}\lambda)$. The corresponding solutions read

$$\mathsf{q}(\lambda) = \mathsf{q}_0 + \lambda\,, \tag{3.3.123}$$

$$p(\lambda) = p_0 - q(\lambda)\Big[\lambda + Q(\lambda)\Big] + \frac{\lambda^2}{2} + q_0 Q_0 \tag{3.3.124}$$

and do not exhibit the periodic nature of the system state (3.3.121). Fixing of the initial positions q_0 simultaneously determines the initial momenta p_0 by means of the energy requirement $H_S(q_0, p_0) + V_S(q_0, p_0, \lambda = 0) = E_S$. That the whole ensemble of single trajectories for all q_0, collectively representing ρ_S, can still show periodic behavior is shown in Fig. 3.11.

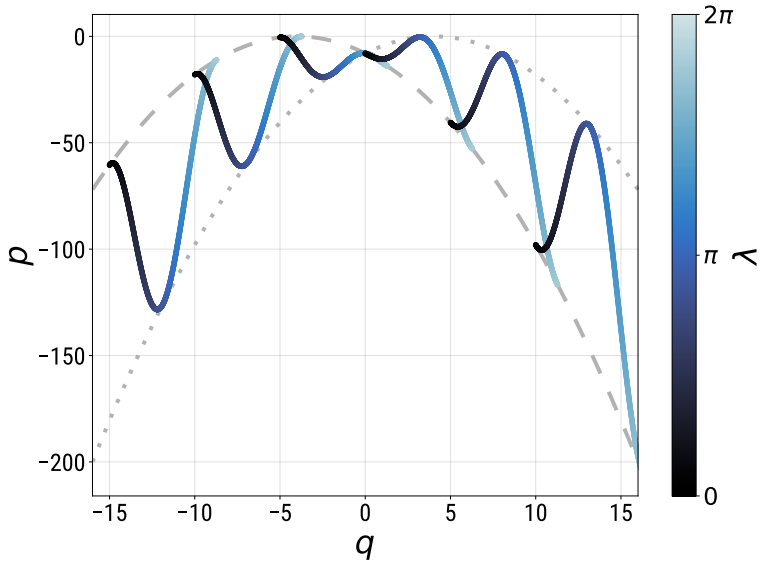

Figure 3.11 – The classical evolution under the system Hamilton function (3.3.122) for single trajectories (continues color scale) and the microcanonical ensemble (3.3.121) (gray lines) is shown for one clock period $T_C = 2\pi$. The global energy value is fixed at $E = 0$. Furthermore, $Q_0 = 4$ sets the initial clock position and the initial position of the system point particle trajectories are taken from the set $q_0 \in \{-15, -10, -5, 0, 5, 10\}$. For a direct comparison of the changing microcanonical ensemble to the collection of single trajectories, the former is plotted for $\lambda = 0$ (dashed lines) and $\lambda = \pi$ (dotted lines).

3.4 Unified formulation

In Section 3.2.5, we introduced a quantum mechanical formulation on phase space in order to be able to directly compare to our results for probability densities in classical mechanics. Such a procedure depends explicitly on the chosen basis in phase space and is, thus, rendered basis-dependent. As demonstrated in the literature, for example in Refs. [225, 266], it is nevertheless useful to compare and to interpret dynamics in both mechanics and to better understand quantum to classical transitions. However, our treatment in Sec. 3.3 has shown the effectiveness and the simplicity of a Hilbert space formulation in classical mechanics. For this reason, we introduce a common basis-independent notation for both theories in terms of vectors $|A\rangle\!\rangle$ in Hilbert space, "... since a good notation can be of great value in helping the development of a theory ..." [267]. It allows us to directly point out the common features in quantum and classical mechanics. Each individual framework, classical or quantum, is obtained by explicitly defining the form of the inner product and the involved operators. This remarkable property has already been pointed out in Ref. [242] with the statement that "this great unity is one of the most striking features of this method".

3.4.1 Inner product and operators

To elaborate, we introduce a general inner product $\langle\!\langle A|B\rangle\!\rangle$, which is either taken to be the classical version (3.3.1) or the quantum mechanical inner product

$$\langle\!\langle A|B\rangle\!\rangle \equiv \mathrm{tr}\left(\hat{A}^\dagger \hat{B}\right) = \langle\!\langle B|A\rangle\!\rangle^* \tag{3.4.1}$$

for two quantum mechanical operators $\hat{A}$ and $\hat{B}$, respectively. Equation (3.4.1) is known as the "Hilbert-Schmidt inner product" [145]. The usual quantum mechanical operators are now considered as vectors and so-called "superoperators" take the place of operators in our unified formalism. An excellent source for details of the quantum mechanical formulation in "Liouville space" [225] is given in Ref. [237]. At this point, the pure state vector formalism of Sec. 3.1 is not used any longer, but readily included in the quantum mechanical density operator formalism.

Furthermore, the derivations in Sections 3.2.3 and 3.3 have shown that Liouville-type operators $\hat{L}_A$ are necessary and, therefore, we take $\hat{L}_A$ to be either (3.3.7) or (3.2.27) in classical and quantum mechanics, respectively. These operators have the properties

$$\left\langle\!\!\left\langle B\middle|\hat{L}_A C\right\rangle\!\!\right\rangle = \left\langle\!\!\left\langle \hat{L}_{A^\dagger} B\middle| C\right\rangle\!\!\right\rangle, \tag{3.4.2}$$

$$\hat{L}_A|B\rangle\!\rangle = -\hat{L}_B|A\rangle\!\rangle\,, \tag{3.4.3}$$

$$\hat{L}_A|\mathbb{1}\rangle\!\rangle = 0\,, \tag{3.4.4}$$

where the Hermitian conjugate reduces to the complex conjugate in the classical framework.

In order to complete the set of necessary elements for our unified formulation, a second class of operators needs to be introduced. As part of the quantum mechanical energy constraint in Section 3.2, Equation (3.2.4) hints at the definition of an operator complementary to the Liouville type operators. In particular, we use $\hat{K}_A \equiv \{\hat{A}, \bullet\}_+/2$ for quantum mechanics and the classical equivalent $\langle\!\langle \mathbf{q},\mathbf{p}|\hat{K}_A B\rangle\!\rangle \equiv \{A(\mathbf{q},\mathbf{p}), B(\mathbf{q},\mathbf{p})\}_+/2 = A(q,p)\,B(q,p)$, matching the multiplicative operators defined in Eq. (3.3.5). In contrast to the Liouville operators, a minus sign is absent in

$$\langle\!\langle B|\hat{K}_A C\rangle\!\rangle = \langle\!\langle \hat{K}_{A^\dagger} B|C\rangle\!\rangle\,, \tag{3.4.5}$$

$$\hat{K}_A|B\rangle\!\rangle = \hat{K}_B|A\rangle\!\rangle\,, \tag{3.4.6}$$

$$\hat{K}_A|\mathbb{1}\rangle\!\rangle = |A\rangle\!\rangle\,, \tag{3.4.7}$$

regardless of a classical or quantum character.

3.4.2 States

Having established the mathematical groundwork, the only missing part is a set of conditions that distinguish Hilbert space vectors $|\rho\rangle\!\rangle$ representing states from the rest. It is straightforward to give the normalization condition as

$$\langle\!\langle \mathbb{1}|\rho\rangle\!\rangle = 1\,, \tag{3.4.8}$$

which should not require any further explanation. In both theories, states possess a non-negativity property. Classical probability densities are required to fulfill $\rho(\mathbf{q},\mathbf{p}) = \langle \mathbf{q},\mathbf{p}|\rho\rangle \geq 0$, whereas (mixed) quantum states $\hat{\rho}$ must have non-negative eigenvalues. In particular, $\mathrm{tr}(|\eta\rangle\langle\eta|\,\hat{\rho}) \geq 0$ must hold for any normalized state $|\eta\rangle\langle\eta|$. However, the last relation can be expanded to include not only pure states $|\eta\rangle\langle\eta|$, but any valid state $\hat{\rho}_1$, such

that $\mathrm{tr}(\hat{\rho}_1\hat{\rho}) \geq 0$ [7]. Along the same line of thought, we recognize that the non-negativity of classical states $\langle\!\langle \mathbf{q},\mathbf{p}|\rho\rangle\!\rangle$ on phase space is also a statement about the inner product of two valid states, because $|\mathbf{q},\mathbf{p}\rangle\!\rangle$ is the state of a classical point particle. Due to this fact, any two general states $|\rho\rangle\!\rangle$ and $|\rho_1\rangle\!\rangle$ must satisfy

$$\langle\!\langle \rho\,|\rho_1\rangle\!\rangle \geq 0\,. \tag{3.4.9}$$

This relation contains the implicit condition that classical states are real-valued functions on phase space and quantum states are Hermitian. Otherwise, the inner product in Eq. (3.4.9) could take on complex values, which are known to possess no order[8]. Using the classical case as an illustration, Eq. (3.4.9) could also be fulfilled for phase space densities that are entirely non-positive, because their product yields non-negative values. Despite this possibility, the normalization condition (3.4.8) enforces the non-negativity. The combination of Eqs. (3.4.8) and (3.4.9) has another interesting consequence concerning the upper limit of the scalar product $\langle\!\langle \rho\,|\rho_1\rangle\!\rangle$ for any two states ρ and ρ_1. In classical mechanics, the probability density can take arbitrary large values on phase space, but for finite-dimensional quantum states the inner product has an upper limit of unity, $\langle\!\langle \rho\,|\rho_1\rangle\!\rangle_{\mathrm{QM}} \leq 1$, due to the non-negativity and the normalization. In other words, the eigenvalues of $\hat{\rho}$ are confined to the range $[0,1]$, as expected.

In addition, Jaffe and Brumer [246] also require for classical mechanics that $\left|\int \mathrm{d}^n\mathbf{q}\,\mathrm{d}^n\mathbf{p}\,A(\mathbf{q},\mathbf{p})\,\rho(\mathbf{q},\mathbf{p})\right| < \infty$ for any measurable function A on phase space [268]. Here, we take the liberty to use the absolute value of the integral, in contrast to its original form in Ref. [246]. This condition can be accommodated in our unified formulation via

$$|\langle\!\langle A|\rho\rangle\!\rangle| < \infty \tag{3.4.10}$$

for any vector $|A\rangle\!\rangle$. The mathematical details of the equivalent for the measurability condition in Ref. [246] shall not be of any concern here, as we do not aim for strict mathematical exactness, but rather for physical understanding.

As an example, we can give the uncertainty relation (3.1.200)

$$\Delta A^2 \cdot \Delta B^2 \geq \frac{1}{4}\left|\left\langle\!\left\langle \rho\,\middle|\,\hat{L}_A B\right\rangle\!\right\rangle\right|^2 + \left|\left\langle\!\left\langle \rho\,\middle|\,\hat{K}_A\hat{K}_B\hat{\mathbb{1}}_S\right\rangle\!\right\rangle - \left\langle\!\left\langle \rho\,\middle|\,\hat{K}_A\mathbb{1}\right\rangle\!\right\rangle \cdot \left\langle\!\left\langle \rho\,\middle|\,\hat{K}_B\mathbb{1}\right\rangle\!\right\rangle\right|^2 \tag{3.4.11}$$

completely in terms of the unified formalism for classical and quantum mechanics with the variances $\Delta A^2 = \langle\!\langle \rho\,|\hat{K}_A^2\mathbb{1}\rangle\!\rangle - \langle\!\langle \rho\,|\hat{K}_A\mathbb{1}\rangle\!\rangle^2 = \langle\!\langle \rho\,|A^2\rangle\!\rangle - \langle\!\langle \rho\,|A\rangle\!\rangle^2$. Moreover, the generalized covariance (3.1.201) from Sec. 3.1.9 reads

$$\mathrm{Cov}(A,B) = \left\langle\!\left\langle \rho\,\middle|\,\hat{K}_A\hat{K}_B\hat{\mathbb{1}}_S\right\rangle\!\right\rangle - \left\langle\!\left\langle \rho\,\middle|\,\hat{K}_A\mathbb{1}\right\rangle\!\right\rangle \cdot \left\langle\!\left\langle \rho\,\middle|\,\hat{K}_B\mathbb{1}\right\rangle\!\right\rangle. \tag{3.4.12}$$

3.4.3 Time emergence

Equipped with the general formulation from above, the important equations for the time emergence can be readily given and, therefore, briefly summarized. The global energy constraints read

$$\left(\hat{K}_H - E\right)|\rho_\Psi\rangle\!\rangle = 0\,, \tag{3.4.13}$$

[7] The validity can be simply proven for two arbitrary states in their respective eigenbasis with $\hat{\rho} = \sum_m a_m\,|a_m\rangle\langle a_m|$ and $\hat{\rho}_1 = \sum_n b_n\,|b_n\rangle\langle b_n|$. The inner product reads $\langle\!\langle \rho_1|\rho\rangle\!\rangle = \mathrm{tr}(\hat{\rho}_1\hat{\rho}) = \sum_{m,n} a_m b_n |\langle a_m|b_n\rangle|^2 \geq 0$ for $0 \leq a_m, b_n \leq 1$.

[8] More specifically, no order exists for the complex field $(\mathbb{C},+,\cdot)$ in the mathematical sense, which can turn it into an ordered field [268].

$$\hat{L}_H|\rho_\Psi\rangle\!\rangle = 0 \tag{3.4.14}$$

and the latter generates the global invariance

$$\exp\left[i\lambda\hat{L}_H\right]|\rho_\Psi\rangle\!\rangle = |\rho_\Psi\rangle\!\rangle\,. \tag{3.4.15}$$

A quantum mechanical pure global state fulfills $\hat{L}_{\rho_\Psi}|\rho_\Psi\rangle\!\rangle_{\mathrm{QM}} = 0$ and $\hat{K}_{\rho_\Psi}|\rho_\Psi\rangle\!\rangle_{\mathrm{QM}} = |\rho_\Psi\rangle\!\rangle_{\mathrm{QM}}$. Based on this observation, we speculate that the energy constraints must be complemented by the requirements

$$\hat{L}_{\rho_\Psi}|\rho_\Psi\rangle\!\rangle = 0\,, \tag{3.4.16}$$
$$\hat{K}_{\rho_\Psi}|\rho_\Psi\rangle\!\rangle = a|\rho_\Psi\rangle\!\rangle \tag{3.4.17}$$

for $a > 0$, if the global state shall be pure. In the classical case, this would correspond to a constant probability density on the support in phase space. The Hamilton function has a constant energy on this support, but the global state must not necessarily be a microcanonical ensemble. Nevertheless, such a state represents an allowed global state under the constraints and is in accordance with previous findings [235, 262, 264], which established a link between energy eigenstates and microcanonical ensembles for ergodic systems. For integrable systems, Wigner functions of quantum mechanical energy eigenstates correspond to constant probability densities on particular tori in the classical limit [235, 262, 264].

Focusing on the system part, the evolution of the relational system state

$$|\rho_{\mathrm{S}}\rangle\!\rangle_{\mathrm{S}} \equiv \frac{\langle\!\langle \rho_{\mathrm{C}}|\rho_\Psi\rangle\!\rangle_{\mathrm{C}}}{\langle\!\langle \mathbb{1}_{\mathrm{S}}, \rho_{\mathrm{C}}|\rho_\Psi\rangle\!\rangle} \tag{3.4.18}$$

follows the differential equation

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_{\mathrm{S}}\rangle\!\rangle_{\mathrm{S}} = \left[\hat{L}_{H_{\mathrm{S}}+V_{\mathrm{S}}} + \hat{K}_{B_{\mathrm{S}}} - \langle\!\langle \rho_{\mathrm{S}}|B_{\mathrm{S}}\rangle\!\rangle_{\mathrm{S}}\right]|\rho_{\mathrm{S}}\rangle\!\rangle_{\mathrm{S}}\,. \tag{3.4.19}$$

As shown in this chapter, the quantities appearing in this equation must be expressed in the eigenbasis of the system, which is determined from

$$\hat{L}_{\rho_{\mathrm{S}}}|\rho_{\nu\mu\zeta}\rangle\!\rangle_{\mathrm{S}} = \nu|\rho_{\nu\mu\zeta}\rangle\!\rangle_{\mathrm{S}}\,, \tag{3.4.20}$$
$$\hat{K}_{\rho_{\mathrm{S}}}|\rho_{\nu\mu\zeta}\rangle\!\rangle_{\mathrm{S}} = \mu|\rho_{\nu\mu\zeta}\rangle\!\rangle_{\mathrm{S}} \tag{3.4.21}$$

with index ζ denoting additional degeneracies. Consequently, the effective system potential reads

$$|V_{\mathrm{S}}\rangle\!\rangle_{\mathrm{S}} = -\sum_{\nu\neq 0}\frac{1}{\nu}\sum_{\mu}\sum_{\zeta}|\rho_{\nu\mu\zeta}\rangle\!\rangle_{\mathrm{S}}\langle\!\langle \rho_{\nu\mu\zeta}|M\rangle\!\rangle_{\mathrm{S}}\,, \tag{3.4.22}$$

while the term

$$|B_{\mathrm{S}}\rangle\!\rangle_{\mathrm{S}} = i\sum_{\mu>0}\frac{1}{\mu}\sum_{\zeta}|\rho_{0\mu\zeta}\rangle\!\rangle_{\mathrm{S}}\langle\!\langle \rho_{0\mu\zeta}|M\rangle\!\rangle_{\mathrm{S}} \tag{3.4.23}$$

generates a non-unitary contribution to the system evolution.

Chapter 4

Temperature emergence

In the beginning of this thesis (Chapter 1) we have alluded to an intriguing connection between time and inverse temperature. Initially, it was recognized through the formal similarity of the real-time propagator $\hat{U}(t) = \exp\left(-it\hat{H}\right)$ and the quantum canonical density operator $\hat{\rho}_{\mathrm{can}}(\beta) = \exp\left(-\beta\hat{H}\right)/Z_{\mathrm{can}}(\beta)$ with $Z_{\mathrm{can}}(\beta) = \mathrm{tr}\exp\left(-\beta\hat{H}\right)$. Except for the prefactor, one can be transformed into the other via the Wick rotation [116] (or analytic continuation of time to imaginary values [269])

$$t \longleftrightarrow -i\beta\,. \tag{4.1}$$

Here, the Boltzmann constant $k_{\mathrm{B}} = 1$ is set to unity. Based on relation (4.1), one also finds the formal similarity of generating functionals in quantum field theory for dynamical and statistical descriptions [116, 270]. Some physicists also prefer the name "Euclidean time" for imaginary time [116, 270, 271], due to the transformation of the Minkowski metric to a Euclidean one under the Wick rotation in special relativity. Another likeness is provided by time-energy (see Sect. 3.1.9) and temperature-energy uncertainties [122, 123, 125, 126]. With the appearance of time emergence frameworks, the link between both descriptions became even stronger, because their origin is based on the same two principles. These are the energy constraint of the global system, postulate **(I)**, and the splitting into subsystems, postulate **(II)**. Therefore, we show in this chapter how and under which conditions the parameter λ can take the role of inverse temperature β. Only reference to inverse temperature is made, rather than temperature, because it connects to time directly via the Wick rotation, is the more natural quantity in terms of thermodynamical Legendre transformations [272] and has a monotonic relationship with the mean energy. The last argument refers to the possible appearance of negative temperatures [273–276] and is illustrated in Fig. 4.1.

We exclusively treat canonical ensembles without (or negligible) interactions between system and complement in this chapter, for which some basics are reviewed in Section 4.1. The Wick rotation (4.1) indicates that one must seek for inverse temperature in the imaginary-time formulation [277–279] for classical and quantum dynamics. Thus, we derive the imaginary-time dynamics in Section 4.2 in an analogous way to the emergence of real-time dynamics and use it as a stepping stone in Section 4.3 to achieve the connection to thermodynamics. The unified formalism from Section 3.4 allows us to investigate the relation to inverse temperature simultaneously for classical and quantum mechanics and, thus, is used in this chapter.

4.1 Inverse temperature and the canonical ensemble

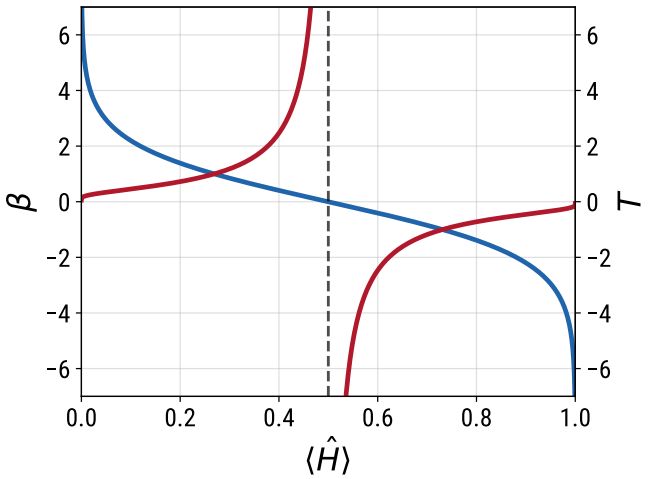

Figure 4.1 – A comparison between the temperature T and the inverse temperature $\beta = 1/T$ is shown for a simple quantum mechanical two-level system with $\hat{H} = \mathrm{diag}(1,0)$ in atomic units. The mean energy reads $\langle\hat{H}\rangle(\beta) = e^{-\beta}/(e^{-\beta}+1)$, and the corresponding temperature and inverse temperature are represented by the red and blue line, respectively. Moreover, the vertical dashed line corresponds to $\langle\hat{H}\rangle(0) = 0.5$ at which the temperature diverges. Even though the system is quite simplistic, the general form of these curves is universal for any bounded energy spectrum. If the energy spectrum is not bound from above, then the mean energy diverges for $\beta \geq 0$.

4.1.1 Derivation

The canonical ensemble (or "Gibbs state") is characterized by a maximal von Neumann entropy [280]

$$S[\rho_S] \equiv \langle\!\langle -\ln\rho_S | \rho_S \rangle\!\rangle_S = \langle\!\langle -\ln\rho_S \rangle\!\rangle_{\rho_S} \stackrel{!}{=} \max \tag{4.1.1}$$

under the constraint of a given fixed mean energy E_S, namely

$$E_S \stackrel{!}{=} \left\langle\!\!\left\langle \mathbb{1}_S \middle| \hat{K}_{H_S}\rho_S \right\rangle\!\!\right\rangle_S = \langle\!\langle H_S | \rho_S \rangle\!\rangle_S \,. \tag{4.1.2}$$

Potential shortcomings of the von Neumann entropy in classical mechanics have already been discussed in Ref. [281], but shall not be of concern here. The variation with respect to ρ_S of

$$W \equiv \langle\!\langle -\ln\rho_S | \rho_S \rangle\!\rangle_S + \alpha\Big(1 - \langle\!\langle \mathbb{1}_S | \rho_S \rangle\!\rangle_S\Big) + \beta\Big(E_S - \langle\!\langle H_S | \rho_S \rangle\!\rangle_S\Big) \tag{4.1.3}$$

with Lagrange multipliers α and β yields

$$|\ln\rho_S\rangle\!\rangle_S = -(1+\alpha)|\mathbb{1}_S\rangle\!\rangle_S - \beta|H_S\rangle\!\rangle_S \tag{4.1.4}$$

$$= -\left|(1+\alpha)\mathbb{1}_S + \beta\hat{K}_{H_S}\mathbb{1}_S\right\rangle\!\!\right\rangle_S \,. \tag{4.1.5}$$

Thus, the canonical ensemble reads

$$\left|\rho_{S,\mathrm{can}}\right\rangle\!\!\right\rangle_S = \frac{1}{Z_{\mathrm{can}}(\beta)}\left|\exp\left(-\beta\hat{K}_{H_S}\right)\mathbb{1}_S\right\rangle\!\!\right\rangle_S \tag{4.1.6}$$

with the partition function $Z_{\mathrm{can}}(\beta) \equiv \langle\!\langle \hat{\mathbb{1}}_S | \exp(-\beta \hat{K}_{H_S}) \mathbb{1}_S \rangle\!\rangle_S = \exp(1+\alpha)$ ensuring the normalization. This state also fulfills $\hat{L}_{H_S} | \rho_{S,\mathrm{can}} \rangle\!\rangle_S = 0$. The inverse temperature β is determined from the energy restriction and yields the equation

$$E_S = \langle\!\langle H_S | \rho_{S,\mathrm{can}} \rangle\!\rangle_S = -\frac{\partial}{\partial \beta} \ln Z_{\mathrm{can}}(\beta) \tag{4.1.7}$$

with the solution $\beta = \beta(E_S)$. Even though the canonical density (4.1.6) is undisputed, its origin in terms of a global state of an enlarged system is not unique. For example, it can be derived as the quantum mechanical reduced density of a microcanonical global mixed state to a fixed global energy E, but also from a "typical" pure global energy eigenstate [117]. In both cases, the complement of the system is assumed to be large. Another example from quantum mechanics is the thermofield method [282–284], which features a global state that is obtained via purification [145] of the canonical density. In this case, the complement is a copy of the original system Hilbert space and once the complement Hamiltonian is chosen as the negative of the system Hamiltonian, the purified state can constitute an eigenstate with $E = 0$. Due to the non-uniqueness of the origin, we inquire about alternative ways of deriving the same state.

For completeness, the canonical ensemble reads

$$\rho_{S,\mathrm{can}}(\mathbf{q},\mathbf{p}) = \frac{\exp\left[-\beta H_S(\mathbf{q},\mathbf{p})\right]}{\int \mathrm{d}^{n_S}\mathbf{q}\, \mathrm{d}^{n_S}\mathbf{p}\, \exp\left[-\beta H_S(\mathbf{q},\mathbf{p})\right]} \tag{4.1.8}$$

and

$$\hat{\rho}_{S,\mathrm{can}} = \frac{\exp\left[-\beta \hat{H}_S\right]}{\mathrm{tr}_S \exp\left[-\beta \hat{H}_S\right]} \tag{4.1.9}$$

in classical and quantum mechanics, respectively [285].

4.1.2 Changes with respect to inverse temperature

For later reference, we also calculate the change of the canonical state for a change in inverse temperature β. The derivative of state (4.1.6) yields

$$-\frac{\mathrm{d}}{\mathrm{d}\beta} | \rho_{S,\mathrm{can}} \rangle\!\rangle_S = \left(\hat{K}_{H_S} - \langle\!\langle \rho_{S,\mathrm{can}} | H_S \rangle\!\rangle_S \right) | \rho_{S,\mathrm{can}} \rangle\!\rangle_S . \tag{4.1.10}$$

Furthermore, the entropy of the canonical ensemble is

$$S[\rho_{S,\mathrm{can}}] = \ln Z_{\mathrm{can}} + \beta \underbrace{\langle\!\langle \rho_{S,\mathrm{can}} | H_S \rangle\!\rangle_S}_{\equiv \langle\!\langle H_S \rangle\!\rangle_{\rho_{S,\mathrm{can}}}} \tag{4.1.11}$$

and has the derivative

$$\frac{\mathrm{d}S[\rho_{S,\mathrm{can}}]}{\mathrm{d}\beta} = \frac{\mathrm{d}\ln Z_{\mathrm{can}}}{\mathrm{d}\beta} + \langle\!\langle H_S \rangle\!\rangle_{\rho_{S,\mathrm{can}}} + \beta \frac{\mathrm{d}\langle\!\langle H_S \rangle\!\rangle_{\rho_{S,\mathrm{can}}}}{\mathrm{d}\beta} = \beta \frac{\mathrm{d}\langle\!\langle H_S \rangle\!\rangle_{\rho_{S,\mathrm{can}}}}{\mathrm{d}\beta} . \tag{4.1.12}$$

In addition, we can determine the mean energy change with

$$-\frac{\mathrm{d}}{\mathrm{d}\beta} \langle\!\langle H_S \rangle\!\rangle_{\rho_{S,\mathrm{can}}} = \langle\!\langle H_S | \left[\hat{K}_{H_S} - \langle\!\langle H_S \rangle\!\rangle_{\rho_{S,\mathrm{can}}} \right] | \rho_{S,\mathrm{can}} \rangle\!\rangle_S = \langle\!\langle H_S^2 \rangle\!\rangle_{\rho_{S,\mathrm{can}}} - \langle\!\langle H_S \rangle\!\rangle^2_{\rho_{S,\mathrm{can}}} \tag{4.1.13}$$

$$= \mathrm{Var}_{\rho_{\mathrm{S,can}}}(H_{\mathrm{S}})\,. \tag{4.1.14}$$

and express the entropy change as

$$\frac{\mathrm{d}S[\rho_{\mathrm{S,can}}]}{\mathrm{d}\beta} = -\beta \mathrm{Var}_{\rho_{\mathrm{S,can}}}(H_{\mathrm{S}})\,. \tag{4.1.15}$$

The fundamental relation

$$\frac{\mathrm{d}S[\rho_{\mathrm{S,can}}]}{\mathrm{d}\,\langle H_{\mathrm{S}}\rangle_{\rho_{\mathrm{S,can}}}} = \beta \tag{4.1.16}$$

derives from Eq. (4.1.12) and is compared to the definition

$$\beta(U) \equiv \frac{\mathrm{d}S_{\mathrm{TD}}(U)}{\mathrm{d}U} \tag{4.1.17}$$

in classical thermodynamics [133–136]. In other words, the inverse temperature β characterizes the change of the entropy S_{TD} under a change of the internal energy U.

4.2 Imaginary time

So far only the real-time dynamics have been shown to emerge from postulates **(I)**, **(II)** and proposition **(III)** (Chapter 3). In contrast, it is the imaginary-time formulation that is indispensable for a time-temperature connection. For this reason, the emergence of imaginary time shall be the main subject of this section. We start with the pure state vector formalism in Sec. 4.2.1 as a first illustration, even though it does not play a part in the thermodynamic setting. Afterward, an equivalent analysis is presented in the unified formalism for classical and quantum mechanics in Sec. 4.2.2. We retain the name "clock" for the complement of the principal system, but use the label "complement" synonymously when we consider inverse temperature later.

4.2.1 Quantum Mechanics - Pure states

The energy constraint from Section 3.1 is unchanged in our analysis and reads

$$(\hat{H} - E)\,|\Psi\rangle = (\hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{C}} - E)\,|\Psi\rangle = 0 \tag{4.2.1}$$

in the case of non-interacting subsystems. In contrast, the required invariance

$$\exp\Big[\lambda(\hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{C}} - E)\Big]|\Psi\rangle = 0, \tag{4.2.2}$$

originates from a Hermitian, rather than a unitary transformation. Instead of using a new symbol for the one-dimensional parameter in this case, λ is kept and understood as the imaginary equivalent of the parameter used in the real-time formalism. Using the same partial projection with an initial clock state $\langle\chi_0|_{\mathrm{C}}$ as in Sec. 3.1 leads to

$$\langle\chi_0|e^{\lambda(\hat{H}_{\mathrm{C}}-E)}|\Psi\rangle_{\mathrm{C}} = e^{-\lambda\hat{H}_{\mathrm{S}}}\,\langle\chi_0|\Psi\rangle_{\mathrm{C}} \tag{4.2.3}$$

and its normalized version

$$|\varphi(\lambda)\rangle_{\mathrm{S}} = \frac{e^{-\lambda\hat{H}_{\mathrm{S}}}\,\langle\chi_0|\Psi\rangle_{\mathrm{C}}}{\sqrt{\langle\Psi|\Big[e^{-2\lambda\hat{H}_{\mathrm{S}}}\otimes|\chi_0\rangle\langle\chi_0|_{\mathrm{C}}\Big]|\Psi\rangle}} \equiv \frac{\langle\chi(\lambda)|\Psi\rangle_{\mathrm{C}}}{\sqrt{\langle\Psi|\chi(\lambda)\rangle\langle\chi(\lambda)|\Psi\rangle}}\,. \tag{4.2.4}$$

Here, the normalized λ-evolved clock state reads

$$|\chi(\lambda)\rangle_C = \frac{e^{\lambda(\hat{H}_C - E)}|\chi_0\rangle_C}{\sqrt{\langle\chi_0|e^{2\lambda(\hat{H}_C-E)}|\chi_0\rangle_C}} = \frac{e^{\lambda\hat{H}_C}|\chi_0\rangle_C}{\sqrt{\langle\chi_0|e^{2\lambda\hat{H}_C}|\chi_0\rangle_C}}, \tag{4.2.5}$$

although a normalization is not strictly needed, due to the normalization factor in the denominator of Eq. (4.2.4). The derivative of the system state with respect to λ is

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}|\varphi(\lambda)\rangle_S = \hat{H}_S|\varphi(\lambda)\rangle_S + \frac{1}{2}|\varphi(\lambda)\rangle_S \frac{\mathrm{d}\langle\Psi|\chi(\lambda)\rangle\langle\chi(\lambda)|\Psi\rangle/\mathrm{d}\lambda}{\langle\Psi|\chi(\lambda)\rangle\langle\chi(\lambda)|\Psi\rangle} \tag{4.2.6}$$

$$= \hat{H}_S|\varphi(\lambda)\rangle_S - |\varphi(\lambda)\rangle_S \frac{\langle\Psi|\chi(\lambda)\rangle_C e^{-\lambda\hat{H}_S}\hat{H}_S e^{-\lambda\hat{H}_S}\langle\chi(\lambda)|\Psi\rangle_C}{\langle\Psi|\chi(\lambda)\rangle\langle\chi(\lambda)|\Psi\rangle} \tag{4.2.7}$$

and we recognize the last term as the system mean energy $\langle\varphi(\lambda)|\hat{H}_S|\varphi(\lambda)\rangle_S$, such that

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}|\varphi(\lambda)\rangle_S = \left[\hat{H}_S - \langle\varphi(\lambda)|\hat{H}_S|\varphi(\lambda)\rangle_S\right]|\varphi(\lambda)\rangle_S\,. \tag{4.2.8}$$

This is the non-linear imaginary-time TDSE, for which λ takes the place of "traditional" imaginary time. Here, the additional term involving the mean energy of the system ensures the normalization of $|\varphi(\lambda)\rangle_S$ for all λ. One may ask why such a term is absent in the real-time TDSE. In fact, it can be easily incorporated in the real-time formalism and yields a differential equation that induces only physical changes in the state, or in more mathematical terms [286], parallel transport in the space of normalized Hilbert space vectors[1]. Furthermore, stationary states (energy eigenstates) actually have a vanishing time derivative instead of an irrelevant global time-dependent phase if the mean energy contribution is included. One could even argue that this additional term should be part of the usual real-time TDSE as a consequence of the aforementioned points.

In contrast to the real-time formalism, the mean energy for a λ-independent Hamiltonian is not constant and changes with

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\hat{H}_S\rangle_\varphi = 2\langle\hat{H}_S^2\rangle_\varphi - 2\langle\hat{H}_S\rangle_\varphi^2 = 2\,\mathrm{Var}_\varphi(\hat{H}_S)\,. \tag{4.2.9}$$

4.2.2 Quantum mechanical density operators and classical probability densities in unified formalism

For general mixed states in the unified formalism, we keep the energy constraints (3.4.13) and (3.4.14) from Sec. 3.4.3. Instead of the invariance (3.4.15) from the real-time formalism, it is the second, somewhat unusual invariance

$$\exp\left[\lambda\hat{K}_{H-E\mathbb{1}}\right]\left|\rho_\Psi\right\rangle\!\right\rangle = \left|\rho_\Psi\right\rangle\!\right\rangle \qquad \forall\lambda\in\mathbb{R} \tag{4.2.10}$$

that is needed for the imaginary-time framework. Similar to our treatments from before, a projection of $\rho_C(0)$ onto the invariance Eq. (4.2.10) yields

$$e^{\lambda\hat{K}_{H_S}}\left\langle\!\left\langle e^{\lambda\hat{K}_{H_C-E\mathbb{1}}}\rho_C(0)\middle|\rho_\Psi\right\rangle\!\right\rangle_C = \langle\!\langle\rho_C(0)|\rho_\Psi\rangle\!\rangle_C\,, \tag{4.2.11}$$

[1] A U(1) principal fiber bundle with the base space being the space of all normalized pure state density operators $|\varphi\rangle\langle\varphi|_S / \langle\varphi|\varphi\rangle_S$ for $\langle\varphi|\varphi\rangle_S \in \mathscr{H}_S\backslash\{0\}$ [286].

and the associated normalized version reads

$$\frac{e^{-\lambda\hat{K}_{H_S}}\langle\!\langle\rho_C(0)|\rho_\Psi\rangle\!\rangle_C}{\left\langle\!\!\left\langle e^{-\lambda\hat{K}_{H_S}}\mathbb{1}_S,\rho_C(0)\middle|\rho_\Psi\right\rangle\!\!\right\rangle}=\frac{\left\langle\!\!\left\langle e^{\lambda\hat{K}_{H_C-E\mathbb{1}}}\rho_C(0)\middle|\rho_\Psi\right\rangle\!\!\right\rangle_C}{\left\langle\!\!\left\langle e^{-\lambda\hat{K}_{H_S}}\mathbb{1}_S,\rho_C(0)\middle|\rho_\Psi\right\rangle\!\!\right\rangle}=\frac{\left\langle\!\!\left\langle e^{\lambda\hat{K}_{H_C-E\mathbb{1}}}\rho_C(0)\middle|\rho_\Psi\right\rangle\!\!\right\rangle_C}{\left\langle\!\!\left\langle\mathbb{1}_S,e^{\lambda\hat{K}_{H_C-E\mathbb{1}}}\rho_C(0)\middle|\rho_\Psi\right\rangle\!\!\right\rangle}\,. \tag{4.2.12}$$

Hence, the system states evolve as

$$|\rho_S(\lambda)\rangle\!\rangle_S=\frac{\langle\!\langle\rho_C(\lambda)|\rho_\Psi\rangle\!\rangle_C}{\langle\!\langle\mathbb{1}_S,\rho_C(\lambda)|\rho_\Psi\rangle\!\rangle}=\frac{e^{-\lambda\hat{K}_{H_S}}|\rho_S(0)\rangle\!\rangle_S}{\langle\!\langle\mathbb{1}_S|e^{-\lambda\hat{K}_{H_S}}\rho_S(0)\rangle\!\rangle_S} \tag{4.2.13}$$

with the normalized λ-evolved clock state

$$|\rho_C(\lambda)\rangle\!\rangle_C\equiv\frac{e^{\lambda\hat{K}_{H_C-E\mathbb{1}}}|\rho_C(0)\rangle\!\rangle_C}{\left\langle\!\!\left\langle\mathbb{1}_C\middle|e^{\lambda\hat{K}_{H_C-E\mathbb{1}}}\rho_C(0)\right\rangle\!\!\right\rangle_C}\,. \tag{4.2.14}$$

The differential equation describing the change of $|\rho_S\rangle\!\rangle_S$ is

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_S(\lambda)\rangle\!\rangle_S=\hat{K}_{H_S}|\rho_S(\lambda)\rangle\!\rangle_S+|\rho_S(\lambda)\rangle\!\rangle_S\frac{\mathrm{d}\langle\!\langle\mathbb{1}_S|e^{-\lambda\hat{K}_{H_S}}\rho_S(0)\rangle\!\rangle_S/\mathrm{d}\lambda}{\left\langle\!\!\left\langle\mathbb{1}_S\middle|e^{-\lambda\hat{K}_{H_S}}\rho_S(0)\right\rangle\!\!\right\rangle_S} \tag{4.2.15}$$

$$=\hat{K}_{H_S}|\rho_S(\lambda)\rangle\!\rangle_S-|\rho_S(\lambda)\rangle\!\rangle_S\frac{\left\langle\!\!\left\langle\mathbb{1}_S\middle|\hat{K}_{H_S}e^{-\lambda\hat{K}_{H_S}}\rho_S(0)\right\rangle\!\!\right\rangle_S}{\left\langle\!\!\left\langle\mathbb{1}_S\middle|e^{-\lambda\hat{K}_{H_S}}\rho_S(0)\right\rangle\!\!\right\rangle_S} \tag{4.2.16}$$

$$=\hat{K}_{H_S}|\rho_S(\lambda)\rangle\!\rangle_S-|\rho_S(\lambda)\rangle\!\rangle_S\underbrace{\langle\!\langle\mathbb{1}_S|\hat{K}_{H_S}\rho_S(\lambda)\rangle\!\rangle_S}_{=\langle\!\langle H_S|\rho_S(\lambda)\rangle\!\rangle_S} \tag{4.2.17}$$

or

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}|\rho_S(\lambda)\rangle\!\rangle_S=\left[\hat{K}_{H_S}-\langle\!\langle H_S\rangle\!\rangle_{\rho_S}\right]|\rho_S(\lambda)\rangle\!\rangle_S \tag{4.2.18}$$

with mean energy $\langle\!\langle H_S\rangle\!\rangle_{\rho_S}\equiv\langle\!\langle\mathbb{1}_S|\hat{K}_{H_S}\rho_S(\lambda)\rangle\!\rangle_S=\langle\!\langle H_S|\rho_S(\lambda)\rangle\!\rangle_S$. Curiously, it has the same form as the pure state version (4.2.8) and the mean energy changes similarly with

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\!\langle H_S\rangle\!\rangle_{\rho_S}=\langle\!\langle H_S^2\rangle\!\rangle_{\rho_S}-\langle\!\langle H_S\rangle\!\rangle_{\rho_S}^2=\mathrm{Var}_{\rho_S}(H_S)\geq 0\,. \tag{4.2.19}$$

As a sanity check for the unified notation, we give the differential equations in both theories. The classical version in phase space coordinates $(\mathbf{q},\mathbf{p})$ is

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}\rho_S(\mathbf{q},\mathbf{p},\lambda)=\left[H_S(\mathbf{q},\mathbf{p})-\int\mathrm{d}^{n_S}\mathbf{q}'\,\mathrm{d}^{n_S}\mathbf{p}'\,H_S(\mathbf{q}',\mathbf{p}')\rho_S(\mathbf{q}',\mathbf{p}',\lambda)\right]\rho_S(\mathbf{q},\mathbf{p},\lambda) \tag{4.2.20}$$

and the quantum mechanical density operator (in the usual meaning) changes as

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{\rho}_S(\lambda)=\frac{1}{2}\left\{\hat{H}_S,\hat{\rho}_S(\lambda)\right\}_+-\mathrm{tr}_S\left(\hat{H}_S\,\hat{\rho}_S(\lambda)\right)\hat{\rho}_S(\lambda)\,. \tag{4.2.21}$$

The mean energy of the system decreases monotonically with increasing λ, due to the non-negativity of the right-hand side of Eq. (4.2.19). In order to uphold the global energy constraint, the clock state (4.2.14) increases in energy. Put differently, an energy flow from system to clock occurs for increasing λ. Even though this is a very counter-intuitive notion, it is an algebraic consequence of our basic assumptions.

4.2.3 Rate of change for mean values

The change of any mean value reads

$$-\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\!\langle A_\mathrm{S}|\rho_\mathrm{S}(\lambda)\rangle\!\rangle_\mathrm{S} = \langle\!\langle A|\Big[\hat{K}_{H_\mathrm{S}} - \langle\!\langle H_\mathrm{S}\rangle\!\rangle_{\rho_\mathrm{S}(\lambda)}\Big]|\rho_\mathrm{S}(\lambda)\rangle\!\rangle \tag{4.2.22}$$

$$= \langle\!\langle A|\hat{K}_{H_\mathrm{S}}|\rho_\mathrm{S}(\lambda)\rangle\!\rangle - \langle\!\langle H_\mathrm{S}\rangle\!\rangle_{\rho_\mathrm{S}(\lambda)}\langle\!\langle A\rangle\!\rangle_{\rho_\mathrm{S}(\lambda)} \tag{4.2.23}$$

$$= \mathrm{Cov}_{\rho_\mathrm{S}(\lambda)}(A_\mathrm{S}, H_\mathrm{S}) \tag{4.2.24}$$

for an arbitrary $|A_\mathrm{S}\rangle\!\rangle_\mathrm{S}$ and is directly connected to the generalized covariance (3.4.12) of A_S and H_S with respect to $|\rho_\mathrm{S}(\lambda)\rangle\!\rangle_\mathrm{S}$.

4.3 Synthesis

Remarkably, already the imaginary-time von Neumann equation (4.2.18) is identical to Eq. (4.1.10), the change of a canonical ensemble with respect to the inverse temperature β. Nevertheless, it is obvious that not every state evolving under Eq. (4.2.18) represent a canonical ensemble and appropriate boundary conditions have to be found. From the outset it is clear that any initial state being a canonical ensemble remains as such, because of the equality of the evolution equation. Even though this represents a valid boundary condition, we investigate the rate of the entropy change instead of the entropy itself. Such an approach corresponds to not knowing the exact form (4.1.6) of the Gibbs state, but only the inverse temperature definition (4.1.17). The review in Sec. 4.1 has shown that the entropy of a canonical ensemble changes in a specific way, namely Eq. (4.1.12). Therefore, we investigate the entropy rate $\mathrm{d}S/\mathrm{d}\lambda$ for the imaginary-time evolution and our task is to find the appropriate conditions in order to justify the connection $\lambda \longleftrightarrow \beta$. The evaluation of a term appearing in the von Neumann entropy is treated first.

4.3.1 Logarithm of system state

A central element of the following treatment is the logarithm of the system state, namely $|\ln\rho_\mathrm{S}(\lambda)\rangle\!\rangle_\mathrm{S}$ for the state (4.2.13). Unfortunately, a general derivation is missing and we have to consider the individual formulas for classical and quantum mechanics. The classical state reads

$$\langle\mathbf{q},\mathbf{p}|\rho_\mathrm{S}(\lambda)\rangle_\mathrm{S} = \frac{1}{Z(\lambda)}e^{-\lambda H_\mathrm{S}(\mathbf{q},\mathbf{p})}\rho_\mathrm{S}(\mathbf{q},\mathbf{p},0) \tag{4.3.1}$$

with the normalization factor $Z(\lambda) \equiv \left\langle \mathbb{1}_\mathrm{S}\middle| e^{-\lambda\hat{K}_{H_\mathrm{S}}}\rho_\mathrm{S}(0)\right\rangle_\mathrm{S} = \int \mathrm{d}^{n_\mathrm{S}}\mathbf{q}\,\mathrm{d}^{n_\mathrm{S}}\mathbf{p}\,\exp[-\lambda H_\mathrm{S}(\mathbf{q},\mathbf{p})]$ $\times\,\rho_\mathrm{S}(\mathbf{q},\mathbf{p},0)$, and its logarithm yields

$$\langle\mathbf{q},\mathbf{p}|\ln\rho_\mathrm{S}(\lambda)\rangle_\mathrm{S} = -\lambda H_\mathrm{S}(\mathbf{q},\mathbf{p}) + \ln\rho_\mathrm{S}(\mathbf{q},\mathbf{p},0) - \ln Z \tag{4.3.2}$$

$$= \langle\mathbf{q},\mathbf{p}|-\lambda H_\mathrm{S} + \ln\rho_\mathrm{S}(0) - \mathbb{1}_\mathrm{S}\ln Z\rangle_\mathrm{S}\,. \tag{4.3.3}$$

The corresponding quantum density operator is expressed as

$$\hat{\rho}_\mathrm{S}(\lambda) = \frac{1}{Z(\lambda)}e^{-\lambda\hat{H}_\mathrm{S}/2}\,\hat{\rho}_\mathrm{S}(0)\,e^{-\lambda\hat{H}_\mathrm{S}/2} \tag{4.3.4}$$

and the logarithm of this product of operators cannot be straightforwardly calculated as in the classical case. For a better grasp of the logarithm term, we use a variant of the Baker-Campbell-Hausdorff formula

$$\ln\left(e^X e^Y\right) = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}\Big(\big[X,[X,Y]\big] + \big[Y,[Y,X]\big]\Big) - \dots , \tag{4.3.5}$$

which is given in Ref. [287] as

$$\begin{aligned}\ln\left(e^{-X}e^Y e^{-X}\right) = -2X + Y - \frac{1}{6}\Big(&\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}X + \hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}Y\Big)\\ &+ \frac{7}{360}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}Y + \frac{1}{360}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}X\\ &+ \frac{4}{360}\hat{L}_X^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}X - \frac{8}{360}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}Y\\ &+ \frac{6}{360}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}X + \frac{12}{360}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_Y^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}\hat{L}_X^{(\mathrm{qm})}Y + \dots\end{aligned} \tag{4.3.6}$$

Thus, the logarithm of the system state reads

$$\ln\hat{\rho}_\mathrm{S}(\lambda) = -\lambda\hat{H}_\mathrm{S} + \ln\hat{\rho}_\mathrm{S}(0) - \ln Z(\lambda)\cdot\hat{\mathbb{1}}_\mathrm{S} + \hat{F}(\lambda) \tag{4.3.7}$$

with the newly defined operator

$$\begin{aligned}\hat{F}(\lambda) \equiv -\frac{\lambda}{6}\Big(&\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{H}_\mathrm{S} + \lambda\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\ln\hat{\rho}_\mathrm{S}(0)\Big)\\ &+ \frac{7\lambda^4}{360}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\ln\hat{\rho}_\mathrm{S}(0) + \frac{\lambda}{360}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{H}_\mathrm{S}\\ &+ \frac{4\lambda^2}{360}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{H}_\mathrm{S} - \frac{8\lambda^3}{360}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\ln\hat{\rho}_\mathrm{S}(0)\\ &+ \frac{6\lambda^3}{360}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{H}_\mathrm{S} + \frac{12\lambda^2}{360}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{\ln\rho_\mathrm{S}(0)}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\ln\hat{\rho}_\mathrm{S}(0)\\ &+ \dots .\end{aligned} \tag{4.3.8}$$

It is important to note that this remainder term depends explicitly on the term $\hat{L}^{(\mathrm{qm})}_{H_\mathrm{S}}\ln\hat{\rho}_\mathrm{S}(0) = \big[\hat{H}_\mathrm{S}, \ln\hat{\rho}_\mathrm{S}(0)\big]$. Overall, we can express the logarithm of system states as

$$|\ln\rho_\mathrm{S}(\lambda)\rangle\!\rangle_\mathrm{S} = |-\lambda H_\mathrm{S}\rangle\!\rangle_\mathrm{S} + |\ln\rho_\mathrm{S}(0)\rangle\!\rangle_\mathrm{S} - \ln Z|\mathbb{1}_\mathrm{S}\rangle\!\rangle_\mathrm{S} + |F\rangle\!\rangle_\mathrm{S}\,, \tag{4.3.9}$$

for which $|F\rangle\!\rangle_\mathrm{S}$ vanishes in classical mechanics.

4.3.2 Entropy and entropy change

The expression (4.3.9) allows us to express the von Neumann entropy as

$$S[\rho_\mathrm{S}(\lambda)] = \lambda\langle\!\langle\rho_\mathrm{S}|H_\mathrm{S}\rangle\!\rangle_\mathrm{S} - \langle\!\langle\rho_\mathrm{S}(\lambda)|\ln\rho_\mathrm{S}(0)\rangle\!\rangle_\mathrm{S} + \ln Z(\lambda) - \langle\!\langle F(\lambda)|\rho_\mathrm{S}(\lambda)\rangle\!\rangle_\mathrm{S}\,, \tag{4.3.10}$$

and its derivative with respect to λ yields

$$\begin{aligned}\frac{\mathrm{d}S[\rho_\mathrm{S}(\lambda)]}{\mathrm{d}\lambda} = \lambda\underbrace{\frac{\mathrm{d}\langle\!\langle\rho_\mathrm{S}(\lambda)|H_\mathrm{S}\rangle\!\rangle_\mathrm{S}}{\mathrm{d}\lambda}}_{=-\mathrm{Var}(H_\mathrm{S})_{\rho_\mathrm{S}(\lambda)}} + \underbrace{\langle\!\langle\rho_\mathrm{S}(\lambda)|H_\mathrm{S}\rangle\!\rangle_\mathrm{S} + \frac{\mathrm{d}\ln Z(\lambda)}{\mathrm{d}\lambda}}_{=0} - \frac{\mathrm{d}\langle\!\langle F(\lambda)|H_\mathrm{S}\rangle\!\rangle_\mathrm{S}}{\mathrm{d}\lambda}\\ + \langle\!\langle\hat{K}_{H_\mathrm{S}}\rho_\mathrm{S}(\lambda)|\ln\rho_\mathrm{S}(0)\rangle\!\rangle_\mathrm{S} - \langle\!\langle H_\mathrm{S}|\rho_\mathrm{S}(\lambda)\rangle\!\rangle_\mathrm{S}\cdot\langle\!\langle\rho_\mathrm{S}(\lambda)|\ln\rho_\mathrm{S}(0)\rangle\!\rangle_\mathrm{S}\,.\end{aligned} \tag{4.3.11}$$

A connection of imaginary time λ to inverse temperature β is only be achieved if the change in entropy matches that of the canonical ensemble, Eq. (4.1.15). Upon closer inspection of the last equation, it is evident that the only undetermined quantity is the initial state $|\rho_S(0)\rangle\!\rangle_S$ and is determined from the premise of matching the entropy change for the canonical ensemble. The first thing to notice is the term involving $F(\lambda)$ and one realizes that it cannot be proportional to $\mathrm{Var}(H_S)_{\rho_S(\lambda)}$, but must vanish. For this to be the case, the term $\langle\!\langle F(\lambda)|H_S\rangle\!\rangle_S$ must be constant for all λ. The form of Eq. (4.3.8) indicates that this is only possible if

$$\hat{L}_{H_S}|\ln\rho_S(0)\rangle\!\rangle_S = 0\,, \tag{4.3.12}$$

which then implies

$$|F\rangle\!\rangle_S = 0 \tag{4.3.13}$$

in quantum and classical mechanics. In turn, the form of the logarithm of the initial state can be expressed as a function of H_S and additional quantum operators or classical phase space functions with $\hat{L}_{H_S}|A_i\rangle\!\rangle_S = 0$, collectively denoted by $A = \{A_1, A_2, \dots\}$. Using $|\ln\rho_S(0)\rangle\!\rangle_S = |f(H_S,A)\rangle\!\rangle_S$ with a function f fulfilling $\hat{L}_{H_S}|f(H_S,A)\rangle\!\rangle_S = 0$, the entropy change reads

$$\begin{aligned}
\frac{\mathrm{d}S[\rho_S(\lambda)]}{\mathrm{d}\lambda} &= -\lambda\mathrm{Var}(H_S)_{\rho_S(\lambda)} + \left\langle\!\!\left\langle \left(\hat{K}_{H_S} - \langle\!\langle H_S\rangle\!\rangle_{\rho_S(\lambda)}\right)\rho_S(\lambda)\middle| f(H_S,A)\right\rangle\!\!\right\rangle_S && (4.3.14)\\
&= \left\langle\!\!\left\langle \left(\hat{K}_{H_S} - \langle\!\langle H_S\rangle\!\rangle_{\rho_S(\lambda)}\right)\rho_S(\lambda)\middle| -\lambda H_S\right\rangle\!\!\right\rangle_S \\
&\qquad + \left\langle\!\!\left\langle \left(\hat{K}_{H_S} - \langle\!\langle H_S\rangle\!\rangle_{\rho_S(\lambda)}\right)\rho_S(\lambda)\middle| f(H_S,A)\right\rangle\!\!\right\rangle_S && (4.3.15)\\
&= \left\langle\!\!\left\langle \left(\hat{K}_{H_S} - \langle\!\langle H_S\rangle\!\rangle_{\rho_S(\lambda)}\right)\rho_S(\lambda)\middle| -\lambda H_S + f(H_S,A)\right\rangle\!\!\right\rangle_S . && (4.3.16)
\end{aligned}$$

In order to match Eq. (4.1.15), the function f must be linear in H_S, i.e.,

$$|f(H_S,A)\rangle\!\rangle_S = -\vartheta_0|H_S\rangle\!\rangle_S - \vartheta_1|\mathbb{1}_S\rangle\!\rangle_S + |g(A)\rangle\!\rangle_S\,. \tag{4.3.17}$$

for constant real numbers $\vartheta_i \in \mathbb{R}$ with a new function g. The second term, ensuring the normalization of $|\rho_S(0)\rangle\!\rangle_S$, always vanishes in Eq. (4.3.16) and, thus,

$$\frac{\mathrm{d}S[\rho_S(\lambda)]}{\mathrm{d}\lambda} = -(\lambda+\vartheta_0)\,\mathrm{Var}_{\rho_S(\lambda)}(H_S) + \mathrm{Cov}_{\rho_S(\lambda)}\big(g(A), H_S\big) \tag{4.3.18}$$

for the state

$$|\rho_S(\lambda)\rangle\!\rangle_S = \frac{e^{-(\lambda+\vartheta_0)\hat{K}_{H_S}}|e^{g(A)}\rangle\!\rangle_S}{\left\langle\!\!\left\langle \mathbb{1}_S\middle| e^{-(\lambda+\vartheta_0)\hat{K}_{H_S}} e^{g(A)}\right\rangle\!\!\right\rangle_S}\,. \tag{4.3.19}$$

Consequently, the remaining task is to show under which conditions for g the covariance term $\mathrm{Cov}_{\rho_S(\lambda)}(g, H_S)$ vanishes. To this end, we exemplarily consider the quantum case and find the condition

$$\mathrm{tr}_S\Big[\hat{g}e^{-\lambda\hat{H}_S+\hat{g}}\Big]\cdot\mathrm{tr}_S\Big[\hat{H}_S e^{-\lambda\hat{H}_S+\hat{g}}\Big] \overset{!}{=} \mathrm{tr}_S\Big[\hat{g}\hat{H}_S e^{-\lambda\hat{H}_S+\hat{g}}\Big]\cdot\mathrm{tr}_S\Big[e^{-\lambda\hat{H}_S+\hat{g}}\Big] \qquad \forall\lambda\,. \tag{4.3.20}$$

Both operators, $\hat{g}$ and $\hat{H}_S$, share a common eigenbasis, because of the vanishing commutator $[\hat{g}, \hat{H}_S] = 0$. Hence,

$$\sum_{m,n} e^{-\lambda(\varepsilon_m+\varepsilon_n)} e^{g_m+g_n} g_m \varepsilon_n \overset{!}{=} \sum_{m,n} e^{-\lambda(\varepsilon_m+\varepsilon_n)} e^{g_m+g_n} g_n \varepsilon_n \qquad \forall\lambda \tag{4.3.21}$$

for the eigenvalues $\{\varepsilon_m\}$ and $\{g_m\}$ in the eigenbasis. Since this equation must hold for all λ, it can only be fulfilled if all summands are equal and implies $g_n \overset{!}{=} g_m$ or

$$\hat{g} = g_0 \hat{\mathbb{1}}_S \,. \tag{4.3.22}$$

However, this form of the operator only induces a scalar factor, which drops out through the normalization factor and we find the condition

$$g = 0 \,. \tag{4.3.23}$$

At last, we get the entropy rate

$$\frac{\mathrm{d}S[\rho_S(\lambda)]}{\mathrm{d}(\lambda+\vartheta_0)} = -(\lambda+\vartheta_0)\,\mathrm{Var}_{\rho_S(\lambda)}(H_S) \tag{4.3.24}$$

with system states

$$|\rho_S(\lambda)\rangle\!\rangle_S = \frac{e^{-(\lambda+\vartheta_0)\hat{K}_{H_S}}|\mathbb{1}_S\rangle\!\rangle_S}{\left\langle\!\left\langle \mathbb{1}_S \middle| e^{-(\lambda+\vartheta_0)\hat{K}_{H_S}} \right\rangle\!\right\rangle_S} \,. \tag{4.3.25}$$

By requiring the entropy rate to match to defining equation (4.1.17) for inverse temperature under the given imaginary-time evolution (4.2.13), we find the inverse temperature to be imaginary time (with a possible offset), i.e.,

$$\beta = \lambda + \vartheta_0 \,. \tag{4.3.26}$$

Like real-valued time, inverse temperature is a manifestation of the entanglement contained in the global state with respect to the subsystem splitting. Simultaneously, the canonical ensembles emerged as the only states giving rise to the demanded entropy rate, as revealed by direct comparison of Eq. (4.1.6) with Eq. (4.3.25). The connection between inverse temperature and imaginary time is made explicit for the first time. Even though the physical derivation differs from traditional approaches, the outcome for the system is the same. By imposing the global energy constraint and the conditional system state formalism, the derived inverse temperature β acquires a dynamical character. Perhaps it should not be too surprising, because we set out to connect a dynamical quantity, imaginary time, with inverse temperature. The complement mean energy retains the property of being increased with increasing λ from the imaginary-time evolution (Sec. 4.2.2). Furthermore, it is not necessary for the complement to be in a canonical ensemble state as well. The particular case of canonical typicality is naturally included by assuming a large complement dimension $d_C \gg d_S$ and by taking the initial complement state as $|\hat{\rho}_C(0)\rangle\!\rangle \propto |\mathbb{1}_C\rangle\!\rangle$. Similar to our remarks in Section 3.1.5.1, it should always be possible to find a clock/complement property that allows us to deparametrize β in terms of a clock/complement mean value. As a result, the abstract quantity β can be substituted by a physical attribute of the complement.

Chapter 5

Consequences

After the successful derivations in the previous two chapters regarding the real and imaginary time formulation and the connections to inverse temperature, we discuss some further consequences of our framework in the current chapter. One of the main elements of this thesis has been the relational system state proposition **(III)**. As demonstrated, it allows to derive the TDSE, even with time-dependent potentials, without resorting to any approximations and, thus, motivates further discussions, which appear in Section 5.1. Even though we have already discussed properties of the dynamical features of our framework in Chapter 3, several important issues remain and we shed some light on these in Section 5.2. Afterward, we discuss the possibility to substitute conventional time propagation methods with a numerical procedure based on our relational formalism in Section 5.3. This chapter concludes with Section 5.4, in which some aspects of the temperature formulation are inspected.

5.1 Relational state formalism

Several aspects of the system state definition as a relational statement deserve further attention. These include the distinguishability relation for clock states and their associated relational system states, a preference for the classical state vectors and, crucially, a discussion about the physical meaning of the relational state.

5.1.1 Distinguishability

The discussion about the energy relations between system and clock in Sec. 3.1.9 already indicated that subsystem relations have a non-trivial structure. One of the simplest quantities to investigate is the overlap between two different pure states. In particular, the magnitude of the overlap of two clock states, $|\chi_1\rangle_C$ and $|\chi_2\rangle_C$, and their associated relational system states, $|\varphi[\chi_1]\rangle_S$ and $|\varphi[\chi_2]\rangle_S$, can be compared via the difference

$$\mathscr{D}_{12} \equiv \left|\langle\chi_1|\chi_2\rangle_C\right|^2 - \left|\langle\varphi[\chi_1]|\varphi[\chi_2]\rangle_S\right|^2 . \tag{5.1.1}$$

Subsequently, the central question concerns the sign of this difference and the simple example shown in Figure 5.1 illustrates that no definite inequality exists. Similar to the energy relations, only for global MES does an equality between the overlaps exist, i.e., $\mathscr{D}_{12} = 0$.

5.1.2 Preference for state formulation in classical mechanics

In Section 3.3 about the classical formulation for time emergence, we have already mentioned that often the probability amplitude of a classical state is used in the definition of

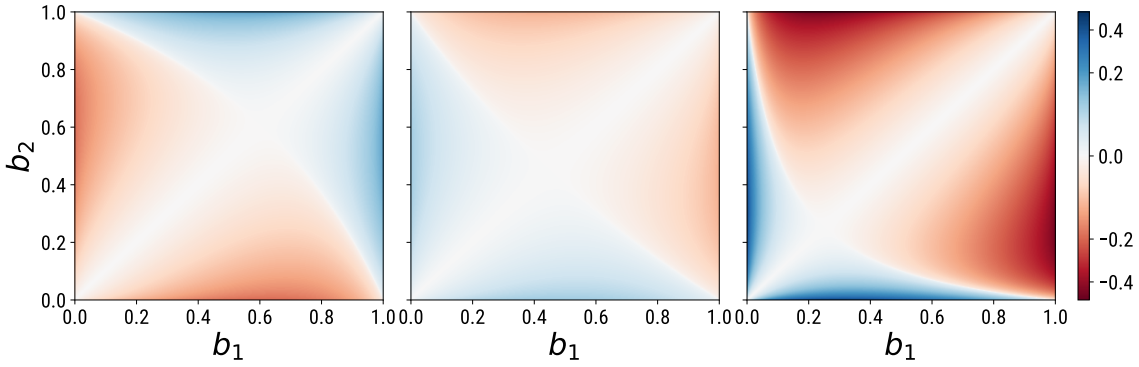

Figure 5.1 – The overlap difference (5.1.1) is shown for a bipartite system, in which each subsystem possesses only two states. Moreover, the global state $|\Psi\rangle = \sqrt{a}\,|{\uparrow_S}{\downarrow_C}\rangle + \sqrt{1-a}\,|{\downarrow_S}{\uparrow_C}\rangle$ is characterized by the single real number $0 \leq a \leq 1$. and the clock states $|\chi_m\rangle_C = \sqrt{1-b_m}\,|{\uparrow}\rangle_C + \sqrt{b_m}\,|{\downarrow}\rangle_C$ have a similar parametrization with $0 \leq b_m \leq 1$. From left to right, the global states correspond to $a \in \{0.3, 0.6, 0.9\}$. As a special case, the global MES corresponds to $a = 0.5$ and exhibits a complete equality between the overlap of different clock and associated systems states.

a state vector representation. However, as we have argued, a formulation in terms of the probability amplitude cannot match conditional statements in terms of Wigner functions, which are known to have a well-defined classical limit. As a result, we find the formulation in terms of the probability density to be singled out by this condition, even though any function ρ^γ fulfills the classical Liouville equation for an arbitrary exponent γ.

5.1.3 Interpretation of relational state

A potential drawback of PW, and, in conjunction, also our proposition **(III)**, is the status of relational states within quantum and classical theory. In Section 3.1.4, we have already alluded to the fact that the relational system state (3.1.5) cannot constitute a measurement in quantum mechanics, i.e., a physical acquisition of information about the state of the clock by the system. But how should this definition be understood, if not as a measurement? We believe that the interpretation of the conditional formalism is a major challenge for the PW approach, even though it is generally not realized as such. Unfortunately, we cannot resolve this issue, but hope for a resolution in the future. In addition, we elucidate that the problem is not exclusively quantum in nature.

Although classical mechanics does not feature the interference of different states known from quantum mechanics, it still upholds the possibility for convex combinations of classical density probabilities. In conjunction with this fact, the measurement problem persists in the classical limit of quantum theory. Specifically, a measurement must constitute the coupling of two subsystems and the accumulation of classical correlation between them through their interaction, which presupposes time. For example, if a classical coin is initially in a state of having an even probability to show either heads or tails, then an interaction with an observing system creates classical correlation (by means of a time evolution). Subsequently, the combined system of coin and observer is in a probabilistic state of observing heads or tails, similar to the quantum mechanical expression (3.1.11). The "self-locating uncertainty" issue [172,173], mentioned in Section 3.1.4, remains in classical mechanics. Clearly, a large overlap on this subject exists in quantum and classical mechanics and, thus, the interpretational issue of the conditional system state is not confined to the quantum realm. Nevertheless, given the successful derivations in this thesis, the

relational formalism certainly has merit to be investigated further.

The nowadays standard use of partially tracing over a global state in order to obtain a quantum mechanical reduced density is usually associated with ignoring any information about the environmental degrees of freedom. In view of relational system state formulation, this statement translates to the conditioning on an environmental state without any structure, i.e., one being invariant under any conceivable unitary transformation and having the least amount of information as determined by the von Neumann entropy. Both interpretations bear a close resemblance with each other and, with this in mind, it may not be too far-fetched to entertain the idea of relational states being physical elements of our theories.

5.2 Dynamics

The emergence of dynamical equations for a purely real time comprises a major part of this thesis and it is remarkable that general system dynamics in quantum and classical mechanics can ensue from a set of only three elementary guiding principles. However, this also raises entirely new questions about the physical nature of our framework. For example, does a mechanism exist which favors an evolution in real time over one in imaginary time? After all, both possibilities are algebraic consequences of our framework. Unfortunately, we cannot provide an answer, but only the phenomenological observation that we perceive an evolution in real, and not in imaginary time.

Even though many important dynamical aspects of our approach have already been discussed, several more are addressed here, which include the quantum nature of the clock, the effective system potential, an inherent asymmetry in our framework, a comparison to open system dynamics, the occurrence of changes in the system entropy and a discussion on the arrow of time.

5.2.1 Quantum nature of clock

One of the most prominent outcomes of Section 3.1 is the full quantum nature of the clock. We are able to derive exact (time-local) dynamical system equations, even in the presence of an interaction $\hat{V}$. An immediate consequence is that, contrary to previous arguments, a clock *need not* be classical or semiclassical. Nonetheless, one can choose to employ a semiclassical approximation based on stationary phase approximations (Sec. 3.1.8.5). The need for a Born-Oppenheimer approximation did not arise and, in addition, we have pointed out flaws in the previous semiclassical treatments. Despite this misconception, we also believe that our semiclassical treatment is more transparent and sleeker in form, but acknowledge that this might lie in the eye of the beholder. More importantly, the conventional semiclassical approach [98,99,102,192,209] is not confined to the field of non-relativistic atomic and molecular physics, but, as stated in Chapter 1, features prominent in research on quantum gravity [75, 85, 89–96]. An interesting and definitive difference in this line of research is the appearance of a functional derivative with respect to a "time-field", instead of a conventional time derivative. The effective dynamical law is therefore not an ordinary Schrödinger equation, but rather a "functional Schrödinger equation" or Tomonaga-Schwinger equation [87, 88, 90]. Having such a distinguished role in gravity research, it should be of academic interest to apply the analytically exact procedure given in this thesis instead of using the Born-Oppenheimer treatment and to further understand the difference in the appearing derivatives.

Furthermore, quantum clocks can live in a finite-dimensional Hilbert space and still provide a continuous notion of time. An intriguing consequence of this fact is the cyclic character of such clocks [288], which is imprinted on the system for which time is provided. Any useful clock must have a much larger natural period than the principal system in order to be able, for example, to provide time for near-recurrent phenomena of the system. Additionally, the dimension d_C of the clock has an influence on the complexity of the possible system dynamics. If we consider a two-level system as an example ($E = 0$), then the unnormalized system state reads

$$|\phi(\lambda)\rangle_\mathrm{S} = \langle\chi(\lambda)|\Psi\rangle_\mathrm{C} = \left(\sum_{k=1}^{d_\mathrm{C}} b_k^* e^{i\lambda\mathscr{E}_k} \langle\mathscr{E}_k|_\mathrm{C}\right)\left(\sum_{j=1}^{d_\mathrm{S}=2}\sum_{l=1}^{d_\mathrm{C}} a_{jl} \left|\varepsilon_j \otimes \mathscr{E}_l\right\rangle\right) \tag{5.2.1}$$

$$= \sum_{j=1}^{d_\mathrm{S}=2}\left(\sum_{k=1}^{d_\mathrm{C}} e^{i\lambda\mathscr{E}_k} b_k^* a_{jk}\right)\left|\varepsilon_j\right\rangle_\mathrm{S} \tag{5.2.2}$$

in terms of energy eigenstates. The dynamical evolution of the system coefficients is a weighted sum of complex phases. In case the clock possesses only two levels as well, i.e., $d_\mathrm{C} = 2$, each system coefficient can only exhibit sinusoidal change. Hence, in order to obtain more complicated behaviors of the energy coefficients, the clock must be high-dimensional. This is a general fact holding true for any system dimension d_S.

5.2.2 Effective system potential

The aforementioned exactness of the derived system TDSE for interacting subsystems provides perfect unitary system evolution and, thus, might shed new light on the arguments given by Marletto and Vedral [128], at least for pure states. They claim that in the presence of an interaction term the clock cannot properly function and that the system evolution "will not be a unitary evolution generated by a *time-independent* Hamiltonian" [128], but rather has the form

$$\frac{\partial\hat{\rho}_\mathrm{S}(\lambda)}{\partial\lambda} = i\left[\hat{\rho}_\mathrm{S}(\lambda), \hat{H}_\mathrm{S}\right] + \text{terms depending on } \lambda \tag{5.2.3}$$

for the state $\hat{\rho}_\mathrm{S}(\lambda)$, adopted to the notation used in this thesis. However, no attempt has been made to actually derive the form of the additional terms. On this basis and the assumption that a time operator $\hat{T}_\mathrm{C}$ with $[\hat{T}_\mathrm{C}, \hat{H}_\mathrm{C}] = i$ exists, their argument is that if a tensor product structure on the global Hilbert space $\mathscr{H}$ exists, in which the interaction term vanishes, then this factorization is unique. First, that a time operator is dispensable has been shown in this thesis. Second, the example of having a global Hamiltonian $\hat{H} = \hat{H}_1\otimes\hat{\mathbb{1}}_2\otimes\hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1\otimes\hat{H}_2\otimes\hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1\otimes\hat{\mathbb{1}}_2\otimes\hat{H}_3$ of three commuting Hamiltonian terms shows that at least two possible factorizations

$$\mathscr{H} = \underbrace{\left(\mathscr{H}_1\otimes\mathscr{H}_2\right)}_{\equiv\mathscr{H}_\mathrm{S}} \otimes \underbrace{\mathscr{H}_3}_{\equiv\mathscr{H}_\mathrm{C}} = \underbrace{\mathscr{H}_1}_{\equiv\mathscr{H}'_\mathrm{S}} \otimes \underbrace{\left(\mathscr{H}_2\otimes\mathscr{H}_3\right)}_{\equiv\mathscr{H}'_\mathrm{C}} \tag{5.2.4}$$

exist for which no subsystem interaction takes places. Regardless of the non-uniqueness issue, it is also possible to have an *exact* time-independent effective Hermitian system Hamiltonian even in the presence of an interaction $\hat{V}$. As an example, we take the clock Hamiltonian to be $\hat{H}_\mathrm{C} = K_1^2/(2\mathrm{M})\otimes\hat{\mathbb{1}}_{\mathrm{C},2}$, which operates on the further partitioned clock Hilbert space $\mathscr{H}_\mathrm{C} = \mathscr{H}_{\mathrm{C},1}\otimes\mathscr{H}_{\mathrm{C},2}$. The interaction term is $\hat{V} = \left(\hat{\mathbb{1}}_{\mathrm{C},1}\otimes\hat{A}_{\mathrm{C},2}\right)\otimes\hat{W}_\mathrm{S}$ for arbitrary clock operator $\hat{A}_{\mathrm{C},2}$ and system operator $\hat{W}_\mathrm{S}$. Taking the initial clock state as $|\chi_0\rangle_\mathrm{C} = \left|\chi_{0,1}\right\rangle_{\mathrm{C},1}\otimes|a\rangle_{\mathrm{C},2}$ with the eigenvector $\hat{A}_{\mathrm{C},2}|a\rangle_{\mathrm{C},2} = a|a\rangle_{\mathrm{C},2}$ yields the system TDSE

$$i\frac{\mathrm{d}}{\mathrm{d}\lambda}|\varphi(\lambda)\rangle_\mathrm{S} = \left[\hat{H}_\mathrm{S} + a\hat{W}_\mathrm{S}\right]|\varphi(\lambda)\rangle_\mathrm{S} \tag{5.2.5}$$

for an arbitrary system Hamiltonian $\hat{H}_S$, because $\langle\chi(\lambda)|\hat{V}|\Psi\rangle_C = a\hat{W}_S\langle\chi(\lambda)|\Psi\rangle_C$. Clearly, the evolution is unitary with a *time-independent* Hamiltonian $\hat{H}_S + a\hat{W}_S$ and thus invalidates the statement in Ref. [128]. Moreover, the authors acknowledge that an effective time-dependent Hermitian system Hamiltonian can exist, but only in a semiclassical approximation. With the determination of the additional terms in Eq. (5.2.3) we have proven that a unitary evolution is also possible without a semiclassical approximation.

5.2.3 Asymmetry of clock and system

Symmetry has played a decisive role in allowing us to base our framework on an invariance of the global state instead of the TISE. Similar to the symmetry of a circle under rotations, the global state is symmetric under the transformations generated by the global constraint operator, because of postulate (I). We note in passing that this set of transformations may rightfully be called the "symmetry group of the universe", in reference to the famous publication by Hartle and Hawking [84]. On the contrary, the emergence of time relies on a strong asymmetry between clock and system. A relational system state is associated with a predetermined clock state and, thus, induces an asymmetry through a directionality in the appearance of states in our framework, a subject closely linked to the interpretational issues in Sec. 5.1.3. As we have previously mentioned in Sec. 3.1.5.1, the conditional system state does not "relate back" to the original clock state in general, except for global MES. The disparity already occurs on the structural level of the framework without reference to a specific global Hamiltonian. Having a coupling between system and clock makes the asymmetry even more pronounced. Our results show that while the clock evolves unitarily under its own inherent Hamiltonian, the system dynamics are governed by an additional clock-dependent potential. In other words, the motion of the clock can influence the dynamics of the system in a significant manner, but any so-called "back-coupling" [98, 99] from the system on the clock is completely absent. Ultimately, the dynamical laws governing a fraction of the whole emerge through a peculiar combination of symmetry and asymmetry and understanding this imbalance between system and clock is one of the open problems of our framework.

5.2.4 Comparison to conventional open system dynamics

In the previous sections, we have mainly addressed cases with pure states, but also the mixed state treatment deserves several remarks. We have already pointed out differences of the relational framework and the conventional theory of open systems in Sec. 3.1.3 in terms of the definition of a system state and the energy content of the global state. Since time is presupposed in open systems theory, the entanglement with respect to the Hilbert space factorization changes in time, whereas it is constant in our framework and is actually a prerequisite for the appearance of subsystem dynamics. Despite the differences, there is a remarkable conceptual similarity in the way the effective system Hamiltonian is determined. This has been nicely demonstrated in the very recent publication by Hayden and Sorce [289], in which they provide a "canonical choice" for the Hamiltonian $\hat{H}_S(\lambda)$ in the quantum master equation

$$\frac{\mathrm{d}\hat{\rho}_S(\lambda)}{\mathrm{d}\lambda} = -i\Big[\hat{H}_S(\lambda), \hat{\rho}_S(\lambda)\Big] + \mathscr{D}_\lambda(\hat{\rho}_S)\,. \tag{5.2.6}$$

The "dissipative piece" $\mathscr{D}_\lambda(\hat{\rho}_S)$ is responsible for dissipative evolution under which the state properties of $\hat{\rho}_S$ are still preserved. In general, infinitely many splittings exist under which Eq. (5.2.6) is form invariant [289], but a unique preference exists. The "principle of minimal dissipation" [290] asserts that the minimization of the dissipative term with an appropriate norm implies a unique choice for the Hamiltonian part. Without going

	Open system theory in Ref. [289]	Time emergence for mixed states
Global state $\hat{\rho}_\Psi$	not energy constrained	energy constrained and pure
System definition	$\hat{\rho}_S = \mathrm{tr}_C(\hat{\rho}_\Psi)$	$\hat{\rho}_S = \mathrm{tr}_C(\hat{\rho}_C\hat{\rho}_\Psi)/\,\mathrm{tr}(\hat{\rho}_C\hat{\rho}_\Psi)$
Entanglement	increasing from zero	constant
Minimization of non-unitary part	averaged over all possible system states	depending on system state
Effective operators	depend on environment	depend on clock

Table 5.1 – The frameworks of conventional open system theory, as presented in Ref. [289], and the one used in this thesis are compared with regard to certain key features.

into detail, the norm of $\mathscr{D}_\lambda(\hat{\rho}_S)$ is based on an average over all possible system states (for a finite-dimensional $\mathscr{H}_S$). This concept of minimization of a non-Hermitian term resembles very closely our procedure for time emergence in quantum mechanics, except that we minimize with respect to the actual system state and not an average. Another interesting parallel concerns the notion of effective system operators depending on the state of the clock/complement, which is not foreign to open systems theory. Usually the initial state is taken as the product $\hat{\rho}_\Psi(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_C(0)$ [291], allowing for the unambiguous identification of the complement state $\hat{\rho}_C(0)$. Consequently, the resulting operators in the quantum master equation (5.2.6) depends specifically on the initial state $\hat{\rho}_C(0)$ [289], very similar to the clock-dependent effective system potential and anti-Hermitian term in Sec. 3.2. The individual characteristics of both approaches are summarized in Table 5.1.

5.2.5 Entropy change of system

In general, the von Neumann entropy (4.1.1) of the system varies for mixed states, due to the presence of an additional term in the system evolution equation (3.4.19), generating non-unitary evolution. This change raises two questions, namely how to reconcile a non-vanishing entropy production rate with the static nature of the global state and how to understand negative rates necessarily occurring for cyclic clocks.

The former is quite puzzling, because the global state $|\Psi\rangle$ is truly static and its entanglement must remain unchanged. A typical measure for entanglement is the entropy of the reduced density of a subsystem. For bipartite total systems, the entropy of the reduced densities is always equal for pure global states, i.e., $S[\mathrm{tr}_S(|\Psi\rangle\langle\Psi|)] = S[\mathrm{tr}_C(|\Psi\rangle\langle\Psi|)]$, regardless of the entropy measure [145, 292]. In addition, they are always constant, since the global state is static. Contrarily, we know that the clock entropy remains constant due to the unitary evolution with the clock Hamiltonian, while the system entropy changes in time. This behavior is certainly in contrast with the aforementioned equality of subsystem entropies. The apparent contradiction can be resolved by recognizing the fundamentally different definition of subsystem states, proposition **(III)** and Eq. (3.4.18). In view of the relational formulation, the reduced subsystem densities correspond to a conditioning on totally mixed states in the associated complement subsystems and, thus, do not match the setting used for time emergence. Nevertheless, it is certainly interesting to further investigate the relation of subsystem entropies and to determine if a constant combination of both entropies can be found.

The second question concerns the change of system entropy in real-valued time. We have not investigated the corresponding equations in Chapter 3, but have shown that for any quantum clock with finite dimension the system must return to its initial state eventually. Consequently, this recurrence is imprinted on the entropy and implies the occurrence of negative entropy rates. How the entropy changes for infinite-dimensional clock Hilbert spaces, or non-cyclic clocks, is unclear and requires further analytical work. A reduction in system entropy is an interesting phenomena in the field of non-equilibrium dynamics of open systems. In this regard, one usually considers the entropy production $\Sigma_S(\lambda)$ [293, 294], which is the sum of system entropy change and the entropy flux from the system to the complement [295]. Its rate $\sigma_S(\lambda) \equiv \mathrm{d}\Sigma_S(\lambda)/\mathrm{d}\lambda$ can be used for a formulation of the second law of thermodynamics [290, 296] in physical situations in which a strict non-negativity exists. Nevertheless, negative entropy production rates can occur, indicating non-Markovian characteristics, and are at the forefront of research on open system dynamics [290, 297–300]. It would be intriguing to subject our framework to a similar analysis in order to find a possibly preferred direction of time. However, the hurdle of correctly translating notions of entropy relations of open systems theory to our framework must be overcome first, as discussed above.

5.2.6 Arrow of time

The nature of time cannot be discussed without addressing the subject of a preferred direction of evolution, commonly known as the ”arrow of time”. To be clear, what we derived in this thesis is a one-dimensional parametrization of the system dynamics and the corresponding differential equations. However, the notion of a distinguished direction of time cannot originate from our basic principles (Chapter 2) and must be deduced from an additional axiom or postulate. A prime candidate is an entropic principle due to its prominent role in the second law of thermodynamics [96, 133, 301], which singles out a preferred arrow of time by demanding ever-increasing entropy. On the one hand, an intriguing possibility is a demand for increasing von Neumann entropy of the system, which can potentially be facilitated by the non-Hermitian term appearing for genuine mixed state (see previous section). On the other hand, the dynamics is always unitary for pure states and does not induce any entropy change. While this choice is rather speculative, another reasoning for the potential origin of the observed arrow of time exists, one which is compatible with our framework. Page states in Ref. [301] that “we cannot know the past except through its records in the present, ...” and such records are stored in separate degrees of freedom, possibly in a redundant manner as dictated by Quantum Darwinism [160–162, 165]. Hence, the Hilbert space $\mathscr{H}_S = \bigotimes_i \mathscr{H}_{S,i}$ must be understood as being composed of many smaller subsystem Hilbert spaces $\{\mathscr{H}_{S,i}\}$, of which some can act as measuring devices to record history. As a consequence, the direction of time arises from a special boundary condition, namely an initial system state with a very low degree of entanglement between its subsystems. This point is also conveyed by Marletto and Vedral in Ref. [128] in the context of time emergence.

5.3 Computational advantage

The timeless formalism allows for a direct computation of a time-evolved pure system state $|\varphi(\lambda)\rangle_S$ by means of the partial projection $\langle\chi(\lambda)|\Psi\rangle_C$. This fact was illustrated by two examples in Sections 3.1.7 and 3.1.8.4, which were of analytical and numerical nature, respectively. Although fascinating, they can only serve as a proof of concept and we briefly discuss the elements necessary for a viable numerical alternative to sequential time propagation. Such an alternative might be particularly promising if it allows to rely on highly parallelizable algorithms.

5.3.1 Global state as ground state and energy deviation

A crucial element of the timeless framework, derived in this thesis, is the global energy eigenstate $|\Psi\rangle$ of the total Hamiltonian $\hat{H}$. Therefore, one of the major challenges for a numerical procedure is, therefore, the determination of the global energy eigenstate $|\Psi\rangle$. A certain energy eigenstate typically plays a special role, namely the ground state. Taking the ground state of $\hat{H}$ is a perfectly reasonable choice for the global state $|\Psi\rangle$. Powerful numerical methods exist for determining ground states to high accuracy and might therefore be useful for a time propagation formalism based on relational states. One just has to ensure that $|\Psi\rangle$ contains the desired initial system state $|\varphi(0)\rangle_S$ as a potential system state (see Sec. 5.3.2). An attempt to use global ground states in a timeless formulation has been undertaken by McClean et al. [302, 303], but has since been criticized to not uphold its promises [304].

It might be difficult in numerical applications to find the exact energy eigenstate. However, often approximations to it are available. For instance, after an imaginary-time evolution of a random initial state for a sufficiently long time, one obtains the ground state in general, but a small component of the first excited state may survive in the superposition. As an example, we take the superposition

$$|\Psi\rangle = \sqrt{1-a}\,|E\rangle + \sqrt{a}\,|E+\Delta E\rangle \tag{5.3.1}$$

of a desired energy state $(\hat{H}-E)\,|E\rangle = 0$ and a component $|E+\Delta E\rangle$ for a nearby energy level $E+\Delta E$. Here, the coefficient $a \in [0,1]$ is real-valued for simplicity, but typically small. If an evolution of duration T is required, then the invariance (3.1.4) is violated by a correction term, namely

$$e^{-i(\hat{H}-E)T}\,|\Psi\rangle = \sqrt{1-a}\,|E\rangle + \sqrt{a}e^{-iT\Delta E}\,|E+\Delta E\rangle \tag{5.3.2}$$

$$= |\Psi\rangle + \sqrt{a}\left[e^{-iT\Delta E}-1\right]|E+\Delta E\rangle\,. \tag{5.3.3}$$

Hence, as a long as the product $T\Delta E$ is small, $|\Psi\rangle$ still serves as a suitable vector for time emergence and, as a result, the correction to the expected system dynamics remains small.

5.3.2 Finding the correct initial system state

In the usual treatment of differential equations such as the TDSE, one can freely choose an initial state and propagate it forward (or backward) in time. In our framework, the initial system states depends explicitly on the choice of $|\Psi\rangle$ and the initial clock state $|\chi_0\rangle_C$. Thus, if a specific initial state $|\overline{\varphi}(0)\rangle_S$ is wanted, then $|\chi_0\rangle_C$ and $|\Psi\rangle$ have to be determined such that $\left||\overline{\varphi}(0)\rangle_S - \langle\chi_0|\Psi\rangle_C / \sqrt{\langle\Psi|\chi_0\rangle\langle\chi_0|\Psi\rangle}\right|$ is minimal. In case the quasi-eigenstate approximation is employed, the clock state $|\chi_0\rangle_C$ is typically fixed and only $|\Psi\rangle$ can be optimized. Nevertheless, the global Hilbert space is large and there is a great freedom to choose the global state. For example, we assume that an orthonormal set $\{|\Psi_i\rangle\}$ of energy eigenstates associated with energies lying in the interval $[E-\Delta E, E+\Delta E]$ can be found. This set translates to a non-orthogonal set $\{|\varphi_i[\chi_0]\rangle_S\}$ of relational system states by means of $|\chi_0\rangle_C$. The system states may not be linearly independent, but the span of all vectors can still be used to construct many different initial system states via superposition and allows for a great variety. Interestingly, different dynamical system evolutions are obtained by simply changing the superposition $|\Psi\rangle = \sum_i c_i\,|\Psi_i\rangle$.

The authors of Refs. [302, 303] used an additional penalty term

$$\hat{C} \equiv \left(\hat{\mathbb{1}}_S - |\overline{\varphi}(0)\rangle\langle\overline{\varphi}(0)|_S\right) \otimes |\chi_0\rangle\langle\chi_0|_C \tag{5.3.4}$$

in their global Hamiltonian to break the degeneracy of the ground state energy and enforce a particular initial system state $|\overline{\varphi}(0)\rangle_S$. Such an additional term might be useful to obtain a global energy eigenstate in our framework that yields the correct initial system state, but can have an undesired side effect. Specifically, the effective system potential features an additional term acting mainly around $\lambda = 0$. As an illustration we assume the quasi-eigenstate approximation (3.1.102) to hold for the interaction $\hat{V} = \hat{V}_0 + \gamma\hat{C}$ ($\gamma \in \mathbb{R}$), in which case the effective potential

$$\hat{V}_S \approx \langle\chi(\lambda)|\hat{V}_0|\chi(\lambda)\rangle_C + \gamma\left|\langle\chi_0|\chi(\lambda)\rangle_C\right|^2 \cdot \left(\hat{\mathbb{1}}_S - |\overline{\varphi}(0)\rangle\langle\overline{\varphi}(0)|_S\right) \tag{5.3.5}$$

features an additional term. The clock overlap $\left|\langle\chi_0|\chi(\lambda)\rangle_C\right|^2$ typically vanishes rapidly for $\lambda \neq 0$, but has support around $\lambda \approx 0$. Assuming also $\hat{V}_0 = 0$ for simplicity, the system undergoes unwanted evolution, if the initial state $|\overline{\varphi}(0)\rangle$ is *not* an eigenstate of $\hat{H}_S$.

5.3.3 Effective system potential

The approximation of a desired system potential $\hat{W}_S(\lambda)$ with the effective system potential $\hat{V}_S(\lambda)$ in Eq. (3.1.48) is a critical part for a successful numerical simulation. Such a task requires careful fine-tuning and a minimization of any deviations, i.e.,

$$\int_0^T \mathrm{d}\lambda \left\|\hat{W}_S(\lambda) - \hat{V}_S[\chi_0, \Psi](\lambda)\right\| \stackrel{!}{=} \min \tag{5.3.6}$$

with a suitable operator norm $\|\bullet\|$ for a simulation up to time T. Despite the difficulties, the quasi-eigenstate approximation (Sec. 3.1.8.1) for appropriate clock states might help greatly to disentangle the effective potential from the influence of the global state.

Certainly, the implementation of such a numerical procedure is far from being straightforward and might not work at all, but an investigation in this direction is without a doubt worth the effort. Once one realizes that the additional complexity of the problem allows also for greater flexibility regarding approximations on a global rather than a local level, one might be even more inclined to look for possible applications. It is an extraordinary property that the global state $|\Psi\rangle$ contains an infinitely large set of possible solutions to system dynamics with different effective potentials, but finding the right one is the crux of the matter.

5.4 Temperature

As a final reflection, we briefly comment on the consequences of the results for temperature emergence in Chapter 4. Once we attach a dynamical meaning to imaginary time as the counterpart to real time, the revealed identification with temperature implies a dynamical quality for this quantity as well. Such a notion seems odd, given that one usually associates a canonical ensemble with an equilibrium situation, a concept in which (macroscopic) change is absent. The peculiar energy flow between system and complement under an evolution in imaginary time only adds to the strangeness of this scenario. For all we know, such a behavior is not part of our physically observed world and does not lend any explanatory power to the imaginary time framework for the description of natural phenomena. In spite of this deficiency, the results in Section 4.3 still contain value from a theoretical point of view. To be clear, we do *not* attempt to prove conventional thermodynamics wrong, neither do we claim to have derived a more fundamental theory for canonical ensembles. Instead, our derivations show that what has been considered mere similarities between thermal and temporal formulations thus far evolves to a direct

relationship, originating from the same set of main principles (Chapter 2). Although the considered physical situation often differs, we can still establish the link between both formulations, because the physical origin is not included in the bare description of a subsystem as a canonical ensemble. Hence, our treatment is able to shed some light on the enigmatic connection of time and temperature.

Chapter 6

Outlook

We have successfully applied the three guiding principles from Chapter 2 in quantum and classical mechanics to elucidate the emergence of subsystem dynamics. Thus, we are not only able to bridge the gap between the two prevailing approaches for time emergence in quantum mechanics, but also to extend the framework to classical mechanics in great generality. In this way, we prove how a static formulation can give rise to the dynamical equations of motions, namely the TDSE, the von Neumann equation and the classical Liouville equation. Using our framework for the emergence of imaginary time has also allowed us to finally unveil the origin of the algebraic connection of Euclidean time to one of the most important quantities in thermodynamics, the temperature of canonical ensembles.

Nevertheless, many new open questions and possible routes for future work have surfaced. To begin with, an investigation of the non-Hermitian term appearing for quantum mixed states and classical probability densities is without a doubt wanted. Not only is it vital to classify under which general conditions such a term vanishes, but also what kind of dynamics it generates. This is closely tied to an examination of the induced entropy change mentioned in Sec. 5.2.5, which would facilitate a deeper understanding of the physical implications. Furthermore, a simple example appears in Sec. 3.2.3, for which the pure state system dynamics are invariant under a change of the initial clock state, because of an additional symmetry of the clock Hamiltonian. A general classification of invariant dynamics and invariant effective system potentials in terms of symmetry properties of the clock and the interaction would be useful, especially in the context of numerical time evolution (see Sec. 5.3). Moreover, a thorough feasibility study of a numerical time propagation scheme based on the relational formalism, in order to bypass sequential time evolution algorithms, is unquestionably in great demand. On a similar note, further investigation of the timeless approach for analytically exact energy eigenstates of multipartite interacting systems could be of considerable interest for the purpose of finding new classes of exact solutions to time-dependent problems (see Sec. 3.1.7). Such examples may be found for any kind of spin chain. At least from a purely numerical perspective, they are suitable candidates for the numerical determination of energy eigenstate since powerful methods for the computation and for the storage of such states exist in the form of tensor networks [305, 306].

Other paths toward greater insight are provided by a more sophisticated error analysis and additional inspections of the time-energy uncertainty relations. The first includes a detailed quantification of the deviation from exact dynamics, due to the semiclassical approximation and, furthermore, the determination of an overall error quantifier complementing the instantaneous one for the quasi-eigenstate approximation (Sec. 3.1.8.1). Such a term might prove beneficial for the alternative time propagation method via relational states (Sec. 3.1.8.4). The second path concerns time-energy uncertainty relations, for

which we did not succeed in finding a general functioning formulation in Sec. 3.1.9. With this in mind, we believe that seeking a working approach is important, especially for non-vanishing interactions $\hat{V} \neq 0$. This includes deriving attainable tighter bounds for mixed states, such as given in Ref. [307], and a conceivable use of entropic uncertainty relations [127, 142, 211]. In particular for the latter, throughout this thesis we have encountered the special role of MES several times with its special properties in our framework. It would be very interesting to further explore its role in time emergence, in particular, how compatible MES are with the requirement of being an energy eigenstate to a specific Hamiltonian and which restrictions arise. Alongside, one could envision a connection to environment-assisted invariance (or "envariance") and to emergence of Born's rule [164, 308]. Another special class of states are pure states in classical mechanics. An analysis of the surmised conditions given in Sec. 3.4 may prove useful to derive a complete analog to the quantum mechanical pure state case, which would guarantee unitary system evolution.

On the conceptual level, several intriguing ideas emerge as well. As a first aspect, we strongly suspect our framework to provide the necessary link between two apparently unrelated perturbation theories, namely a connection between a global *time-independent* perturbation theory and a *time-dependent* perturbation theory for system states. Furthermore, we point out resemblances of our framework to open systems theory and decoherence theory, for which a closer study might reveal useful mathematical cross-overs, also from the field of "quantum steering" [309–311]. Moreover, the fact that a general pure state of a bipartite system usually has non-vanishing entanglement is well-known and has been extensively used in this thesis. However, the restrictions on entanglement by the global energy constraint for a general Hamiltonian are not entirely understood [312–314], but rather an open research problem. A further understanding of the interplay between entanglement and energy would also be advantageous for additional insight on the obtainable dynamics in the time emergence framework [127]. In light of the global symmetry, another very intriguing line of thought can be pursued. If we abandon the concept of a continuous notion of time, then the global state can still be invariant under a *discrete* symmetry group. Our relational framework applies nonetheless in this case and leads to stroboscopic changes in the clock state, which implies an evolution of the system in *discrete time*. Astonishingly, this result depends crucially on the invariance perspective employed in this thesis and cannot be obtained with previous approaches, because the concept of a global TISE does not exist in this case and a system TDSE does not either. Entertaining this possibility, one would need to replace the energy constraint in postulate **(I)** with a statement about the global symmetry.

Probably one of the greatest issues of the PW approach and of our generalized framework is the interpretation of the conditional system state, given that it does *not* correspond to a measurement of the clock by the system (Sec. 3.1.4). Such an understanding is however critical for the time emergence approach to manifest itself as a serious theory and must be addressed in subsequent works. Our results certainly render future studies in this direction worthwhile.

By showing that our three basic principles can be applied to derive imaginary time, we also found a gateway to connect to inverse temperature in canonical ensembles. As is common in thermodynamical settings, we assumed the interaction between subsystems to be negligible. Such a simplification does not always hold in practice and a derivation of imaginary time for generally coupled subsystems with $\hat{V} \neq 0$ would broaden the scope of our framework. This is especially true for thermodynamics, where the treatment of non-negligible interactions is still an open problem [126, 315–320]. Just as there is no genuine time operator, a legitimate temperature operator does not exist either, but only tempera-

ture estimators [321, 322]. An examination of the possible connection of these estimators to time estimators, in the form of age operators (Sec. 3.1.5.1 and App. E), may allow to further reinforce the link between time and temperature. So far we have only treated time exclusively along the real or the imaginary axis, but arbitrary paths through the complex plane provide another interesting extension of our framework. Complex time paths usually arise in semiclassical approximations for tunneling dynamics [277, 323, 324] and an embedding of this process into our framework could help to obtain a better understanding of such a mechanism. The extension to complex time is straightforward for pure quantum states, contrary to mixed quantum states and classical probability densities, which need different generators for real and imaginary time for the global invariance.

Entanglement is arguably one of the most fascinating aspects of quantum theory and has been a cornerstone for the emergence of *time*. In a similar fashion, it is hypothesized that entanglement may also be the foundation for the emergence of *space* [112, 114]. Thus, we close with the mesmerizing idea of searching for a joint origin of *space-time* in abstract quantum mechanics [325, 326].

Appendix A

Effective system potential

A.1 Determination from variational procedure

The variational approach has led to the equation

$$\langle\chi|\Big(\hat{P}_\Psi\hat{V}+\hat{V}\hat{P}_\Psi\Big)|\chi\rangle_\mathrm{C}=\langle\phi|\phi\rangle_\mathrm{S}\Big(\hat{P}_\varphi\hat{V}_\mathrm{S}+\hat{V}_\mathrm{S}\hat{P}_\varphi\Big), \tag{A.1.1}$$

from which we determine $\hat{V}_\mathrm{S}$. Using the complementary projector $\hat{\bar{P}}_\varphi=\hat{\mathbb{1}}_\mathrm{S}-P_\varphi$ helps us to bring the effective system potential to the block form

$$\hat{V}_\mathrm{S}=\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi+\hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi+\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi+\hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi=\left(\begin{array}{c|c}\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi & \hat{P}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi\\ \hline \hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi & \hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi\end{array}\right). \tag{A.1.2}$$

As we have stated in the main text, the hermitian term $\hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi$ does not affect the dynamics of the system. Eq. (A.1.1) does not provide means to evaluate this term and, for this reason, we set it to zero, i.e., $\hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi=0$. Even though it does not influence the system dynamics either, the term $\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi$ is kept in $\hat{V}_\mathrm{S}$, as it ensures Hermiticity. The remaining three terms can be extracted with the use of

$$\hat{P}_\varphi\hat{V}_\mathrm{S}+\hat{V}_\mathrm{S}\hat{P}_\varphi=2\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi+\hat{\bar{P}}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi+\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi \tag{A.1.3}$$

and the appropriate projections from the left and right onto Eq. (3.1.43). In particular, the diagonal block reads

$$\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{P}_\varphi=\frac{1}{\langle\phi|\phi\rangle_\mathrm{S}}\,\mathrm{Re}\left\{\hat{P}_\varphi\,\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_\mathrm{C}\,\hat{P}_\varphi\right\} \tag{A.1.4}$$

$$=\frac{|\phi\rangle\langle\phi|_\mathrm{S}}{\langle\phi|\phi\rangle_\mathrm{S}^3}\,\mathrm{Re}\Big\{\,\langle\Psi|\hat{P}_\chi|\Psi\rangle\,\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle\,\Big\} \tag{A.1.5}$$

$$=\hat{P}_\varphi\,\mathrm{Re}\left\{\frac{\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}\right\}=\hat{P}_\varphi\,\mathrm{Re}(a)\,. \tag{A.1.6}$$

Here, we use the definition of the complex scalar $a(\lambda)\equiv\langle\Psi|\hat{V}\hat{P}_\chi(\lambda)|\Psi\rangle\,/\,\langle\Psi|\hat{P}_\chi(\lambda)|\Psi\rangle\in\mathbb{C}$ from the main text. In a similar manner, we determine the off-diagonal blocks to be

$$\hat{P}_\varphi\hat{V}_\mathrm{S}\hat{\bar{P}}_\varphi=\frac{1}{\langle\phi|\phi\rangle_\mathrm{S}}\hat{P}_\varphi\,\langle\chi|\Big(\hat{P}_\Psi\hat{V}+\hat{V}\hat{P}_\Psi\Big)|\chi\rangle_\mathrm{C}\,\hat{\bar{P}}_\varphi \tag{A.1.7}$$

$$=\frac{1}{\langle\phi|\phi\rangle_\mathrm{S}}\underbrace{\hat{P}_\varphi\,\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_\mathrm{C}}_{=\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_\mathrm{C}}\hat{\bar{P}}_\varphi \tag{A.1.8}$$

$$= \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle}\hat{P}_\varphi \tag{A.1.9}$$

$$= \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - \frac{|\phi\rangle\langle\phi|_S}{\langle\phi|\phi\rangle_S}\frac{\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} \tag{A.1.10}$$

$$= \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - \hat{P}_\varphi\frac{\langle\Psi|\hat{V}\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} \tag{A.1.11}$$

$$= \frac{\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - a\,\hat{P}_\varphi \tag{A.1.12}$$

and

$$\hat{\bar{P}}_\varphi\hat{V}_S\hat{P}_\varphi = \left(\hat{P}_\varphi\hat{V}_S\hat{\bar{P}}_\varphi\right)^\dagger = \frac{\langle\chi|\hat{V}\hat{P}_\Psi|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - a^*\,\hat{P}_\varphi\,. \tag{A.1.13}$$

Finally, we put the results together and find the optimal effective system potential

$$\hat{V}_S = \mathrm{Re}(a)\hat{P}_\varphi + \frac{\langle\chi|\left(\hat{V}\hat{P}_\Psi + \hat{P}_\Psi\hat{V}\right)|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - (a+a^*)\hat{P}_\varphi \tag{A.1.14}$$

$$= \frac{\langle\chi|\left(\hat{V}\hat{P}_\Psi + \hat{P}_\Psi\hat{V}\right)|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} - \mathrm{Re}(a)\hat{P}_\varphi\,, \tag{A.1.15}$$

for which the remainder vector becomes

$$|\Delta\rangle_{S,\min} = \langle\chi|\hat{V}|\Psi\rangle_C - \hat{V}_S\,|\phi\rangle_S \tag{A.1.16}$$

$$= \langle\chi|\hat{V}|\Psi\rangle_C - \left[\hat{P}_\varphi\hat{V}_S\hat{P}_\varphi + \hat{\bar{P}}_\varphi\hat{V}_S\hat{P}_\varphi\right]|\phi\rangle_S \tag{A.1.17}$$

$$= \langle\chi|\hat{V}|\Psi\rangle_C - \left[\mathrm{Re}(a)\,|\phi\rangle_S + \underbrace{\frac{\langle\chi|\hat{V}\hat{P}_\Psi|\chi\rangle_C}{\langle\phi|\phi\rangle_S}\,|\phi\rangle_S}_{=\langle\chi|\hat{V}|\Psi\rangle_C} - a^*\,|\phi\rangle_S\right] \tag{A.1.18}$$

$$= -i\,\mathrm{Im}(a)\,|\varphi\rangle_S\,. \tag{A.1.19}$$

A.2 Alternative form of TDSE

Making use of the TISE (3.1.3) and the freedom to subtract $\mathrm{Re}(a)\hat{\bar{P}}_\varphi$ allows us to express the effective system potential in the alternative form

$$\hat{V}_S = E - \left\{\hat{H}_S, \hat{P}_\varphi\right\}_+ - \frac{\langle\chi|\left\{\hat{H}_C, \hat{P}_\Psi\right\}_+|\chi\rangle_C}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle} + \langle\varphi|\hat{H}_S|\varphi\rangle_S + \mathrm{Re}\,\frac{\langle\Psi|\hat{H}_C\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}\,. \tag{A.2.1}$$

Here, $\{\hat{A},\hat{B}\}_+$ denotes the anti-commutator. Interestingly, the knowledge of $\hat{V}$ is not needed to characterize the effective potential. The necessary information about $\hat{V}$ is encoded in the global state $|\Psi\rangle$. When applied to the system state, as in the system TDSE, we find

$$\left[\hat{H}_S + \hat{V}_S\right]|\varphi\rangle_S = \left[E - \frac{\langle\chi|\left\{\hat{H}_C, \hat{P}_\Psi\right\}_+|\chi\rangle_C}{\langle\Psi|\hat{P}_\chi|\Psi\rangle} + \mathrm{Re}\,\frac{\langle\Psi|\hat{H}_C\hat{P}_\chi|\Psi\rangle}{\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle}\right]|\varphi\rangle_S\,. \tag{A.2.2}$$

This expression does not depend on $\hat{H}_S$ and $\hat{V}$ any longer.

Appendix B

Hermite polynomials

The Hermite polynomials read

$$H_n(x) = n! \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(-1)^m}{m!(n-2m)!} (2x)^{n-2m} \tag{B.1}$$

for $n \geq 0$ in explicit form and constitute a set of orthogonal polynomials by means of

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2} H_m(x) H_n(x) = \sqrt{\pi} 2^n n! \delta_{nm} \,. \tag{B.2}$$

Some of their characteristic properties are used to solve integrals in the following and we list them in the next section.

B.1 Properties

First, they transform as

$$H_n(-x) = (-1)^n H_n(x) \tag{B.1.1}$$

under parity transformations, which is a useful property for the evaluation of integrals with symmetric or antisymmetric integrands. Second, Hermite polynomials can be constructed from lower order ones through the recurrence relation

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x) \,. \tag{B.1.2}$$

Third, a Taylor expansion yields the finite sum

$$H_n(x+y) = \sum_{k=0}^{n} \binom{n}{k} H_k(x) (2y)^{n-k} \tag{B.1.3}$$

due to the polynomial nature. Fourth, we need the generating function

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \tag{B.1.4}$$

in Sec. B.2 for the calculation of Fourier transformations involving Hermite polynomials.

An important integral containing Hermite polynomials is given in Ref. [327] as

$$I'_{nm} \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-2a^2x^2} H_n(x) H_m(x) \tag{B.1.5}$$

$$= \sqrt{2}^{m+n-1}\,\Gamma\left(\frac{m+n+1}{2}\right)\cdot\frac{\sqrt{1-2a^2}^{n+m}}{a^{n+m+1}}\cdot{}_2F_1\left(-m,-n;\frac{1-n-m}{2};\frac{a^2}{2a^2-1}\right) \tag{B.1.6}$$

for $\mathrm{Re}\,a^2 > 0$, $a^2 \neq \frac{1}{2}$ and $m+n$ being even. Here, we denote hypergeometric functions by ${}_2F_1$ and the integral yields zero for an odd sum $m+n$. For our purpose, we need the substitution $2a^2 \to a$, to get

$$I_{nm} \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ax^2} H_n(x) H_m(x) \tag{B.1.7}$$

$$= \frac{2^{m+n}}{\sqrt{a}}\,\Gamma\left(\frac{m+n+1}{2}\right)\cdot\sqrt{\frac{1-a}{a}}^{n+m}\cdot{}_2F_1\left(-m,-n;\frac{1-n-m}{2};\frac{a}{2(a-1)}\right). \tag{B.1.8}$$

B.2 Fourier transform of Hermite polynomial

In order to determine an important Fourier transformation of a term including the product of a Hermite polynomial and a Gaussian function, we first derive a simpler version and, subsequently, use the same underlying procedure to evaluate the full expression.

B.2.1 Simple form

To this end, we consider the generating function

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x)\,\frac{t^n}{n!} \tag{B.2.1}$$

for all complex x and t. Multiplying by $\exp\left(-x^2/2\right)$ and taking the Fourier transformation on both sides yields

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} e^{-x^2/2+2xt-t^2} = \sqrt{2\pi}\, e^{-k^2/2+t^2-2itk} \tag{B.2.2}$$

$$= \sqrt{2\pi}\, e^{-k^2/2} e^{2k(-it)-(-it)^2} \tag{B.2.3}$$

$$= \sqrt{2\pi}\, e^{-k^2/2} \sum_{n=0}^{\infty} H_n(k)\,\frac{(-it)^n}{n!} \tag{B.2.4}$$

$$\overset{!}{=} \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} e^{-x^2/2} H_n(x). \tag{B.2.5}$$

By comparison of different orders of t, we get the desired Fourier transform

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} e^{-x^2/2} H_n(x) = \sqrt{2\pi}\,(-i)^n\, e^{-k^2/2}\, H_n(k). \tag{B.2.6}$$

B.2.2 Advanced form

The integral necessary for the calculation of a relational system state in Sec. 3.1.7 requires a more complicated integral. Nevertheless, the procedure from above allows us to solve it in a similar way. Again, we start from the generating function (B.1.4), but multiply both sides by $\exp\left(-x^2/(2a^2)\right)$ for $a > 0$ instead. Fourier transforming the equations yields

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} e^{-x^2/(2a^2)+2xt-t^2} = \sqrt{2\pi}a\, e^{-a^2(k+2it)^2/2-t^2} \tag{B.2.7}$$

$$= \sqrt{2\pi}a\, e^{-a^2k^2/2+(2a^2-1)t^2-2ia^2tk} \tag{B.2.8}$$

$$= \sqrt{2\pi}a\, e^{-a^2k^2/2} e^{2\frac{a^2}{\sqrt{2a^2-1}}k(-it\sqrt{2a^2-1})-(-it\sqrt{2a^2-1})^2} \tag{B.2.9}$$

$$= \sqrt{2\pi}a\, e^{-a^2k^2/2} \sum_{n=0}^{\infty} H_n\left(k\frac{a^2}{\sqrt{2a^2-1}}\right) \frac{(-it\sqrt{2a^2-1})^n}{n!} \tag{B.2.10}$$

$$\stackrel{!}{=} \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} e^{-x^2/(2a^2)} H_n(x) \tag{B.2.11}$$

and we find

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} e^{-x^2/(2a^2)} H_n(x) = \sqrt{2\pi}a\,(-i\sqrt{2a^2-1})^n\, e^{-a^2k^2/2}\, H_n\left(k\frac{a^2}{\sqrt{2a^2-1}}\right) \tag{B.2.12}$$

$$= \sqrt{2\pi}a\,\sqrt{1-2a^2}^n\, e^{-a^2k^2/2}\, H_n\left(k\frac{a^2}{\sqrt{2a^2-1}}\right). \tag{B.2.13}$$

Moreover, we need to solve the integral

$$I_n \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikx} \cdot e^{-x^2/2} \cdot H_n\big(ax+y\big). \tag{B.2.14}$$

For this purpose, we use the linear transformation

$$z \equiv ax+y \qquad \Rightarrow \qquad x = \frac{z-y}{a}. \tag{B.2.15}$$

and a straightforward calculation yields

$$I_n = \frac{1}{a} e^{iky/a} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikz/a} \cdot e^{-(z-y)^2/(2a^2)} \cdot H_n(z) \tag{B.2.16}$$

$$= \frac{1}{a} e^{iky/a} e^{-y^2/(2a^2)} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ikz/a} e^{zy/a^2} \cdot e^{-z^2/(2a^2)} \cdot H_n(z) \tag{B.2.17}$$

$$= \frac{1}{a} e^{iky/a} e^{-y^2/(2a^2)} \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-iz\left(k/a+iy/a^2\right)} \cdot e^{-z^2/(2a^2)} \cdot H_n(z) \tag{B.2.18}$$

$$= \sqrt{2\pi}\, e^{iky/a} e^{-y^2/(2a^2)}\, \sqrt{1-2a^2}^n\, e^{-(ak+iy)^2/(2a^2)}\, H_n\left(\frac{ak+iy}{\sqrt{2a^2-1}}\right) \tag{B.2.19}$$

$$= \sqrt{2\pi}\,\sqrt{1-2a^2}^n\, e^{-k^2/2}\, H_n\left(\frac{ak+iy}{\sqrt{2a^2-1}}\right) \tag{B.2.20}$$

with the result from above. In particular, the case $n=1$ gives

$$I_{n=1} = \sqrt{2\pi}\,\sqrt{1-2a^2}\, e^{-k^2/2} \cdot 2\frac{ak+iy}{\sqrt{2a^2-1}}. \tag{B.2.21}$$

Appendix C

Coupled harmonic oscillators

C.1 Global Hamiltonian and energy eigenstate

For completeness, we state some important formulas from the main text again, namely the Hamiltonian

$$\hat{H} = \underbrace{\frac{\hat{p}_r^2}{2} + \frac{\cos^2\theta}{2}\hat{r}^2}_{=\hat{H}_\mathrm{C}} + \underbrace{\frac{\hat{p}_s^2}{2} + \frac{\sin^2\theta}{2}\hat{s}^2}_{=\hat{H}_\mathrm{S}} \underbrace{- \frac{\sin(2\theta)}{2}\cdot\hat{s}\otimes\hat{r}}_{=\hat{V}}, \tag{C.1.1}$$

and the corresponding energy eigenstates

$$\Psi_{n,k}(r,s) = \frac{1}{\pi^{1/4}\sqrt{2^{n+1}\pi n!}} e^{-ik(s\cos\theta + r\sin\theta)} H_n\Big(r\cos\theta - s\sin\theta\Big) e^{-(r\cos\theta - s\sin\theta)^2/2}. \tag{C.1.2}$$

In particular, the wavefunction reads

$$\Psi_{1,k}(r,s) = \frac{1}{\pi^{1/4}\sqrt{\pi}} e^{-ik(s\cos\theta + r\sin\theta)} \Big(r\cos\theta - s\sin\theta\Big) e^{-(r\cos\theta - s\sin\theta)^2/2} \tag{C.1.3}$$

for $n = 1$.

C.2 Clock state

In the main text, the clock states rely on the coherent states

$$\alpha(r,\lambda,\omega,r_0) = \left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} e^{-i\Big(\omega\lambda + r_\mathrm{cl}(\lambda)\cdot p_\mathrm{cl}(\lambda)\Big)/2} \cdot e^{-\omega\Big(r - r_\mathrm{cl}(\lambda)\Big)^2/2} \cdot e^{ir\cdot p_\mathrm{cl}(\lambda)} \tag{C.2.1}$$

evolving under the Hamiltonian $\hat{H}_\mathrm{osc} = (\hat{p}_r^2 + \omega^2\hat{r}^2)/2$ with the classical trajectories $r_\mathrm{cl}(\lambda) = r_0\cos(\omega\lambda)$ and $p_\mathrm{cl}(\lambda) = -\omega r_0\sin(\omega\lambda)$. For later reference in the derivation of relational system states, we give the definition

$$\langle\chi(\lambda)|r\rangle_\mathrm{C} \equiv \alpha^*(r,\lambda,\omega_r,r_0)\cdot\exp\Big[-i\lambda E\Big] \tag{C.2.2}$$

of the clock state once more, in which the complex conjugated form

$$\alpha^*(r,\lambda,\omega,r_0) = \left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} e^{i\Big(\omega\lambda + r_\mathrm{cl}(\lambda)\cdot p_\mathrm{cl}(\lambda)\Big)/2} e^{-ir\cdot p_\mathrm{cl}(\lambda)} e^{-\omega\Big(r - r_\mathrm{cl}(\lambda)\Big)^2/2} \tag{C.2.3}$$

has to be used.

C.3 Conditional system state

In the following, we solve the integral appearing in the unnormalized conditional system states

$$\phi_{n,k}(s,\lambda) = \left\langle s \otimes \chi(\lambda) \middle| \Psi_{n,k} \right\rangle \tag{C.3.1}$$

$$\begin{aligned} &= \frac{1}{\pi^{1/4}\sqrt{2^{n+1}\pi n!}} \left(\frac{\cos\theta}{\pi}\right)^{1/4} e^{-iE\lambda} e^{i\left(\lambda\cos\theta + r_{\mathrm{cl}}(\lambda)\cdot p_{\mathrm{cl}}(\lambda)\right)/2} e^{-iks\cos\theta} \\ &\quad \cdot \int_{-\infty}^{\infty} \mathrm{d}r\, e^{-\cos\theta\left(r - r_{\mathrm{cl}}(\lambda)\right)^2/2} e^{-ir\left(k\sin\theta + p_{\mathrm{cl}}(\lambda)\right)} \cdot e^{-(r\cos\theta - s\sin\theta)^2/2} \\ &\quad \cdot H_n\big(r\cos\theta - s\sin\theta\big) \end{aligned} \tag{C.3.2}$$

in position basis. To this end, we restructure the exponents with

$$\cos\theta(r - r_{\mathrm{cl}})^2 + (r\cos\theta - s\sin\theta)^2$$

$$= r^2(\cos\theta + \cos^2\theta) - 2r\cos\theta(r_{\mathrm{cl}} + s\sin\theta) + r_{\mathrm{cl}}^2\cos\theta + s^2\sin^2\theta \tag{C.3.3}$$

$$= \left(r\sqrt{\cos\theta + \cos^2\theta} - (r_{\mathrm{cl}} + s\sin\theta)\frac{\cos\theta}{\sqrt{\cos\theta + \cos^2\theta}}\right)^2 - (r_{\mathrm{cl}} + s\sin\theta)^2\frac{\cos\theta}{1+\cos\theta} + r_{\mathrm{cl}}^2\cos\theta + s^2\sin^2\theta \tag{C.3.4}$$

$$\begin{aligned} &= \left(r\sqrt{\cos\theta(1+\cos\theta)} - (r_{\mathrm{cl}} + s\sin\theta)\sqrt{\frac{\cos\theta}{1+\cos\theta}}\right)^2 \\ &\quad + r_{\mathrm{cl}}^2\cos\theta\frac{(1+\cos\theta)-1}{1+\cos\theta} + s^2\sin^2\theta\frac{1+\cos\theta-\cos\theta}{1+\cos\theta} \\ &\quad - 2sr_{\mathrm{cl}}\cdot\frac{\sin\theta\cos\theta}{1+\cos\theta} \end{aligned} \tag{C.3.5}$$

$$\begin{aligned} &= \left(r\sqrt{\cos\theta(1+\cos\theta)} - (r_{\mathrm{cl}} + s\sin\theta)\sqrt{\frac{\cos\theta}{1+\cos\theta}}\right)^2 \\ &\quad + \underbrace{\frac{1}{1+\cos\theta}\big(s\sin\theta - r_{\mathrm{cl}}\cos\theta\big)^2}_{=(1-\cos\theta)\cdot(s - r_{\mathrm{cl}}\cot\theta)^2}. \end{aligned} \tag{C.3.6}$$

The modified momentum

$$\mathsf{K} \equiv k\sin\theta + p_{\mathrm{cl}} \tag{C.3.7}$$

allows for a compact notation and we get the expression

$$\begin{aligned} \phi_{n,k} = &\frac{\cos^{1/4}\theta}{\sqrt{2^{n+1}\pi^2 n!}} e^{-iE\lambda} e^{i\left(\lambda\cos\theta + r_{\mathrm{cl}}\cdot p_{\mathrm{cl}}\right)/2} e^{-iks\cos\theta}\ e^{-(s\sin\theta - r_{\mathrm{cl}}\cos\theta)^2/[2(1+\cos\theta)]} \\ &\int_{-\infty}^{\infty} \mathrm{d}r\, e^{-ir\mathsf{K}} \cdot e^{-\left(r\sqrt{\cos\theta(1+\cos\theta)} - \frac{(r_{\mathrm{cl}} + s\sin\theta)\sqrt{\cos\theta}}{\sqrt{1+\cos\theta}}\right)^2/2} H_n\big(r\cos\theta - s\sin\theta\big). \end{aligned} \tag{C.3.8}$$

Using the linear transformation

$$z \equiv r\sqrt{\cos\theta(1+\cos\theta)} - \frac{(r_{\mathrm{cl}} + s\sin\theta)\sqrt{\cos\theta}}{\sqrt{1+\cos\theta}} \tag{C.3.9}$$

and the inverse form

$$r = \frac{z}{\sqrt{\cos\theta(1+\cos\theta)}} + \frac{r_{\mathrm{cl}} + s\sin\theta}{1+\cos\theta} \tag{C.3.10}$$

results in

$$r\cos\theta - s\sin\theta = z\sqrt{\frac{\cos\theta}{1+\cos\theta}} + \frac{r_{\mathrm{cl}}\cos\theta + s\sin\theta\cos\theta}{1+\cos\theta} - s\sin\theta \tag{C.3.11}$$

$$= z\sqrt{\frac{\cos\theta}{1+\cos\theta}} + \frac{r_{\mathrm{cl}}\cos\theta - s\sin\theta}{1+\cos\theta}\,. \tag{C.3.12}$$

Consequently, the unnormalized system state takes the form

$$\begin{aligned}\phi_{n,k} = {} & \frac{\cos^{1/4}\theta}{\sqrt{\cos\theta(1+\cos\theta)2^{n+1}\pi^2 n!}} e^{-iE\lambda} e^{i\left(\lambda\cos\theta + r_{\mathrm{cl}}\cdot p_{\mathrm{cl}}\right)/2} \\ & \cdot e^{-iks\cos\theta}\, e^{-(s\sin\theta - r_{\mathrm{cl}}\cos\theta)^2/[2(1+\cos\theta)]}\, e^{-i\mathsf{K}(r_{\mathrm{cl}} + s\sin\theta)/(1+\cos\theta)} \\ & \cdot \int_{-\infty}^{\infty} \mathrm{d}z\, e^{-iz\mathsf{K}/\sqrt{\cos\theta(1+\cos\theta)}} \cdot e^{-z^2/2} H_n\left(z\sqrt{\frac{\cos\theta}{1+\cos\theta}} + \frac{r_{\mathrm{cl}}\cos\theta - s\sin\theta}{1+\cos\theta}\right)\end{aligned} \tag{C.3.13}$$

with $\mathrm{d}r = \mathrm{d}z/\sqrt{\cos\theta(1+\cos\theta)}$. The solution to the integral is given as Eq. (B.2.20) in Appendix B, with which we find

$$\begin{aligned}&\int_{-\infty}^{\infty} \mathrm{d}z\, e^{-iz\mathsf{K}/\sqrt{\cos\theta(1+\cos\theta)}} \cdot e^{-z^2/2} H_n\left(z\sqrt{\frac{\cos\theta}{1+\cos\theta}} + \frac{r_{\mathrm{cl}}\cos\theta - s\sin\theta}{1+\cos\theta}\right) \\ &\quad = \sqrt{2\pi}\, e^{-\mathsf{K}^2/[2\cos\theta(1+\cos\theta)]} \sqrt{\frac{1-\cos\theta}{1+\cos\theta}}^{\,n} \\ &\qquad \cdot H_n\left[\sqrt{\frac{1+\cos\theta}{1-\cos\theta}}\left(\frac{r_{\mathrm{cl}}\cos\theta - s\sin\theta}{1+\cos\theta} - i\frac{\mathsf{K}}{1+\cos\theta}\right)\right] \qquad \text{(C.3.14)} \\ &\quad = \sqrt{2\pi}\, e^{-\mathsf{K}^2/[2\cos\theta(1+\cos\theta)]} \tan^n\left(\frac{\theta}{2}\right) H_n\left[\frac{r_{\mathrm{cl}}\cos\theta - s\sin\theta - i\mathsf{K}}{\sin\theta}\right] \qquad \text{(C.3.15)} \\ &\quad = \sqrt{2\pi}\, e^{-\mathsf{K}^2/[2\cos\theta(1+\cos\theta)]} \tan^n\left(\frac{\theta}{2}\right) H_n\Big[r_{\mathrm{cl}}\cot\theta - s - i\underbrace{\left(k + \frac{p_{\mathrm{cl}}}{\sin\theta}\right)}_{\equiv \mathsf{L}}\Big] \qquad \text{(C.3.16)} \\ &\quad = (-1)^n\sqrt{2\pi}\, e^{-(1-\cos\theta)\mathsf{L}^2/(2\cos\theta)} \tan^n\left(\frac{\theta}{2}\right) H_n\Big[s - r_{\mathrm{cl}}\cot\theta + i\mathsf{L}\Big]. \qquad \text{(C.3.17)}\end{aligned}$$

The penultimate line features the newly defined modified momentum $\mathsf{L} \equiv \mathsf{K}/\sin\theta$ and we use the parity relation (B.1.1) to arrive at the final solution. Upon substitution of the integral solution, the wavefunction reads

$$\begin{aligned}\phi_{n,k} = {} & \frac{\cos^{1/4}\theta}{\sqrt{\cos\theta(1+\cos\theta)2^{n+1}\pi^2 n!}} e^{-iE\lambda} e^{i\left(\lambda\cos\theta + r_{\mathrm{cl}}\cdot p_{\mathrm{cl}}\right)/2} \\ & \cdot e^{-iks\cos\theta}\, e^{-(s\sin\theta - r_{\mathrm{cl}}\cos\theta)^2/[2(1+\cos\theta)]}\, e^{-i\mathsf{L}(r_{\mathrm{cl}}/\sin\theta + s)/(1+\cos\theta)} \\ & \cdot (-1)^n\sqrt{2\pi}\, e^{-(k\sin\theta + p_{\mathrm{cl}})^2/[2\cos\theta(1+\cos\theta)]} \tan^n\left(\frac{\theta}{2}\right) H_n\Big[s - r_{\mathrm{cl}}\cot\theta + i\mathsf{L}\Big]\end{aligned} \tag{C.3.18}$$

$$\begin{aligned}= {} & \frac{(-1)^n\tan^n(\theta/2)}{\cos^{1/4}\theta\,\sqrt{(1+\cos\theta)2^n\pi n!}} e^{-iE\lambda} e^{i\left(\lambda\cos\theta + r_{\mathrm{cl}}\cdot p_{\mathrm{cl}}\right)/2} \\ & \cdot \exp\left[-is\left(k + p_{\mathrm{cl}}\underbrace{\frac{\sin\theta}{1+\cos\theta}}_{=\tan(\theta/2)}\right)\right] \cdot \exp\left[-i\frac{r_{\mathrm{cl}}(p_{\mathrm{cl}} + k\sin\theta)}{1+\cos\theta}\right]\end{aligned}$$

$$\cdot\, e^{-(1-\cos\theta)(s-r_{\mathrm{cl}}\cot\theta)^2/2}\, e^{-(k\sin\theta+p_{\mathrm{cl}})^2/[2\cos\theta(1+\cos\theta)]}\, H_n\Big[s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big]. \tag{C.3.19}$$

For a simplified form, we introduce the variables

$$\mathcal{N}_{n,k}(\lambda) \equiv \frac{(-1)^n \tan^n(\theta/2)}{\cos^{1/4}\theta\sqrt{(1+\cos\theta)2^n\pi n!}} \exp\left[-\frac{(k\sin\theta+p_{\mathrm{cl}}(\lambda))^2}{2\cos\theta(1+\cos\theta)}\right] \in \mathbb{R} \tag{C.3.20}$$

$$= -\frac{\tan(\theta/2)}{\sqrt{2n}}\mathcal{N}_{n-1,k}(\lambda), \tag{C.3.21}$$

$$\zeta(\lambda) \equiv \left(E-\frac{\cos\theta}{2}\right)\lambda - \frac{p_{\mathrm{cl}}(\lambda)r_{\mathrm{cl}}(\lambda)}{2} + \frac{\Big(k\sin\theta+p_{\mathrm{cl}}(\lambda)\Big)r_{\mathrm{cl}}(\lambda)}{1+\cos\theta} \in \mathbb{R} \tag{C.3.22}$$

and express the unnormalized system states as

$$\phi_{n,k}(s,\lambda) = \mathcal{N}_{n,k}(\lambda)\, e^{-i\zeta(\lambda)} \exp\left[-\frac{(1-\cos\theta)}{2}\big(s-r_{\mathrm{cl}}(\lambda)\cot\theta\big)^2\right]$$
$$\cdot \exp\left[-is\left(k+p_{\mathrm{cl}}(\lambda)\tan\frac{\theta}{2}\right)\right] H_n\Big[s-r_{\mathrm{cl}}(\lambda)\cot\theta+i\mathsf{L}(\lambda)\Big]. \tag{C.3.23}$$

In addition, we can use recurrence relation (B.1.2) to find

$$\phi_{n+1,k} = -\frac{2\tan(\theta/2)}{\sqrt{2(n+1)}}\mathcal{N}_{n,k}\, e^{-i\zeta}\, e^{-is\left(k+p_{\mathrm{cl}}\tan\frac{\theta}{2}\right)} e^{-\frac{(1-\cos\theta)}{2}\left(s-r_{\mathrm{cl}}\cot\theta\right)^2}$$
$$\cdot\left\{\Big(s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big)H_n\Big[s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big] - n\,H_{n-1}\Big[s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big]\right\} \tag{C.3.24}$$

$$= -\sqrt{\frac{2}{n+1}}\tan\left(\frac{\theta}{2}\right)\left[\Big(s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big)\phi_{n,k} + \sqrt{\frac{n}{2}}\tan\left(\frac{\theta}{2}\right)\phi_{n-1,k}\right] \tag{C.3.25}$$

$$= -\sqrt{\frac{2}{n+1}}\tan\left(\frac{\theta}{2}\right)\Big(s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big)\phi_{n,k} - \sqrt{\frac{n}{n+1}}\tan^2\left(\frac{\theta}{2}\right)\phi_{n-1,k} \tag{C.3.26}$$

or, expressed in state vector form,

$$\big|\phi_{n+1,k}\big\rangle_{\mathrm{S}} = -\sqrt{\frac{2}{n+1}}\tan\left(\frac{\theta}{2}\right)\Big(\hat{s}-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big)\big|\phi_{n,k}\big\rangle_{\mathrm{S}} - \sqrt{\frac{n}{n+1}}\tan^2\left(\frac{\theta}{2}\right)\big|\phi_{n-1,k}\big\rangle_{\mathrm{S}}\,. \tag{C.3.27}$$

For example, choosing $n=0$ yields

$$\big|\phi_{1,k}\big\rangle_{\mathrm{S}} = -\sqrt{2}\tan\left(\frac{\theta}{2}\right)\Big(\hat{s}-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\Big)\big|\phi_{0,k}\big\rangle_{\mathrm{S}}\,. \tag{C.3.28}$$

C.3.1 Mean position

An evaluation of the mean position for any $\big|\phi_{n,k}\big\rangle_{\mathrm{S}}$ leads to

$$\big\langle\phi_{n,k}\big|\,\hat{s}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}} \propto \int_{-\infty}^{\infty} \mathrm{d}s\, e^{-(1-\cos\theta)(s-r_{\mathrm{cl}}\cot\theta)^2}\, s\,|H_n(s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L})|^2 \tag{C.3.29}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}s\, e^{-(1-\cos\theta)s^2}\,(s+r_{\mathrm{cl}}\cot\theta)\,|H_n(s+i\mathsf{L})|^2 \tag{C.3.30}$$

$$\propto r_{\mathrm{cl}} \cot\theta \left\langle \phi_{n,k} \middle| \phi_{n,k} \right\rangle_{\mathrm{S}} + \ldots \underbrace{\int_{-\infty}^{\infty} \mathrm{d}s\, e^{-(1-\cos\theta)s^2}\, s\, |H_n(s+i\mathsf{L})|^2}_{=0} . \tag{C.3.31}$$

The antisymmetry of the integrand implies the vanishing of the last integral. Closer inspection of the result already shows that the system does not exhibit its natural frequency $\omega_s = \sin\theta$, but takes on the periodicity $\omega_r = \cos\theta$ of the clock through the classical trajectory $r_{\mathrm{cl}}(\lambda)$. Furthermore, the result does not depend on n or k.

C.3.2 Momentum operator

Another useful expression is the action of $\hat{p}_s$ on the unnormalized system states. Therefore, we calculate

$$\left\langle s \middle| \hat{p}_s \middle| \phi_{n,k} \right\rangle_{\mathrm{S}} = -i\partial_s \phi_{n,k} \tag{C.3.32}$$

$$= -i\partial_s \mathcal{N}_{n,k}\, e^{-i\zeta}\, e^{-(1-\cos\theta)(s-r_{\mathrm{cl}}\cot\theta)^2/2} e^{-is\mathsf{M}}\, H_n\Big[s - r_{\mathrm{cl}}\cot\theta + i\mathsf{L}\Big] \tag{C.3.33}$$

$$\begin{aligned} &= -\Big\{\mathsf{M} - i(1-\cos\theta)\big(s - r_{\mathrm{cl}}\cot\theta\big)\Big\}\phi_{n,k} \\ &\quad - i\mathcal{N}_{n,k}\, e^{-i\zeta}\, e^{-(1-\cos\theta)(s-r_{\mathrm{cl}}\cot\theta)^2/2} e^{-is\mathsf{M}} \cdot \underbrace{\partial_s H_n\Big[s - r_{\mathrm{cl}}\cot\theta + i\mathsf{L}\Big]}_{=2nH_{n-1}\left[s-r_{\mathrm{cl}}\cot\theta+i\mathsf{L}\right]} \end{aligned} \tag{C.3.34}$$

$$= -\Big\{\mathsf{M} - i(1-\cos\theta)\big(s - r_{\mathrm{cl}}\cot\theta\big)\Big\}\phi_{n,k} + i\sqrt{2n}\tan\left(\frac{\theta}{2}\right)\phi_{n-1,k}\,, \tag{C.3.35}$$

which reads

$$\hat{p}_s \left|\phi_{n,k}\right\rangle_{\mathrm{S}} = -\Big\{\mathsf{M} - i(1-\cos\theta)\big(\hat{s} - r_{\mathrm{cl}}\cot\theta\big)\Big\}\left|\phi_{n,k}\right\rangle_{\mathrm{S}} + i\sqrt{2n}\tan\left(\frac{\theta}{2}\right)\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}} \tag{C.3.36}$$

in bra-ket notation.

C.3.3 Normalization factor

In order to obtain the *normalized* system state

$$\left|\varphi_{n,k}\right\rangle_{\mathrm{S}} = \frac{\left\langle \chi \middle| \Psi_{n,k} \right\rangle_{\mathrm{C}}}{\sqrt{\left\langle \Psi_{n,k} \middle| \chi \right\rangle\!\left\langle \chi \middle| \Psi_{n,k} \right\rangle}} = \frac{\left|\phi_{n,k}\right\rangle_{\mathrm{S}}}{\sqrt{\left\langle \phi_{n,k} \middle| \phi_{n,k} \right\rangle_{\mathrm{S}}}}, \tag{C.3.37}$$

one needs to evaluate the norm

$$\left\langle \phi_{n,k} \middle| \phi_{n,k} \right\rangle_{\mathrm{S}} = \int_{-\infty}^{\infty} \mathrm{d}s \left|\phi_{n,k}(s)\right|^2 \tag{C.3.38}$$

$$= \mathcal{N}_{n,k}^2 \int_{-\infty}^{\infty} \mathrm{d}s\, e^{-(1-\cos\theta)(s-r_{\mathrm{cl}}\cot\theta)^2} |H_n(s - r_{\mathrm{cl}}\cot\theta + i\mathsf{L})|^2 \tag{C.3.39}$$

$$\overset{s-r_{\mathrm{cl}}\cot\theta\to s}{=} \mathcal{N}_{n,k}^2 \int_{-\infty}^{\infty} \mathrm{d}s\, e^{-(1-\cos\theta)s^2} |H_n(s+i\mathsf{L})|^2 \tag{C.3.40}$$

$$\equiv \mathcal{N}_{n,k}^2 \int_{-\infty}^{\infty} \mathrm{d}s\, e^{-us^2} H_n(s+i\mathsf{L})\, H_n(s-i\mathsf{L})\,. \tag{C.3.41}$$

Here, the auxiliary variable is defined as $u \equiv 1-\cos\theta$. Before providing a general derivation, we give two exemplary solutions. The system norm reads

$$\langle \phi_{0,k} | \phi_{0,k} \rangle_S = \mathcal{N}_{0,k}^2 \sqrt{\frac{\pi}{u}} = \mathcal{N}_{0,k}^2 \sqrt{\frac{\pi}{1-\cos\theta}} \tag{C.3.42}$$

for $n = 0$, while $n = 1$ yields

$$\langle \phi_{1,k} | \phi_{1,k} \rangle_S = 2\mathcal{N}_{1,k}^2 \frac{\sqrt{\pi}}{u^{3/2}} \left(2\mathrm{L}^2 u + 1\right) = \mathcal{N}_{1,k}^2 \sqrt{\frac{\pi}{u}} \left((2\mathrm{L})^2 + \frac{2}{u}\right) \tag{C.3.43}$$

$$= \sqrt{\frac{\pi}{1-\cos\theta}} \mathcal{N}_{1,k}^2 \left((2\mathrm{L})^2 + \frac{2}{1-\cos\theta}\right) \tag{C.3.44}$$

$$= \underbrace{\frac{\mathcal{N}_{1,k}^2}{\mathcal{N}_{0,k}^2}}_{=\tan^2(\theta/2)/2} \langle \phi_{0,k} | \phi_{0,k} \rangle_S \left((2\mathrm{L})^2 + \frac{2}{1-\cos\theta}\right) \tag{C.3.45}$$

$$= \langle \phi_{0,k} | \phi_{0,k} \rangle_S \frac{(2\mathrm{L})^2(1-\cos\theta)+2}{2(1+\cos\theta)} . \tag{C.3.46}$$

Using the Taylor expansion (B.1.3) for

$$H_n(s \pm i\mathrm{L}) = \sum_{m=0}^{n} \binom{n}{m} H_m(s) (\pm 2i\mathrm{L})^{n-m} , \tag{C.3.47}$$

allows us to express the norm as

$$\langle \phi_{n,k} | \phi_{n,k} \rangle_S = \mathcal{N}_{n,k}^2 \sum_{l,m=0}^{n} \binom{n}{m} \binom{n}{l} (2i\mathrm{L})^{n-m} (-2iL)^{n-l} \int_{-\infty}^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) \tag{C.3.48}$$

$$= \mathcal{N}_{n,k}^2 \sum_{l,m=0}^{n} \binom{n}{m} \binom{n}{l} (2L)^{2n-(l+m)} i^{l-m} \underbrace{\int_{-\infty}^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s)}_{\equiv F_{l,m}} . \tag{C.3.49}$$

A further examination requires the evaluation of the integral $F_{l,m}$, which is symmetric, i.e. $F_{l,m} = F_{m,l}$. First, we use the symmetry property of the integrand under parity transformations to show

$$F_{l,m} = \int_0^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) + \int_{-\infty}^{0} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) \tag{C.3.50}$$

$$\overset{\text{Eq. (B.1.1)}}{=} \int_0^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) + \int_0^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(-s) H_l(-s) \tag{C.3.51}$$

$$= \int_0^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) + (-1)^{l+m} \int_0^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) \tag{C.3.52}$$

$$= \left[1 + (-1)^{l+m}\right] \int_0^{\infty} \mathrm{d}s\, e^{-u^2 s^2} H_m(s) H_l(s) \tag{C.3.53}$$

$$= \begin{cases} F_{l,m}, & \text{for } l+m \text{ even} \\ 0, & \text{for } l+m \text{ odd} \end{cases} . \tag{C.3.54}$$

For the case of $m+l$ being even, the result of the integral is given by Eq. (B.1.8) and reads

$$F_{l,m} = \frac{2^{m+n}}{\sqrt{u}}\,\Gamma\!\left(\frac{m+n+1}{2}\right)\cdot\sqrt{\frac{1-u}{u}}^{n+m}\cdot{}_2F_1\!\left(-m,-n;\frac{1-n-m}{2};\frac{u}{2(u-1)}\right) \tag{C.3.55}$$

$$= \frac{2^{m+n}}{\sqrt{1-\cos\theta}}\,\Gamma\!\left(\frac{m+n+1}{2}\right)\cdot\sqrt{\frac{\cos\theta}{1-\cos\theta}}^{n+m} \cdot{}_2F_1\!\left(-m,-n;\frac{1-n-m}{2};\frac{\cos\theta-1}{2\cos\theta}\right). \tag{C.3.56}$$

Finally, the norm becomes

$$\left\langle\phi_{n,k}\middle|\phi_{n,k}\right\rangle_{\mathrm{S}} = \mathcal{N}_{n,k}^2 \sum_{\substack{l,m=0\\ l+m\,\text{even}}}^{n}\binom{n}{m}\binom{n}{l}(2L)^{2n-(l+m)}\,i^{l-m}\,F_{l,m} \tag{C.3.57}$$

$$= \frac{\mathcal{N}_{n,k}^2}{\sqrt{1-\cos\theta}} \sum_{\substack{l,m=0\\ l+m\,\text{even}}}^{n}\binom{n}{m}\binom{n}{l}(2\mathrm{L})^{2n-(l+m)}\,i^{l-m}\,2^{m+l}\,\Gamma\!\left(\frac{m+l+1}{2}\right) \cdot\sqrt{\frac{\cos\theta}{1-\cos\theta}}^{l+m}\,{}_2F_1\!\left(-m,-l;\frac{1-l-m}{2};\frac{\cos\theta-1}{2\cos\theta}\right) \tag{C.3.58}$$

with the prefactor

$$\mathcal{N}_{n,k}^2 = \frac{\tan^{2n}(\theta/2)}{2^n\pi n!(1+\cos\theta)\sqrt{\cos\theta}}\,e^{-(k\sin\theta+p_{\mathrm{cl}})^2/[\cos\theta(1+\cos\theta)]} \tag{C.3.59}$$

$$= \frac{\tan^2(\theta/2)}{2n}\,\mathcal{N}_{n-1,k}^2 = \frac{\tan^{2n}(\theta/2)}{2^n n!}\,\mathcal{N}_{0,k}^2\,. \tag{C.3.60}$$

In the main text, we consider the example $n=1$ and, therefore, give the explicit expression

$$\mathcal{N}_{1,k}^2 = \frac{\tan^2(\theta/2)}{2\pi(1+\cos\theta)\sqrt{\cos\theta}}\,e^{-(k\sin\theta+p_{\mathrm{cl}})^2/[\cos\theta(1+\cos\theta)]}\,. \tag{C.3.61}$$

For later use, we also provide

$$\left\langle\phi_{0,k}\middle|\phi_{0,k}\right\rangle_{\mathrm{S}} = \mathcal{N}_{0,k}^2\sqrt{\frac{\pi}{1-\cos\theta}}\cdot\underbrace{{}_2F_1\!\left(0,0;\frac{1}{2};\frac{\cos\theta-1}{2\cos\theta}\right)}_{=1} \tag{C.3.62}$$

for $n=0$ and

$$\left\langle\phi_{1,k}\middle|\phi_{1,k}\right\rangle_{\mathrm{S}} = \frac{\mathcal{N}_{1,k}^2}{\sqrt{1-\cos\theta}} \sum_{\substack{l,m=0\\ l+m\,\text{even}}}^{1}\binom{1}{m}\binom{1}{l}(2\mathrm{L})^{2-(l+m)}\,2^{m+l}\,\Gamma\!\left(\frac{m+l+1}{2}\right) \cdot\sqrt{\frac{\cos\theta}{1-\cos\theta}}^{l+m}\,{}_2F_1\!\left(-m,l;\frac{1-l-m}{2};\frac{\cos\theta-1}{2\cos\theta}\right) \tag{C.3.63}$$

$$= \frac{\mathcal{N}_{1,k}^2}{\sqrt{1-\cos\theta}}\Bigg[\sqrt{\pi}(2\mathrm{L})^2\underbrace{{}_2F_1\!\left(0,0;\frac{1}{2};\frac{\cos\theta-1}{2\cos\theta}\right)}_{=1} + 2\sqrt{\pi}\frac{\cos\theta}{1-\cos\theta}\cdot\underbrace{{}_2F_1\!\left(-1,-1;-\frac{1}{2};\frac{\cos\theta-1}{2\cos\theta}\right)}_{=1/\cos\theta}\Bigg] \tag{C.3.64}$$

$$= \mathcal{N}_{1,k}^2\sqrt{\frac{\pi}{1-\cos\theta}}\left[(2\mathrm{L})^2+\frac{2}{1-\cos\theta}\right] \tag{C.3.65}$$

for $n=1$ with the specific hypergeometric function ${}_2F_1(-1,-1;-1/2;x)=1-2x$.

C.3.4 Normalized state

Using the derived norm expression from above, one can express the normalized system states

$$\varphi_{n,k}(s) = \frac{\langle s|\phi_{n,k}\rangle_S}{\sqrt{\langle\phi_{n,k}|\phi_{n,k}\rangle_S}} \tag{C.3.66}$$

in full generality. However, the expressions are bulky and we provide only the two cases $n=0$ and $n=1$, for which we find

$$\varphi_{0,k}(s) = \left(\frac{1-\cos\theta}{\pi}\right)^{1/4} e^{-i\zeta}\, e^{-(1-\cos\theta)(s-r_{\rm cl}\cot\theta)^2/2}\, e^{-is[k+p_{\rm cl}\tan(\theta/2)]} \tag{C.3.67}$$

and

$$\varphi_{1,k}(s) = -\left(\frac{1-\cos\theta}{\pi}\right)^{1/4} e^{-i\zeta}\, e^{-(1-\cos\theta)(s-r_{\rm cl}\cot\theta)^2/2}\, e^{-is[k+p_{\rm cl}\tan(\theta/2)]} \cdot \frac{\sqrt{2(1-\cos\theta)}\left[s-r_{\rm cl}\cot\theta+i\mathsf{L}\right]}{\sqrt{2\mathsf{L}^2(1-\cos\theta)+1}}. \tag{C.3.68}$$

Both states are related by

$$\left|\varphi_{1,k}\right\rangle_S = -\sqrt{2}\sqrt{\frac{\langle\phi_{0,k}|\phi_{0,k}\rangle_S}{\langle\phi_{1,k}|\phi_{1,k}\rangle_S}}\tan\left(\frac{\theta}{2}\right)\left(\hat{s}-r_{\rm cl}\cot\theta+i\mathsf{L}\right)\left|\varphi_{0,k}\right\rangle_S \tag{C.3.69}$$

$$= -\sqrt{\frac{2(1-\cos\theta)}{2\mathsf{L}^2(1-\cos\theta)+1}}\left(\hat{s}-r_{\rm cl}\cot\theta+i\mathsf{L}\right)\left|\varphi_{0,k}\right\rangle_S. \tag{C.3.70}$$

and, thus, the $n=1$ pure state density reads

$$\left|\varphi_{1,k}\right\rangle\!\left\langle\varphi_{1,k}\right|_S = \frac{2(1-\cos\theta)}{2\mathsf{L}^2(1-\cos\theta)+1}\left(\hat{s}-r_{\rm cl}\cot\theta+i\mathsf{L}\right)\left|\varphi_{0,k}\right\rangle\!\left\langle\varphi_{0,k}\right|_S\left(\hat{s}-r_{\rm cl}\cot\theta-i\mathsf{L}\right). \tag{C.3.71}$$

C.3.5 Effective system potential

As mentioned in the main text, we only consider the case $|\Psi\rangle = \left|\Psi_{n,k}\right\rangle$ for simplicity, but superpositions of different $\left|\Psi_{n,k}\right\rangle$ allow for analytical calculations as well. The effective system potential features the term

$$\langle\chi|\hat{V}\hat{P}_\Psi|\chi\rangle_C = \underbrace{-\frac{\sin(2\theta)}{2}}_{=-\sin\theta\cos\theta}\hat{s}\,\langle\chi|\hat{r}\hat{P}_\Psi|\chi\rangle_C \tag{C.3.72}$$

and its Hermitian conjugate $\langle\chi|\hat{P}_\Psi\hat{V}|\chi\rangle_C$. Specifically, one needs to determine

$$\sin(2\theta)\left\langle s\otimes r\middle|\hat{r}\middle|\Psi_{n,k}\right\rangle \propto \frac{r\sin(2\theta)}{\sqrt{2^{n+1}n!}}H_n\left(r\cos\theta-s\sin\theta\right) \tag{C.3.73}$$

$$= \frac{2\sin\theta\cos\theta}{\sqrt{2^{n+1}n!}\cos\theta}\left(r\cos\theta-s\sin\theta+s\sin\theta\right)H_n\left(r\cos\theta-s\sin\theta\right). \tag{C.3.74}$$

Using the recurrence relation (B.1.2) helps us to express the term from above as

$$\sin(2\theta)\left\langle s\otimes r\middle|\hat{r}\middle|\Psi_{n,k}\right\rangle \propto \frac{2\sin\theta}{\sqrt{2^{n+1}n!}}\left[\frac{1}{2}H_{n+1}\left(r\cos\theta-s\sin\theta\right)+nH_{n-1}\left(r\cos\theta-s\sin\theta\right)\right]$$

$$+\frac{2s\sin^2\theta}{\sqrt{2^{n+1}n!}}\cdot H_n\big(r\cos\theta-s\sin\theta\big) \tag{C.3.75}$$

$$=\sin\theta\Bigg[\frac{\sqrt{2(n+1)}}{\sqrt{2^{n+2}(n+1)!}}H_{n+1}\big(r\cos\theta-s\sin\theta\big) +\frac{\sqrt{2n}}{\sqrt{2^n(n-1)!}}H_{n-1}\big(r\cos\theta-s\sin\theta\big)\Bigg] +\frac{2s\sin^2\theta}{\sqrt{2^{n+1}n!}}\cdot H_n\big(r\cos\theta-s\sin\theta\big) \tag{C.3.76}$$

and it follows that

$$\sin(2\theta)\left\langle s\otimes r\middle|\hat{r}\middle|\Psi_{n,k}\right\rangle=\sqrt{2(n+1)}\sin\theta\,\Psi_{n+1,k}(r,s)+\sqrt{2n}\sin\theta\,\Psi_{n-1,k}(r,s) +2s\sin^2\theta\,\Psi_{n,k}(r,s)\,. \tag{C.3.77}$$

Utilizing this result in the bra-ket notation

$$\sin(2\theta)\,\hat{r}\left|\Psi_{n,k}\right\rangle=\sqrt{2(n+1)}\sin\theta\,\left|\Psi_{n+1,k}\right\rangle+\sqrt{2n}\sin\theta\,\left|\Psi_{n-1,k}\right\rangle+2\sin^2\theta\,\hat{s}\,\left|\Psi_{n,k}\right\rangle\,, \tag{C.3.78}$$

we find the essential term

$$\left\langle\chi\middle|\hat{V}\middle|\Psi_{n,k}\right\rangle_{\mathrm{C}}=-\frac{\sin(2\theta)}{2}\,\hat{s}\left\langle\chi\middle|\hat{r}\middle|\Psi_{n,k}\right\rangle_{\mathrm{C}} \tag{C.3.79}$$

$$=-\sqrt{\frac{(n+1)}{2}}\big(\sin\theta\,\hat{s}\big)\left|\phi_{n+1,k}\right\rangle_{\mathrm{S}}-\sqrt{\frac{n}{2}}\big(\sin\theta\,\hat{s}\big)\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}} -\big(\sin\theta\,\hat{s}\big)^2\left|\phi_{n,k}\right\rangle_{\mathrm{S}}\,. \tag{C.3.80}$$

Instead of using three different system states, we use the recurrence relation (C.3.27) to express one of them in terms of the other two, i.e.,

$$-\sqrt{\frac{(n+1)}{2}}\big(\sin\theta\,\hat{s}\big)\left|\phi_{n+1,k}\right\rangle_{\mathrm{S}}=(1-\cos\theta)\Big\{\hat{s}\big(\hat{s}-r_{\mathrm{cl}}\cot\theta+i\mathrm{L}\big)\left|\phi_{n,k}\right\rangle_{\mathrm{S}} +\sqrt{\frac{n}{2}}\tan\frac{\theta}{2}\,\hat{s}\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}}\Big\}\,. \tag{C.3.81}$$

It reduces the previous expression to a form with only two system states, namely

$$\left\langle\chi\middle|\hat{V}\middle|\Psi_{n,k}\right\rangle_{\mathrm{C}}=-\sqrt{\frac{n}{2}}\sin\theta\,\hat{s}\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}}-\sin^2\theta\,\hat{s}^2\left|\phi_{n,k}\right\rangle_{\mathrm{S}} +\sin\theta\,\hat{s}\Big\{\tan\Big(\frac{\theta}{2}\Big)\big(\hat{s}-r_{\mathrm{cl}}\cot\theta+i\mathrm{L}\big)\left|\phi_{n,k}\right\rangle_{\mathrm{S}} +\sqrt{\frac{n}{2}}\tan^2\Big(\frac{\theta}{2}\Big)\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}}\Big\} \tag{C.3.82}$$

$$=-\underbrace{\Big\{1-\tan^2\Big(\frac{\theta}{2}\Big)\Big\}\sin\theta}_{=2\cot\theta(1-\cos\theta)}\sqrt{\frac{n}{2}}\,\hat{s}\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}} -\Big\{\underbrace{\sin^2\theta}_{=1-\cos^2\theta}\,\hat{s}^2-\underbrace{\tan\Big(\frac{\theta}{2}\Big)\sin\theta}_{=1-\cos\theta}\,\hat{s}\big(\hat{s}-r_{\mathrm{cl}}\cot\theta+i\mathrm{L}\big)\Big\}\left|\phi_{n,k}\right\rangle_{\mathrm{S}} \tag{C.3.83}$$

$$=-\sqrt{2n}\cot\theta(1-\cos\theta)\,\hat{s}\left|\phi_{n-1,k}\right\rangle_{\mathrm{S}}$$

$$-(1-\cos\theta)\Big\{\cos\theta\,\hat{s}^2+\big(r_{\mathrm{cl}}\cot\theta-i\mathsf{L}\big)\hat{s}\Big\}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}} \tag{C.3.84}$$

$$=-(1-\cos\theta)\Big[\Big\{\cos\theta\,\hat{s}^2+\big(r_{\mathrm{cl}}\cot\theta-i\mathsf{L}\big)\hat{s}\Big\}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}} + \sqrt{2n}\cot\theta\,\hat{s}\,\big|\phi_{n-1,k}\big\rangle_{\mathrm{S}}\Big] \tag{C.3.85}$$

$$=-(1-\cos\theta)\hat{s}\Big[\Big\{\cos\theta\,\hat{s}+r_{\mathrm{cl}}\cot\theta-i\mathsf{L}\Big\}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}}+\sqrt{2n}\cot\theta\,\big|\phi_{n-1,k}\big\rangle_{\mathrm{S}}\Big] \tag{C.3.86}$$

$$=-\underbrace{(1-\cos\theta)\cot\theta}_{=\tan(\theta/2)\cos\theta}\,\hat{s}\Big[\Big\{\sin\theta\,\hat{s}+r_{\mathrm{cl}}-i\mathsf{L}\tan\theta\Big\}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}}+\sqrt{2n}\,\big|\phi_{n-1,k}\big\rangle_{\mathrm{S}}\Big]. \tag{C.3.87}$$

Moreover, another useful form exists for the term $\big\langle\chi\big|\hat{V}\big|\Psi_{n,k}\big\rangle_{\mathrm{C}}$ and is based on the momentum operator relation

$$\Big[r_{\mathrm{cl}}\cos\theta-i\frac{\sin\theta}{1-\cos\theta}(\hat{p}_s+\mathsf{M})\Big]\big|\phi_{n,k}\big\rangle_{\mathrm{S}}=\sin\theta\,\hat{s}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}}+\sqrt{2n}\,\big|\phi_{n-1,k}\big\rangle_{\mathrm{S}}\,, \tag{C.3.88}$$

which is given in Section C.3.2. Thus, the crucial term for the effective system potential also reads

$$\big\langle\chi\big|\hat{V}\big|\Psi_{n,k}\big\rangle_{\mathrm{C}}=-(1-\cos\theta)\cot\theta\,\hat{s}\Big[\frac{-i\sin\theta}{1-\cos\theta}(\hat{p}_s+\mathsf{M})\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}} + \Big\{r_{\mathrm{cl}}(1+\cos\theta)-i\mathsf{L}\tan\theta\Big\}\,\big|\phi_{n,k}\big\rangle_{\mathrm{S}}\Big] \tag{C.3.89}$$

$$=-\hat{s}\Big[-i\cos\theta(\hat{p}_s+\mathsf{M})+\Big\{r_{\mathrm{cl}}\sin\theta\cos\theta-i\mathsf{L}(1-\cos\theta)\Big\}\Big]\big|\phi_{n,k}\big\rangle_{\mathrm{S}} \tag{C.3.90}$$

$$=-\hat{s}\Big[r_{\mathrm{cl}}\sin\theta\cos\theta-i\Big\{\cos\theta(\hat{p}_s+\mathsf{M})+\mathsf{L}(1-\cos\theta)\Big\}\Big]\big|\phi_{n,k}\big\rangle_{\mathrm{S}} \tag{C.3.91}$$

$$=\Big[\underbrace{-\hat{s}\,r_{\mathrm{cl}}\frac{\sin(2\theta)}{2}}_{=\langle\chi|\hat{V}|\chi\rangle_{\mathrm{C}}}+i\,\hat{s}\Big\{\cos\theta\,\hat{p}_s+k+p_{\mathrm{cl}}\sin\theta\Big\}\Big]\big|\phi_{n,k}\big\rangle_{\mathrm{S}}\,. \tag{C.3.92}$$

Interestingly, we are able to find a formulation in which $\langle\chi|\hat{V}|\chi\rangle_{\mathrm{C}}$ appears as part of the effective system potential. Employing the alternative form (C.3.92), the additional scalar $\mathrm{Re}\,a$ in the effective potential can be efficiently calculated to yield

$$\mathrm{Re}\,a=\mathrm{Re}\left\{\frac{\big\langle\Psi_{n,k}\big|\hat{V}\hat{P}_\chi\big|\Psi_{n,k}\big\rangle}{\big\langle\Psi_{n,k}\big|\hat{P}_\chi\big|\Psi_{n,k}\big\rangle}\right\}=\mathrm{Re}\left\{\frac{\big\langle\Psi_{n,k}\big|\hat{P}_\chi\hat{V}\big|\Psi_{n,k}\big\rangle}{\big\langle\Psi_{n,k}\big|\hat{P}_\chi\big|\Psi_{n,k}\big\rangle}\right\} \tag{C.3.93}$$

$$=\frac{1}{\big\langle\phi_{n,k}\big|\phi_{n,k}\big\rangle_{\mathrm{S}}}\mathrm{Re}\Big\{-r_{\mathrm{cl}}\frac{\sin(2\theta)}{2}\big\langle\phi_{n,k}\big|\hat{s}\big|\phi_{n,k}\big\rangle_{\mathrm{S}}+\underbrace{i(k+p_{\mathrm{cl}}\sin\theta)\big\langle\phi_{n,k}\big|\hat{s}\big|\phi_{n,k}\big\rangle_{\mathrm{S}}}_{\in i\mathbb{R}} + i\cos\theta\,\big\langle\phi_{n,k}\big|\hat{s}\hat{p}_s\big|\phi_{n,k}\big\rangle_{\mathrm{S}}\Big\} \tag{C.3.94}$$

$$=\frac{1}{\big\langle\phi_{n,k}\big|\phi_{n,k}\big\rangle_{\mathrm{S}}}\mathrm{Re}\Big\{-r_{\mathrm{cl}}\frac{\sin(2\theta)}{2}\big\langle\phi_{n,k}\big|\hat{s}\big|\phi_{n,k}\big\rangle_{\mathrm{S}}+\frac{i}{2}\cos\theta\,\big\langle\phi_{n,k}\big|\underbrace{\big(\hat{s}\hat{p}_s-\hat{p}_s\hat{s}\big)}_{=i}\big|\phi_{n,k}\big\rangle_{\mathrm{S}}\Big\} \tag{C.3.95}$$

$$= -r_{\mathrm{cl}} \frac{\sin(2\theta)}{2} \underbrace{\langle \varphi_{n,k} | \hat{s} | \varphi_{n,k} \rangle_{\mathrm{S}}}_{= r_{\mathrm{cl}} \cot\theta} - \frac{\cos\theta}{2} \tag{C.3.96}$$

$$= -r_{\mathrm{cl}}^2 \cos^2\theta - \frac{\cos\theta}{2} \tag{C.3.97}$$

regardless of the values of n and k. Substituting the aforementioned results into the general form (3.1.48) for the effective system potential leads to

$$\hat{V}_{\mathrm{S}} = -r_{\mathrm{cl}} \frac{\sin(2\theta)}{2} \left(\hat{P}_\varphi \hat{s} + \hat{s} \hat{P}_\varphi \right) + \left(r_{\mathrm{cl}}^2 \cos^2\theta + \frac{\cos\theta}{2} \right) + i \left[\hat{s} \Big(\cos\theta \hat{p}_s + k + p_{\mathrm{cl}} \sin\theta \Big) \hat{P}_\varphi - \hat{P}_\varphi \Big(\cos\theta \hat{p}_s + k + p_{\mathrm{cl}} \sin\theta \Big) \hat{s} \right] \tag{C.3.98}$$

or

$$\hat{V}_{\mathrm{S}} = -r_{\mathrm{cl}} \frac{\sin(2\theta)}{2} \left(\hat{P}_\varphi \hat{s} + \hat{s} \hat{P}_\varphi \right) + \left(r_{\mathrm{cl}}^2 \cos^2\theta + \frac{\cos\theta}{2} \right) - \cos\theta \hat{P}_\varphi + i \left[\hat{s} \Big(\cos\theta \hat{p}_s + k + p_{\mathrm{cl}} \sin\theta \Big), \hat{P}_\varphi \right] \tag{C.3.99}$$

$$= -r_{\mathrm{cl}} \frac{\sin(2\theta)}{2} \left(\hat{P}_\varphi \hat{s} + \hat{s} \hat{P}_\varphi \right) + \left(r_{\mathrm{cl}}^2 \cos^2\theta + \frac{\cos\theta}{2} \right) - \cos\theta \hat{P}_\varphi + i \Big(k + p_{\mathrm{cl}} \sin\theta \Big) \Big[\hat{s}, \hat{P}_\varphi \Big] + \frac{i}{2} \cos\theta \Big[\big(\hat{s} \hat{p}_s + \hat{p}_s \hat{s} \big), \hat{P}_\varphi \Big] \tag{C.3.100}$$

with $\big[\hat{s}, \big(\cos\theta \hat{p}_s + k + p_{\mathrm{cl}} \sin\theta \big) \big] = i \cos\theta$. Applied to the system state, we find

$$\hat{V}_{\mathrm{S}} | \varphi_{n,k} \rangle_{\mathrm{S}} = \left\{ - r_{\mathrm{cl}} \frac{\sin(2\theta)}{2} \hat{s} - \frac{\cos\theta}{2} + i \Big(k + p_{\mathrm{cl}} \sin\theta \Big) \Big[\hat{s}, \hat{P}_\varphi \Big] + i \cos\theta \Big[\big(\hat{s} \hat{p}_s + \hat{p}_s \hat{s} \big), \hat{P}_\varphi \Big] \right\} | \varphi_{n,k} \rangle_{\mathrm{S}} \,, \tag{C.3.101}$$

expressed in a way that preserves Hermiticity.
Without the use of the momentum operator, the effective system potential reads

$$\hat{V}_{\mathrm{S}} = -\tan\frac{\theta}{2} \cos\theta \left[\hat{s} \Big(\sin\theta \hat{s} + r_{\mathrm{cl}} - i\mathsf{L} \tan\theta \Big) \hat{P}_\varphi + \hat{P}_\varphi \Big(\sin\theta \hat{s} + r_{\mathrm{cl}} + i\mathsf{L} \tan\theta \Big) \hat{s} + \sqrt{2n} \left\{ \hat{s} \frac{| \phi_{n-1,k} \rangle\langle \phi_{n,k} |_{\mathrm{S}}}{\langle \phi_{n,k} | \phi_{n,k} \rangle_{\mathrm{S}}} + \frac{| \phi_{n,k} \rangle\langle \phi_{n-1,k} |_{\mathrm{S}}}{\langle \phi_{n,k} | \phi_{n,k} \rangle_{\mathrm{S}}} \hat{s} \right\} \right] - \mathrm{Re}\, a \,. \tag{C.3.102}$$

In particular, the main text features the case $n = 1$, for which we find

$$\langle \chi | \hat{V} \hat{P}_\Psi | \chi \rangle_{\mathrm{C}} = 2 \tan^2\left(\frac{\theta}{2} \right) \hat{s} \Big[\cos\theta - (1 - \cos\theta) \Big(\cos\theta \hat{s} + r_{\mathrm{cl}} \cot\theta - i\mathsf{L} \Big) \cdot \Big(\hat{s} - r_{\mathrm{cl}} \cot\theta + i\mathsf{L} \Big) \Big] | \phi_{0,k} \rangle\langle \phi_{0,k} |_{\mathrm{S}} \Big(\hat{s} - r_{\mathrm{cl}} \cot\theta - i\mathsf{L} \Big) \tag{C.3.103}$$

with the recurrence relation (C.3.27). This term allows us to obtain the position representation

$$\langle s | \hat{V}_{\mathrm{S}} | s' \rangle_{\mathrm{S}} = \frac{\langle s, \chi | \{ \hat{V}, \hat{P}_\Psi \} | s', \chi \rangle}{\langle \phi_{1,k} | \phi_{1,k} \rangle_{\mathrm{S}}} - \mathrm{Re}\, a \delta(s - s') \tag{C.3.104}$$

$$= \underbrace{2\tan^2\left(\frac{\theta}{2}\right)\frac{\langle\phi_{0,k}|\phi_{0,k}\rangle_S}{\langle\phi_{1,k}|\phi_{1,k}\rangle_S}}_{=(1-\cos\theta)/[2L^2(1-\cos\theta)+1]}\langle s|\hat{P}_{\varphi_0}|s'\rangle_S$$
$$\cdot\Big\{s\Big[\cos\theta-(1-\cos\theta)\Big(\cos\theta\, s+r_{cl}\cot\theta-iL\Big)\Big(s-r_{cl}\cot\theta+iL\Big)\Big]$$
$$\cdot\Big(s'-r_{cl}\cot\theta-iL\Big)+\Big(s-r_{cl}\cot\theta+iL\Big)s'\Big[\cos\theta-(1-\cos\theta)$$
$$\cdot\Big(\cos\theta\, s'+r_{cl}\cot\theta+iL\Big)\Big(s'-r_{cl}\cot\theta-iL\Big)\Big]\Big\}-\mathrm{Re}\,a\delta(s-s') \quad \text{(C.3.105)}$$

$$= \frac{2(1-\cos\theta)}{2L^2(1-\cos\theta)+1}\langle s|\hat{P}_{\varphi_0}|s'\rangle_S\Big\{\cos\theta\Big[2ss'-r_{cl}\cot\theta(s+s')-iL(s-s')\Big]$$
$$-(1-\cos\theta)\Big[s\Big(\cos\theta\, s+r_{cl}\cot\theta-iL\Big)\Big(s-r_{cl}\cot\theta+iL\Big)$$
$$\cdot\Big(s'-r_{cl}\cot\theta-iL\Big)$$
$$+\Big(s-r_{cl}\cot\theta+iL\Big)s'\Big(\cos\theta\, s'+r_{cl}\cot\theta+iL\Big)\Big(s'-r_{cl}\cot\theta-iL\Big)\Big]\Big\}$$
$$-\mathrm{Re}\,a\delta(s-s') \quad \text{(C.3.106)}$$

$$= \frac{2(1-\cos\theta)}{2L^2(1-\cos\theta)+1}\langle s|\hat{P}_{\varphi_0}|s'\rangle_S\Big\{\cos\theta\Big[2ss'-r_{cl}\cot\theta(s+s')-iL(s-s')\Big]$$
$$-(1-\cos\theta)\Big(s-r_{cl}\cot\theta+iL\Big)\Big(s'-r_{cl}\cot\theta-iL\Big)\Big[\cos\theta\,(s^2+s'^2)$$
$$+r_{cl}\cot\theta(s+s')-iL(s-s')\Big]\Big\}-\mathrm{Re}\,a\delta(s-s') \quad \text{(C.3.107)}$$

of $\hat{V}_S$. As a last step, we use the $n=0$ projector

$$\langle s|\hat{P}_{\varphi_0}|s'\rangle_S = \sqrt{\frac{1-\cos\theta}{\pi}}e^{-(1-\cos\theta)\Big[(s-r_{cl}\cot\theta)^2+(s'-r_{cl}\cot\theta)^2\Big]/2}e^{-i(s-s')M} \quad \text{(C.3.108)}$$

in position basis in order to derive the final expression

$$\langle s|\hat{V}_S|s'\rangle_S = \frac{2\sqrt{1-\cos\theta}^3}{\sqrt{\pi}(2L^2(1-\cos\theta)+1)}e^{-(1-\cos\theta)\Big[(s-r_{cl}\cot\theta)^2+(s'-r_{cl}\cot\theta)^2\Big]/2}e^{-i(s-s')M}$$
$$\cdot\Big\{\cos\theta\Big[2ss'-r_{cl}\cot\theta(s+s')-iL(s-s')\Big]-(1-\cos\theta)$$
$$\cdot\Big(s-r_{cl}\cot\theta+iL\Big)\Big(s'-r_{cl}\cot\theta-iL\Big)\Big[\cos\theta\,(s^2+s'^2)$$
$$+r_{cl}\cot\theta(s+s')-iL(s-s')\Big]\Big\}-\mathrm{Re}\,a\delta(s-s')\,. \quad \text{(C.3.109)}$$

Appendix D

Atomic units

For a simplification of the analytical treatment of problems in atomic and molecular physics, atomic units are often employed. They are based on setting the important typical scales to unity and, therefore, provide means for dimensionless numerical calculations. A list of the essential constants is shown in Table D.1.

Quantity	Atomic units	SI units
Bohr radius a_0	1	5.29×10^{-11} m
Reduced Planck's constant $\hbar$	1	1.06×10^{-34} J
Electron mass m_e a_0	1	9.10×10^{-31} kg
Electric charge $\|e\|$	1	1.60×10^{-16} C
Vacuum permittivity ϵ_0	$1/4\pi$	8.85×10^{-12} F/m
Vacuum speed of light c_{light}	137.0	3×10^{8} m/s

Table D.1 – The four most relevant constants of atomic physics define the atomic unit system and their value is fixed to unity. Two additional frequently occurring constants are also shown. In addition, the last column features the corresponding SI units for all considered quantities [183].

Appendix E

Age operator

E.1 Original age operator

The subsequent treatment is a summary of the content of Ref. [188]. Instead of following the pedagogical derivation in the original publication, we only present the results, for which Planck's reduced constant $\hbar$ appears explicitly. Matching the presentation in Ref. [188], t is exclusively used in this appendix, instead of λ.

E.1.1 Definition

For simplicity, we assume non-degenerate energy-levels and set the ground state energy $E_0 = 0$ to zero. The number $L+1$ of physically accessible or essential states during the whole dynamics of a system is the sum of all energy levels that are populated at some point of time [188]. All these energy states are denoted by $|E_k\rangle$ in order of increasing energy, and the corresponding time-independent Hamiltonian shall be

$$\hat{H}_L = \sum_{k=0}^{L} E_k \, |E_k\rangle\langle E_k| \, . \tag{E.1.1}$$

This form derives from the general Hamiltonian $\hat{H}$ through projection into the subspace spanned by $\{|E_k\rangle\}$, namely $\hat{H}_L = \hat{P}_L \hat{H} \hat{P}_L$ with projectors $\hat{P}_L \equiv \sum_{k=0}^{L} |E_k\rangle\langle E_k|$. An essential element of Pegg's derivation constitutes the (smallest) time period T after which any state returns to its initial state. In order to determine this period, we assume all energy ratio to be rational numbers, such that

$$\frac{E_k}{E_1} = \frac{C_k}{B_k} \tag{E.1.2}$$

features the coprime integers B_k and C_k, which do not possess a common factor. The lowest common multiple of all B_k shall be denoted by r_1 and one finds

$$T = r_1 \cdot \frac{2\pi\hbar}{E_1} \, . \tag{E.1.3}$$

Any operator tracking the evolution must necessarily respect this inherent periodicity. Pegg defines the operator

$$\hat{\alpha}(\alpha_0) \equiv \frac{1}{T} \int_{\alpha_0}^{\alpha_0+T} \mathrm{d}\alpha \, \alpha \, |\overline{\alpha}\rangle\langle\overline{\alpha}| \tag{E.1.4}$$

for some initial α_0 and the non-orthogonal vectors

$$|\overline{\alpha}\rangle \equiv \sum_{k=0}^{L} \exp\left(-\frac{iE_k\alpha}{\hbar}\right) |E_k\rangle \, , \tag{E.1.5}$$

which also provide a resolution of identity in the effective space of essential states, i.e.,

$$\hat{\mathbb{1}}_L = \hat{P}_L \hat{\mathbb{1}} \hat{P}_L = \int_{\alpha_0}^{\alpha_0+T} \frac{\mathrm{d}\alpha}{T} |\overline{\alpha}\rangle\langle\overline{\alpha}| \,. \tag{E.1.6}$$

The vectors $|\overline{\alpha}\rangle$ correspond to unnormalized states with a uniform distribution across all accessible energy levels and form an overcomplete basis, similar to coherent states. For completeness, we provide the normalized version $|\alpha\rangle = |\overline{\alpha}\rangle / \sqrt{L+1}$ as well.

E.1.2 Age of a quantum state

Subsequently, the "age" of a state $|\psi(t)\rangle = \sum_{k=0}^{L} c_k \exp(-itE_k/\hbar)\,|E_k\rangle$ is defined [188] as

$$\langle\hat{\alpha}(\alpha_0)\rangle(t) \equiv \langle\psi(t)|\hat{\alpha}(\alpha_0)|\psi(t)\rangle \tag{E.1.7}$$

$$\equiv \int_{\alpha_0}^{\alpha_0+T} \mathrm{d}\alpha\, \alpha\, P(\alpha, t) \tag{E.1.8}$$

with the time-dependent probability

$$P(\alpha, t) \equiv \frac{1}{T} |\langle\psi(t)|\overline{\alpha}\rangle|^2 \,. \tag{E.1.9}$$

Its rate of change reads

$$\frac{\mathrm{d}\,\langle\hat{\alpha}(\alpha_0)\rangle(t)}{\mathrm{d}t} = \frac{i}{\hbar} \langle\psi(t)|\Big[\hat{H}_L, \hat{\alpha}(\alpha_0)\Big]|\psi(t)\rangle \,, \tag{E.1.10}$$

in which the commutator has the form

$$\Big[\hat{H}_L, \hat{\alpha}(\alpha_0)\Big] = i\hbar\Big(|\overline{\alpha}_0\rangle\langle\overline{\alpha}_0| - \hat{\mathbb{1}}_L\Big) \tag{E.1.11}$$

and, thus, is close to the desired commutation relation for a sought-after time operator. The right-hand side vanishes under the trace operation, as it should for commutators of operators in finite-dimensional Hilbert spaces. Consequently, rate (E.1.10) becomes

$$\frac{\mathrm{d}\,\langle\hat{\alpha}(\alpha_0)\rangle(t)}{\mathrm{d}t} = 1 - |\langle\overline{\alpha}_0|\psi(t)\rangle|^2 = 1 - TP(\alpha_0, t) \,. \tag{E.1.12}$$

Due to the inherent periodic nature of these quantum states, the age must be cyclic as well and, therefore, returns to previous values during the course of its evolution. The last term in Eq. (E.1.12) ensures this behavior. For an illustration, we consider a harmonic oscillator with frequency ω which is energy restricted up to a certain energy eigenstate $|n = n_{\max}\rangle \equiv |n = L\rangle$. Every state of a harmonic oscillator returns to its initial value after $T = 2\pi/\omega$, because all energy levels are equidistant. Choosing the initial state $|\psi(0)\rangle = |\overline{\alpha} = 0\rangle / \sqrt{L+1}$, we find

$$TP(\alpha_0, t) = \left| \frac{1}{\sqrt{L+1}} \left(\sum_{m=0}^{L} \langle m|\, e^{i\omega n \alpha_0} \right) \cdot \left(\sum_{n=0}^{L} e^{-i\omega n t} e^{-i\omega t/2} \,|n\rangle \right) \right|^2 \tag{E.1.13}$$

$$= \frac{1}{L+1} \left| \frac{1 - e^{i\omega(L+1)(\alpha_0 - t)}}{1 - e^{i\omega(\alpha_0 - t)}} \right|^2 \tag{E.1.14}$$

$$= \frac{1}{L+1} \cdot \frac{1 - \cos\big[\omega(L+1)(t-\alpha_0)\big]}{1 - \cos\big[\omega(t-\alpha_0)\big]} \,, \tag{E.1.15}$$

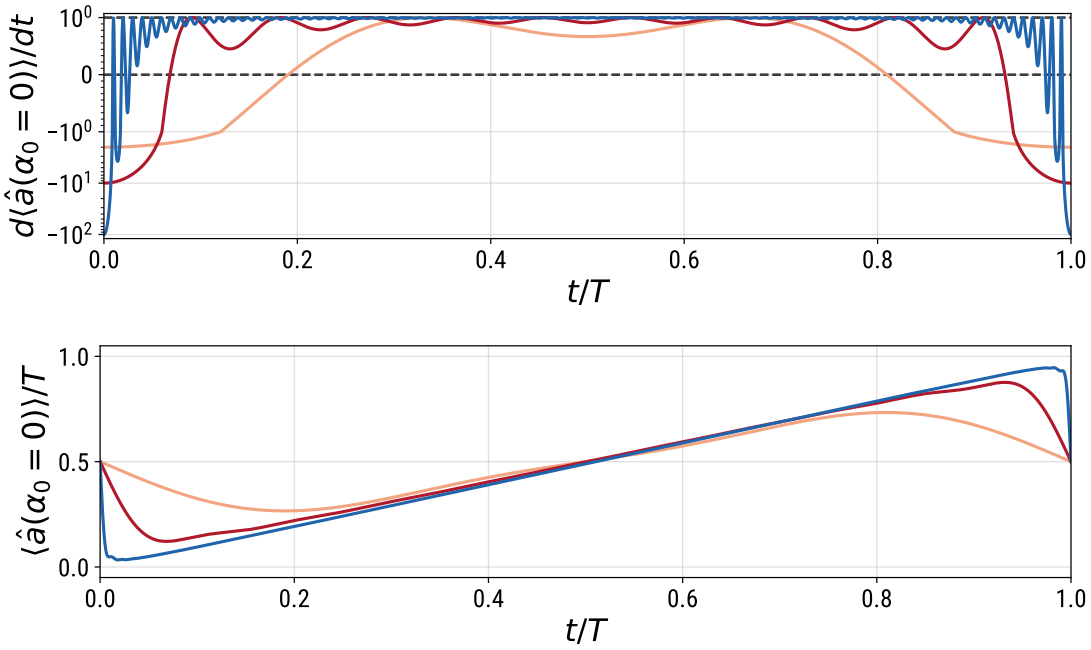

Figure E.1 – For a harmonic oscillator, the rate (E.1.12) and the age (E.1.8) are shown in the upper and lower panel, respectively. Here, the initial state consists of an equally weighted superposition of the lowest $L+1$ energy eigenstates, such that $|\psi(0)\rangle = |\alpha_0\rangle$. The parameters are $L = 2$ (orange), $L = 10$ (red), $L = 100$ (blue), $\alpha_0 = 0$ and $\omega = 1$ in atomic units (Appendix D).

which is finite for $t = \alpha_0$, i.e., $TP(\alpha_0, t = \alpha_0) = L + 1$. This already indicates that the rate $\mathrm{d}\langle\hat{\alpha}(\alpha_0)\rangle(t)/\mathrm{d}t\,\big|_{t=\alpha_0} = -L$ equals a large negative value at $t = \alpha_0$. For $\alpha_0 = 0$, the initial age at $t = 0$ has the analytic expression

$$\frac{\mathrm{d}\langle\hat{\alpha}(\alpha_0=0)\rangle}{\mathrm{d}t}\Big|_{t=0} \overset{x=\alpha\omega}{=} \frac{T}{(2\pi)^2(L+1)} \underbrace{\int_0^{2\pi} \mathrm{d}x\, x \frac{1-\cos[(L+1)x]}{1-\cos x}}_{=(L+1)2\pi^2} \tag{E.1.16}$$

$$= \frac{T}{2} \tag{E.1.17}$$

In Figure E.1, the age and its rate of change are presented for two effective dimensions L.

E.1.3 Uncertainty relation

Pegg has shown [188] that age and energy, by means of the Hamiltonian, have the uncertainty relation

$$(\Delta E)^2(\Delta\alpha)^2 \geq \left|\langle\psi|\Big(\hat{H}_L - \big\langle\hat{H}_L\big\rangle\Big)\Big(\hat{\alpha}(\alpha_0) - \langle\hat{\alpha}(\alpha_0)\rangle\Big)|\psi\rangle\right|^2 \tag{E.1.18}$$

$$= \frac{1}{4}\left|\Big\langle\Big[\hat{H}_L, \hat{\alpha}(\alpha_0)\Big]\Big\rangle\right|^2 + \left[\frac{1}{2}\Big\langle\big\{\hat{H}_L, \hat{\alpha}(\alpha_0)\big\}_+\Big\rangle - \big\langle\hat{H}_L\big\rangle\langle\hat{\alpha}(\alpha_0)\rangle\right]^2 \tag{E.1.19}$$

$$\geq \frac{\hbar^2}{4}\Big(1 - |\langle\overline{\alpha}_0|\psi\rangle|^2\Big). \tag{E.1.20}$$

The variances are defined as $(\Delta E)^2 = \mathrm{Var}_\psi(\hat{H}_L)$ and $(\Delta\alpha)^2 = \int_{\alpha_0}^{\alpha_0+T} \mathrm{d}\alpha\, P(\alpha,t)\big(\alpha - \langle\hat{\alpha}(\alpha_0)\rangle\big)^2$ in Ref. [188]. The second relation denotes the variance of the classical probability distribution $P(\alpha, t)$. In contrast, the variance $\mathrm{Var}_\psi[\hat{\alpha}(\alpha_0)]$ does not equal $(\Delta\alpha)^2$, due to the

non-orthogonality of the $|\overline{\alpha}\rangle$'s, but can be used in the same inequality instead of $(\Delta\alpha)^2$. As argued in Sec. 3.1.9 and with the relation given in footnote 3 on page 52, the uncertainty relation for mixed states $\hat{\rho}$ reads

$$\begin{aligned}
&\mathrm{Var}_{\hat{\rho}}(\hat{H}_L)\cdot\mathrm{Var}_{\hat{\rho}}[\hat{\alpha}(\alpha_0)] \\
&\qquad \geq \left|\mathrm{tr}\left[\hat{\rho}\left(\hat{H}_L-\langle\hat{H}_L\rangle\right)\left(\hat{\alpha}(\alpha_0)-\langle\hat{\alpha}(\alpha_0)\rangle\right)\right]\right|^2 && \text{(E.1.21)}\\
&\qquad = \frac{1}{4}\left|\left\langle\left[\hat{H}_L,\hat{\alpha}(\alpha_0)\right]\right\rangle\right|^2+\left[\frac{1}{2}\left\langle\left\{\hat{H}_L,\hat{\alpha}(\alpha_0)\right\}_+\right\rangle-\langle\hat{H}_L\rangle\langle\hat{\alpha}(\alpha_0)\rangle\right]^2 && \text{(E.1.22)}\\
&\qquad \geq \frac{\hbar^2}{4}\left(1-\langle\overline{\alpha}_0|\hat{\rho}|\overline{\alpha}_0\rangle\right) && \text{(E.1.23)}
\end{aligned}$$

with mean values $\langle\hat{A}\rangle=\mathrm{tr}\left(\hat{\rho}\hat{A}\right)$.

E.1.4 Classes of aging states

A drawback of Pegg's age operator is the uncertainty about which classes of states allow for a proper tracking by the age operator. Instead of doing an analytical investigation, we examine states for which the coefficients $c_k \equiv r_k\exp(i\gamma_k)$ are randomly distributed. All magnitudes r_k are uniformly drawn from the interval $[0,1]$ and a subsequent division by $\sum_k r_k$ ensures the state normalization. We consider two distinct states, which are characterized by the distribution of their phases. In particular, we either set all γ_k to zero or randomly draw them from a uniform distribution over the range $[0,2\pi]$. The resulting rates and age values are shown in Figure E.2 and are compared to the previous result, for which all r_k are equal and all phases vanish. For purely positive real-valued coefficients, the rate has a smaller slope, but still displays linearly behavior. In contrast, the age operator fails to track the evolution of a state with completely random coefficients. To deal with such states, we propose a modified age operator, which relies on the autocorrelation function in the next section.

E.2 Alternative age operator

E.2.1 Definition

We have noted above that Pegg's $|\alpha\rangle$ states correspond to time-evolved states with equal population on all accessible energy levels. Hence, the age operator $\hat{\alpha}(\alpha_0)$ depends on a specific initial state. This insight motivates us to define the modified age operator

$$\hat{\alpha}_\psi(\alpha_0)\equiv\frac{1}{D_\psi T_\psi}\int_{\alpha_0}^{\alpha_0+T_\psi}\mathrm{d}\alpha\,\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)| \qquad \text{(E.2.1)}$$

with $|\psi(\alpha)\rangle=\sum_m c_m\exp\left[-i\alpha E_m/\hbar\right]|E_m\rangle$ and an undetermined scaling factor D_ψ. The period T_ψ is the smallest time after which $|\psi(t)\rangle$ returns to its initial state and we also define the corresponding frequency $\Omega_\psi\equiv 2\pi/T_\psi$, for which $(E_k-E_m)/\Omega\in\mathbb{Z}$ for all k,m. There is no restriction on which c_m are allowed and, thus, we do not distinguish explicitly between populated and unpopulated levels. Without loss of generality, we assume all energy levels to be non-degenerate. Crucially, this modified age operator depends explicitly on the state $|\psi(\alpha)\rangle$ and, thus, should only be applied in context of $|\psi(t)\rangle$. This seems quite restraining, but Pegg already noted [188] that his age operator depends on the state of the system via the number of accessible states. Moreover, we seek an operator that accurately tracks the evolution of a specific state and not a universal tracking operator.

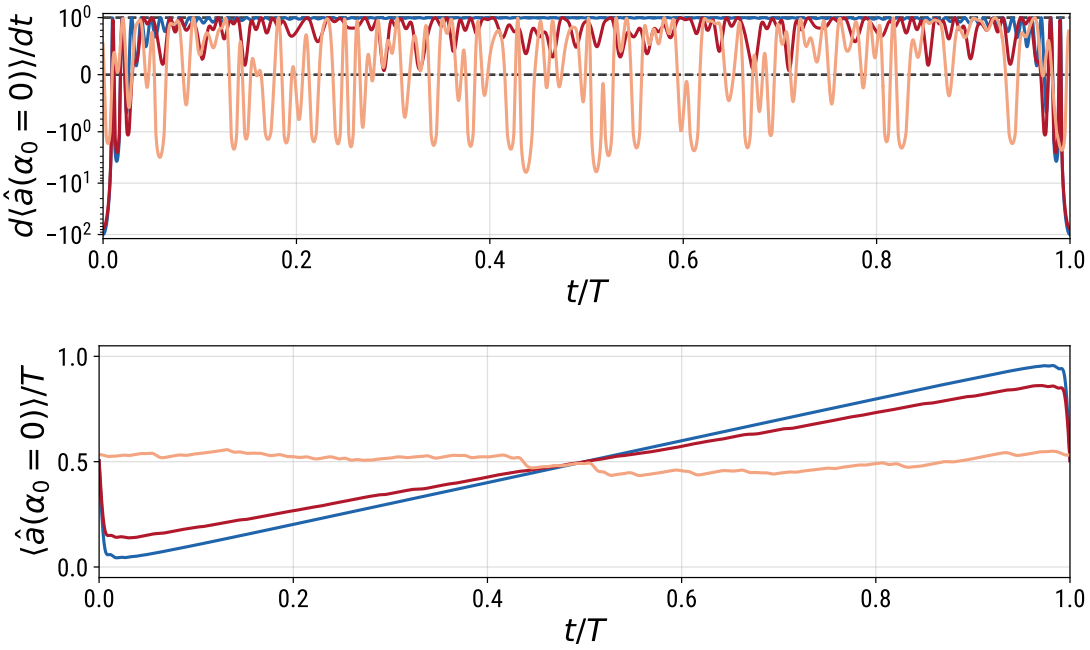

Figure E.2 – The rate of change (upper panel) and the age (lower panel) of harmonic oscillator states, restricted to the first $L+1 = 101$ energy levels, are displayed. All coefficients of the initial state $|\psi(0)\rangle = \sum_{k=0}^{L} c_k |E_k\rangle$ are randomly drawn according to the procedure given in Section E.1.4. While the red line corresponds to positive real-valued $c_k \in \mathbb{R}_+$, the orange line results from random complex variables $c_k \in \mathbb{C}$. For comparison, the previous results (blue line) for $c_k = 1/\sqrt{L+1}$ are plotted as well. The values $\alpha_0 = 0$ and $\omega = 1$ in atomic units (Appendix D) are used, as in Figure E.1.

E.2.2 Age and rate

The mean value, or "modified age", reads

$$\langle\psi(t)|\hat{\alpha}_\psi(\alpha_0)|\psi(t)\rangle = \frac{1}{D_\psi T_\psi}\int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, \alpha\, C_\psi(t-\alpha) \tag{E.2.2}$$

with the periodic and symmetric absolute squared autocorrelation function

$$C_\psi(t) \equiv |\langle\psi(0)|\psi(t)\rangle|^2 = \left|\sum_m |a_m|^2 e^{-itE_m/\hbar}\right|^2 = C_\psi(-t) = C_\psi(t+kT_\psi) \qquad k\in\mathbb{Z}\,. \tag{E.2.3}$$

This quantity is non-negative and upper-bounded by unity. Not only is the commutation relation with the Hamiltonian crucial for the rate of change, but also for the uncertainty relation. For this reason, we commence with the calculation of the mean value

$$\langle\psi(t)|\Big[\hat{H},\hat{\alpha}_\psi(\alpha_0)\Big]|\psi(t)\rangle = \frac{1}{D_\psi T_\psi}\int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, \alpha\, \mathrm{tr}\Big(|\psi(t)\rangle\langle\psi(t)|\Big[\hat{H},|\psi(\alpha)\rangle\langle\psi(\alpha)|\Big]\Big) \tag{E.2.4}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, \alpha\, \partial_\alpha C_\psi(\alpha-t) \tag{E.2.5}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\left[\alpha\, C_\psi(\alpha-t)\Big|_{\alpha_0}^{\alpha_0+T_\psi} - \int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, C_\psi(\alpha-t)\right] \tag{E.2.6}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\Bigg[(\alpha_0+T_\psi)\underbrace{C_\psi(\alpha_0+T_\psi-t)}_{=C_\psi(\alpha_0-t)} - \alpha_0\, C_\psi(\alpha_0-t) - \int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, C_\psi(\alpha-t)\Bigg] \tag{E.2.7}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\Bigg[T_\psi\, C_\psi(\alpha_0-t) - \int_{\alpha_0+t}^{\alpha_0+t+T_\psi} \mathrm{d}\alpha\, C_\psi(\alpha)\Bigg] \tag{E.2.8}$$

$$= \frac{-i\hbar}{D_\psi}\Bigg[\frac{1}{T_\psi}\int_0^{T_\psi} \mathrm{d}\alpha\, C_\psi(\alpha) - C_\psi(t-\alpha_0)\Bigg]. \tag{E.2.9}$$

The first term in squared brackets is the averaged autocorrelation function over one period and does not depend on t, whereas the second term typically remains small for $\lambda \neq \alpha_0$. In order to match the form of Pegg's version (E.1.12), we adopt the prefactor

$$D_\psi \equiv \frac{1}{T_\psi}\int_0^{T_\psi} \mathrm{d}\alpha\, C_\psi(\alpha) = \sum_{k,m} |c_k|^2 |c_m|^2 \int_0^{T_\psi} \frac{\Omega_\psi\, \mathrm{d}\alpha}{2\pi} e^{i\alpha(E_m-E_k)} \tag{E.2.10}$$

$$\overset{\alpha\equiv\Omega_\psi x}{=} \sum_{k,m} |c_k|^2 |c_m|^2 \underbrace{\frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}x\, e^{ix(E_m-E_k)/\Omega_\psi}}_{=\delta_{km}} \tag{E.2.11}$$

$$= \sum_k |c_k|^4, \tag{E.2.12}$$

which represents an inverse participation ratio. This allows us to define the probability

$$P_\psi(\alpha,t) \equiv \frac{C_\psi(t-\alpha)}{\int_0^{T_\psi}\mathrm{d}x\, C_\psi(x)} = \frac{1}{D_\psi}|\langle\psi(t)|\psi(\alpha)\rangle|^2. \tag{E.2.13}$$

and to express the modified age as

$$\langle\psi(t)|\hat{\alpha}_\psi(\alpha_0)|\psi(t)\rangle = \int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, \alpha\, P_\psi(\alpha,t). \tag{E.2.14}$$

In close analogy to Ref. [188], the mean value of the commutator with the Hamiltonian reads

$$\langle\psi(t)|\Big[\hat{H},\hat{\alpha}_\psi(\alpha_0)\Big]|\psi(t)\rangle = -i\hbar\Bigg[1-\frac{1}{D_\psi}C_\psi(t-\alpha_0)\Bigg]. \tag{E.2.15}$$

Such a relation suggests the commutator

$$\Big[\hat{H},\hat{\alpha}_\psi(\alpha_0)\Big] \overset{?}{=} \hat{\mathbb{1}} - \frac{1}{D_\psi}|\psi(\alpha_0)\rangle\langle\psi(\alpha_0)|, \tag{E.2.16}$$

which is a false statement however, as we show below. A direct evaluation of the commutator yields

$$\Big[\hat{H},\hat{\alpha}_\psi(\alpha_0)\Big] = \frac{1}{D_\psi T_\psi}\int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, \alpha\Big[\hat{H},|\psi(\alpha)\rangle\langle\psi(\alpha)|\Big] \tag{E.2.17}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\, \alpha\, \partial_\alpha\, |\psi(\alpha)\rangle\langle\psi(\alpha)| \tag{E.2.18}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\left[\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)|\Big|_{\alpha_0}^{\alpha_0+T_\psi} - \int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)|\right] \tag{E.2.19}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\Bigg[(\alpha_0+T_\psi)\underbrace{|\psi(\alpha_0+T_\psi)\rangle\langle\psi(\alpha_0+T_\psi)|}_{=|\psi(\alpha_0)\rangle\langle\psi(\alpha_0)|} - \alpha_0\,|\psi(\alpha_0)\rangle\langle\psi(\alpha_0)| - \int_{\alpha_0}^{\alpha_0+T_\psi} \mathrm{d}\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)|\Bigg] \tag{E.2.20}$$

$$= \frac{i\hbar}{D_\psi T_\psi}\left[T_\psi\,|\psi(\alpha_0)\rangle\langle\psi(\alpha_0)| - \int_{\alpha_0+t}^{\alpha_0+t+T_\psi} \mathrm{d}\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)|\right] \tag{E.2.21}$$

$$= -i\hbar\left[\frac{1}{D_\psi T_\psi}\int_0^{T_\psi} \mathrm{d}\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)| - \frac{1}{D_\psi}\,|\psi(\alpha_0)\rangle\langle\psi(\alpha_0)|\right]. \tag{E.2.22}$$

We express the first term in brackets in the energy basis as

$$\frac{1}{D_\psi T_\psi}\int_0^{T_\psi} \mathrm{d}\alpha\,|\psi(\alpha)\rangle\langle\psi(\alpha)| \overset{\alpha\equiv\Omega_\psi x}{=} \frac{1}{D_\psi 2\pi}\sum_{k,m} c_k c_m^*\,|E_k\rangle\langle E_m|\underbrace{\int_0^{2\pi}\mathrm{d}x\,e^{ix(E_m-E_k)/\Omega}}_{=2\pi\delta_{km}} \tag{E.2.23}$$

$$= \frac{1}{D_\psi}\sum_m |c_m|^2\,|E_m\rangle\langle E_m| \neq \hat{\mathbb{1}} \tag{E.2.24}$$

which yields the commutator

$$\left[\hat{H},\hat{\alpha}_\psi(\alpha_0)\right] = -i\hbar\left[\frac{1}{D_\psi}\sum_m |c_m|^2\,|E_m\rangle\langle E_m| - \frac{1}{D_\psi}\,|\psi(\alpha_0)\rangle\langle\psi(\alpha_0)|\right]. \tag{E.2.25}$$

In any case, only mean values are important and the exact form of the operator does not matter. Lastly, we obtain Pegg's age operator $\hat{\alpha}(\alpha_0)$ as a limiting case for $|\psi(0)\rangle = \sum_{k=0}^{L}|E_k\rangle/\sqrt{L+1}$. Figure E.3 provides a numerical example for a direct comparison with the original age operator.

E.2.3 Uncertainty relation

Using the results from above, the uncertainty relation becomes

$$\mathrm{Var}_\psi[\hat{H}]\cdot\mathrm{Var}_\psi[\hat{\alpha}_\psi(\alpha_0)] \tag{E.2.26}$$

$$\geq \frac{1}{4}\left|\left\langle\left[\hat{H},\hat{\alpha}_\psi(\alpha_0)\right]\right\rangle\right|^2 + \frac{1}{4}\left[\left\langle\left\{\hat{H},\hat{\alpha}_\psi(\alpha_0)\right\}_+\right\rangle - 2\left\langle\hat{H}\right\rangle\cdot\left\langle\hat{\alpha}_\psi(\alpha_0)\right\rangle\right]^2 \tag{E.2.27}$$

$$\geq \frac{\hbar^2}{4}\left(1-\frac{1}{D_\psi}C_\psi(t-\alpha_0)\right)^2 + \frac{1}{4}\left[\left\langle\left\{\hat{H},\hat{\alpha}_\psi(\alpha_0)\right\}_+\right\rangle - 2\left\langle\hat{H}\right\rangle\cdot\left\langle\hat{\alpha}_\psi(\alpha_0)\right\rangle\right]^2 \tag{E.2.28}$$

$$\geq \frac{\hbar^2}{4}\left(1-\frac{1}{D_\psi}C_\psi(t-\alpha_0)\right)^2. \tag{E.2.29}$$

E.2.4 Mixed states

The previous treatment also works for mixed states $\hat{\rho}(t)$ with the modified age operator

$$\hat{\alpha}_\rho(\alpha_0) \equiv \frac{1}{D_\rho T_\rho}\int_{\alpha_0}^{\alpha_0+T_\rho} \mathrm{d}\alpha\,\alpha\,\hat{\rho}(\alpha) \tag{E.2.30}$$

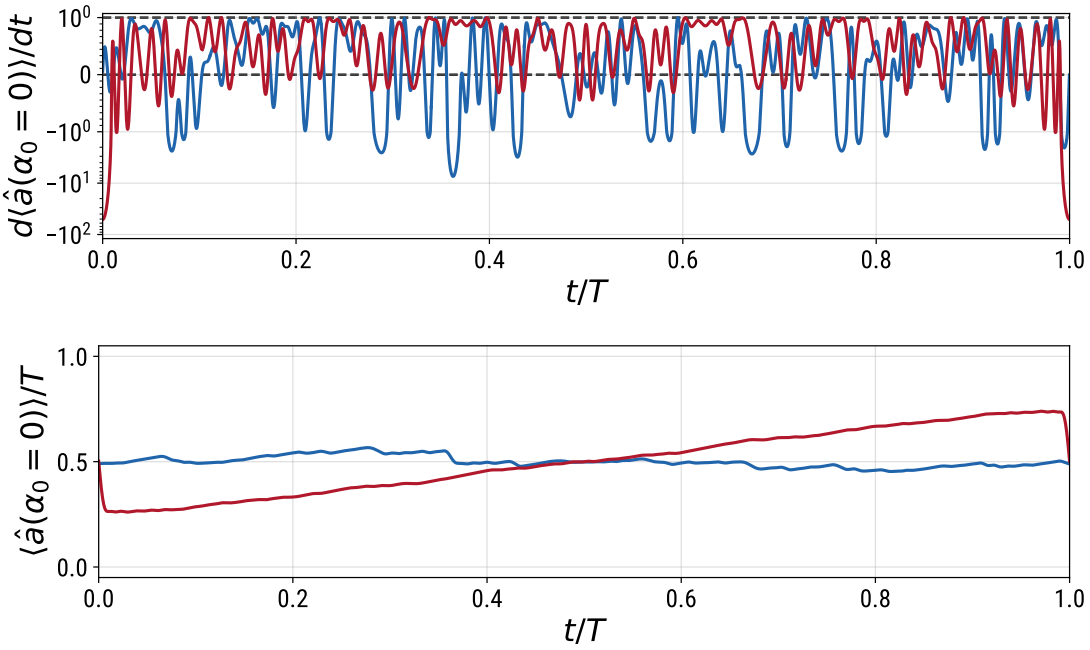

Figure E.3 – Pegg's age operator (blue line) is compared to the modified age operator (E.2.1) (red line). For a harmonic oscillator restricted to its first $L+1=101$ energy levels, the upper and lower panel show the rate of change and the age of a state $|\psi(t)\rangle$, respectively. Each complex coefficient c_k of the initial state $|\psi(0)\rangle=\sum_{k=0}^{L} c_k|E_k\rangle$ is randomly drawn from the unit disc in the complex plane and later normalized, such that $\langle\psi(0)|\psi(0)\rangle=1$. Identically to the previous numerical examples, the parameters are chosen as $\alpha_0=0$ and $\omega=1$ in atomic units (Appendix D).

with $i\hbar\partial_t\hat{\rho}(t)=\left[\hat{H},\hat{\rho}(t)\right]$. In the energy basis, the initial state reads

$$\hat{\rho}(0)=\sum_{m,n} b_{mn}\,|E_m\rangle\langle E_n| \tag{E.2.31}$$

with $b_{mn}=b_{nm}^*$. As a generalization of Eq. (E.2.2), the modified age is

$$\mathrm{tr}\Big[\hat{\rho}(t)\,\hat{\alpha}_\rho(\alpha_0)\Big]=\frac{1}{D_\rho\,T_\rho}\int_{\alpha_0}^{\alpha_0+T_\rho}\mathrm{d}\alpha\,\alpha\,C_\rho(t-\alpha) \tag{E.2.32}$$

with the absolute squared periodic autocorrelation

$$C_\rho(t)\equiv\mathrm{tr}\Big[\hat{\rho}(0)\,\hat{\rho}(t)\Big]=\sum_{m,n}|b_{mn}|^2e^{-it(E_m-E_n)/\hbar} \tag{E.2.33}$$

$$=\frac{1}{2}\left[\sum_{m,n}|b_{mn}|^2e^{-it(E_m-E_n)/\hbar}+\sum_{m,n}|b_{mn}|^2e^{-it(E_m-E_n)/\hbar}\right] \tag{E.2.34}$$

$$=\frac{1}{2}\left[\sum_{m,n}|b_{mn}|^2e^{-it(E_m-E_n)/\hbar}+\sum_{m,n}\underbrace{|b_{nm}|^2}_{=|b_{mn}|^2}e^{it(E_m-E_n)/\hbar}\right] \tag{E.2.35}$$

$$=\sum_{m,n}|b_{mn}|^2\cos\left(\frac{t(E_m-E_n)}{\hbar}\right) \tag{E.2.36}$$

$$=C_\rho(-t)=C_\rho(t+kT_\rho)\qquad k\in\mathbb{Z}\,. \tag{E.2.37}$$

for mixed states. Using the same reasoning as before, the scaling factor D_ρ is chosen as

$$D_\psi \equiv \frac{1}{T_\rho}\int_0^{T_\rho} \mathrm{d}\alpha\, C_\rho(\alpha) = \sum_{m,n} |b_{mn}|^2 \int_0^{2\pi/\Omega_\rho} \frac{\Omega_\psi\, \mathrm{d}\alpha}{2\pi} e^{i\alpha(E_m - E_n)} \tag{E.2.38}$$

$$\overset{x\equiv\alpha/\Omega_\psi}{=} \sum_{m,n} |b_{mn}|^2 \underbrace{\frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}x\, e^{ix(E_m-E_n)/\Omega_\rho}}_{=\delta_{mn}} = \sum_m |b_{mm}|^2\,, \tag{E.2.39}$$

which allows to for the definition of the probability

$$P_\rho(\alpha, t) \equiv \frac{1}{D_\psi}\,\mathrm{tr}\Big[\hat\rho(t)\,\hat\rho(\alpha)\Big] = \frac{1}{D_\psi} C_\rho(\alpha - t)\,. \tag{E.2.40}$$

In addition, the commutator mean value has the same form as before, namely

$$\mathrm{tr}\Big(\hat\rho(t)\Big[\hat H, \hat\alpha_\rho(\alpha_0)\Big]\Big) = -i\hbar\left[1 - \frac{1}{D_\psi} C_\psi(t - \alpha_0)\right], \tag{E.2.41}$$

and the uncertainty relation

$$\mathrm{Var}_\rho[\hat H]\cdot \mathrm{Var}_\rho[\hat\alpha_\psi(\alpha_0)] \geq \frac{\hbar^2}{4}\left(1 - \frac{1}{D_\rho} C_\rho(t-\alpha_0)\right)^2 \tag{E.2.42}$$

holds as well. For illustration, Figure E.4 displays a numerical example with a comparison to Pegg's age operator for mixed states.

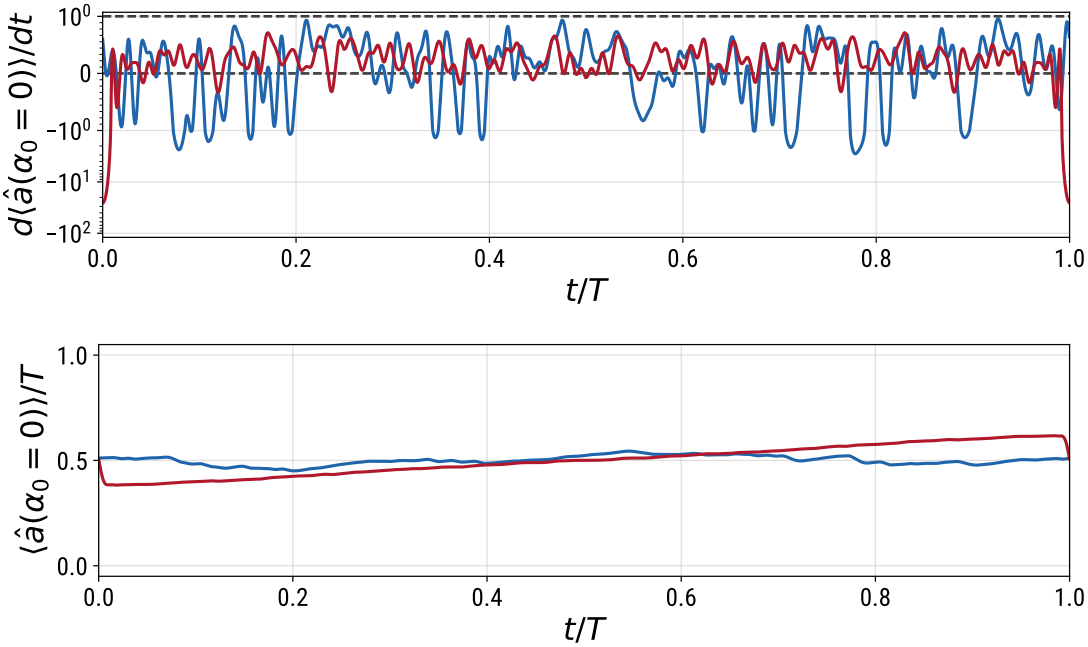

Figure E.4 – The original (blue) and the modified age operator (red) are compared for a mixed state, taken as an incoherent mixture $\hat{\rho}(0) \propto \sum_{m=0}^{2} |\psi_m(0)\rangle\langle\psi_m(0)|$ of three randomly drawn pure states $|\psi_m(0)\rangle = \sum_{k=0}^{L} c_{m,k} |E_k\rangle$. Here, the energy states $|E_k\rangle$ correspond to the lowest $L + 1 = 101$ levels of a harmonic oscillator. Similar to before, the rate of change (upper panel) and the age (lower panel) are used to reveal the difference between both formulations. Instead of the probability (E.1.9) for pure state, we use $P_{\text{Pegg},\rho}(\alpha, t) = \langle\overline{\alpha}|\hat{\rho}(t)|\overline{\alpha}\rangle / T$ for Pegg's formalism. The specific parameter values are $\alpha_0 = 0$ and $\omega = 1$ in atomic units (D).

Appendix F

Wigner representation

All results below are based on the treatments given in Ref. [328].

F.1 Transformation and inverse transformation

The definitions

$$W_\rho(q,p) \equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}x \left\langle q-\frac{x}{2}\middle|\hat{\rho}\middle|q+\frac{x}{2}\right\rangle e^{ipx/\hbar}, \tag{F.1.1}$$

$$\overline{W}_A(q,p) \equiv \int_{-\infty}^{\infty} \mathrm{d}x \left\langle q-\frac{x}{2}\middle|\hat{A}\middle|q+\frac{x}{2}\right\rangle e^{ipx/\hbar} \tag{F.1.2}$$

for the Wigner representation of states $\hat{\rho}$ and operators $\hat{A}$ shall be provided here for quick reference. In addition, the back-transformation from the phase space representation to the original operator form is facilitated by

$$\hat{D}(q,p) \equiv \int \mathrm{d}x \left|q+\frac{x}{2}\middle\rangle\middle\langle q-\frac{x}{2}\right| e^{ipx/\hbar}, \tag{F.1.3}$$

which originates from $\overline{W}_A(q,p) = \mathrm{tr}\big(\hat{A}\hat{D}(q,p)\big)$. This important operator has the properties $\int \mathrm{d}p\, \hat{D}(q,p) = 2\pi\hbar\, |q\rangle\langle q|$ and $\mathrm{tr}\,\hat{D}(q,p) = 1$. Moreover, any density and general operators are recovered via

$$\hat{\rho} = \int \mathrm{d}q \int \mathrm{d}p\; W_\rho(q,p)\,\hat{D}(q,p), \tag{F.1.4}$$

$$\hat{A} = \frac{1}{2\pi\hbar}\int \mathrm{d}q \int \mathrm{d}p\; \overline{W}_A(q,p)\,\hat{D}(q,p). \tag{F.1.5}$$

F.2 Properties of $\hat{D}$

In this section, we derive some of the properties of $\hat{D}(q,p)$. First, the trace of two $\hat{D}$-operators reads

$$\mathrm{tr}\Big(\hat{D}(q,p)\,\hat{D}(q',p')\Big) \tag{F.2.1}$$

$$= \int \mathrm{d}x \int \mathrm{d}y\; e^{i(px+p'y)/\hbar}\,\mathrm{tr}\left(\left|q+\frac{x}{2}\middle\rangle\middle\langle q-\frac{x}{2}\right| \cdot \left|q'+\frac{y}{2}\middle\rangle\middle\langle q'-\frac{y}{2}\right|\right) \tag{F.2.2}$$

$$= \int \mathrm{d}x \int \mathrm{d}y\; e^{i(px+p'y)/\hbar}\,\delta\left(\frac{y+x}{2}-(q-q')\right)\delta\left(\frac{y+x}{2}+(q-q')\right) \tag{F.2.3}$$

$$= 4 \int \mathrm{d}x \int \mathrm{d}y \; e^{i(px+p'y)/\hbar}\, \delta\big(y+x-2(q-q')\big)\, \delta\big(y+x+2(q-q')\big) \tag{F.2.4}$$

$$= 4 \int \mathrm{d}x \; e^{i(p-p')x/\hbar}\, e^{2ip'(q-q')/\hbar}\, \delta\big(2(q-q')\big) \tag{F.2.5}$$

$$= 2\pi\hbar\, \delta(p-p')\, \delta(q-q'), \tag{F.2.6}$$

as is expected, because

$$W_\rho(q,p) = \frac{1}{2\pi\hbar}\, \mathrm{tr}\big(\hat{\rho}\hat{D}(q,p)\big) \tag{F.2.7}$$

$$= \frac{1}{2\pi\hbar} \int \mathrm{d}q' \int \mathrm{d}p' \; W_\rho(q',p')\, \mathrm{tr}\big(\hat{D}(q,p)\hat{D}(q',p')\big) \tag{F.2.8}$$

can only be solved if Eq. (F.2.6) holds. Second, for the Wigner representation of the product of two arbitrary operators, the trace of three $\hat{D}$-operators is needed. Such a term evaluates to

$$\mathrm{tr}\Big(\hat{D}(q,p)\,\hat{D}(q',p')\,\hat{D}(q'',p'')\Big)$$

$$= \int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \; e^{i(px+p'y+p''z)/\hbar}\, \mathrm{tr}\Big\{\Big|q+\frac{x}{2}\Big\rangle\Big\langle q-\frac{x}{2}\Big| \cdot \Big|q'+\frac{y}{2}\Big\rangle\Big\langle q'-\frac{y}{2}\Big| \cdot \Big|q''+\frac{z}{2}\Big\rangle\Big\langle q''-\frac{z}{2}\Big|\Big\} \tag{F.2.9}$$

$$= \int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \; e^{i(px+p'y+p''z)/\hbar} \Big\langle q-\frac{x}{2}\Big|q'+\frac{y}{2}\Big\rangle \Big\langle q'-\frac{y}{2}\Big|q''+\frac{z}{2}\Big\rangle \Big\langle q''-\frac{z}{2}\Big|q+\frac{x}{2}\Big\rangle \tag{F.2.10}$$

$$= \int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \; e^{i(px+p'y+p''z)/\hbar}\, \delta\Big(\frac{x+y}{2}-(q-q')\Big)\, \delta\Big(\frac{y+z}{2}-(q'-q'')\Big) \cdot \delta\Big(\frac{x+z}{2}-(q''-q)\Big) \tag{F.2.11}$$

$$= 2^3 \int \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \; e^{i(px+p'y+p''z)/\hbar}\, \delta\big(x+y-2(q-q')\big)\, \delta\big(y+z-2(q'-q'')\big) \cdot \delta\big(x+z-2(q''-q)\big) \tag{F.2.12}$$

$$= 2^3\, e^{2ip''(q'-q'')/\hbar} \int \mathrm{d}x\,\mathrm{d}y \; e^{ipx/\hbar}\, e^{iy(p'-p'')/\hbar}\, \delta\big(x+y-2(q-q')\big) \cdot \delta\big(x-y+2(q+q')-4q''\big) \tag{F.2.13}$$

$$= 2^2 e^{2ip''(q'-q'')/\hbar}\, e^{2i(p'-p'')(q-q')/\hbar} \int \mathrm{d}x \; e^{ix(p-p'+p'')/\hbar}\, \delta\big(x-2(q''-q')\big) \tag{F.2.14}$$

$$= 2^2 e^{2ip''(q'-q'')/\hbar}\, e^{2i(p'-p'')(q-q')/\hbar}\, e^{2i(p-p'+p'')(q''-q')/\hbar} \tag{F.2.15}$$

$$= 2^2 \exp\Big[\frac{2i}{\hbar}\Big\{p(q''-q')+p'(q-q'')+p''(q'-q)\Big\}\Big]. \tag{F.2.16}$$

Equipped with this result, we express the Wigner representation of $\hat{A}\hat{B}$ as

$$\overline{W}_{AB}(q,p) = \mathrm{tr}\big[\hat{A}\hat{B}\,\hat{D}(q,p)\big] \tag{F.2.17}$$

$$= \frac{1}{(2\pi\hbar)^2} \int \mathrm{d}q'\,\mathrm{d}q''\,\mathrm{d}p'\,\mathrm{d}p'' \; \overline{W}_A(q',p')\, \overline{W}_B(q'',p'') \cdot \mathrm{tr}\big[\hat{D}(q,p)\,\hat{D}(q',p')\,\hat{D}(q'',p'')\big] \tag{F.2.18}$$

$$= \frac{1}{(\pi\hbar)^2}\int \mathrm{d}q'\,\mathrm{d}q''\,\mathrm{d}p'\,\mathrm{d}p''\,\overline{W}_A(q',p')\,\overline{W}_B(q'',p'') \cdot e^{2i\left[p(q''-q')+p'(q-q'')+p''(q'-q)\right]/\hbar} \tag{F.2.19}$$

$$\overset{\substack{x\equiv q''-q\\ k\equiv p''-p}}{=} \frac{1}{(\pi\hbar)^2}\int \mathrm{d}q'\,\mathrm{d}x\,\mathrm{d}p'\,\mathrm{d}k\,\overline{W}_A(q',p')\,\overline{W}_B(q+x,p+k)\,e^{2i\left[x(p-p')+k(q'-q)\right]/\hbar} \tag{F.2.20}$$

$$= \frac{1}{(\pi\hbar)^2}\int \mathrm{d}q'\,\mathrm{d}x\,\mathrm{d}p'\,\mathrm{d}k\,\overline{W}_A(q',p')\,e^{2i\left[x(p-p')+k(q'-q)\right]/\hbar}\,e^{(k\overrightarrow{\partial}_p+x\overrightarrow{\partial}_q)}\,\overline{W}_B(q,p)\,. \tag{F.2.21}$$

In the last line, we use the formal Taylor expansion

$$\overline{W}_B(q+x,p+k) = \exp\left[k\overrightarrow{\partial}_p + x\overrightarrow{\partial}_q\right]\overline{W}_B(q,p)\,, \tag{F.2.22}$$

in which the arrows indicate the action of the derivative operators on the right. It allows us to utilize

$$e^{2i(xp-qk)/\hbar}\exp\left[k\overrightarrow{\partial}_p + x\overrightarrow{\partial}_q\right] = e^{2i(xp-qk)/\hbar}\exp\left[\frac{i\hbar}{2}\left(\overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)\right], \tag{F.2.23}$$

in which $\overleftarrow{\partial}_i$ denotes derivatives acting on the left. Subsequently, the Wigner representation reads

$$\overline{W}_{AB}(q,p) = \frac{1}{(\pi\hbar)^2}\int \mathrm{d}q'\,\mathrm{d}x\,\mathrm{d}p'\,\mathrm{d}k\,\overline{W}_A(q',p')\,e^{2i\left[x(p-p')+k(q'-q)\right]/\hbar} \cdot e^{i\hbar\left(\overleftarrow{\partial}_q\overrightarrow{\partial}_p-\overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)/2}\,\overline{W}_B(q,p) \tag{F.2.24}$$

$$= \frac{(2\pi\hbar)^2}{(\pi\hbar)^2}\int \mathrm{d}q'\,\mathrm{d}p'\,\overline{W}_A(q',p')\,\delta\big(2(p-p')\big)\,\delta\big(2(q'-q)\big) \cdot e^{i\hbar\left(\overleftarrow{\partial}_q\overrightarrow{\partial}_p-\overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)/2}\,\overline{W}_B(q,p) \tag{F.2.25}$$

$$= \int \mathrm{d}q'\,\mathrm{d}p'\,\overline{W}_A(q',p')\,\delta(p-p')\,\delta\big(q-q'\big)\,e^{i\hbar\left(\overleftarrow{\partial}_q\overrightarrow{\partial}_p-\overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)/2}\,\overline{W}_B(q,p) \tag{F.2.26}$$

$$= \overline{W}_A(q,p)\,e^{i\hbar\left(\overleftarrow{\partial}_q\overrightarrow{\partial}_p-\overleftarrow{\partial}_p\overrightarrow{\partial}_q\right)/2}\,\overline{W}_B(q,p) \tag{F.2.27}$$

$$\equiv \overline{W}_A(q,p)\,e^{i\hbar\overleftrightarrow{\Lambda}/2}\,\overline{W}_B(q,p)\,. \tag{F.2.28}$$

Here, we define the Poisson bracket operator [235]

$$\overleftrightarrow{\Lambda} \equiv \overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q\,, \tag{F.2.29}$$

which can also be used to define the classical Poisson bracket

$$\big\{A(q,p),B(q,p)\big\} \equiv A(q,p)\overleftrightarrow{\Lambda}B(q,p) = \frac{\partial A(q,p)}{\partial q}\frac{\partial B(q,p)}{\partial p} - \frac{\partial A(q,p)}{\partial p}\frac{\partial B(q,p)}{\partial q}\,. \tag{F.2.30}$$

F.3 Several representations

An important formula is the Wigner representation

$$\overline{W}_{AB}(q,p) = \overline{W}_A(q,p)\,e^{i\hbar\overleftrightarrow{\Lambda}/2}\,\overline{W}_B(q,p) = \overline{W}_B(q,p)\,e^{-i\hbar\overleftrightarrow{\Lambda}/2}\,\overline{W}_A(q,p) \tag{F.3.1}$$

for products of operators [329]. Immediately, the Wigner function for the commutator $[\hat{A},\hat{B}]$ is given by [328]

$$\overline{W}_{[A,B]}(q,p) = \overline{W}_A(q,p)\, e^{i\hbar\overleftrightarrow{\Lambda}/2}\, \overline{W}_B(q,p) - \overline{W}_B(q,p)\, e^{i\hbar\overleftrightarrow{\Lambda}/2}\, \overline{W}_A(q,p) \tag{F.3.2}$$

$$= \overline{W}_A(q,p)\left(e^{i\hbar\overleftrightarrow{\Lambda}/2} - e^{-i\hbar\overleftrightarrow{\Lambda}/2}\right)\overline{W}_B(q,p) \tag{F.3.3}$$

$$= 2i\,\overline{W}_A(q,p)\,\sin\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right)\overline{W}_B(q,p)\,. \tag{F.3.4}$$

In addition, the anti-commutator representation reads

$$\overline{W}_{\{A,B\}_+}(q,p) = 2\,\overline{W}_A(q,p)\,\cos\left(\frac{\hbar}{2}\overleftrightarrow{\Lambda}\right)\overline{W}_B(q,p)\,. \tag{F.3.5}$$

F.4 Partial trace and relation system state

For the Wigner representation of the relational system state, an expression for the partial trace over clock Hilbert space in Wigner representation is needed. To this end, we use

$$|\Psi\rangle = \sum_m |\bar{\varphi}_m \otimes \chi_m\rangle \tag{F.4.1}$$

for an arbitrary orthonormal clock basis $\{|\chi_m\rangle_{\mathrm{C}}\}$ and a non-orthonormal set $\{|\bar{\varphi}_m\rangle_{\mathrm{S}}\}$ of system states. As a result, the corresponding Wigner function reads

$$W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K}) = \frac{1}{(2\pi)^{n_{\mathrm{S}}+n_{\mathrm{C}}}}\,\mathrm{tr}\Big(|\Psi\rangle\langle\Psi|\,\hat{D}_{\mathrm{S}}(\mathbf{q},\mathbf{p})\,\hat{D}_{\mathrm{C}}(\mathbf{Q},\mathbf{K})\Big) \tag{F.4.2}$$

$$= \frac{1}{(2\pi)^{n_{\mathrm{S}}+n_{\mathrm{C}}}}\sum_{m,n}\mathrm{tr}_{\mathrm{S}}\Big(|\bar{\varphi}_m\rangle\langle\bar{\varphi}_n|_{\mathrm{S}}\,\hat{D}_{\mathrm{S}}(\mathbf{q},\mathbf{p})\Big)\,\mathrm{tr}_{\mathrm{C}}\Big(|\chi_m\rangle\langle\chi_n|_{\mathrm{C}}\,\hat{D}_{\mathrm{C}}(\mathbf{Q},\mathbf{K})\Big) \tag{F.4.3}$$

$$= \frac{1}{(2\pi)^{n_{\mathrm{S}}}}\sum_{m,n}\overline{W}_{|\bar{\varphi}_m\rangle\langle\bar{\varphi}_n|_{\mathrm{S}}}(\mathbf{q},\mathbf{p})\,\overline{W}_{|\chi_m\rangle\langle\chi_n|_{\mathrm{C}}}(\mathbf{Q},\mathbf{K}) \tag{F.4.4}$$

and can be used for the derivation of the system Wigner function

$$W_{\rho_{\mathrm{S}}}(\mathbf{q},\mathbf{p}) = \frac{1}{(2\pi)^{n_{\mathrm{S}}}}\,\mathrm{tr}_{\mathrm{S}}\big(\hat{\rho}_{\mathrm{S}}\hat{D}_{\mathrm{S}}(\mathbf{q},\mathbf{p})\big) \tag{F.4.5}$$

$$= \frac{1}{(2\pi)^{n_{\mathrm{S}}}\,\langle\Psi|\hat{\rho}_{\mathrm{C}}|\Psi\rangle}\,\mathrm{tr}\big(\hat{\rho}_{\mathrm{C}}\,|\Psi\rangle\langle\Psi|\,\hat{D}_{\mathrm{S}}(\mathbf{q},\mathbf{p})\big) \tag{F.4.6}$$

$$= \frac{1}{(2\pi)^{n_{\mathrm{S}}}\,\langle\Psi|\hat{\rho}_{\mathrm{C}}|\Psi\rangle}\sum_{m,n}\mathrm{tr}_{\mathrm{C}}\big(\hat{\rho}_{\mathrm{C}}\,|\chi_m\rangle\langle\chi_n|_{\mathrm{C}}\big)\,\mathrm{tr}_{\mathrm{S}}\big(|\bar{\varphi}_m\rangle\langle\bar{\varphi}_n|_{\mathrm{S}}\,\hat{D}_{\mathrm{S}}(\mathbf{q},\mathbf{p})\big) \tag{F.4.7}$$

$$= \frac{1}{(2\pi)^{n_{\mathrm{S}}}\,\langle\Psi|\hat{\rho}_{\mathrm{C}}|\Psi\rangle}\sum_{m,n}\overline{W}_{|\bar{\varphi}_m\rangle\langle\bar{\varphi}_n|_{\mathrm{S}}}(\mathbf{q},\mathbf{p}) \cdot\int \mathrm{d}^{n_{\mathrm{C}}}\mathbf{Q}\,\mathrm{d}^{n_{\mathrm{C}}}\mathbf{K}\,W_{\rho_{\mathrm{C}}}(\mathbf{Q},\mathbf{K})\,\overline{W}_{|\chi_m\rangle\langle\chi_n|_{\mathrm{C}}}(\mathbf{Q},\mathbf{K}) \tag{F.4.8}$$

$$= \frac{1}{\langle\Psi|\hat{\rho}_{\mathrm{C}}|\Psi\rangle}\int \mathrm{d}^{n_{\mathrm{C}}}\mathbf{Q}\,\mathrm{d}^{n_{\mathrm{C}}}\mathbf{K}\,W_{\rho_{\mathrm{C}}}(\mathbf{Q},\mathbf{K})\,W_{|\Psi\rangle\langle\Psi|}(\mathbf{q},\mathbf{p},\mathbf{Q},\mathbf{K})\,. \tag{F.4.9}$$

Appendix G

Maximally entangled global state

A MES $|\Psi\rangle$ for a bipartite system is characterized by reduced density operators which equal the identity operators on their subsystems, representing maximally mixed subsystem states. In our notation, the global state $|\Psi\rangle$ must fulfill

$$\mathrm{tr}_\mathrm{S}\,|\Psi\rangle\langle\Psi| = \frac{1}{d_\mathrm{C}}\hat{\mathbb{1}}_\mathrm{C}\,, \tag{G.1}$$

$$\mathrm{tr}_\mathrm{C}\,|\Psi\rangle\langle\Psi| = \frac{1}{d_\mathrm{S}}\hat{\mathbb{1}}_\mathrm{S} \tag{G.2}$$

in order to constitute a MES and a necessary requirement for these equations to hold is the matching of both subsystems dimensions, namely $d_\mathrm{C} = d_\mathrm{S}$ (Sec. 3.1.5.1).

G.1 Relations between states

Furthermore, from

$$\langle\Psi|\chi\rangle\langle\chi|\Psi\rangle = \langle\chi|\mathrm{tr}_\mathrm{S}\Big(|\Psi\rangle\langle\Psi|\Big)|\chi\rangle_\mathrm{C} = \frac{1}{d_\mathrm{C}}\langle\chi|\chi\rangle_\mathrm{C} = \frac{1}{d_\mathrm{C}} \tag{G.1.1}$$

follows that the normalized system state is $|\varphi\rangle_\mathrm{S} = \sqrt{d_\mathrm{C}}\,\langle\chi|\Psi\rangle_\mathrm{C}$. In general, it only holds for MES that the conditional system state relates back to the clock state on which it is conditioned, i.e.,

$$\sqrt{d_\mathrm{S}}\,\langle\varphi[\chi]|\Psi\rangle_\mathrm{S} = |\chi\rangle_\mathrm{C}\,. \tag{G.1.2}$$

In addition, the use of MESs implies the equation

$$\langle\Psi|\hat{A}_\mathrm{C}\hat{P}_\chi|\Psi\rangle = \frac{1}{d_\mathrm{C}}\langle\chi|\hat{A}_\mathrm{C}|\chi\rangle_\mathrm{C} \tag{G.1.3}$$

for any clock operator $\hat{A}_\mathrm{C}$ and the equality of state overlaps in different subsystems as well, i.e.,

$$\langle\varphi_1|\varphi_2\rangle_\mathrm{S} = d_\mathrm{C}\,\langle\Psi|\chi_1\rangle\langle\chi_2|\Psi\rangle = \langle\chi_1|\chi_2\rangle_\mathrm{C}\,. \tag{G.1.4}$$

These relations do not hold for general $|\Psi\rangle$, which are not MESs.

G.2 Energy relations

For MESs, the effective system potential becomes

$$\hat{V}_\mathrm{S} = d_\mathrm{C}\,\langle\chi|\Big\{E-\hat{H}_\mathrm{S}-\hat{H}_\mathrm{C},\hat{P}_\Psi\Big\}_+|\chi\rangle_\mathrm{C} - d_\mathrm{C}\,\mathrm{Re}\,\langle\Psi|\Big(E-\hat{H}_\mathrm{S}-\hat{H}_\mathrm{C}\Big)\hat{P}_\chi|\Psi\rangle \tag{G.2.1}$$

$$= 2E\hat{P}_\varphi - \hat{H}_\mathrm{S}\hat{P}_\varphi - \hat{P}_\varphi\hat{H}_\mathrm{S} - d_\mathrm{C}\,\langle\chi|\left\{\hat{H}_\mathrm{C},\hat{P}_\Psi\right\}_+|\chi\rangle_\mathrm{C} - E + \langle\varphi|\hat{H}_\mathrm{S}|\varphi\rangle_\mathrm{S} + \langle\chi|\hat{H}_\mathrm{C}|\chi\rangle_\mathrm{C} \tag{G.2.2}$$

and yields

$$\left(\hat{H}_\mathrm{S}+\hat{V}_\mathrm{S}\right)|\varphi\rangle_\mathrm{S} = E\,|\varphi\rangle_\mathrm{S} + \langle\chi|\hat{H}_\mathrm{C}|\chi\rangle_\mathrm{C}\,|\varphi\rangle_\mathrm{S} - \underbrace{d_\mathrm{C}^{3/2}\,\langle\chi|\left\{\hat{H}_\mathrm{C},\hat{P}_\Psi\right\}_+\hat{P}_\chi|\Psi\rangle_\mathrm{C}}_{=\sqrt{d_\mathrm{C}}\langle\chi|\hat{H}_\mathrm{C}|\Psi\rangle_\mathrm{C}+\langle\chi|\hat{H}_\mathrm{C}|\chi\rangle_\mathrm{C}|\varphi\rangle_\mathrm{S}} \tag{G.2.3}$$

$$= E\,|\varphi\rangle_\mathrm{S} - \sqrt{d_\mathrm{C}}\,\langle\chi|\hat{H}_\mathrm{C}|\Psi\rangle_\mathrm{C}\,. \tag{G.2.4}$$

Immediately, the energy relation

$$\langle\varphi|\left(\hat{H}_\mathrm{S}+\hat{V}_\mathrm{S}\right)|\varphi\rangle_\mathrm{S} = E - \langle\chi|\hat{H}_\mathrm{C}|\chi\rangle_\mathrm{C} \tag{G.2.5}$$

between system and clock follows. The mean value of the squared system Hamiltonian

$$\langle\varphi|\left(\hat{H}_\mathrm{S}+\hat{V}_\mathrm{S}\right)^2|\varphi\rangle_\mathrm{S} = E^2 - d_\mathrm{C}E\Big(\langle\Psi|\hat{P}_\chi\hat{H}_\mathrm{C}|\Psi\rangle + \langle\Psi|\hat{H}_\mathrm{C}\hat{P}_\chi|\Psi\rangle\Big) + d_\mathrm{C}\,\langle\Psi|\hat{H}_\mathrm{C}\hat{P}_\chi\hat{H}_\mathrm{C}|\Psi\rangle \tag{G.2.6}$$

$$= \langle\chi|\left(\hat{H}_\mathrm{C}-E\right)^2|\chi\rangle_\mathrm{C} \tag{G.2.7}$$

implies the equality of subsystem energy variances as well, namely

$$\mathrm{Var}_\varphi\left(\hat{H}_\mathrm{S}+\hat{V}_\mathrm{S}\right) = \langle\chi|\left(\hat{H}_\mathrm{C}-E\right)^2|\chi\rangle_\mathrm{C} - \langle\chi|\left(\hat{H}_\mathrm{C}-E\right)|\chi\rangle_\mathrm{C}^2 \tag{G.2.8}$$

$$= \mathrm{Var}_\chi(\hat{H}_\mathrm{C})\,. \tag{G.2.9}$$

Since the clock energy does not change through the evolution under $\hat{H}_\mathrm{C}$, the system energy variance remains constant as well, even though a λ-dependent system potential exists. This is an interesting behavior and could be further investigated.

G.3 Purity relations for mixed states

In this section, we consider mixed clock and system states. For a MES $|\Psi\rangle$, the *normalized* system state reads $\hat{\rho}_\mathrm{S} = d_\mathrm{C}\,\mathrm{tr}_\mathrm{C}(\hat{\rho}_\mathrm{C}\hat{P}_\Psi)$. Instead of trying to evaluate the von Neumann entropy, it is easier to calculate the purity $\mathscr{P} \equiv \mathrm{tr}\,\hat{\rho}^2$ of a density operator [330], a quantity closely related to entropy [146]. Using the invariance of the trace under cyclic permutations shows that the clock purity

$$\mathscr{P}_\mathrm{C}[\hat{\rho}_\mathrm{C}(\lambda)] = \mathrm{tr}_\mathrm{C}\left(\hat{\rho}_\mathrm{C}^2(\lambda)\right) = \mathrm{tr}_\mathrm{C}\left(e^{-i\lambda\hat{H}_\mathrm{C}}\,\hat{\rho}_\mathrm{C}^2(0)\,e^{i\lambda\hat{H}_\mathrm{C}}\right) = \mathrm{tr}_\mathrm{C}\left(\hat{\rho}_\mathrm{C}^2(0)\right) = \mathrm{const} \tag{G.3.1}$$

stays constant for all λ. The associated purity of the relational system state reads

$$\mathscr{P}_\mathrm{S}[\hat{\rho}_\mathrm{S}] = \mathrm{tr}_\mathrm{S}(\hat{\rho}_\mathrm{S}^2) = d_\mathrm{C}^2\,\mathrm{tr}_\mathrm{S}\Big[\mathrm{tr}_\mathrm{C}(\hat{P}_\Psi\hat{\rho}_\mathrm{C})\,\mathrm{tr}_\mathrm{C}(\hat{\rho}_\mathrm{C}\hat{P}_\Psi)\Big] \tag{G.3.2}$$

$$= d_\mathrm{C}^2\sum_{kmn}\langle\varphi_k\otimes\chi_m|\Psi\rangle\,\langle\Psi|\hat{\rho}_\mathrm{C}\,|\chi_m\rangle\langle\chi_n|_\mathrm{C}\,\hat{\rho}_\mathrm{C}|\Psi\rangle\,\langle\Psi|\varphi_k\otimes\chi_n\rangle \tag{G.3.3}$$

$$= d_\mathrm{C}\sum_{kmn}\langle\Psi|\varphi_k\otimes\chi_n\rangle\,\langle\chi_n|\hat{\rho}_\mathrm{C}^2|\chi_m\rangle_\mathrm{C}\,\langle\varphi_k\otimes\chi_m|\Psi\rangle \tag{G.3.4}$$

$$= d_\mathrm{C}\,\langle\Psi|\hat{\rho}_\mathrm{C}^2|\Psi\rangle = \mathrm{tr}_\mathrm{C}(\hat{\rho}_\mathrm{C}^2) = \mathscr{P}_\mathrm{C}[\hat{\rho}_\mathrm{C}] \tag{G.3.5}$$

and remains constant as well. It immediately implies that the system evolution must be entirely unitary and the system Hamiltonian cannot contain any non-Hermitian terms.

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Statement of authorship

I hereby certify that I have authored this Dissertation entitled *The emergence of time with interactions in quantum and classical mechanics* independently and without undue assistance from third parties. No other than the resources and references indicated in this thesis have been used. I have marked both literal and accordingly adopted quotations as such. There were no additional persons involved in the intellectual preparation of the present thesis. I am aware that violations of this declaration may lead to subsequent withdrawal of the degree.

Dresden, 28th August 2023

Sebastian Gemsheim