

Time dependence in quantum mechanics

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Abstract. It is shown that the time-dependent equations (Schrödinger and Dirac) for a quantum system can be derived from the time-independent equation for the larger object of the system interacting with its environment, in the limit that the dynamical variables of the environment can be treated semiclassically. The time which describes the quantum evolution is then provided parametrically by the classical evolution of the environment variables. The method used is a generalization of that known for a long time in the field of ion-atom collisions, where it appears as a transition from the full quantum mechanical *perturbed stationary states* to the impact parameter method in which the projectile ion beam is treated classically.

PACS. 03.65.Bz Foundations, theory of measurement, miscellaneous theories (including Aharonov-Bohm effect, Bell inequalities, Berry's phase) – 34.10.+x General theories and models of atomic and molecular collisions and interactions (including statistical theories, transition state, stochastic and trajectory models, etc.) – 03.65.Sq Semiclassical theories and applications

1 Introduction

Originally Schrödinger [1] proposed his wave equation in time-independent form as an eigenvalue equation for the time-independent Hamilton operator, *i.e.*

$$(H - E)\Psi = 0, \quad (1)$$

the time-independent Schrödinger equation (TISE). Subsequently, this was generalized to consider quantum systems as being described by state vectors in Hilbert space and observables by Hermitian operators. Pairs of canonically conjugate operators satisfy Heisenberg commutation rules and thereby fulfill corresponding Heisenberg uncertainty relations. In a later paper [2] Schrödinger introduced a time-dependent Schrödinger equation (TDSE) and this version has found much wider application than the TISE even for time-independent Hamiltonians. On the one hand this is due to the technical reason that it is easier to solve the initial value problem of the TDSE than the boundary value problem of the TISE. On the other hand there is the deeper reason that our experience based on the classical world still conditions us to think in terms of physical processes proceeding from some initial state and developing in time to some final state.

Initially, Schrödinger postulated a TDSE involving the second time derivative of a real wavefunction. Indeed, his

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motivation was to derive a wave equation in direct analogy to electrodynamics based upon de Broglie's hypothesis of the wave – like behavior of microscopic material particles. Subsequently he realized that by admitting complex wavefunctions the TDSE need only involve the first time derivative. For a quantum system with time-independent Hamiltonian H_S the TDSE is

$$\left(H_S - i\hbar \frac{\partial}{\partial t} \right) \psi_S(x, t) = 0, \quad (2)$$

where $\{x\}$ are the system variables. Very quickly this form was generalized to include a time-dependent interaction Hamiltonian H_I

$$\left(H_S + H_I(t) - i\hbar \frac{\partial}{\partial t} \right) \psi_S(x, t) = 0. \quad (3)$$

Schrödinger arrived at the TDSE equation (2) by beginning with the TISE equation (1) and postulating that the wavefunction for a free particle should be a function of the argument $(px - Et)/\hbar$, where p is the linear momentum. Again this is clearly based on the analogy to plane-wave solutions of the classical wave equation. Many text books follow this “derivation” of the TDSE by beginning with the TDSE of the form equation (2) for a free particle and then simply postulating a generalization to the form of equation (3). Other text books rely on the fact that both of the pairs (p, x) and (E, t) are *classically* conjugate variables and by analogy to the operator replacement

$$p \rightarrow -i\hbar \frac{\partial}{\partial x} \quad (4)$$

make the replacement

$$E \rightarrow -i\hbar \frac{\partial}{\partial t} \quad (5)$$

to derive equation (2) from equation (1).

Since the TDSE equation (2) admits solutions which are linear superpositions of eigenstates of different energy, whilst the TISE equation (1) does not, (except when the coefficients of the superposition are real) and since equation (1) can be derived from equation (2) by a simple phase transformation, the TDSE is usually considered to be more “fundamental” than the TISE. Nevertheless, despite the intuitive appeal of the TDSE, there are several problems connected with its derivation and application to quantum-mechanical systems. The first is the non-equivalence in quantum mechanics of the replacements equation (4) and equation (5). Although p and $-i\hbar\partial/\partial x$ are operators in Hilbert space, whose expectation value gives the momentum, and H is also such an operator whose expectation value gives the energy E , the expression $-i\hbar\partial/\partial t$ is not such an operator. Rather, it is a parametric differentiation with respect to the c -number representing (classical) time. Correspondingly, although several authors have contrived to define one [3,4], there is no simple obvious definition of a Hilbert space operator T corresponding to time which would satisfy the canonical commutation relation

$$[H, T] = -i\hbar. \quad (6)$$

In view of this unsatisfactory situation, over the years many authors have suggested alternative derivations of an energy-time uncertainty relation [4]. All of them, however, rely upon the validity of the TDSE equation (2) for an isolated quantum system.

This brings us to the next point, namely, the interpretation of equation (2) involving a time-independent Hamiltonian. Clearly, the phase-transformation

$$\tilde{\psi}_{\mathcal{S}}(x, t) = \exp(i/\hbar E_{\mathcal{S}} t) \psi_{\mathcal{S}}(x) \quad (7)$$

in equation (3) leads to the TISE

$$(H_{\mathcal{S}} - E_{\mathcal{S}})\psi_{\mathcal{S}}(x) = 0. \quad (8)$$

It is sometimes stated (*e.g.* by Feynman and Hibbs [6]), that, “for this special solution the wavefunction oscillates with a definite frequency... which corresponds, in classical physics, to the energy”. This is suspect since the energy is not absolute, the zero can be placed arbitrarily. The question then arises, with which frequency (a positive number) does the wavefunction oscillate? This point troubled Schrödinger from the outset. Note, however, that any observable measured on a system described by equation (7) is time-independent. Hence, for a closed quantum system with a time-independent Hamiltonian (and hence of fixed energy) only the TISE is relevant to its description. The question of linear superposition of states of different energy is more subtle and will be discussed later in the paper.

When a time-dependent interaction is introduced as in equation (3) the TDSE *is* clearly the relevant equation. However, as was recognized by Born, Heisenberg and Jordan [7] at the dawn of quantum mechanics, time-dependent interactions always imply coupling to an external *classical* source. Hence, although this is not usually mentioned, the TDSE equation (3) is a mixed quantum-classical equation.

Here, we offer an alternative derivation of the TDSE which (i) explains its mixed quantum-classical nature, and (ii) avoids the problems described which arise when the TDSE is simply postulated. From the point of view of quantum mechanics we postulate only the validity of the TISE equation (1) for a closed quantum object in which only time-independent Hilbert space operators are defined, *i.e.*, all the interactions are also expressed in terms of time-independent Hilbert space operators. The closed quantum object is divided into two parts, the system \mathcal{S} and its environment \mathcal{E} . In the limit that the environment is so large (precisely what this means depends upon the object under discussion) that \mathcal{E} is practically unchanged in its interaction with \mathcal{S} , it can be treated *semiclassically*. In this limit the variables of the environment undergo a time development described by classical equations involving a classical time parameter as measured by a clock. In the same approximation the system \mathcal{S} develops in time governed by the TDSE with an effective time-dependent Hamiltonian whose time dependence arises from the interaction with \mathcal{E} *via* the implicit time-dependence of the classical environment variables. In this way time always arises in quantum mechanics as an externally defined classical parameter and time-dependent Hamiltonians from the interaction with a classical environment. The most important example of the interaction of a quantum system \mathcal{S} with an environment is the act of observation or measurement, when time is defined by the classical (macroscopic) measuring device. Furthermore, since all measurements ultimately involve the detection of charged particles, photons, or heat (phonons) these are the types of environment we shall consider. Their classical motion is described by Newton or classical wave equations and hence the time parameter introduced into the TDSE for the quantum system is *identical* with that entering the classical equations.

In deriving a TDSE from the TISE of a composite system, we will separate the environment \mathcal{E} from the system \mathcal{S} adiabatically. Adiabatic separation has a long tradition in several areas of theoretical physics, probably it is best known as the Born-Oppenheimer approximation in the context of molecular problems. However, also in collision physics it can be traced through the “perturbed stationary states” (PSS) method of Mott and Massey [8] to the original 1931 paper of Mott [9], where he showed the essential equivalence of the time-independent PSS and time-dependent impact parameter approaches in the limit of high beam velocities, with the time defined by the variables of the *particle beam*. The PSS method is a generalization of the Born-Oppenheimer method. Interestingly, this method of molecular physics has become very popular recently in defining time in quantum gravity. Here time

is introduced into the time-independent Wheeler-de Witt equation by treating gravitation semi-classically but the matter field quantum mechanically, in a procedure that is similar to that used in the case of atomic collisions [10].

Starting with the TISE of equation (1) for $\mathcal{E} \otimes \mathcal{S}$ we will *derive* the TDSE equation (3) for \mathcal{S} . Thereby we will show that the *parametric* time derivative can be attributed to the action of the environment *operators* on the system. Similarly, we can relate the energy-time “uncertainty relation” for \mathcal{S} to a true (operator based) uncertainty relation for \mathcal{E} . Furthermore, it will be shown that the time-dependence $H_I(t)$ arises in a well-defined way from the interaction of \mathcal{S} with \mathcal{E} and that the time which arises is precisely the time describing the classical motion of \mathcal{E} *i.e.* the classical environment provides the clock for the quantum system.

It is clear that the procedure can now be continued in that \mathcal{S} , described by the TISE equation (8), can be considered as composed of \mathcal{S}' and \mathcal{E}' to define time and a TDSE for \mathcal{S}' . The extent to which the subdivision is valid depends on the accuracy with which the dynamics of \mathcal{E}' may be approximated (semi-) classically. More pragmatically, one might say that the position of the interface between the quantum and the classical worlds depends upon the degree of precision set (or achieved) by the measurement.

In Section 2 the interaction of a quantum system with a material environment is considered. The TDSE is derived by generalizing the procedure due to Briggs and Macek [5] who considered the particular case of an atom interacting with a particle beam. Then it is shown how the energy-time uncertainty relation arises. In Section 3 the general procedure is illustrated by the three generic examples of a system \mathcal{S} interacting with a particle beam or with a set of quantum oscillators (photons or phonons) as environment \mathcal{E} . Finally, the same procedure can be applied to transform the time-independent Dirac equation (TIDE) into the time-dependent Dirac equation (TDDE). Here it is interesting to observe that the time component of the spacetime of the quantum system actually arises from the implicit time variation of the *classical environment* variables, *i.e.* again it is this variation that provides the clock for the quantum system. The case of a linear superposition of energy eigenstates is considered in Section 4.

2 The emergence of time

We begin by decomposing the total Hamiltonian H for the large object in equation (1) into

$$H = H_{\mathcal{E}} + H_I + H_{\mathcal{S}} \tag{9}$$

with the Hamiltonians $H_{\mathcal{E}}$ for the environment and $H_{\mathcal{S}}$ for the quantum system. For convenience we assume a coordinate representation for \mathcal{E} with a standard form of $H_{\mathcal{E}} = K + V_{\mathcal{E}}$ where the potential energy is a function of coordinates only, $V_{\mathcal{E}} = V_{\mathcal{E}}(R)$ and the kinetic energy is written in mass scaled coordinates $R = (R_1, R_2, \dots)$ as a

sum over all degrees of freedom, $i = 1, \dots, n$:

$$K = -\frac{\hbar^2}{2M} \sum_i^n \frac{\partial^2}{\partial R_i^2}. \tag{10}$$

Almost all relevant environments can be cast into this form as will be illustrated in Section 3. In equation (9) H_I describes the coupling between \mathcal{S} and \mathcal{E} . However, as a consequence of the environment being “large” compared to the quantum system, the coupling is asymmetric in the sense that the state χ of the environment \mathcal{E} depends negligibly on the variables $\{x\}$ of the system \mathcal{S} while the system state ψ depends on the environment variables $\{R\}$. Accordingly, we write the total wavefunction Ψ in equation (1) as

$$\Psi(x, R) = \chi(R)\psi(x, R). \tag{11}$$

Having defined the wavefunction of the system we can express what a “large” environment means in terms of an *asymmetry condition*. It defines and distinguishes, in the decomposition of H , environment \mathcal{E} and system \mathcal{S} through the respective energy expectation values by

$$\langle \chi | H_{\mathcal{E}} | \chi \rangle_R \equiv E_{\mathcal{E}} \gg E_{\mathcal{S}} \equiv \langle \chi | U_{\mathcal{S}} | \chi \rangle_R, \tag{12}$$

where

$$U_{\mathcal{S}}(R) = \langle \psi(x, R) | H - V_{\mathcal{E}} | \psi(x, R) \rangle_x. \tag{13}$$

A more detailed discussion of the requirements for the validity of equation (11) and a derivation of the form of $U_{\mathcal{S}}(R)$ in equation (13) is given in the Appendix, starting from a formally exact “entangled” wavefunction $\Psi(x, R) = \sum_n \chi_n(R)\psi_n(x, R)$ for the complete object composed of system and environment. It will be shown there that the asymmetry condition equation (12) justifies *a posteriori* the form equation (11) of the wavefunction. As is well-known from adiabatic approximations in other contexts a wavefunction of the form equation (11) can only be justified *a posteriori* if a condition such as equation (12) is fulfilled.

Backed by the asymmetry condition (Eqs. (12, 13)) we determine χ from the eigenvalue equation

$$(H_{\mathcal{E}} + U_{\mathcal{S}}(R) - E)\chi(R) = 0. \tag{14}$$

The term $U_{\mathcal{S}}$ represents the very small influence \mathcal{S} has on the state of the environment. The environment is taken to be a large, quasiclassical system so that its state vector χ can be approximated by a semiclassical wavefunction

$$\chi(R) = A(R) \exp(iW/\hbar), \tag{15}$$

where $W(R, E)$ is the (time-independent) action of the *classical* Hamiltonian $H_{\mathcal{E}}$.

Inserting equations (9, 11) into equation (1) we get using equation (14)

$$\chi [U_{\mathcal{S}}(R) - H_{\mathcal{S}} - H_I] \psi(x, R) = \frac{\hbar}{i} \sum_i C_i \frac{\partial \psi(x, R)}{\partial R_i}, \tag{16}$$

where the operator C_i is given by

$$C_i = \chi \frac{1}{2M} \frac{\hbar}{i} \frac{\partial}{\partial R_i} + \frac{1}{M} \frac{\hbar}{i} \frac{\partial \chi}{\partial R_i}. \quad (17)$$

In accordance with the asymmetry condition equation (12) we have assumed that

$$[H_I, \chi] = 0. \quad (18)$$

Note that equation (16) is an equation for the wavefunction ψ while χ , already fixed in equation (14) acts like a potential, *i.e.* an operator.

With the form of equation (15) for χ we can write for the operator C_i of equation (17)

$$C_i = \chi \left[\frac{1}{2M} \frac{\hbar}{i} \left(\frac{\partial}{\partial R_i} + \frac{2}{A} \frac{\partial A}{\partial R_i} \right) + \frac{1}{M} \frac{\partial W}{\partial R_i} \right] \quad (19)$$

where $(\partial W / \partial R_i) M^{-1} = P_i / M = dR_i / dt$ is the *classical* momentum vector of the environment \mathcal{E} . The most important step to turn equation (16) into a TDSE for the system \mathcal{S} and its wavefunction ψ is to keep only the term of lowest order in \hbar in equation (19) which reduces the operator C_i to

$$C_i \approx \chi \frac{1}{M} \frac{\partial W}{\partial R_i} = \chi \frac{P_i}{M} = \chi \frac{dR_i}{dt}. \quad (20)$$

From this approximation for C_i emerges the classical time on the right hand side of equation (16) through

$$\sum_i C_i \frac{\partial}{\partial R_i} = \chi \sum_i \frac{dR_i}{dt} \frac{\partial}{\partial R_i} = \chi \frac{d}{dt}. \quad (21)$$

Since the R_i are reduced to classical variables $R_i(t)$, equation (16) can be written

$$(H_S + H_I(t) - i\hbar \left. \frac{\partial}{\partial t} \right|_x - U_S(t)) \psi(x, t) = 0, \quad (22)$$

where $H_I = H_I(t)$ is now an explicitly time-dependent interaction. Here we emphasize that the time derivative is to be taken with $\{x\}$ fixed since it arises from the derivative w.r.t. the independent (quantum) variables $\{R\}$. Since, from equation (13), the potential U_S (unlike H_I) is independent of the system variables, a phase or gauge transformation

$$\psi = \exp[i/\hbar \int_{-\infty}^t (U_S(t')) dt'] \tilde{\psi} \quad (23)$$

leads to the TDSE for the quantum system alone,

$$(H_S + H_I(t) - i\hbar \frac{\partial}{\partial t}) \tilde{\psi}(x, t) = 0. \quad (24)$$

Having accepted equation (24), the whole structure of time-dependent quantum mechanics, *e.g.*, the transition to Heisenberg and interaction pictures, time-dependent perturbation theory, the derivation of a Liouville equation etc., can be developed as usual. Indeed, Briggs and

Macek [5] show explicitly that, in the same approximations that lead to equation (24), the time-independent T -matrix element for the system plus environment reduces to a time-dependent transition amplitude for the system alone. Similarly, a precise consideration of the nature of the interaction $H_I(t)$ should allow one to derive the many variations of stochastic Schrödinger equations that have been proposed to model the interaction of a quantum system with an environment or measuring device.

One further observation must be made. This is the question of the “uncertainty relation” for energy and time. Since there is no canonical operator for time there is no uncertainty relation in the sense of Heisenberg. That quoted in many books arises from the basic property of the Fourier transform from energy space to time space in which time appears as a mathematical, rather than a mechanical (physical) variable. However, within the approximation of the environment as a classical object a time-energy relation for the quantum system can be *derived* from the uncertainty relation for the environment, since it is the position variable of the environment that defines the classical time. First treating the environment quantum-mechanically, for any two operators related to the environment, one has

$$\Delta A \Delta B \geq \frac{1}{2i} \langle [A, B] \rangle. \quad (25)$$

In particular if $A = H_{\mathcal{E}}$ and $B = R_i$, then

$$\Delta H_{\mathcal{E}} \Delta R_i \geq \hbar/2 \frac{\langle P_i \rangle}{M}. \quad (26)$$

Now, in the classical limit for the environment variables, $\Delta R_i = v_i \Delta t$ and $v_i = P_i / M = \langle P_i \rangle / M$, so that we obtain

$$\Delta E_{\mathcal{E}} \Delta t \geq \hbar/2. \quad (27)$$

However, from equations (14, 13) $E = E_{\mathcal{E}} + E_{\mathcal{S}}$ where E is the fixed total energy. Hence, $|\Delta E_{\mathcal{E}}| = |\Delta E_{\mathcal{S}}|$ and equation (27) becomes

$$\Delta E_{\mathcal{S}} \Delta t \geq \hbar/2, \quad (28)$$

i.e. the energy-time uncertainty for the quantum system emerges from the fluctuations in the expectation values of the environment variables.

Note that for the derivation and application of this uncertainty relation it is necessary that the quantum system interacts with the environment through the potential H_I . It is this interaction that leads to the uncertainty in the system energy $E_{\mathcal{S}}$. In the same way the uncertainty in the time Δt arises from the time development described by equation (24) where the time is the classical time defined by the classical time-development of the environment.

3 Specific examples

To illustrate the general approach of Section 2 in more detail we will consider three examples which represent the

most common ways in which quantum systems are probed and measured. First we will discuss the interaction of the quantum system with a particle beam, then we will describe the interaction with a “bath” of oscillators, *e.g.* photons or phonons. Finally, we will show that also in a relativistic environment the time-dependent Dirac equation (TDDE) can be derived from the time-independent Dirac equation (TIDE) in a way analogous to the non-relativistic case.

3.1 A particle beam as environment

A particle beam of fixed momentum $\mathbf{P} = \hbar\mathbf{K}$ interacting with a quantum system was considered by Briggs and Macek [5]. The asymmetry condition equation (12), necessary to separate environment and quantum system, is achieved when the beam kinetic energy $P^2/2M$ is much greater than the energy differences ΔE_S in the system states populated as a result of the interaction. The (semi-) classical limit for the environment, necessary to justify equation (15), is reached when \mathbf{P} is so large that the de Broglie wavelength is far shorter than the extent of the quantum system. In this case the WKB-wavefunction for a free beam-particle is the exact quantum solution. We may choose a coordinate system with the z -axis along the beam direction,

$$\chi(X, Y, Z) = (2\pi)^{-3/2} \exp(iP_Z Z/\hbar), \quad (29)$$

where $\mathbf{P} = (0, 0, P_Z)$ is the classical momentum of the beam. Since equation (29) is of the form equation (15) it leads directly to the emergence of time according to equation (21),

$$\frac{P_Z}{M} \frac{\partial}{\partial Z} = \frac{dZ}{dt} \frac{\partial}{\partial Z} = \frac{d}{dt}. \quad (30)$$

3.2 A quantized field as environment

In the second example the environment comprises a collection of quantum oscillators with mode frequencies ω_k , *i.e.* photons or phonons. Then the Hamiltonian H_E can be written as a sum over field modes

$$H_E = \sum_k \left[\frac{P_k^2}{2m_k} + \frac{\omega_k^2 Q_k^2}{2} \right], \quad (31)$$

where $m_k = 1$ for photons. The field operators satisfy the usual commutation relations

$$[Q_k, P_{k'}] = i\hbar\delta_{kk'} \quad (32)$$

with

$$P_k = -i\hbar \frac{\partial}{\partial Q_k}. \quad (33)$$

The energy E_E is the eigenenergy of equation (31) and $\chi(Q)$ is an eigenvector in the Q -representation which need

not be specified further here. Then, using equation (11), we write

$$\Psi(x, Q) = \chi(Q)\psi(x, Q). \quad (34)$$

Substitution of Ψ into equation (1) leads as before to equation (16). The quasiclassical field limit leads now for the operator C_i in equation (16) to the replacement

$$C_i = \frac{P_k}{m_k} \chi \rightarrow \chi \frac{dQ_k}{dt} \quad (35)$$

where $Q_k(t)$ is now a *classical* field amplitude. Since equation (35) is of the same form as equation (20) time emerges as in equation (21) and the TDSE is established for the case of a quasi-classical field as environment.

3.3 An example of relativistic dynamics

Finally, we consider how the relativistic generalization of the transition from the TISE to TDSE occurs for fermions, *i.e.* how a time-independent Dirac equation (TIDE) for system plus environment becomes a time-dependent Dirac equation for the system. To keep the derivation simple we restrict ourselves to a quantum object of two fermions whose spins are uncoupled and where the energies are such that pair production can be neglected. In this case the classical limit will be where the relativistic mass M of the environment fermion becomes much greater than that of the system fermion m . The TIDE can be written formally as in equation (1) with the Hamiltonian equation (9) whose elements are now defined as,

$$H_E = c\alpha_E \mathbf{P}_E + V_E(\mathbf{R}) + \beta_E M c^2 \quad (36)$$

$$H_S = c\alpha_S \mathbf{P}_S + V_S(\mathbf{x}) + \beta_S m c^2. \quad (37)$$

The potentials V_E, V_S are potentials acting separately on environment and system particles, respectively and can be neglected in what follows, *i.e.* we consider two free fermions interacting through a coupling Hamiltonian H_I . The total wavefunction Ψ is then written as in equation (11) but is now a product of a spinor $\chi(\mathbf{R})$ representing the spin state of \mathcal{E} and a spinor $\psi(\mathbf{x}, \mathbf{R})$ representing the spin state of the system but depending parametrically on the space variables of the environment.

The analogue of equation (16) now becomes

$$[\chi(E_E - E + H_S + H_I) - c\alpha_E \chi \mathbf{P}_E] \psi(\mathbf{x}, \mathbf{R}) = 0. \quad (38)$$

However, the operator $c\alpha_E$ is just the velocity operator [11] which for positive energy solutions has the form $c^2 \mathbf{P}_E / E_E$. For free motion the exact solution is the same as the semiclassical one. However, Jensen and Bernstein [12] have shown that even when potentials as in equations (36, 37) are retained, in lowest order semiclassical approximation the *form* of the velocity operator is unchanged. Then, in this limit, with $E_E = M c^2$ one has

$$\mathbf{P}_E / M = \mathbf{v}_E = \frac{d\mathbf{R}}{dt} \quad (39)$$

so that equation (38) becomes

$$[H_S + H_I - i\hbar \mathbf{v}_\varepsilon \nabla_R] \psi(\mathbf{x}, \mathbf{R}(t)) = U_S \psi(\mathbf{x}, \mathbf{R}(t)) \quad (40)$$

or

$$\left[H_S + H_I - i\hbar \frac{\partial}{\partial t} \Big|_x \right] \psi(\mathbf{x}, t) = U_S(t) \psi(\mathbf{x}, t). \quad (41)$$

With the phase transformation equation (23) one has

$$\left[H_S + H_I - i\hbar \frac{\partial}{\partial t} \right] \tilde{\psi}(\mathbf{x}, t) = 0, \quad (42)$$

the time dependent Dirac equation. Here, it is interesting to note that the time coordinate of the *quantum system* spacetime arises from the space coordinate of the *classical environment*.

4 Superposition of eigenstates

It must be emphasized that the appearance of $-i\hbar\partial/\partial t$ and $H_I(t)$ in equation (24) are completely coupled; either they both appear or neither do. Hence, it is inconsistent to put $H_I(t) = H_I$ in equation (24) to zero. If this is done, however, then the Hamiltonian of the system becomes time-independent and a transition to the TISE of equation (8) can be made, removing the term $-i\hbar\partial/\partial t$ and illustrating its direct coupling to $H_I(t)$.

Indeed, were H_I zero, the TDSE equation (24) cannot be derived, since the Hamiltonian equation (9) is then fully separable in x and R and instead of the *approximation* equation (11) one has an *exact* solution of the form $\Psi(x, R) = \chi(R)\psi(x)$. However, if H_I is not identically zero, for all R , then in the approximation described one can derive the TDSE equation (24) for the quantum system.

Note that at the level of equation (24), energy conservation between system and environment has been abandoned. The energy of the classical environment is viewed as not being changed by the coupling to the quantum system. This means that the environment can act as an infinite source or sink of energy for the system and the coupling $H_I(t)$ invokes transitions between different energy states of the system.

To re-iterate, if $H_I(x, R)$ is not identically zero then, in the approximations described above, one can derive the TDSE equation (24) for the quantum system alone. However, this *does not* preclude the possibility that $H_{\mathcal{E}\mathcal{S}}(x, R)$ is zero for some R , corresponding in the classical limit to $H_I(t)$ being zero for some times. In times when $H_I(t)$ is zero, the solution of equation (24) would imply that $\tilde{\psi}(x, t)$ could be a linear combination of eigenstates of H_S , each component of this combination acquiring a phase accumulation as $\exp(-iE_m t/\hbar)$, where E_m is some eigenvalue of H_S alone. That is, although the interaction with the environment is switched off, there appears to be still a time dependence. This is not inconsistent with our derivation however, since such effects of free time propagation are

only physically detectable if the system is first prepared in some state by a pulse $V_1(x, t)$ of interaction and probed later by a further pulse $V_2(x, t)$. That is $H_I(t)$ is not identically zero for all times. It is very important to realize that this experiment must be considered as a whole and hence, as a time-dependent problem where time is defined externally by the pulses and in particular the time interval between them. The full Hamiltonian equation (22) can be written as

$$H_S + H_I(t) \equiv H_S + V_1(x, t) + V_2(x, t). \quad (43)$$

To speak of free propagation without preparation and detection is meaningless. Situations where such two-pulse interactions occur are in beam-foil spectroscopy (first interaction, preparation by the foil; second interaction, detection of the emitted photon) or in pump-probe femtosecond spectroscopy, for example. In both cases a linear superposition of eigenstates is prepared, then follows a period of free propagation and then detection. However, the period is determined in the first example by the time-of-flight of the (classical) particle beam, in the second example by the externally fixed delay between pump and probe pulse. Hence, in both cases the classical environment defines the period of time. We can conclude that in our approach the superposition of eigenstates is always the result of a time-dependent interaction and must be described correspondingly.

5 Summary

We began our considerations with a time-independent stationary state of a complete object comprising system and environment described by the fully quantum mechanical TISE. The semiclassical treatment of the environment \mathcal{E} with the requirement that its own state and energy to zeroth order are unaffected by the quantum system \mathcal{S} , has led to a TDSE for this system in which the quantum variables of the environment are replaced by classical variables. The interaction with the environment then appears as explicitly time-dependent and the motion of the environment provides a time derivative which monitors the development of the quantum system. This demonstrates that the TDSE is in fact a mixed quantum-classical equation. If the interaction with the environment is ignored *i.e.* the quantum system is closed, then time is reduced to a mere mathematical variable and can be removed entirely by the simple phase transformation equation (7) leading to the TISE of equation (8). This has the consequence that system and environment are fully decoupled implying that the environment can no longer provide time for the system. Formally, one can see this from the uncertainty relation equation (28). As $H_I \rightarrow 0$, the energy exchange between environment and system vanishes and \mathcal{E} and \mathcal{S} separately become isolated without uncertainty in their respective energy. Hence, in equation (28) with $\Delta E_S \rightarrow 0$ we get $\Delta t \rightarrow \infty$. In this sense time arises and is meaningful for a quantum system only when interaction with a quasi-classical external environment defines a clock with which the time development is monitored.

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Appendix

In the following we will show under what approximations and with which consequences an exact or “entangled” wavefunction,

$$\Psi(x, R) = \sum_n \chi_n(R) \psi_n(x, R) \quad (44)$$

for the large object described by the Hamiltonian H in equation (1), leads to the product wavefunction equation (11). This form of the wavefunction describes a state of $H = H_{\mathcal{E}} + H_{\mathcal{S}} + H_{\mathcal{I}}$ if the system \mathcal{S} and the environment \mathcal{E} are weakly coupled under the asymmetry condition equation (12). Without loss of generality we may assume the ψ_n to be orthonormal for each R , *i.e.* $\langle \psi_n | \psi_m \rangle = \delta_{nm}$, where here and in the following brackets $\langle | \rangle$ denote integration over system variables x only.

We first proceed exactly as in the Born-Oppenheimer, or better, perturbed stationary states (PSS) approximation of molecular physics [8] where equation (44) is substituted in $H_{\mathcal{E}} + H_{\mathcal{S}} + H_{\mathcal{I}} - E|\Psi\rangle = 0$ and a projection is made onto a particular state ψ_m to give

$$\sum_n \langle \psi_m | H_{\mathcal{E}} + H_{\mathcal{S}} + H_{\mathcal{I}} - E | \psi_n \rangle \chi_n = 0. \quad (45)$$

Making use of the explicit form of $H_{\mathcal{E}}$ given in equation (10) we see that equation (45) describes a state χ_m of the environment “closely coupled” to all other states χ_n :

$$\begin{aligned} H_{\mathcal{E}} \chi_m + \sum_n \langle \psi_m | H_{\mathcal{S}} + H_{\mathcal{I}} | \psi_n \rangle \chi_n \\ - \sum_{n,i} \left[\langle \psi_m | \frac{\hbar^2}{2M} \frac{\partial^2}{\partial R_i^2} | \psi_n \rangle + \langle \psi_m | \frac{\partial}{\partial R_i} | \psi_n \rangle \frac{\hbar^2}{2M} \frac{\partial}{\partial R_i} \right] \chi_n \\ = E \chi_m. \end{aligned} \quad (46)$$

This is the full quantum equation for the environment whose states χ_n are mixed by the “back-coupling” from the system. The first set of coupling terms on the l.h.s. of equation (46) are called potential couplings and usually the ψ_n are chosen to diagonalize these terms. The remaining terms are the “dynamical couplings”, since their off-diagonal matrix elements describe changes in the state of the quantum system induced by the motion of the environment. Clearly, in order to fulfill the conditions that we demand for separation of environment and system, it is necessary that all off-diagonal couplings are small, *i.e.* the environment is insensitive to changes in the state of the system. Then equation (46) reduces to the single-channel equation

$$(H_{\mathcal{E}} + E_m(R) - E) \chi_m(R) = \sum_i \langle \psi_m | \frac{\partial}{\partial R_i} | \psi_m \rangle \frac{\hbar^2}{2M} \frac{\partial \chi_m}{\partial R_i} \quad (47)$$

where

$$E_m(R) = \langle \psi_m | H_{\mathcal{S}} + H_{\mathcal{I}} - \sum_i \frac{\hbar^2}{2M} \frac{\partial^2}{\partial R_i^2} | \psi_m \rangle. \quad (48)$$

The dynamical coupling involving the second derivatives $\partial^2/\partial R_i^2$ has been incorporated formally in $E_m(R)$. However, in connection with the semiclassical approximation for χ_m which must be made to derive the TDSE for the system, it is consistent to neglect this term. This is shown explicitly in Section 2 in the reduction of the operator C_i . Note that this forces a choice of the environment such that the major R -dependence is contained in the χ_m and the ψ_m are slowly varying functions of R . Then, since

$$\langle \psi_m | \frac{\partial^2}{\partial R_i^2} | \psi_m \rangle = \sum_n |\langle \psi_m | \frac{\partial}{\partial R_i} | \psi_n \rangle|^2, \quad (49)$$

the requirement that the term on the l.h.s. of this equation is small ensures that the off-diagonal dynamical couplings in equation (46) are also small.

If the ψ_m can be chosen real, the dynamical coupling terms on the r.h.s. of equation (47) vanish. If the ψ_m are complex, these terms give rise only to geometric (or Berry) phases that can be accounted for by a phase transformation of the χ_n . Effectively, then equation (47) reduces to the eigenvalue equation

$$(H_{\mathcal{E}} + E_m(R) - E) \chi_m(R) = 0 \quad (50)$$

for the state of the environment when the quantum system is in the state ψ_m . Note that the environment is still coupled to the system in that the different states of the system provide separate potential surfaces $E_m(R)$ for the motion of the environment. The complete independence of the environment from the precise state of the system is achieved in the approximation that the *different* $E_m(R)$ can be replaced by an average potential leading to a common R dependence for all $\chi_m(R)$, *i.e.*, $\chi_m = a_m \chi$, where the a_m are constants. This gives the simplified form of equation (44)

$$\Psi(x, R) = \chi(R) \sum_n a_n \psi_n(x, R) \equiv \chi(R) \psi(x, R) \quad (51)$$

corresponding to the ansatz of equation (11). Similarly equation (50) becomes identical to equation (14), where the averaged potential $U_{\mathcal{S}}$ of equation (13) assumes the form

$$U_{\mathcal{S}}(R) = \langle \psi | H - V_{\mathcal{E}}(R) | \psi \rangle = \sum_m |a_m|^2 E_m(R) \quad (52)$$

with $E_m(R)$ from equation (48).

Note that the product ansatz equation (51) (Eq. (11) of the text) and the environment equation (14) evaluated in the lowest order WKB approximation lead directly to the TDSE equation (24) for the quantum system. The analysis of this appendix shows how the environment must be chosen “large enough” so that it is insensitive to the back-coupling from the system. This insensitivity is necessary to derive an effective TDSE from the TISE for the composite object of system coupled to environment.

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