Decay Rates and Survival Probabilities in Open Quantum Systems

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(Received 3 September 2002; published 6 December 2002)

We provide the first statistical analysis of the decay rates of strongly driven 3D atomic Rydberg states. The distribution of the rates exhibits universal features due to Anderson localization, while universality of the time dependent decay requires particular initial conditions.

DOI: 10.1103/PhysRevLett.89.263601 PACS numbers: 42.50.Za, 05.45.Mt, 05.60.Gg, 72.15.Rn

The macroscopic transport properties of classical and quantum systems sensitively depend on the dynamics of their microscopic constituents. Whereas regular Hamiltonian dynamics implies the quasiperiodic confinement of phase space density, chaotic motion and disorder generically induce diffusionlike probability transport exploring all accessible phase space at sufficiently long times. In low-dimensional, disordered quantum systems Anderson localization efficiently inhibits diffusive transport through quantum interference, as first predicted by Anderson for the charge transfer across disordered solid state samples. Later on it was realized that chaos can substitute for disorder in Anderson’s scenario, leading to dynamical localization [1,2] of quantum probability transport. However, as a further complication, quantum systems with classically nonintegrable Hamiltonian dynamics (or, in the absence of a clear classical analog, with strongly coupled degrees of freedom) most often do not feature purely chaotic but rather mixed regular chaotic dynamics: besides the chaotic component of phase space the latter also comprises regular regions separated from the chaotic domain by fractal structures such as cantori [3]. Hence, dynamically localized quantum transport may be amended by quantum tunneling from regular regions or by semiclassical localization in the vicinity of partial phase space barriers [4].

A rather robust measure of transport is the transmission or decay probability of some initial probability distribution across or from a confined region Ω of phase space. Whereas the transmission problem immediately suggests a scattering approach, decay is most conveniently described by the norm || PΩ · U |φ0⟩ || of the time evolved initial state |φ0⟩ upon projection PΩ on the phase space domain we want to characterize. If Ω is confined by an absorbing boundary, attached to some leads which allow for transport to infinity, or coupled to some continuum of states, then || PΩ · U |φ0⟩ || will decrease monotonically in time, for generic |φ0⟩ [5–8]. Given the spectral decomposition of the Hamiltonian, this finite leakage from Ω can be accounted for by associating nonvanishing (exponential) decay rates Γj with eigenstates |ei⟩ with nonvanishing support on Ω. Given some initial |φ0⟩ = PΩ |φ0⟩, the survival probability within the domain Ω boils down to [6]

\[ P_{\text{surv}}(t) = \| P_{\Omega} \cdot U |\phi_0 \rangle \| = \sum_j w_j \exp(-\Gamma_j t). \tag{1} \]

All information on the decay process is now encoded [9] (i) in the set of decay rates—which is a global spectral property of the problem—and (ii) in the expansion coefficients wj = |〈φ0|ei⟩|^2 of the initial wave packet in the eigenbasis, what is a specific representation of the initial condition, and a local property to the extent that |φ0⟩ is localized. With these premises, our initial assertion on the crucial importance of microscopic dynamics for macroscopic transport leads to the guiding question of our present contribution [9,10]: How do classically mixed regular-dynamics affect these global and local spectral properties, and, consequently, the time dependence of Psurv? While, recently, a considerable corpus of literature has addressed this problem within the context of simple models of mesoscopic transport [10,11], we shall here underpin our rather general answer by a numerically exact treatment of highly excited three-dimensional Rydberg states under strong microwave driving [12]. These are paradigmatic objects to (theoretically and experimentally) study [6,9,12,13] quantum probability decay in the presence of tunneling as well as semiclassical and dynamical localization, and allow a natural and clean definition of Psurv and the associated projection PΩ, without any approximations.

Let us start with a brief reminder of dynamical localization in periodically driven hydrogen Rydberg atoms, to establish the analogy between the general transport problem depicted above and our specific choice of its physical realization: The atoms are initially prepared in an unperturbed atomic eigenstate |φ0⟩ = |n0ℓ0m0⟩ labeled by the principal quantum number n0, the angular momentum ℓ0, and the angular momentum projection m0. For linearly polarized coherent driving (which we treat in dipole approximation) of amplitude F at frequency ω, m0 is a good quantum number inherited from the rotational symmetry of the problem, and the atomic excitation process proceeds through the subsequent absorption and/or emission of photons from/into the field, along a sequence of near resonantly coupled states |nℓ⟩. Provided F is
large enough compared to the attractive force exerted on the electron by the nucleus, the classical dynamics of the driven Rydberg electron initially launched along a Kepler orbit turns chaotic, leading to an efficient energy absorption also on the quantum level, which finally leads to the ionization of the atom. Hence, we define the electronic survival probability as the remaining bound state population after an interaction time $t$, with $P_{\Omega}$ the projector on the bound state component of Hilbert space. The $\Gamma_j$ in Eq. (1) then become the ionization rates of the Floquet eigenstates $|\epsilon_j\rangle$ of the atom in the field, and the $\omega_j$ the associated overlaps (averaged over one field cycle [6]) of $|\phi_0\rangle$ with $|\epsilon_j\rangle$. With some theoretical and numerical effort, all these quantities can be extracted from the fundamental Floquet eigenvalue problem, for typical parameter values of state of the art laboratory experiments [13].

The atomic ionization process is mapped on the Anderson model through the atomic localization parameter $L = \xi/\eta$ [2], with $\xi$ the localization length in units of the photon energy. $\eta$ is the ionization potential of $|\phi_0\rangle$, measured in units of $\omega$, and is completely determined by $n_0$, due to the angular momentum degeneracy of the hydrogen spectrum. Provided that $n_0$ — through its correspondence with the principal action of the classical dynamics — is chosen within the chaotic component of phase space (possibly garnished by nonlinear resonance islands and remnants of classically regular motion immersed in the “chaotic sea”), $\eta$ can be conceived as a measure of the extension of the domain of complex transport along the energy axis. If we identify $\eta$ with the sample length in the original Anderson problem and average over different realizations of a fixed value of $L \ll 1$, quantum suppression of transport through exponentially localized eigenfunctions over the quasiresonantly coupled states on the energy axis [2,7,14] implies a distribution $P(\Gamma) \sim 1/\Gamma$ of the ionization rates entering Eq. (1), in accord with the current theory [11] on open Anderson insulators.

Statistically independent realizations of a fixed localization parameter can be generated by simultaneous variation of $F$ and $\omega$, due to the relation $L \approx 6.66F^2n_0^2/\omega^{7/3}$ from the original theory on dynamical localization [2] in periodically driven, one-dimensional hydrogen atoms. While this theory has no quantitative predictive power [6,12], it is nonetheless known to give qualitatively correct predictions, even for 3D Rydberg states with not too large values of the angular momentum quantum number $\ell$. In the sequel we therefore use this quantity to guide our choice of $F$ and $\omega$ values.

Figure 1 shows the distribution of ionization rates $\Gamma$ of real 3D hydrogen Rydberg states and of a one-dimensional model atom (where the Rydberg electron is confined to 1D configuration space $z > 0$ defined by the polarization axis, with the Coulomb singularity at the origin [6,9]) exposed to a microwave field, within a Floquet zone (of width $\omega$ on the energy axis [6,13]) centered around the $n_0 = 70$ (3D) and $n_0 = 100$ (1D) Rydberg manifold. The different values of $L = 0.25 \ldots 2.0$ are realized by sampling the spectra over frequency ranges $\omega/2\pi = 13.16 \ldots 16.45$ GHz (1D) and $35.5 \ldots 36.1$ GHz (3D), within a Floquet zone of width $\omega$ centered around $n_0 = 70$ (3D) and $n_0 = 100$ (1D), respectively.

For small localization parameter $L = 0.25$, both the 1D model atom as well as the real object do exhibit ionization rates distributed according to the $\Gamma^{-1}$ law, over approximately 7 orders of magnitude from $\Gamma \approx 10^{-15}$ to $\Gamma \approx 10^{-8}$ a.u., in nice agreement with the prediction for decay from a disordered solid [11]. However, as the localization parameter is increased (by systematically increasing $F$ over the entire frequency range indicated above) to $L = 1.0$, we observe a depletion of the distribution at small rates, balanced by a decrease of the slope of $P(\Gamma)$ in an intermediate range $\Gamma \approx 10^{-10} \ldots 10^{-8}$ a.u. Such behavior is clearly incompatible with the simple picture of exponentially localized probability densities along the energy axis (due to dynamical localization of the eigenstates over the chaotic phase space component) [2,7,14], and suggests the presence of alternative transport mechanisms which compete with dynamically localized.

![Figure 1](image)

**FIG. 1.** Distribution of the ionization rates $\Gamma$ of microwave-driven (a) 1D and (b) 3D $m_0 = 0$ Rydberg states of atomic hydrogen, for three different values of the localization parameter $L = 0.25$ (diamonds), 0.5 (stars), 1.0 (circles), and 2.0 (pyramids; only in (a), because of the high cost of 3D calculations at the corresponding high field amplitudes). The distributions were generated, at fixed $L$, by sampling the Floquet spectra over the frequency (and corresponding amplitude, $F$) ranges $\omega/2\pi = 13.16 \ldots 16.45$ GHz (1D) and $35.5 \ldots 36.1$ GHz (3D), within a Floquet zone of width $\omega$ centered around $n_0 = 70$ (3D) and $n_0 = 100$ (1D), respectively.
diffusion [9,10]. As already anticipated in the introduction, such observation does not come as a surprise, since periodically driven Rydberg states exhibit a mixed regular chaotic phase space. Indeed, it is known from experimental as well as exact theoretical/numerical studies [9,12,15] of strongly perturbed atomic Rydberg systems, and, more recently, from mesoscopic systems with decay [10], that the eigenstates of such quantum systems can be classified according to their localization [9,10,16] (i) on regular and/or elliptic regions, (ii) along remnants of regular motion immersed in the chaotic sea (“separatrix/hierarchical states” living on “cantori”), and (iii) in the chaotic domain of phase space. Furthermore, elliptic regions as well as remnants of invariant tori are rather robust under changes of some control parameter such as $F$ in our present case [9].

Accordingly, the localization properties as well as the decay rates of the associated eigenstates tend to be less sensitive when changing $F$, whereas those states localized in the chaotic domain, with their decay rates essentially sensitive when changing $F$. Hence, we attribute the deviation from the $L^2$ law at large values of $F$ in Fig. 1 to the rapid increase of the decay rates of class (iii) states with $L$ (corresponding to the effective destruction of dynamical localization), whereas class (i) and (ii) states accumulate at intermediate $L$ values at the largest $L$ values considered here (we verified this assertion by inspection of the Husimi phase space representations of the Floquet eigenstates of the 1D problem [9]). At small values of $L$, the latter exhibit extremely small ionization rates below $\Gamma \approx 10^{-13}$ a.u. (or even below $\Gamma \approx 10^{-15}$ a.u., this is below our numerical precision, hence the plot does not extend into that domain), which leads to isolated, extremely narrow resonances in experimental or numerical photoionization cross sections [9,15]. Therefore, in this parameter regime, $P(\Gamma)$ is dominated by the decay rates of the dynamically localized class (iii) states, in agreement with the Anderson scenario. Let us also comment on the apparently distinct weight of class (i) and (ii) states in the 1D and the 3D situation, which is born out in Fig. 1: the depletion of the low-$\Gamma$ part is less pronounced for the real atom, and equally so the region of decreased slope at intermediate $\Gamma$ values. This is due to the contribution of high $\ell$ states (at fixed $m_0$) to the rate distribution — unavailable in 1D — which exhibit vanishing decay rates and do not contribute to the plotted distribution at small $L$. As $L$ is increased, these states contribute to $P(\Gamma)$ in the range $\Gamma < 10^{-11}$ a.u., such as to compensate for the reshuffling of low-$\ell$ states from small to intermediate $\Gamma$’s. This smooths the 3D distribution as compared to the 1D result.

Hence, we have seen how chaotic transport can mimic signatures of disorder in the quantum decay rate distribution, and induce amendments thereof due to peculiar structures of mixed regular chaotic dynamics. As is obvious from Eq. (1), $P(\Gamma)$ does not determine the (experimentally often very easily accessible [6,9,13]) survival probability alone, but only in conjunction with the expansion coefficients $w_j$. Starting from a general form $P(\Gamma) \sim \Gamma^{-\alpha}$, many authors infer a “universal” time dependence $P_{\text{surv}} \sim 1/\Gamma^{2-\alpha}$, leaning on the additional assumption $w_j \sim \Gamma_j$ [7,8]. The latter is nonetheless only justified if the initial state $|\phi_0\rangle$, which represents a local probe of the spectrum, is localized close to the boundary of $\Omega$ — which is the “edge of the sample” in a language adapted to the Anderson scenario, and the last near resonantly coupled bound state below threshold in the atomic problem. For a generic choice of $|\phi_0\rangle$ “within the sample,” i.e., somewhere within $\Omega$, this basic assumption is utterly misleading, as illustrated in Fig. 2. In Fig. 2(a), we show the distribution of the $w_j$ and of the corresponding $\Gamma_j$, on a double logarithmic plot, for $|\phi_0\rangle = |n_0 = 70, \ell_0 = 0\rangle$ in driven 3D hydrogen. The essentially uncorrelated $w_j$ and $\Gamma_j$ nicely correlate with the earlier finding that phase space localization properties and decay rates of strongly driven Rydberg atoms are not unambiguously related [9], and clearly devalidate the above proportionality assumption. On the other hand, it can easily be shown within a simple, one-dimensional Anderson model.
FIG. 3. Survival probability $P_{\text{surv}}(t)$ obtained from distributions as in Figs. 1 and 2 via Eq. (1). (a) 1D hydrogen, initial state $|\tilde{n}_0 = 100\rangle$, driving frequencies and localization parameters $\omega/2\pi = 16.45$ GHz, $L = 1.0$ (full line), $13.16$ GHz and 2.0 (dashed); (b) 3D hydrogen, $n_0 = 70$, $m_0 = 0$, $\ell_0 = 0$ (solid line), 15 (dashed), 45 (dotted), $\omega/2\pi = 35.6$ GHz, $L = 1.0$. In this latter case, different $w_j$ distributions are realized by changing the angular momentum $\ell_0$ of the initial atomic state, always leading to near-algebraic decay (like in 1D), though with distinct (and nonuniversal) decay exponents. Only fictitious expansion coefficients $w_j = \Gamma_j/\langle \Gamma \rangle$ induce asymptotically “universal” decay $P_{\text{surv}}(t) \sim t^{-\gamma}$ (dash-dotted line), $\gamma = 2 - \alpha \approx 1.1$ (indicated by the full line), with $\Gamma_j$, $\langle \Gamma \rangle$, and $\alpha \approx 0.9$ extracted from the $\Gamma < 10^{-10}$ a.u. part of the $L = 1.0$ data in Fig. 1(b).

how the generic situation of Fig. 2(a) continuously evolves into the situation of strongly correlated $w_j$ and $\Gamma_j$, as illustrated in Fig. 2(b): There, we calculated the decay rates of the eigenstates of a 1D tight binding Hamiltonian of length $N = 1000$, with diagonal disorder. Decay is introduced in this model by absorbing boundary conditions at one end, whereas a reflecting wall is imposed at the other. If $|\phi_{0j}\rangle$ is placed well inside the sample, expansion coefficients and decay rates are uncorrelated, though the distribution collapses onto a straight line $w_j \sim \Gamma_j$ as $|\phi_{0j}\rangle$ is shifted towards the open end (site $n_i = 1000$) of the sample. It is this latter situation which was realized in recent numerical calculations on periodically driven hydrogen atoms additionally subjected to an intense static electric field [7].

Given the results illustrated in Fig. 2, we can no longer hope for a universal decay law for the survival probability $P_{\text{surv}}(t)$—despite the rather universal features of $P(\Gamma)$. This is finally illustrated in Fig. 3, where we show $P_{\text{surv}}(t)$ for 1D and 3D hydrogen in the case of large $L$. While algebraic decay of $P_{\text{surv}}(t) \sim t^{-\gamma}$ is generic (even if modulated by local fluctuations [18]), simply due to the broad distribution of the $w_j$ and $\Gamma_j$, as illustrated in Figs. 1 and 2, the universal decay exponent $\gamma = 2 - \alpha$ is observed only in accidental cases—or if we reschedule the expansion coefficients of Fig. 2(a) according to $w_j \rightarrow \Gamma_j/\langle \Gamma \rangle$, with $\langle \Gamma \rangle$ the average rate over the entire spectrum, as illustrated in Fig. 3(b). In this, however, unrealistic case, $P_{\text{surv}}(t)$ asymptotically decays with $\gamma \approx 1.1$, which perfectly matches the prediction $\gamma = 2 - \alpha$, with $\alpha \approx 0.9$ extracted from the small $\Gamma (< 10^{-10}$ a.u.) part of the corresponding data set in Fig. 1(b). Therefore, universal features of the statistics of the decay rates of classically chaotic quantum systems do generically not carry over to the time dependent decay of the survival probability of some initial state prepared at an arbitrary location in phase space. This simply expresses the essential decorrelation of the phase space localization properties of the eigenstates of chaotic quantum systems and of their asymptotics—which alone determine their decay.

Support from EU Program QTRANS RTN-1999-08400, is gratefully acknowledged (S.W.).