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Recurrences in Driven Quantum Systems

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Abstract

We consider an initially bound quantum particle subject to an external time-dependent field. When the external field is large, the particle shows a tendency to repeatedly return to its initial state, irrespective of whether the frequency of the field is sufficient for escape from the well. These recurrences, which are absent in a classical calculation, arise from the system evolving primarily like a free particle in the external field.

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A very common experimental probe of a physical system is the study of its response to an imposed time-dependent perturbation. The behavior of quantum systems subject to strong time-dependent forces is of fundamental interest to a variety of situations such as field-enhanced decay in nuclei [1], highly excited atoms in microwave fields [2] and rf-driven Josephson junctions [3]. For weak external forces, a very successful approach is standard perturbation theory, where the response of a physical system is calculated in terms of correlation functions evaluated in the absence of the external perturbation. However, there are a steadily increasing number of experimental situations where the probe is so invasive that one does not expect perturbative approaches to provide even a qualitative picture of the behavior of the system. For example, the use of high intensity lasers in a variety of experiments during the last few years has revealed novel phenomena like the decreasing of ionization probability with increasing laser intensity [4]. In these situations, there is no simple theoretical picture akin to perturbation theory and so the analysis of quantum systems under strong driving remains an unsolved problem.

We consider the following problem: a quantum particle is in the ground state of a Hamiltonian whose spectrum is partly discrete and partly continuous. It is then subjected to a spatially uniform, time-dependent force. We are interested in the subsequent behavior of the system, particularly at strong driving. We avoid analysis in terms of quasienergies as is done in the Floquet method [5], as that method can only be used if the external forces are purely periodic.

We solve the time-dependent Schrodinger equation numerically and monitor the probability for the system to remain in its initial state as a function of time. We find that in regions of the parameter space characterized by strong driving, the system repeatedly exhibits a tendency to return to its initial state, leading to a series of recurrences in the initial state occupation probability; this effect is enhanced if the excitation frequency is above the threshold for ionization. These recurrences appear to have no classical analog.

Quantum recurrences in the dynamics of wavepackets in time-*independent* situations have been extensively discussed in the chemical literature [6], and have also been studied in

the context of quantum chaos [7]. For time-dependent Hamiltonians, Hogg and Huberman [8] have established a recurrence theorem: a system described by a Hamiltonian with a discrete spectrum subject to a nonresonant, bounded and time-periodic potential will return arbitrarily close to its initial configuration infinitely often. In our case, the Hamiltonian has a partly discrete and a partly continuous spectrum and so the above theorem does not apply.

We study a particle of mass m in a one dimensional potential under the influence of an external force, $F(t)$. For technical reasons, we use a vector potential to represent the forcing term. The Hamiltonian is

$$\mathcal{H} = \hbar\omega_0\left[-x_0^2\frac{\partial^2}{\partial x^2} + \frac{V}{\hbar\omega_0} + \frac{2}{(\hbar/x_0)}\int F(t)dt\left(\frac{x_0}{i}\frac{\partial}{\partial x}\right)\right] \tag{1}$$

where we have introduced length and frequency scales x_0 and ω_0 with $\hbar^2/2m = \hbar\omega_0 x_0^2$, and dropped an irrelevant time-dependent constant from the right hand side of Eq. (1). Hereafter, we work in dimensionless units and choose $F(t) = F_0\cos(\omega t)$. The Hamiltonian becomes

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + V - iS\mathcal{G}(t)\frac{\partial}{\partial x}, \tag{2}$$

where $S \equiv 2F_0/\omega$ is a dimensionless measure of the strength of the forcing term and $\mathcal{G}(t) = \sin(\omega t)$.

The numerical method that we adopt to solve this problem begins with an expansion of the wavefunction in a set of time-*dependent* basis states $\eta_k(t)$:

$$\Psi(t) = \sum_k X_k(t)\,\eta_k(t) \tag{3}$$

In order to account exactly for the influence of the external force, we choose these basis states such that they evolve according to the field-dependent piece of the Hamiltonian

$$i\frac{\partial\eta_k}{\partial t} = -iS\mathcal{G}(t)\frac{\partial\eta_k}{\partial x}. \tag{4}$$

The advantage of this procedure is that the choice of the basis at $t = 0$, $\eta_k(0)$, is dictated entirely by numerical convenience. We choose $\eta_k(0) = \exp(ikx)$, so that $\eta_k(t) =$

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$\eta_k(0) \exp(-iS\gamma(t)k)$ where $\gamma(t) = \int_0^t \mathcal{G}(t')dt'$. These considerations lead to a set of equations for the amplitudes $X_k(t)$:

$$i\dot{X}_k = k^2 X_k + \int \frac{dk'}{2\pi} \tilde{V}(k-k') e^{iS\gamma(t)(k-k')} X_{k'} \tag{5}$$

where $\tilde{V}(k)$ is the Fourier transform of $V(x)$.

For our numerical studies, we choose a smoothly varying potential, $V(x) = -\lambda \operatorname{sech}^2(x)$. For $\lambda = 0.75$, this potential admits one bound state $\psi_b(x) = \pi^{-1/2} \operatorname{sech}^{1/2}(x)$, with energy $E_b = -0.25$. We integrate Eq. (5) numerically using the Crank–Nicholson algorithm [9] to ensure unitarity and monitor the probability to return to the ground state, $P(t) \equiv |\langle\psi(0)|\psi(t)\rangle|^2$.

For low strengths ($S \lesssim 0.5$) we find that our numerical results agree with the predictions of first-order perturbation theory. For example, for frequencies above threshold ($\omega > 0.25$), we find that the probability of remaining in the ground state decays exponentially with a decay rate given exactly by Fermi's Golden Rule. Closer examination of the decay curve shows that superimposed on the exponential decay is a small periodic ripple whose frequency is twice that of the external force. The amplitude of this modulation drops rapidly as the strength of the external force is decreased. This small periodic term arises from coupling between the continuum states induced by the external force and is dropped in the typical Golden Rule calculation when the "rotating wave" approximation is made.

In the high strength regime the new phenomenon of recurrences appears. Figure 1, which shows the ground state occupation probability as a function of time for different values of the excitation frequency, clearly shows that perturbation theory fails to describe this situation. While we would intuitively expect rapid and complete decay, we see a surprising sequence of recurrences in the initial state occupation probability after nearly complete depletion. The recurrences become more pronounced at frequencies larger than the ionization threshold, although we expect that a particle supplied with sufficient energy to overcome the attractive potential should escape. Contrary to intuition, the system comes back to its initial state even though the density of sufficiently energetic quanta is substantial at these forcing strengths.

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We will now focus on the origin of these above threshold recurrences. At $S = 10$, the potential is clearly overwhelmed by the driving term. The system behaves largely like a quantum free particle subjected to the forcing field, the potential being responsible only for minor corrections to that behavior. We therefore proceed by first solving the problem of the free particle in the forcing field exactly and then adding in the potential through a Born approximation.

The momentum space wavefunction $\tilde{\psi}_f(k, t)$ of a free particle in the external field can be found from Eq. (2) with $V = 0$ as

$$\tilde{\psi}_f(k, t) = \tilde{\psi}(k, 0) \exp[-i(k^2 t + S\gamma(t)k)], \tag{6}$$

where the initial wavefunction, given by the Fourier transform of $\psi_b(x, 0)$, is $\tilde{\psi}(k, 0) = (1/\pi\sqrt{2})|\Gamma(1/4 + ik/2)|^2$.

A first Born approximation to the correct solution (valid in the case when the potential is small compared to the driving term) is a solution ψ_B of

$$i\frac{\partial \psi_B}{\partial t} - [k^2 + S\mathcal{G}(t)k]\psi_B = V\psi_f, \tag{7}$$

where the approximation lies in including only ψ_f instead of ψ_B on the right hand side. We solve this linear differential equation for ψ_B numerically and evaluate the approximate ground state occupation probability. Figure 2(a) compares the complete solution with the solution obtained by letting the initial wavepacket evolve under the influence of the forcing field only, while Fig. 2(b) shows the improvement gained with the Born correction. We see that most of the behavior of the exact solution is reproduced by the free particle result $|\langle\psi(0)|\psi_f(t)\rangle|^2$. The bimodal structures present in the full problem are missed, but the overall size of the recurrences is well reproduced. So the existence of decaying recurrences is primarily due to the dynamics of wavepacket evolution in the external field and is relatively independent of the potential.

While the results we have shown here are for a potential with only one bound state, we have also studied the potential $V(x) = -6\,\text{sech}^2(x)$, which has two bound states at $E_b = -4$

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and $E_b = -1$. For this problem we see qualitatively similar recurrences at $S = 10$, although with more structure, for excitation frequencies of $\omega = 3$, 4, and 5.61. Note that only the last frequency is above threshold, and the first one is the resonant frequency for the transition between the two bound states.

To study the dependence of the recurrences on the form of the initial state, we examine the behavior of a free particle under the influence of the external force for an initial state given by a Gaussian wavepacket, $\psi_G(x) \propto \exp(-x^2/4a^2 + ik_0 x)$, of width a and momentum k_0. The recurrence probability $P_G(t)$ is given by

$$P_G(t) = \frac{2}{\sqrt{4 + t^2/a^4}} \exp\left[-\frac{(S\gamma(t) + 2k_0 t/a)^2}{4 + t^2/a^4}\right]. \tag{8}$$

In Fig. 3 we show the behavior of Eq. (8) for $k_0 = 1$ and $a = 1$. These results are quite similar to those of Fig. 2 and clearly show that recurrences are generic features of strongly driven quantum systems. We also see from Eq. (8) that recurrences will appear when the impulse given the particle in one cycle of the external field $S\gamma(t)$ dominates the characteristic momentum of the particle. Furthermore, the decay of the recurrence height is controlled by the prefactor in Eq. (8) which arises from spreading of the wavepacket. In general, as we can see from Eq. (6), if the argument of the exponential is stationary for k values where $\tilde{\psi}_f(k, 0)$ is large, then the wave function has a large overlap with the initial state and the particle shows recurrences.

One further question that naturally arises is whether these recurrences have a classical analog. This is particularly interesting since Davis and Heller [10] have studied wavepacket evolution in several model potentials in time-independent situations and conclude that there is indeed very good correspondence between the time average of the quantum overlap $|\langle \psi(0)|\psi(t)\rangle|^2$ and its classical analog. Furthermore, a classical mechanism involving the return of an electron to the origin which then scatters out a second electron has been invoked [11] in a model for strong-field double ionization of atoms [12].

To compare the classical and quantum dynamics, we consider [10,13] a cloud of classical particles whose initial conditions are chosen so that their probability distribution mimics

$|\psi_0|^2$ as much as possible. Since we have chosen an energy eigenfunction as an initial state, we have several choices for the initial distribution of the classical cloud. We studied two different classical distributions. In one, we fixed the position probability density to match $|\psi(x)|^2$ and determined the momenta from the fixed energy, giving positive and negative momenta equal weight. In the second case, we generated initial conditions with position and momentum probability densities corresponding to Gaussians; the width of the initial position distribution was matched with that of the initial quantum state. In either case, we could represent the analog of the quantum overlap by using either the overlap of the time evolved position probability density with the initial one, $\int dx\, \rho(x,0)\rho(x,t)$, or an overlap integral [10] in phase space, $\text{Tr}\,[\rho(0)\,\rho(t)]$.

We find that in all cases there are no similarities between the classical and quantum results; the classical distributions fail to show recurrences for the same values of the parameters of the forcing term. We thus conclude that the recurrences discussed here are purely quantum mechanical in nature, and that the classical model for the recurrence used in studying the double-ionization of atoms [11] dramatically underestimates the amplitude for an electron to return to its original bound state, which may explain the discrepancy between the classical model and the experimental results [12].

To examine whether the phenomenon of recurrences in strong driving fields exists in higher dimensional phase spaces, we have also considered an effective 2D problem: the hydrogen atom in its ground state subject to linearly polarized radiation. We observe that recurrences in the ground state occupation probability do exist at strong driving above the ionization threshold, even though they are much smaller. This work shall be reported elsewhere.

We also expect recurrences even when the external force is not purely periodic. The crucial parameter that determines whether the external force is strong is the coefficient of the momentum operator in the last term in Eq. (1), $\int F(t)dt/(\hbar/x_o)$, which can be interpreted as the impulse delivered to the system in one cycle in units of the characteristic momentum of a particle in the potential. For above threshold excitation, when this number exceeds the

strength of the potential, the system will behave like a free quantum wavepacket and show all resulting effects described here.

We have therefore shown that whenever a quantum system is subject to a uniform force varying sinusoidally in time with a strength parameter that overwhelms the potential, above threshold excitation will lead to a set of decaying recurrences in the initial state occupation probability. While the exact nature of the potential and the shape of the initial packet determine the detailed behavior and the long time decay in the magnitude of the recurrences, the existence of the recurrences is relatively insensitive to these features of the problem. While qualitatively similar decaying recurrences have been observed [6,7] in time-independent situations, the ones we describe are more startling; the quantum system repopulates the ground state even when more than enough energy is available from the external field for escape from the well.

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FIGURES

FIG. 1. Probability of initial state occupation as a function of reduced time. $T = 2\pi/\omega$ is the period of the forcing function. Note that $\omega/\omega_0 = 0.25$ corresponds to threshold excitation.

FIG. 2. Agreement between approximate and exact calculations for above threshold excitation. $T = 2\pi/\omega$ is the period of the forcing function. The exact calculation is shown in both figures by the solid line, while the dashed line shows (a) the free particle result $|\langle\psi(0)|\psi_f(t)\rangle|^2$ from Eq. (6) and (b) the Born approximation $|\langle\psi(0)|\psi_B(t)\rangle|^2$ from Eq. (7).

FIG. 3. Recurrences in the time evolution of a Gaussian wavepacket subject to an external field, according to Eq. (8) with $k_0 = a = 1$ for two different driving freqencies.