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Control of Wave Packet Revivals Using Geometric Phases

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Wave packets in a system governed by a Hamiltonian with a generic nonlinear spectrum typically exhibit both full and fractional revivals. It is shown that, by varying the parameters in the Hamiltonian cyclically with a period T and thus inducing suitable geometric phases in the states, fractional revivals can be eliminated at the relevant times $T, 2T,...$. Further, with the introduction of this time step T, the occurrence of *near* full revivals can be mapped onto that of Poincaré recurrences in an irrational rotation map of the circle. The distinctive recurrence statistics of the latter can thus serve as a clear signature of the dynamics of wave packet revivals.

KEY WORDS: Fractional revivals; coherent wave packet; geometric phases; near revivals; rotation map; recurrence statistics.

1. INTRODUCTION

There has been considerable interest in the dynamics of wave packets right from the early days of quantum mechanics.(1) In recent years this subject has gained further impetus from a variety of experiments in molecular systems,(2) Rydberg wave packets,(3) semiconductor quantum wells,(4) etc., which require a detailed understanding of wave packet evolution—e.g., investigations in molecular physics (using femtosecond laser pulse techniques) based on the phenomena of full and fractional revivals(5) of a vibrational wave packet.

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Consider the evolution of an initial state $|\psi(0)\rangle$ of a system governed by a Hamiltonian H. In general, if $|\psi(0)\rangle$ is not an eigenstate of H, the correlation or overlap function

$$\mathscr{C}(t) = |\langle \psi(0) \mid \psi(t) \rangle|^2 \tag{1.1}$$

will decrease from its initial value of unity as t increases. Under special circumstances, however, $\mathscr{C}(t)$ may return to its initial value at some particular instant of time, and a revival is said to occur. One might therefore expect that revivals would be facilitated if the system is prepared in an initial state $|\psi(0)\rangle$ which is a superposition (a "wave packet") of stationary states of H, sharply peaked about some energy eigenvalue E_{n_0}. (We consider, for simplicity, the one-dimensional case.) In the *linear* case of an equally-spaced spectrum, it is easy to show that revivals are a consequence of a simple periodicity. In general, however, E_n is a *nonlinear* function of n. On expanding E_n in a Taylor series about E_{n_0}, it turns out that the revival times depend on the coefficients of the linear and quadratic terms in this expansion.[(6)] Cubic and higher order terms lead to (rare) "super-revivals"[(7)] and can be neglected in most realistic situations, if the wave packet is peaked sufficiently sharply about E_{n_0}. The quadratic term in the Taylor expansion leads to so-called *fractional* revivals that could occur between two full revivals: the initial wave packet evolves to a state that can be described as a collection of a small number of spatially distributed sub-packets, each of which closely reproduces the initial state.[(8)] Experiments with NaI molecules display complex wave packet evolution that suggests fractional revivals of molecular wave packets.[(9, 10)]

Revivals and fractional revivals of a wave packet are, of course, a manifestation of the interference between the constituent basis states, each of which acquires a different phase during its temporal evolution. In general, the occurence of fractional revivals is contingent on delicate arithmetic properties of the numerical values of the parameters that appear in the Hamiltonian, e.g., the closeness of certain ratios of these parameters to rational numbers. The question that arises then is whether one can make the phenomenon of revivals more "robust" by suppressing the plethora of fractional or partial revivals in favour of clearly-signalled full (or nearly full) revivals, even though the spectrum is nonlinear. We shall show that this is indeed feasible, by exploiting the possibility of inducing *geometric* (Berry) phases in the states over and above the dynamical (or secular) ones acquired by unitary evolution. As is well known, such phases may occur if at least two parameters in the Hamiltonian are varied cyclically (with a period T, say) and adiabatically (the original, simplest setting for Berry phases[(11)]). This variation can be tailored so as to eliminate fractional revivals in a generic nonlinear Hamiltonian at certain definite times, *by arranging for a suitable cancellation between appropriate terms in the geometric and secular phases, respectively*. These times are fixed by the following fact: the cycling of parameters implies that it is only at instants of time separated by an interval T that the Hamiltonian returns to its original self. Therefore, with the introduction of this time step T into the problem, it is natural to speak of possible revivals of a state (in the strict sense of the term) only at the instants $T, 2T, \ldots$. It turns out that *nearly* full revivals ("near revivals") are still possible after this discretization of time. Moreover, the statistical distribution of these events is found to be precisely that of Poincaré recurrences in the rotation map on a circle.

The plan of this paper is as follows: In the next section, we give a brief review of wave packet revivals with particular emphasis on fractional revivals. In Section 3 we show that by inducing suitable geometric phases in the basis states, we can eliminate all fractional revivals. The formalism is also illustrated explicitly. Finally, in Section 4 we indicate briefly how the statistics of near revivals in the reduced problem can be mapped onto that of recurrences in an irrational rotation of the circle.

2. FRACTIONAL REVIVALS: REVIEW

Consider a system with a time-independent hermitian Hamiltonian H, with spectrum $\{E_n\}$ and eigenstates $\{|\phi_n\rangle\}$. Let the system be prepared in an initial state $|\psi(0)\rangle$ that is a superposition of the $\{|\phi_n\rangle\}$, sharply peaked about some n_0. As mentioned earlier, we expand E_n as

$$E_n = E_{n_0} + (n - n_0)\, E'_{n_0} + (1/2)(n - n_0)^2\, E''_{n_0} + \cdots \tag{2.1}$$

As we wish to analyze only revivals and fractional revivals, we retain only terms up to the second order in Eq. (2.1) and shift n by n_0 for notational simplicity, to arrive at the quadratic form

$$E_n = C_0 + C_1 n + C_2 n^2 \tag{2.2}$$

The coefficients C_i evidently depend on the parameters that occur in H. We shall assume that $C_1, C_2 > 0$. (The modifications necessary in other cases are easily worked out.) In the $|\phi_n\rangle$-basis the time evolution operator $U(t) = \exp[-iHt/\hbar]$ has the representation

$$U(t) = \sum_n^{\infty} \exp[-i(C_0 + C_1 n + C_2 n^2)\, t/\hbar]\, |\phi_n\rangle\langle\phi_n| \tag{2.3}$$

For a full revival ($\mathscr{C}(t)=1$) to occur at time t, $U(t)$ must reduce to the unit operator (apart from a possible overall phase factor), i.e., $(C_1 n + C_2 n^2)\, t$ must be an integer multiple of $2\pi\hbar$ for every n in the summation. The following cases arise:

(i) $C_1 \neq 0$, $C_2 = 0$ (equi-spaced or linear spectrum): Revivals of an initial state occur with a period $T_{rev} = 2\pi\hbar/C_1$.

(ii) $C_1 = 0$, $C_2 \neq 0$: Revivals occur with a period $T_{rev} = 2\pi\hbar/C_2$.

(iii) $C_1, C_2 \neq 0$, $C_1/C_2 =$ a rational number r/s: Once again, full revivals occur with a fundamental revival time $T_{rev} = 2\pi\hbar s/C_2$. A specific example is provided by the Hamiltonian $a^{\dagger 2} a^2 = a^\dagger a (a^\dagger a - 1)$ that is relevant to wave packets propagating in a Kerr medium.[12] It is evident that, in this case, E_n is proportional to $n(n-1)$ which is an even integer for every n.

(iv) $C_1, C_2 \neq 0$, C_1/C_2 irrational (the generic case): As the condition $(C_2 n^2 + C_1 n)\, t = 2\pi\hbar m$ ($m =$ integer) cannot be satisfied for *all* n at any value of t, full revivals are no longer possible. However, at certain instants of time the quantity $\mathscr{C}(t)$ could come *arbitrarily* close to unity, producing a near revival.

Between occurrences of full (or near) revivals, the wave packet breaks up into a finite sum of subsidiary packets at specific instants of time, *provided* the spectrum is nonlinear, i.e., $C_2 \neq 0$.[8] These fractional revivals occur at times t given by $t = \pi\hbar r/C_2 s$ where r and s are mutually prime integers. It can be shown that at these instants the evolution operator U can be expressed as a finite sum of operators U_p, in each of which the phase factor multiplying the projection operator $|\phi_n\rangle\langle\phi_n|$ is linear in n: That is,

$$U(\pi\hbar r/C_2 s) = \sum_{p=0}^{l-1} a_p^{(r,s)}\, U_p \tag{2.4}$$

with

$$a_p^{(r,s)} = (1/l) \sum_{k=0}^{l-1} \exp[-(i\pi k^2 r/s) + (2i\pi k p/l)] \tag{2.5}$$

and

$$U_p = \sum_{n=0}^{\infty} \exp(-in\theta_p)\, |\phi_n\rangle\langle\phi_n|, \qquad \theta_p = \pi[(C_1 r/C_2 s) + (2p/l)] \tag{2.6}$$

It is this decomposition of U which is responsible for fractional revivals, as can be seen by investigating the action of the operator U_p on the initial state. For instance, if the initial state $|\psi(0)\rangle$ is the "coherent state" $|z\rangle$ given by

$$|z\rangle = \exp(-|z|^2/2) \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |\phi_n\rangle, \qquad z \in \mathbb{C} \tag{2.7}$$

Eqs. (2.4)–(2.6) yield

$$|\psi(\pi\hbar r/C_2 s)\rangle = \exp(-i\pi C_0 r/C_2 s) \sum_{p=0}^{l-1} a_p^{(r,s)} |z \exp(-i\theta_p)\rangle \tag{2.8}$$

The state at time $\pi\hbar r/C_2 s$ is therefore a weighted sum of wave packets, each of which has the same form as the initial state $|z\rangle$.

It is clear from the foregoing that (i) fractional revivals arise from the quadratic dependence of E_n on n, and (ii) a whole host of such revivals of varying intensities can appear in a given case, depending on the numerics, i.e., the precise values of C_2 and the integers r and s for which these revivals are detectable. In the next two sections we show that, by inducing suitable geometric phases in the basis states $|\phi_n\rangle$, we can eliminate these partial revivals and restore near revivals at specific instants of time.

3. SUPPRESSION OF FRACTIONAL REVIVALS

We now consider the situation in which the Hamiltonian contains a set of "slow" parameters $\mathbf{R}$ that can be varied adiabatically and cyclically with period T, as in Berry's original setting for the geometric phase: i.e., $\mathbf{R}_T = \mathbf{R}_0$.

In order to keep track of the parameter dependence in the basis states as well, we denote by $|\phi_n, \mathbf{R}\rangle$ the nth eigenstate of the instantaneous Hamiltonian $H(\mathbf{R})$. Then, at the end of each cycle of period T, $|\phi_n, \mathbf{R}\rangle$ picks up a geometric phase γ_n (over and above the E_n-dependent dynamical phase factor), given by the expression[11]

$$\gamma_n = i \oint \langle \phi_n, \mathbf{R}| \, (\nabla_{\mathbf{R}} |\phi_n, \mathbf{R}\rangle) \cdot d\mathbf{R} \tag{3.1}$$

where the integral runs over the corresponding closed loop in parameter space. Substituting for $|\phi_n, \mathbf{R}\rangle$ at the end of a cycle, the time evolution operator at time T therefore becomes

$$U(T) = \sum_n \exp\left[i\gamma_n - (i/\hbar) \int_0^T dt \, E_n(\mathbf{R}_t) \right] |\phi_n, \mathbf{R}_0\rangle\langle\phi_n, \mathbf{R}_0| \tag{3.2}$$

To proceed, we need to know the n-dependence of γ_n. For a general nonlinear spectrum E_n, one may expect a dependence of the form

$$\gamma_n = \Theta_0 + \Theta_1 n + \Theta_2 n^2 + \cdots \tag{3.3}$$

This is generic, as it only requires that γ_n be a regular function of n (see Eqs. (3.13), (3.14) *ff.* below). As in the expansion of E_n, only terms up to $O(n^2)$ in Eq. (3.3) are relevant for our present purposes. The coefficients Θ_i will clearly depend on the manner in which the parameters $\mathbf{R}$ are varied. We now substitute for γ_n and E_n in Eq. (3.2) from Eqs. (3.3) and (2.2), respectively, taking into account the fact that the coeffcients C_i are now time-dependent owing to the variation of parameters in H. Moreover, in each cycle of period T the state $|\phi_n, \mathbf{R}\rangle$ picks up the same additional geometric and dynamical phase. Hence the time evolution operator at time kT (where $k = 1, 2,...$) is given by

$$U(kT) = \sum_n \exp[ik(v_0 + v_1 n + v_2 n^2)]\ |\phi_n, \mathbf{R}_0\rangle\langle\phi_n, \mathbf{R}_0| \tag{3.4}$$

where

$$v_i = \Theta_i - (1/\hbar)\int_0^T C_i(t)\, dt, \qquad (i = 0, 1, 2) \tag{3.5}$$

From the discussion in Section 2, it is clear that fractional revivals of a wave packet will be eliminated if the coefficient v_2 of n^2 in the foregoing expression for $U(kT)$ vanishes: this happens if we arrange the variation of the parameters such that the contribution from the geometric phase cancels that from the dynamical phase, i.e., if

$$\Theta_2 = (1/\hbar)\int_0^T C_2(t)\, dt \tag{3.6}$$

Once this is done, the exponent in $U(kT)$ has only terms that are linear in n. Hence, at the relevant times kT ($k = 1, 2,...$), the wave packet will no longer exhibit fractional revivals.

To see in a little more detail how a geometric phase γ_n of the desired form may be generated,[13] consider first the classical one-freedom Hamiltonian

$$H'(x', p') = Ap'^2 + CV(x') \tag{3.7}$$

where A and C are positive constants, and $V(x')$ is a potential that supports bounded, periodic motion. We assume that the quantum mechanical version, with a self-adjoint Hamiltonian H', has a non-degenerate, discrete spectrum $\{E_n\}$ with normalized eigenstates $\{|\chi_n\rangle\}$. The position-space wavefunction $\langle x' \mid \chi_n\rangle = \chi_n(x')$ can be chosen to be a real function, from which it follows that the Berry phase γ_n that one may expect from the possible variation of A and C vanishes identically. Reverting to the classical case, consider now the canonical transformation $(x', p') \to (x, p)$ where

$$x = x', \qquad p = p' - (B/A)\, f(x') \tag{3.8}$$

where B is a constant and the function $f(x)$ is to be specified. The transformed Hamiltonian is

$$H(x, p) = Ap^2 + B[\, pf(x) + f(x)\, p] + CV(x) + (B^2/A)\, f^2(x) \tag{3.9}$$

where we have written the cross terms in symmetric form in anticipation of quantization. Let $f(x)$ be chosen such that the phase trajectories corresponding to H continue to represent bounded, periodic motion. Quantum mechanically, H is obtained by the action upon H' of the unitary operator

$$W = \exp(-iB\hbar F(x)/A), \qquad F(x) = \int^x f(x)\, dx \tag{3.10}$$

Provided that this leads to a self-adjoint Hamiltonian H, it follows that H and H' are isospectral. The normalized eigenstates of H are given by $|\phi_n\rangle = U\,|\chi_n\rangle$. Under an adiabatic, cyclic variation of parameters $\mathbf{R} = (A, B, C)$, the Berry phase acquired by $|\phi_n\rangle$ is

$$\gamma_n = i \oint \langle \phi_n |\, (\nabla_{\mathbf{R}}\, |\phi_n\rangle) \cdot d\mathbf{R} \tag{3.11}$$

As $|\phi_n\rangle$ is normalized, this simplifies to

$$\gamma_n = i \oint \langle \phi_n |\, (\nabla_{\mathbf{R}}\, U)\, |\chi_n\rangle \cdot d\mathbf{R} \tag{3.12}$$

Using the unitarity of U, this yields

$$\gamma_n = (1/\hbar) \oint \langle F \rangle_n\, \nabla_{\mathbf{R}} (B/A) \cdot d\mathbf{R} \tag{3.13}$$

where

$$\langle F \rangle_n = \int_{-\infty}^{\infty} F(x)\, \chi_n^2(x)\, dx \tag{3.14}$$

Therefore the n-dependence of the Berry phase γ_n can be tailored by choosing the transformation function $f(x)$ appropriately, even though $\{E_n\}$ remains the same for all acceptable choices of $f(x)$.

An explicit example is provided by the Pöschl–Teller Hamiltonian[14]

$$H' = Ap^2 - C\,\mathrm{sech}^2\, x \qquad (A,\, C > 0) \tag{3.15}$$

which is unitarily transformed by $W = \exp[-(iB/A\hbar) \ln \cosh x]$ to $H = WH'W^\dagger$ where

$$H = Ap^2 + B[\,p(\tanh x) + (\tanh x)\, p\,] - [\,C + (B^2/A)\,]\,\mathrm{sech}^2\, x + (B^2/A) \tag{3.16}$$

Writing $\eta = (1 + 4C/A\hbar^2)^{1/2}$, the spectrum of H is given by

$$E_n = -A\hbar^2(\eta - 1 - 2n)^2/4 \tag{3.17}$$

where $n = 0, 1, ..., [\frac{1}{2}(\eta - 1)]$ ($[\xi]$ stands for the largest integer contained in ξ). As E_n is quadratic in n, a wave packet whose evolution is governed by H will exhibit fractional revivals. Applying Eq. (2.4) to the case at hand, we can now identify the instants at which such revivals occur as $\pi r/A\hbar s$, where r and s are mutually prime integers.

To induce a geometric phase γ_n in the eigenstate $|\phi_n\rangle$ of H, it suffices in the present instance to vary just the two parameters A and B with a period T. It can be shown[15] that the geometric phase in this case is precisely of the form

$$\gamma_n = \Theta_0 + \Theta_1 n + \Theta_2 n^2 \tag{3.18}$$

Putting in the exact expression for Θ_2 in this instance, the condition (3.6) for the cancellation of fractional revivals then reads

$$\int [\nabla_{\mathbf{R}}(1/\eta^2) \times \nabla_{\mathbf{R}}(B/A)] \cdot d\mathbf{S} = \hbar^2 \int_0^T A(t)\, dt \tag{3.19}$$

where the integral on the left runs over the surface bounded by the closed loop in the (A, B) plane along which A and B are varied.

Once fractional revivals are eliminated in the manner just described, we are left with linear n-dependences for both E_n and γ_n. But, owing to the discretization of time in steps of T, this no longer implies trivial periodicity, i.e., that full revivals would automatically occur at integral multiples of T. However, as we shall show, *near* revivals will now occur generically without any further fine tuning of the parameters concerned.

4. STATISTICS OF NEAR REVIVALS

After the cancellation of the quadratic (n^2) term in the phase factors in Eq. (3.4), the effective time development operator at time kT ($k = 1, 2,...$) is of the form

$$U(kT) = \exp(ikv_0) \sum_n \exp(iknv_1) \, |\phi_n, \mathbf{R}_0\rangle \langle \phi_n, \mathbf{R}_0| \tag{4.1}$$

Therefore an initial coherent state $|\psi(0)\rangle = |z\rangle$ given by Eq. (2.7) evolves to

$$|\psi(kT)\rangle = |z \exp(ikv_1)\rangle \tag{4.2}$$

Correspondingly, the correlation function given by Eq. (1.1) becomes

$$\mathscr{C}(kT) = \exp[2 \, |z|^2 \, (\cos kv_1 - 1)] \tag{4.3}$$

Thus, if kv_1 happens to be an integer multiple of 2π (recall that v_1 depends on T, cf. Eq. (3.5)), then full revivals occur with $T_{rev} = kT$ as the basic revival time. In general, however, v_1 is an irrational number (modulo 2π). Therefore, if θ_0 is the phase of the complex number z labelling the initial state $|\psi(0)\rangle$, and θ_k that of the corresponding number at time kT, Eq. (4.2) shows that the (discrete time) evolution of the state is entirely equivalent to the circle map

$$\theta_k = \theta_{k-1} + v_1 \qquad (\text{mod } 2\pi) \tag{4.4}$$

corresponding to a rigid "irrational" rotation. As is well known,[16] this map has no periodic orbits, is ergodic, and has a uniform invariant density. Given an ε-neighborhood I_ε of the initial phase θ_0, we have a Poincaré recurrence to I_ε at time kT if $\theta_k \in I_\varepsilon$. This corresponds to a near revival of the original wave packet, because it is easily shown that we then have

$$\mathscr{C}(kT) > 1 - |z|^2 \, \varepsilon^2 \tag{4.5}$$

The recurrence statistics for the rotation map is already known from certain "gap theorems,"[17] and has found applications in the study of level spacings of oscillator systems[18] and recurrences in the coarse grained dynamics of quasiperiodic flow on a two-torus.[19] In earlier work,[20] we have discussed the application of these theorems to near revivals of coherent states of a deformed (displaced, squeezed) oscillator, and these results can now be taken over directly to the problem at hand. While the mean time between successive near revivals turns out to be simply $2\pi T/\varepsilon$ in accordance with the ergodic theorem (the measure of I_ε being $\varepsilon/2\pi$), the probability distribution of this time interval is quite remarkable. It is typically concentrated at three specific values $k_1 T$, $k_2 T$ and $(k_1 + k_2)\,T$, regardless of the values of ν_1 and ε. The actual values of the integers k_1 and k_2, and the relative frequencies of occurrence of the three different revival times, are of course dependent on ν_1 and ε.[20]

We have thus established an interesting link between revivals, anholonomies and recurrences. These are manifestations, respectively, of quantum interference efffects, non-trivial topology in parameter space, and ergodic behavior in a discrete-time classical dynamical system. The distinctive nature of the generic distribution of near revival times that we have predicted should provide a clear signature, from the experimental point of view, for testing the validity of our formulation of certain aspects of wave packet evolution.

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