Control of Wave Packet Revivals Using Geometric Phases

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Abstract

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 the latter can be eliminated by inducing suitable geometric phases in the states, by varying the parameters in the Hamiltonian cyclically with a period $T$. Further, with the introduction of this natural time step $T$, the occurrence of near revivals can be mapped onto that of Poincaré recurrences in an irrational rotation map of the circle. The distinctive recurrence time 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. In recent years this subject has gained further impetus from a variety of experiments in molecular systems, Rydberg wave packets, semiconductor quantum wells, 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 of a vibrational wave packet.

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

$$C(t) = |\langle \psi(0) | \psi(t) \rangle|^2$$

(1.1)

will decrease from its initial value of unity as $t$ increases. Under special circumstances, however, $C(t)$ 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. Cubic and higher order terms lead to (rare) “super-revivals” 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.

Experiments with NaI molecules display complex wave packet evolution that suggests fractional revivals of molecular wave packets.

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 occurrence 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 non-linear. 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 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\textsuperscript{11}). This variation can be tailored so as to cancel out all fractional revivals in a generic nonlinear Hamiltonian. The cycling of parameters, however, means 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 natural time step $T$ into the problem, it is only meaningful to speak of possible revivals of a state at the instants $T, 2T, \cdots$. 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

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

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

$$E_n = C_0 + C_1 n + C_2 n^2. \quad (2.2)$$

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 $U(t) = \exp \left[-i H t / \hbar \right]$ has the representation

$$U(t) = \sum_n^\infty \exp\left[-i (C_0 + C_1 n + C_2 n^2) t / \hbar \right] |\phi_n\rangle \langle \phi_n|. \quad (2.3)$$
For a full revival \((C(t) = 1)\) to occur at time \(t\), \(U(t)\) must reduce to the unit operator (apart from a possible overall phase factor), i.e., \((C_1n + C_2n^2)\) 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 \(T_{\text{rev}} = 2\pi\hbar/C_1\).

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

(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 \(T_{\text{rev}} = 2\pi\hbar s/C_2\). A specific example is provided by the Hamiltonian \(a^\dagger a^2 = a^\dagger a(a^\dagger a - 1)\) 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 \((C_2n^2 + C_1n)\) 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 \(C(t)\) 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,

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

with

\[
a_p^{(r,s)} = \left(1/l\right) \sum_{k=0}^{l-1} \exp\left[-i\pi k^2 r/s + (2i\pi kp/l)\right] ,
\]

and

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

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

\[
|z\rangle = \exp\left(-|z|^2/2\right) \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \ |\phi_n\rangle , \ z \in \mathbb{C} ,
\]

Eqs. (2.4)-(2.6) yield

\[
|\psi(\pi\hbar r/C_2 s)\rangle = \exp\left(-i\pi C_0 r/C_2 s\right) \sum_{p=0}^{l-1} a_p^{(r,s)} \ z \exp(-i \theta_p) .
\]
The state at time $\pi hr/C_2 s$ 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 $R$ that can be varied adiabatically and cyclically with period $T$, as in Berry’s original setting for the geometric phase: i.e., $R_T = R_0$.

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

$$\gamma_n = i \oint \langle \phi_n, R |(\nabla_R |\phi_n, R\rangle) \cdot dR,$$

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

$$U(T) = \sum_n \exp \left[ i\gamma_n - (i/\hbar) \int_0^T dt E_n(R_t) \right] |\phi_n, R_0\rangle \langle \phi_n, R_0|.$$

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

$$\gamma_n = \Theta_0 + \Theta_1 n + \Theta_2 n^2 + \cdots$$

This is generic, as it only requires that $\gamma_n$ 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 $\Theta_i$ will clearly depend on the manner in which the parameters $R$ are varied. We now substitute for $\gamma_n$ and $E_n$ in Eq. (3.2) from Eqs. (3.3) and (2.2), respectively, taking into account the fact that the coefficients $C_i$ are now time-dependent owing to the variation of parameters in $H$. Moreover, in each
cycle of period $T$ the state $|\phi_n, R\rangle$ picks up the same additional geometric and dynamical phase. Hence the time evolution operator at time $kT$ (where $k = 1, 2, \cdots$) is given by

$$U(kT) = \sum_n \exp\left[i(k\nu_0 + \nu_1 n + \nu_2 n^2)\right] |\phi_n, R_0\rangle \langle \phi_n, R_0|$$

(3.4)

where

$$\nu_i = \Theta_i - (1/\hbar) \int_0^T C_i(t) \, dt, \quad (i = 0, 1, 2).$$

(3.5)

From the discussion in Section 2, it is clear that all fractional revivals of a wave packet will be eliminated if the coefficient $\nu_2$ of $n^2$ in the foregoing expression for $U(kT)$ vanishes: this happens if we arrange the variation of the parameters such that

$$\Theta_2 = (1/\hbar) \int_0^T C_2(t) \, dt.$$

(3.6)

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

To see in a little more detail how a geometric phase $\gamma_n$ of the desired form may be generated, consider first the classical one-freedom Hamiltonian

$$H'(x', p') = Ap'^2 + CV(x')$$

(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 $\langle x'|\chi_n\rangle = \chi_n(x')$ can be chosen to be a real function, from which it follows that the Berry phase $\gamma_n$ that one may expect from the possible variation of $A$ and $C$ vanishes identically. Reverting to the classical case, consider now the canonical transformation $(x', p') \rightarrow (x, p)$ where

$$x = x', \quad p = p' - (B/A) f(x')$$

(3.8)

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

$$H(x, p) = Ap^2 + B[p f(x) + f(x)p] + CV(x) + (B^2/A) f^2(x),$$

(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

$$W = \exp \left( -i B \hbar F(x)/A \right), \quad F(x) = \int^x f(x) \, dx.$$  \hfill (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 $R = (A, B, C)$, the Berry phase acquired by $|\phi_n\rangle$ is

$$\gamma_n = i \oint \langle \phi_n | (\nabla_R |\phi_n\rangle) \cdot dR.$$  \hfill (3.11)$$

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

$$\gamma_n = i \oint \langle \phi_n | (\nabla_R U)|\chi_n\rangle \cdot dR.$$  \hfill (3.12)$$

Using the unitarity of $U$, this yields

$$\gamma_n = (1/\hbar) \oint \langle F_n | \nabla_R (B/A) \cdot dR,$$

where

$$\langle F_n \rangle = \int_{-\infty}^{\infty} F(x) \chi_n^2(x) \, dx.$$  \hfill (3.14)$$

Therefore the $n$-dependence of the Berry phase $\gamma_n$ 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

$$H' = Ap^2 - C \text{sech}^2 x \quad (A, C > 0)$$  \hfill (3.15)$$

which is unitarily transformed by $W = \exp \left[ -(i B/\hbar) \ln \cosh x \right]$ to $H = W H' W^\dagger$ where

$$H = A p^2 + B[p(\tanh x) + (\tanh x)p] - \left[ C + (B^2/A) \right] \text{sech}^2 x + (B^2/A).$$  \hfill (3.16)$$

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

$$E_n = -A\hbar^2 \left( \eta - 1 - 2n \right)^2/4$$  \hfill (3.17)$$

where $n = 0, 1, \cdots, \lfloor \eta/2 \rfloor$ ($\lfloor \xi \rfloor$ stands for the largest integer contained in $\xi$). 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 $\pi r/\hbar s$, where $r$ and $s$ are mutually prime integers.
To induce a geometric phase $\gamma_n$ 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\textsuperscript{15)} that the geometric phase in this case is precisely of the form

$$\gamma_n = \Theta_0 + \Theta_1 n + \Theta_2 n^2.$$  

Putting in the exact expression for $\Theta_2$ in this instance, the condition (3.6) for the cancellation of fractional revivals then reads

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

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 $\gamma_n$. 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 $kT$ ($k = 1, 2, \cdots$) is of the form

$$U(kT) = \exp(ik\nu_0) \sum_n \exp(ikn\nu_1) |\phi_n, \mathbf{R}_0\rangle \langle \phi_n, \mathbf{R}_0|. $$ \hfill (4.1)

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

$$|\psi(kT)\rangle = |z \exp(ik\nu_1)\rangle. $$ \hfill (4.2)

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

$$\mathcal{C}(kT) = \exp \left[ 2|z|^2 \left( \cos k\nu_1 - 1 \right) \right]. $$ \hfill (4.3)

Thus, if $kn_1$ happens to be an integer multiple of $2\pi$ (recall that $\nu_1$ depends on $T$, cf. Eq. (3.5)), then full revivals occur with $T_{\text{rev}} = kT$ as the basic revival time. In general, however, $\nu_1$ is an irrational number (modulo $2\pi$). Therefore, if $\theta_0$ is the phase of the complex number $z$ labelling the initial state $|\psi(0)\rangle$, and $\theta_k$ 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

$$\theta_k = \theta_{k-1} + \nu_1 \pmod{2\pi} $$ \hfill (4.4)
corresponding to a rigid “irrational” rotation. As is well known,\textsuperscript{16} this map has no periodic orbits, is ergodic, and has a uniform invariant density. Given an $\epsilon$-neighborhood $I_\epsilon$ of the initial phase $\theta_0$, we have a Poincaré recurrence to $I_\epsilon$ at time $kT$ if $\theta_k \in I_\epsilon$. This corresponds to a near revival of the original wave packet, because it is easily shown that we then have

$$C(kt) > 1 - |z|^2 \epsilon^2.$$  \hspace{1cm} (4.5)

The recurrence statistics for the rotation map is already known from certain “gap theorems”,\textsuperscript{17} and has found applications in the study of level spacings of oscillator systems\textsuperscript{18} and recurrences in the coarse grained dynamics of quasiperiodic flow on a two-torus.\textsuperscript{19} In earlier work,\textsuperscript{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 $2\pi T/\epsilon$ in accordance with the ergodic theorem (the measure of $I_\epsilon$ being $\epsilon/2\pi$), the probability distribution of this time interval is quite remarkable. It is typically concentrated at three specific values $k_1T$, $k_2T$ and $(k_1+k_2)T$, regardless of the values of $\nu_1$ and $\epsilon$. 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 $\nu_1$ and $\epsilon$.\textsuperscript{20}

We have thus established an interesting link between revivals, anholonomies and recurrences. These are manifestations, respectively, of quantum interference effects, 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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