Geometric phase effects for wavepacket revivals

C. Jarzynski

Institute for Nuclear Theory, University of Washington
Seattle, WA 98195

(April 1, 2022)

Abstract

The study of wavepacket revivals is extended to the case of Hamiltonians which are made time-dependent through the adiabatic cycling of some parameters. It is shown that the quantal geometric phase (Berry's phase) causes the revived packet to be displaced along the classical trajectory, by an amount equal to the classical geometric phase (Hannay's angle), in one degree of freedom. A physical example illustrating this effect in three degrees of freedom is mentioned.

PACS numbers: 03.65.Bz, 31.50.+w
Ordinarily, a quantal wavepacket following a classical trajectory spreads irreversibly, until it completely loses its integrity as a localized packet. However, when the underlying classical trajectory is stable and periodic, the dispersed wavepacket eventually “puts itself together again” and for a time continues, localized, along the classical trajectory. The argument for this comes from an examination of the dynamical phases \( \exp(-iE_n t/\hbar) \) acquired by the energy eigenstates whose superposition makes up the wavepacket.\(^1\)\(^3\) Such wavepacket revivals — which have been observed experimentally in Rydberg atoms\(^1\) as well as one-atom masers\(^3\) — are intriguing because they represent the seemingly spontaneous resurrection of classical behaviour in a quantal system. The study of wavepacket revivals has so far been restricted to systems where the Hamiltonian is time-independent. The present paper extends the theory to the case of slowly time-dependent Hamiltonians, where, as will be shown, Berry’s phase adds a new and interesting twist to the picture.

Specifically, in this paper I consider wavepacket evolution under an adiabatically cycled Hamiltonian, that is, a parameter-dependent Hamiltonian \( \hat{H}(R) \), where the parameter \( R \) is made to slowly trace out a closed loop in parameter space. I will restrict myself to systems of one degree of freedom, although parameter space is multi-dimensional. Thus the underlying classical motion (assumed bounded) is periodic for fixed \( R \). When \( R \) is made to change slowly with time, the classical motion is nearly periodic: a trajectory goes round and round a slowly changing closed curve in the two-dimensional phase space. At any instant, this curve is an energy shell — a level surface — of the instantaneous Hamiltonian, and is determined by the requirement that the action \( \oint pdq \) over one “period” is an invariant (see e.g. Ref.\(^6\) for details). The analysis that follows shows that, as in the time-independent case, there will be a revival of the wavepacket: the standard argument for revivals is easily extended to the case of a slowly time-dependent Hamiltonian, only the dynamical phases now have the form \( \exp(-(i/\hbar) \int E_n(t) \, dt) \). However, this is only part of the story. As demonstrated by Berry\(^7\), an energy eigenstate evolving under an adiabatically cycled Hamiltonian acquires not only a dynamical phase, but also a geometric phase, determined by the loop traced out in \( R \)-space. A proper analysis of wavepacket evolution in this situation must take this
phase into account. I show that, if the time at which the parameter returns to its initial value is chosen to coincide with the revival time, then the net effect of Berry’s phase is to cause a displacement of the location at which the revived wavepacket appears. Moreover, the amount of this displacement is given by Hannay’s angle \[\theta\], the classical analogue of Berry’s phase. As the analysis will show, this effect is generic in one degree of freedom; at the end of the paper I briefly mention a physical example in three degrees of freedom which illustrates the same effect.

To demonstrate what has been stated above, it is useful to first review a result concerning wavepacket evolution under a time-independent Hamiltonian \(H\); this result is summarized by Eq.\(1\) below. Imagine a quantal wavepacket \(\psi_0\) localized around some point \((q_0, p_0)\) in phase space. (That is, the configuration-space representation is localized around \(q_0\), the momentum-space representation around \(p_0\). More formally, one could represent the quantal state directly in phase space, using a Wigner transform.) Expressing \(\psi_0\) as a superposition of energy eigenstates \(|u_n\rangle\), the non-vanishing coefficients \(a_n\) are confined to some finite range of values of \(n\), centered, say, around \(\bar{n}\). Assume the semiclassical regime: \(\bar{n} \gg 1\). Under time evolution, the coefficients in this superposition acquire phases: 

\[
\psi(t) = \sum_n \exp(i\alpha_n a_n |u_n\rangle),
\]

where \(\alpha_n = -\frac{E_n}{\hbar} t\). It is the process of “de-phasing” — the fact that the \(\alpha_n\)’s grow at different rates — which determines how the wavepacket moves and spreads. The Correspondence Principle, however, dictates that in the semiclassical limit (\(\bar{n} \to \infty\)), the packet is propelled along a classical trajectory. Let us consider this more closely.

A Taylor expansion of \(E_n\) around \(\bar{n}\) yields:

\[
\alpha_n = -\frac{1}{\hbar} E_n t - \Delta n \frac{1}{\hbar} E'_n t - \frac{1}{2\hbar} (\Delta n)^2 E''_n t - \cdots,
\]

(1)

where \(\Delta n \equiv n - \bar{n}\), and \(E'_n \equiv dE_n/d\bar{n}\), (and similarly for the second derivative \(E''_n\), and higher derivatives \(E^{(s)}_n\).) Using \(1/\bar{n}\) as an ordering parameter, \(E^{(s)}_n\) is \(O(1/\bar{n}^s)\), and \(\hbar\) is \(O(1/\bar{n})\) (in comparison with the relevant “macroscopic” quantities \(E_{\bar{n}}\) and \(I_{\bar{n}} \equiv (1/2\pi) \int p\,dq\), with the latter calculated for a classical orbit of energy \(E_{\bar{n}}\)). The first term on the right side of Eq.\(1\), \(-E_n t/\hbar\) (which scales as \(\bar{n}\)), contributes an external phase to the wavepacket. The
second term ($\sim \tilde{n}^0$) describes the \textit{linear} (in $\Delta n$) de-phasing between the components $|u_n\rangle$ of $\psi_0$, the third term ($\sim 1/\bar{n}$) the \textit{quadratic} de-phasing, and so forth.

In the semiclassical limit, in which the wavepacket follows a classical trajectory, the first two terms dominate:

\[
\psi(t) \cong \exp(-iE_\bar{n}t/\hbar) \sum_n \exp(-i\Delta n E'_\bar{n}t/\hbar)a_n|u_n\rangle \\
\equiv e^{i\alpha_n} \sum_n e^{i\beta_n a_n|u_n\rangle}.
\]  

Thus, disregarding the external phase $\alpha_\bar{n}$, the phases

\[
\beta_n = -\Delta n E'_\bar{n}t/\hbar
\]

specify a wavepacket that evolves along a classical trajectory. (Note in particular that this evolution is periodic.) This result is valid for times of order unity: $t \sim \tilde{n}^0$ (by which is meant that the ratio of $t$ to the relevant macroscopic time scale — the period of an orbit of energy $E_\bar{n}$ — is held fixed as $\bar{n} \to \infty$). At longer times, the quadratic and higher-order de-phasing terms become appreciable, and are responsible for the spreading of the packet. Now, WKB theory gives us

\[
\frac{1}{\hbar}E'_\bar{n} \approx \frac{\partial H}{\partial I},
\]

where $\partial H/\partial I$ is the derivative of the classical Hamiltonian with respect to the classical action, evaluated at energy $E_\bar{n}$. The correction to Eq.4 is $O(1/\bar{n}^2)$ (the $O(1/\bar{n})$ correction is identically zero). In terms of \textit{action-angle variables} ($\theta, I$) \cite{4}, $\partial H/\partial I$ is simply the rate of change of the angle variable $\theta$ along a classical trajectory. Thus, neglecting the $O(1/\bar{n}^2)$ correction to Eq.4, we get

\[
\beta_n = -\Delta n \Delta \theta,
\]

where $\Delta \theta = (\partial H/\partial I)t$ is the change in $\theta$ associated with classical evolution for time $t$. We therefore conclude that, if we modify a semiclassical wavepacket $\psi_0$ by tacking on linear de-phasing factors $\exp(-i\Delta n \Delta \theta)$ to the terms in the superposition, then the effect is to
shift the location of the wavepacket along a classical trajectory, by a change in the angle variable equal to the amount of (linear) de-phasing, $\Delta \theta$. Symbolically,

$$\{a_n \rightarrow e^{-i\Delta n \Delta \theta a_n}\} \implies (\theta, I) \rightarrow (\theta + \Delta \theta, I).$$

(6)

Let us now move on to adiabatically driven systems. Consider a parameter-dependent Hamiltonian $\hat{H}(R)$, and imagine again an initial wavepacket $\psi_0$ localized at $(q_0, p_0)$. Now, however, let the packet evolve under the time-dependent Hamiltonian obtained by making $R$ slowly trace out a closed loop $\Gamma$ in parameter space. Denote the initial (and final) point on this loop by $R_0$, and the initial and final times by $t = 0$ and $t = T_\Gamma$.

Assuming $dR/dt$ slow enough that the quantal adiabatic theorem holds, the wavefunction at time $t$ is

$$\psi(t) = \sum_n e^{i\phi_n(t)}a_n|u_n(R(t))\rangle,$$

(7)

where the $\phi_n$’s are real, the coefficients $a_n$ are time-independent, and the $|u_n(R)\rangle$’s are the eigenstates of $\hat{H}(R)$. Thus, when $R(t)$ returns to $R_0$ at time $T_\Gamma$, we have a state identical to $\psi_0$, except that the expansion coefficients have acquired phases: $a_n \rightarrow e^{i\phi_n(T_\Gamma)}a_n$.

Before the discovery of Berry’s phase [7], one might have guessed that the phases $\phi_n(T_\Gamma)$ are given by

$$\phi_n(T_\Gamma) = -\frac{1}{\hbar} \int_0^{T_\Gamma} dt E_n(t),$$

(8)

where $E_n(t)$ is the $n$th eigenstate of $\hat{H}(R(t))$. For the time being, assume Eq.8 is correct. Expanding as in Eq.8 above, we get

$$\phi_n(T_\Gamma) = -\frac{b_0(T_\Gamma)}{\hbar} - \Delta n \frac{b_1(T_\Gamma)}{\hbar} - (\Delta n)^2 \frac{b_2(T_\Gamma)}{2\hbar} - \cdots,$$

(9)

where

$$b_s(T_\Gamma) = \int_0^{T_\Gamma} dt E_n^{(s)}(t).$$

(10)

The sizes of the terms in Eq.9 are determined by a competition between the largeness of $T_\Gamma$ and the smallness of $1/\bar{n}$. For instance, suppose we take $\bar{n} \rightarrow \infty$, while letting $T_\Gamma$ scale
as unity: \( T\Gamma \sim \bar{n}^0 \) (in the sense defined earlier). This is the limit in which classical behavior persists over the entire time of observation. On the other hand, in this limit \( b_\mathbf{b}(T\Gamma) \sim 1/\bar{n}^s \), so the quadratic and higher-order de-phasing terms in Eq.4 are negligible. Thus, as in the time-independent case, we associate linear de-phasing with classical propagation, and the higher-order terms with spreading.

The regime of interest in this paper is that for which \( T\Gamma \) is large enough that the first three terms of Eq.4 are significant, while terms of order \((\Delta n)^3\) and higher are not. (Formally: \( \bar{n} \rightarrow \infty, T\Gamma \sim \bar{n} \).) In this regime the spreading of the wavepacket becomes important, and wavepacket revivals appear.

As mentioned, a revival occurs when a packet — after having lost its localized structure — reassembles itself, continues for a while along a classical trajectory, then again spreads and dissolves. (Such revivals repeat themselves regularly, in a pattern of “quantum beats” [1]. Additionally, there are fractional revivals [4], but these will not be discussed here.) To show that revivals appear in adiabatically cycled systems, suppose we choose \( T\Gamma \) so that \( b_\mathbf{b}(T\Gamma)/2\hbar = 2\pi \). Then at time \( T\Gamma \) the effect of the quadratic de-phasing term in Eq.4 will be null, and the wavefunction will reflect only the external phase \( \exp(i\phi_n) \) and the linear de-phasing term

\[
- \Delta n \frac{b_1(T\Gamma)}{\hbar} = -\Delta n \int_0^{T\Gamma} dt \frac{\partial H}{\partial I}(t).
\]

(We have discarded a correction that scales like \( 1/\bar{n} \).) Here \( \partial H/\partial I \) at time \( t \) is evaluated at the energy shell of \( H(R(t)) \) which corresponds to the eigenstate \( \bar{n} \), in other words at constant \( I \), even as \( H \) slowly changes. According to Eq.4, Eq.11 describes a wavepacket which has shifted from its original position in phase space, \((q_0, p_0)\), along a classical trajectory of \( \dot{H}(R_0) \), by a change in the angle variable given by

\[
\Delta \theta = \int_0^{T\Gamma} dt \frac{\partial H}{\partial I}(t).
\]

Eq.12 seems to place the revived wave packet at the point in phase space which the classical trajectory would have reached after time \( T\Gamma \). That is, since \( \dot{\theta} = \partial H/\partial I \) in the
time-independent case, and since in the adiabatic limit the action $I$ is an invariant \cite{10}, it appears at first glance evident that the classical change in $\theta$ after time $T$ should be given by Eq.\ref{12} with $\partial H/\partial I$ evaluated at constant $I$. This picture, however, is erroneous: as demonstrated by Hannay \cite{6}, the classical trajectory experiences an additional shift in $\theta$:

$$\Delta \theta = \int_{0}^{T} dt \frac{\partial H}{\partial I}(t) + \Delta \theta_H.$$  \hfill (13)

This “extra” shift $\Delta \theta_H$, Hannay’s angle, is geometric: it is determined by the loop $\Gamma$ in parameter space. I will now show that the source of the discrepancy — the reason Hannay’s angle did not appear in Eq.\ref{12} — is the neglect of Berry’s phase in Eq.\ref{8}.

In Ref. \cite{7}, Berry showed that the correct phase acquired by an adiabatically cycled eigenstate consists of both the dynamical phase of Eq.\ref{8}, and a geometric phase $\gamma_n$ (determined by the loop $\Gamma$):

$$\phi_n(T) = -\frac{1}{\hbar} \int_{0}^{T} dt E_n(t) + \gamma_n.$$  \hfill (14)

Calculating the effect of Berry’s phase on the evolution of a wavepacket launched from $(q_0, p_0)$ is simple. First, Eq.\ref{7} gathers the extra terms

$$\gamma_n + \Delta n \frac{d\gamma_n}{d\bar{n}} + \frac{1}{2}(\Delta n)^2 \frac{d^2\gamma_n}{d\bar{n}^2} + \cdots.$$  \hfill (15)

Now, $\gamma_n \sim \bar{n}$ (see e.g. Eq.[30] of Ref. [11]), so $d^s \gamma_n/d\bar{n}^s \sim \bar{n}^{1-s}$. Thus, in the limit $\bar{n} \to \infty$ only the first two terms in Eq.\ref{15} survive. Let us again choose $T$ so that $b_2(T)/2\hbar = 2\pi$. In the notation of Eq.\ref{2}, the wavepacket at time $T$ is then given by:

$$\psi(T) = e^{i\alpha_n} \sum_n e^{i\beta_n} a_n |u_n\rangle,$$  \hfill (16)

where now

$$\alpha_n = -\frac{1}{\hbar} \int_{0}^{T} dt E_n(t) + \gamma_n$$  \hfill (17)

$$\beta_n = -\Delta n \left[ \int_{0}^{T} dt \frac{\partial H}{\partial I}(t) - \frac{d\gamma_n}{d\bar{n}} \right].$$  \hfill (18)

This describes a wavepacket whose position in phase space is specified by both the “dynamical” shift of Eq.\ref{12}, and an extra shift $-d\gamma_n/d\bar{n}$ in the angle variable:
\[
\Delta \theta = \int_0^{T_f} dt \frac{\partial H(t)}{\partial I} - \frac{d\gamma_n}{dn}.
\] (19)

To complete the connection with the classical result, Eq.13, we invoke the central result of Ref. [11], which states that Hannay’s angle \(\Delta \theta_H\) and Berry’s phase \(\gamma_n\) are related semiclassically by:

\[
\Delta \theta_H = -\frac{d\gamma_n}{dn}.
\] (20)

Thus, the revival described by Eqs.16 - 18 does indeed appear where a proper classical analysis suggests it ought to. Specifically, the dynamical quantal phases \(\int E_n dt\) are responsible for the “dynamical” shift in the angle variable (Eq.12), while the geometric quantal phases \(\gamma_n\) further boost the packet by an amount equal to the classical geometric shift \(\Delta \theta_H\).

(A word about the sizes of terms in Eq.13. Although the first term on the right side scales like \(\bar{n}\), whereas the second term is order unity, the two nevertheless have a comparable effect on the location of the wavepacket, since for this purpose their values are only relevant \(modulo\) \(2\pi\). On the other hand, the leading-order correction to the first term scales like \(1/\bar{n}\) — since corrections to Eq.4 are \(O(1/\bar{n}^2)\) — thus its effect is genuinely small.)

Eq.19 embodies the central result of this paper; combined with Eq.20, it reveals the effect of Berry’s phase on wavepacket revivals in adiabatically cycled systems. In addition to this result, the formalism used in this paper provides a simple interpretation of the semiclassical relationship between Berry’s phase and Hannay’s angle (Eq.20). Namely, if we modify a wavepacket \(\psi_0 = \sum_n a_n |u_n(R_0)\rangle\) by tacking on Berry’s phases \(\exp i\gamma_n\) to the terms in the superposition, then the effect is to shift the packet along a classical trajectory of \(H(R_0)\), by a change in the angle variable equal to Hannay’s angle, \(\Delta \theta_H\). This follows directly from Eqs.13 and 20, without any need for a discussion of revivals. (Alternatively, one could stand the argument on its head and derive Eq.20 by considering the semiclassical evolution of a wavepacket under \(\hat{H}(R(t))\) and invoking Eq.14.) This “wavepacket interpretation” of Eq.20 is similar in spirit to arguments presented by Hannay [6]; its novelty resides in that it offers an easy visualization of the relationship between the two geometric quantities, Berry’s phase (quantal) and Hannay’s angle (classical).
It has been assumed in the preceding analysis that the value of $T_\Gamma$ is chosen so that a revival occurs just as $R(t)$ concludes its circuit in parameter space. Suppose now that we are less restrictive with the value of $T_\Gamma$, but still within the regime of wavepacket revivals (i.e. $b_2(T_\Gamma)/2\hbar$ is order unity, but not necessarily $2\pi$). A straightforward calculation reveals that a revival then occurs (along the classical trajectory) at time $T_R$ satisfying $b_2(T_R)/2\hbar = 2\pi$, even though the Hamiltonian at $t = T_R$ is different from that at $t = 0$. Thus, revivals are as generic in adiabatically driven systems as in time-independent ones. However, only when the revival time $T_R$ coincides with the cycling time $T_\Gamma$ is it meaningful to discuss the effect of Berry’s phase on the revived wavepacket, since Berry’s phase (as well as Hannay’s angle) is well-defined only for closed circuits in parameter space.

The effect of Berry’s phase on the revival location of wavepackets has been illustrated here in one degree of freedom. It would of course be very desirable to find a physical (three-dimensional) system which exhibits this effect. One candidate, suggested in conversation by M. Nauenberg, is a Rydberg atom in a weak magnetic field $B$; here the classical motion is characterized by the precession of the Kepler orbit at the Larmor frequency, and with a proper choice of $|B|$ a wavepacket launched upon the orbit will experience a revival \[3\]. Now suppose that, upon launching the packet, we let the direction of $B$ adiabatically trace out a loop which encloses a solid angle $\Omega$ in $B$-space, so that at the revival time the field is back to its initial orientation. Then as a result of Berry’s phase, the revived wavepacket appears at a location which differs from where it would have appeared had $B$ remained constant. The difference is simply a rotation by $\Omega$ \[12\] around the initial direction of $B$. \[13\] This is essentially an atomic version of the Foucault pendulum, and if experimentally observable \[14\], would constitute a vivid demonstration of the geometric phase effects illustrated in the present paper.
ACKNOWLEDGEMENTS

I would like to thank Mark Mallalieu, Jim Morehead, Michael Nauenberg, and Steve Tomsovic for extended discussions which clarified crucial issues during the preparation of this manuscript. This work was supported by the Department of Energy under Grant No. DE-FG06-90ER40561.
REFERENCES

[1] J.Parker and C.R.Stroud, Jr., Phys.Rev.Lett. 56, 716 (1986).

[2] I.Sh.Averbukh and N.F.Perelman, Phys.Lett. 139A, 449 (1989).

[3] M.Nauenberg, J.Phys.B 23, L385 (1990).

[4] M.Nauenberg, C.Stroud, and J.Yeazell, Scientific American, June, 1994, p. 44, and references therein.

[5] G.Rempe, H.Walther, and N.Klein, Phys.Rev.Lett. 58, 353 (1987).

[6] J.H.Hannay, J.Phys.A 18, 221 (1985).

[7] M.V.Berry, Proc.Roy.Soc.Lond.A 392, 45 (1984).

[8] That these derivatives are well-defined is not immediately obvious, but generally true in one degree of freedom. This follows from a semiclassical extension of WKB theory beyond the leading order, as carried out in O.Bohigas, S.Tomsovic, and D.Ullmo, Phys.Rep. 223, 43 (1993).

[9] H.Goldstein, Classical Mechanics, 2nd ed. Addison-Wesley, 1980. Section 10-5.

[10] V.I.Arnold, Mathematical Methods of Classical Mechanics, Springer, 1978. Section 52.

[11] M.V.Berry, J.Phys.A 18, 15 (1985).

[12] Ω in this example constitutes Hannay’s angle; see Sec. 4 of Ref. [6].

[13] This result follows from the formalism developed by M.Kugler and S.Shtrikman, Phys.Rev.D 37, 934 (1988), and generalized by J.M.Robbins, J.Phys.A 27, 1179 (1994).

[14] Revivals in Rydberg atoms have recently been observed in the presence of external fields; see L.Marmet et al, Phys.Rev.Lett. 72, 3779 (1994), and J.Wals et al, Phys.Rev.Lett. 72, 3783 (1994).