Exact wave functions and nonadiabatic Berry phases of a time-dependent harmonic oscillator

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Exact Schrödinger wave functions of a time-dependent harmonic oscillator are found in analytically closed forms for the eigenstates of the generalized invariant and the instantaneous Hamiltonian. The cyclic initial state (CIS) and corresponding nonadiabatic Berry phase are also found exactly for a τ -periodic Hamiltonian. There may exist $N\tau$ -periodic CISs and corresponding Berry phases, but the cases with unstable classical motions do not have CISs in which cases Berry phases do not exist.

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I. INTRODUCTION

Time-dependent systems in quantum mechanics have been an interesting subject for a long time and the generalized invariant method introduced by Lewis and Riesenfeld (LR) gives a typical and powerful method to study these problems [1,2]. The time-dependent harmonic oscillator is a good example of an exactly solved model and has applications in many areas of physics. On the other hand, the Berry phase [3] and its nonadiabatic generalizations [4] have been another interesting subject.

In order to find the Berry phase of a quantum state we should know its exact wave function up to the timedependent phase. However, the wave functions found in [2] using the LR invariant method do not satisfy the Schrödinger equation, since their time-dependent phases are fixed under the following condition: $\langle 0 | \frac{\partial}{\partial t} | 0 \rangle$ vanish in the limit that the auxiliary function ρ becomes a constant, where the auxiliary function ρ determines the LR invariant and its eigenfunctions. As far as we know the Schrödinger wave function of an eigenstate of the LR invariant in most general cases where mass and frequency are both time-dependent, is found in Refs. [5] and [6]. However, the wave function in [5] satisfies the Schrödinger equation only when the mass is constant and in which case the equivalent wave function also appears in Ref. [7]. Furthermore, some time-dependent phase is missing in the wave function of [6].

In this paper, we find the exact wave function of a timedependent harmonic oscillator using the Heisenberg pic-

ture approach previously developed [8]. The wave func-

Refs. [5,7] for the case with constant mass. However, for the general case where mass is also time-dependent, it is new and different from that of [5]. We examine carefully the wave function for the τ -periodic Hamiltonian, and we find the cyclic initial state (CIS) and the corresponding Berry phase. There may exist $N\tau$ -periodic CISs and corresponding Berry phases. In addition, there exist systems which do not have the CISs, and therefore those systems cannot possess the Berry phase although the Hamiltonians are periodic. They correspond to the systems with unstable classical motions.

tion found in this paper is in agreement with those in

II. GENERALIZED INVARIANT AND ITS EIGENSTATES

For the Hamiltonian of a time-dependent harmonic oscillator system

$$H(t) = \frac{1}{2M(t)}p^{2}(t) + \frac{1}{2}M(t)\omega^{2}(t)q^{2}(t), \qquad (2.1)$$

the following form of the LR invariant is well known:

$$I(t) = g_{-}(t)\frac{p^{2}}{2} + g_{0}(t)\frac{pq + qp}{2} + g_{+}(t)\frac{q^{2}}{2}, \qquad (2.2)$$

where $g_i(t)(i=-,0,+)$ satisfy the linear system of differential equations

$$\dot{g}_{-}(t) = -\frac{2}{M(t)}g_{0}(t),
\dot{g}_{0}(t) = M(t)\omega^{2}(t)g_{-}(t) - \frac{1}{M(t)}g_{+}(t),
\dot{g}_{+}(t) = 2M(t)\omega^{2}(t)g_{0}(t).$$
(2.3)

Moreover, in its most general solutions, $g_{-}(t)$ has the following form [8]:

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$$g_{-}(t) = c_1 f_1^2(t) + c_2 f_1(t) f_2(t) + c_3 f_2^2(t), \tag{2.4}$$

and $g_0(t)$ and $g_+(t)$ are obtained from the first two equations of (2.3) by direct differentiations, where c_i (i=1,2,3) are arbitrary constants and $f_1(t)$ and $f_2(t)$ are two linearly independent solutions of a classical equation of motion:

$$\ddot{f}_{1,2}(t) + \frac{\dot{M}(t)}{M(t)}\dot{f}_{1,2}(t) + \omega^2(t)f_{1,2}(t) = 0. \tag{2.5}$$

We demand that $g_{-}(t)$ is always positive definite because the creation and the annihilation operator of the LR invariant should not be singular (see below). Then, the LR invariant can be written in the form

$$I(t) = \frac{1}{2}\bar{P}^{2}(t) + \frac{1}{2}\omega_{I}^{2}\bar{Q}^{2}(t), \qquad (2.6)$$

where $\omega_I = [g_+(t)g_-(t) - g_0^2(t)]^{1/2}$ and the new canonical variables $\bar{P}(t)$ and $\bar{Q}(t)$ are obtained by two successive time-dependent unitary transformations:

$$U_1(t) = \exp\left(i\frac{g_0(t)}{2g_-(t)}q^2\right)$$
 (2.7)

and

$$U_2(t) = \exp\left(\frac{i}{4} (PQ + QP) \ln g_-(t)\right),$$
 (2.8)

as $Q = U_1^{-1}qU_1 = q$, $P = U_1^{-1}pU_1 = p + \frac{g_0}{g_-}q$, and $\bar{Q} = U_2^{-1}QU_2 = \frac{1}{\sqrt{g_-}}Q$, $\bar{P} = U_2^{-1}PU_2 = \sqrt{g_-}P$, respectively.

From the form of (2.6) one defines the annihilation and creation operator as

$$\begin{split} A(t) &= \sqrt{\frac{\omega_I}{2}} \bar{Q}(t) + \frac{i}{\sqrt{2\omega_I}} \bar{P}(t), \\ A^{\dagger}(t) &= \sqrt{\frac{\omega_I}{2}} \bar{Q}(t) - \frac{i}{\sqrt{2\omega_I}} \bar{P}(t). \end{split} \tag{2.9}$$

Their time evolutions are found from the Heisenberg equation of motion of quantum operators [8],

$$A^{\dagger}(t) = e^{i \int_{t_0}^{t} \frac{\omega_I}{M(t)g_{-}(t)} dt} A^{\dagger}(t_0),$$

$$A(t) = e^{-i \int_{t_0}^{t} \frac{\omega_I}{M(t)g_{-}(t)} dt} A(t_0).$$
(2.10)

Moreover, the invariant (2.6) can be rewritten as $I = \omega_I \left(A^\dagger A + \frac{1}{2} \right)$, where A and A^\dagger are the creation and annihilation operators at an initial time t_0 . Now, the eigenstates of the generalized invariant are the number states

$$I|n\rangle_{I} = \left(n + \frac{1}{2}\right)\omega_{I}|n\rangle_{I}, \ n = 0, 1, 2, \dots,$$
 (2.11)

where $|n\rangle_I = \frac{A^{\dagger n}}{\sqrt{n!}} |0\rangle_I$ and $A|0\rangle_I = 0$.

III. SCHRÖDINGER WAVE FUNCTIONS

Now comparing (2.6), (2.10), and (2.11) with the equations of the time-independent harmonic oscillator it is

easy to find

$$\langle \bar{Q}, t | n \rangle_{I} = e^{-i\left(n + \frac{1}{2}\right) \int^{t} \frac{\omega_{I}}{M(t)g_{-}(t)} dt} \varphi_{n}(\xi), \qquad (3.1)$$

where $\xi = \sqrt{\omega_I} \bar{Q}$ and

$$\varphi_n(\xi) = \frac{1}{\sqrt{2^n n!}} \left(\frac{\omega_I}{\pi}\right)^{1/4} e^{-\frac{\xi^2}{2}} H_n(\xi), \tag{3.2}$$

where $H_n(\xi)$ is a Hermite polynomial. Now it is easy to represent the wave function in terms of the original coordinate variable

$$\langle q|\psi_n(t)\rangle_I \equiv \psi_n(q,t) \equiv \langle q,t|n\rangle_I$$
. (3.3)

It follows from the Eqs. (2.7) and (2.8) that [9]

$$\langle q, t | = e^{-i\frac{g_0(t)}{2g_-(t)}q^2} \langle Q, t |$$

$$= (g_-(t))^{-1/4} e^{-i\frac{g_0(t)}{2g_-(t)}q^2} \langle \bar{Q}, t |, \qquad (3.4)$$

and therefore the result is

$$\psi_n(q,t) = (g_-(t))^{-1/4} e^{-i\frac{g_0(t)}{2g_-(t)}q^2} \langle \bar{Q}, t|n \rangle_I$$
 (3.5)

and it can be written in the original coordinate variable as

$$\psi_{n}(q,t) = \frac{1}{\sqrt{2^{n} n!}} \left(\frac{\omega_{I}}{\pi g_{-}(t)}\right)^{\frac{1}{4}} e^{-i\frac{g_{0}(t)}{2g_{-}(t)}q^{2}} \times e^{-i\int dt \frac{\omega_{I}}{M(t)g_{-}(t)} (n+\frac{1}{2})} e^{-\frac{\omega_{I}}{2g_{-}(t)}q^{2}} \times H_{n}\left(\sqrt{\frac{\omega_{I}}{g_{-}(t)}}q\right). \tag{3.6}$$

By directly substituting Eq. (3.6) into the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi_n(q,t) = H(t)\psi_n(q,t),$$
 (3.7)

and after taking some cancellations using (2.3), we get the ordinary differential equation (see the Appendix)

$$\left(-\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\xi^2\right)\varphi_n(\xi) = \left(n + \frac{1}{2}\right)\varphi_n(\xi) , \qquad (3.8)$$

which shows that (3.6) indeed satisfies the Schrödinger equation.

When the mass is constant, i.e., M(t)=m, our wave function (3.6) becomes the one of Ref. [5] with setting $g_{-}(t)=\frac{\omega_{I}\rho^{2}(t)}{m}$, and the one of Ref. [7] with setting $\omega_{I}=\Omega$ and $g_{-}(t)=f_{1}^{2}(t)+f_{2}^{2}(t)$, where $f_{1}(t)=\rho(t)\cos\gamma(t)$ and $f_{2}(t)=\rho(t)\sin\gamma(t)$ are two linearly independent solutions of the classical equation of motion. However, our result is more general than that of Ref. [7] because ours includes time-varying mass. We also note that the wave function of Ref. [5] does not agree with ours in the time-varying mass case. Their wave function seems to be not correct because it includes the term $\dot{M}(t)/M(t)$ only once. Its time derivative in the Schrödinger equation produces the $\ddot{M}(t)$ term, but there is no other $\ddot{M}(t)$

term which cancels that away. Finally, the missing phase factor in the wave function of [6] is $\exp\left(-i\frac{g_0(t)}{2g_-(t)}q^2\right)$.

Now we can construct the eigenfunction of the instantaneous Hamiltonian at some time, say t_0 . To find eigenstates of the instantaneous Hamiltonian $H(t_0)$, the only thing to do is to find I(t) such that $I(t_0) = H(t_0)$ and this is accomplished by setting three parameters so that $g_-(t_0) = 1/M(t_0)$, $g_0(t_0) = 0$, and $g_+(t_0) = M(t_0)\omega^2(t_0)$. Now it is clear that $|n\rangle_I = |n\rangle_{H(t_0)}$ and therefore the eigenstate of the instantaneous Hamiltonian can be written

$$H(t_0)|n\rangle_{H(t_0)} = E_n(t_0)|n\rangle_{H(t_0)},$$
 (3.9)

where $E_n(t_0) = \omega(t_0)(n+1/2)$. Now we have found an eigenstate of the instantaneous Hamiltonian at t_0 and its time-dependent Schrödinger wave function (3.6).

IV. EXISTENCE OF CYCLIC INITIAL STATES AND NONADIABATIC BERRY PHASES

Consider the nonadiabatic Berry phase of a general quantum system with τ -periodic Hamiltonian. The evolution of an initial state $\psi(t_0)$ is found by solving the time-dependent Schrödinger equation (3.7). Choosing the initial state to be cyclic immediately gives us the overall phase; as $\psi(t_0 + \tau) = e^{i\chi}\psi(t_0)$, we call such an initial state a cyclic initial state. The price we have to pay in making this generalization is that the cyclic initial states are no longer (in general) eigenvectors of the initial Hamiltonian $H(t_0)$ [10]. The overall phase is simply given by χ , and the generalization of dynamical phase is the time integral of the instantaneous expectation value of the Hamiltonian,

$$\delta = -\int_0^\tau \langle \psi_n(t) | H(t) | \psi_n(t) \rangle dt. \tag{4.1}$$

Aharonov and Anandan [4] show that $\beta = \chi - \delta$ is a purely geometrical property of the evolution in the sense that it only depends on the path followed by the system in projective Hilbert space.

In this section, in a τ -periodic Hamiltonian system:

$$M(t+\tau) = M(t), \ \omega(t+\tau) = \omega(t), \tag{4.2}$$

we find the CIS and calculate the corresponding Berry phase in a closed form using classical solutions of (2.5). We consider the cyclic initial state such that

$$\psi_n(t+\tau') = e^{i\chi_n(\tau')}\psi_n(t), \tag{4.3}$$

which is, in general, no longer an eigenstate of the initial Hamiltonian $H(t_0)$. Moreover, a minimal period τ' may not be equal to τ .

Inspecting closely the form of wave function (3.6), we find that the necessary and sufficient condition for the existence of CISs is the existence of periodic auxiliary functions. By Floquet's theorem [11], we have two independent solutions such that

$$f_1(t) = e^{\alpha t} r_1(t), \ f_2(t) = e^{-\alpha t} r_2(t),$$
 (4.4)

where α is a constant and $r_1(t), r_2(t)$ are τ -periodic func-

tions. With these solutions prepared, we examine that the positive τ -periodic auxiliary function can be constructed from them.

Case 1. α is pure imaginary. We set $\alpha=i\alpha_{im}$ (where α_{im} is real). Case 1-1. $\alpha=im\pi/N'\tau$ ($m,\ N'=1$) integers). For N' = 1, $f_1^2(t)$, $f_1(t)f_2(t)$, and $f_2^2(t)$ are τ -periodic and so is any $g_{-}(t)$, and in this case we can always find the CISs which are the eigenstates of both the invariant I(t) and initial Hamiltonian $H(t_0)$. We will consider the case $N' \neq 1$ in a later section. Case 1-2. Otherwise, the real and imaginary parts of $r_1(t)e^{i\alpha_{im}t}$ are two independent solutions and they are aperiodic. In this case, the general auxiliary functions are also aperiodic, and the eigenstates are not CISs. However, we have a τ periodic auxiliary function of the form $g_{-}(t) = c|r_{1}(t)|^{2}$, which is positive definite since $|r_1(t)|$ cannot vanish (if it does, the Wronskian should vanish, and this contradicts the linear independency of two solutions). Furthermore, it cannot be monotonically increasing or decreasing since $g_{-}(t)$ is periodic. Therefore, we have $g_{-}(t)/dt = 0$ at some times $t = t_0 + n\tau$, where we find $I(t) \propto H(t_0)$ using (2.2) and (2.3). Then the eigenstate of $H(t_0)$ is also a CIS. However, it does not mean that we can construct the CISs, at any time, which are also the eigenstates of the instantaneous Hamiltonian.

Case 2. $\alpha = \alpha_{re} + i\alpha_{im}$ has a real part $(\alpha_{re} \neq 0)$. In this case, we can take two independent solutions to be a real (or imaginary) part of (4.4), as $e^{\alpha_{re}t}s_1(t)$ and $e^{-\alpha_{re}t}s_2(t)$, where $s_1(t)$ and $s_2(t)$ are real (or imaginary) parts of $e^{i\alpha_{im}t}r_1(t)$ and $e^{-\alpha_{im}t}r_2(t)$, respectively. Therefore, the only possibility that $g_-(t)$ is τ -periodic is such that $g_-(t) = c_2f_1(t)f_2(t) = c_2s_1(t)s_2(t)$. However, this spoils the positiveness of $g_-(t)$, since the oscillation parts, $s_1(t)$ and $s_2(t)$, have zeros [12]. Therefore it is impossible to construct CISs for the system which has classically unstable motions. The unstable solutions of the Mathieu equation [13] are good examples.

When $g_{-}(t)$ is τ -periodic, all the eigenstates of the generalized invariant are CISs with

$$\chi_n(\tau) = -\left(n + \frac{1}{2}\right) \int_0^{\tau} \frac{\omega_I}{M(t)g_-(t)} dt \tag{4.5}$$

and the nonadiabatic Berry phase is obtained by removing the dynamical phase from (4.5) as

$$\beta_n(\tau) \equiv \chi_n(\tau) + \int_0^\tau \langle \psi_n(t) | H(t) | \psi_n(t) \rangle dt. \tag{4.6}$$

Using $\langle \psi_n(t)|H(t)|\psi_n(t)\rangle=(n+1/2)[h_0(t)/2]$ [8] , where $h_0(t)=[g_0^2(t)+M^2(t)\omega^2(t)g_-^2(t)+\omega_I^2]/[M(t)g_-(t)\omega_I]$, and (2.3) we get

$$\beta_n(\tau) = \frac{1}{2} \left(n + \frac{1}{2} \right) \int_0^{\tau} \frac{g_-(t)}{\omega_I} \frac{d}{dt} \left(\frac{g_0(t)}{g_-(t)} \right) dt. \tag{4.7}$$

The partial integration using the periodicity of $g_i(t)$ and the first equation of (2.3) lead to

$$\beta_n(\tau) = -\left(n + \frac{1}{2}\right) \int_0^{\tau} \frac{g_0^2(t)}{M(t)g_-(t)\omega_I} dt.$$
 (4.8)

Thus we presented the Berry phase for the CIS in a simple closed form.

V. DISCUSSION

We derived the exact wave function of the eigenstate of the LR invariant using the unitary transformations and the Heisenberg operator evolutions. Futhermore, we discussed the wave functions of the instantaneous Hamiltonian and the CISs. Finally we found the nonadiabatic Berry phase of the CIS in terms of classical motions. Two remarkable results are found in relations to the Berry phase. (i) There may exist $N\tau$ -periodic CISs and corresponding Berry phases: when $\alpha = im\pi/N'\tau(N' \neq 1)$, we can easily notice that $g_-(t)$ is periodic with minimal period $N\tau$ (N=N'/2 for even N', N=N' for odd N') and there exist $N\tau$ -periodic CISs such that

$$\psi_n^{(N)}(t + N\tau) = e^{i\chi_n^{(N)}}\psi_n^{(N)}(t), \tag{5.1}$$

where

$$\chi_n^{(N)} = -\left(n + \frac{1}{2}\right) \int_0^{N\tau} \frac{\omega_I}{M(t)g_-(t)} dt$$
 (5.2)

and the nonadiabatic Berry phase for this CIS is

$$\beta_n^{(N)}(\tau) = -\left(n + \frac{1}{2}\right) \int_0^{N\tau} \frac{g_0^2(t)}{M(t)g_-(t)\omega_I} dt.$$
 (5.3)

(ii) The system with unstable classical motions possesses no CIS and therefore there exists no Berry phase.

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APPENDIX: DERIVATION OF (3.8) FROM (3.6)

We are concerned here with the derivation of (3.8) from (3.6). For the simplicity of calculation, we write

$$\psi_n(q,t) = T(q,t)\varphi_n(\xi),\tag{A1}$$

where

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$$T(q,t) = g_{-}(t)^{-\frac{1}{4}} e^{-i\frac{g_{0}(t)}{2g_{-}(t)}q^{2}} e^{-i\int dt \frac{\omega_{I}}{M(t)g_{-}(t)} (n+\frac{1}{2})}.$$
 (A2)

First, let us consider the left-hand side of the Schrödinger equation (3.7):

$$i\frac{\partial}{\partial t}\psi_{n}(q,t) = i\frac{\partial T}{\partial t}\varphi_{n} - iT\sqrt{\frac{\omega_{I}}{g_{-}}}\frac{\dot{g}_{-}}{2g_{-}}q\frac{d}{d\xi}\varphi_{n}, \quad (A3)$$

where we have used $\xi = \sqrt{\omega_I/g_-}q$ and a dot denotes a time derivative. We insert the time derivative of (A2) into (A3) and eliminate \dot{g}_- and \dot{g}_0 by using the first and second equation of (2.3), respectively, we get

$$\begin{split} i\frac{\partial}{\partial t}\psi_{n}(q,t) &= \frac{ig_{0}}{2Mg_{-}}T\varphi_{n} \\ &+ \left(\frac{M\omega^{2}}{2} - \frac{g_{+}}{2Mg_{-}} + \frac{g_{0}^{2}}{Mg_{-}^{2}}\right)q^{2}T\varphi_{n} \\ &+ \left(n + \frac{1}{2}\right)\frac{\omega_{I}}{Mg_{-}}T\varphi_{n} \\ &+ iT\sqrt{\frac{\omega_{I}}{g_{-}}}\frac{g_{0}}{Mg_{-}}q\frac{d}{d\xi}\varphi_{n}. \end{split} \tag{A4}$$

Now we calculate the first term of right-hand side of (3.7):

$$\begin{split} \frac{1}{2M}\frac{\partial^2}{\partial q^2}\psi_n(q,t) &= \frac{1}{2M}\left[-\left(\frac{g_0}{g_-}\right)^2q^2 - i\frac{g_0}{g_-}\right]T\varphi_n \\ &\quad -\frac{i}{M}\frac{g_0}{g_-}q\sqrt{\frac{\omega_I}{g_-}}T\frac{d}{d\xi}\varphi_n \\ &\quad +\frac{1}{2M}\frac{\omega_I}{g_-}T\frac{d^2}{d\xi^2}\varphi_n. \end{split} \tag{A5}$$

From (A4) and (A5), eliminating g_+ by using the identity $\omega_I^2 = g_+g_- - g_0^2$, we get the final result:

$$\begin{split} 0 &= \left(i\frac{\partial}{\partial t} - H(t)\right) \psi_n(q,t) \\ &= \left(i\frac{\partial}{\partial t} + \frac{1}{2M(t)} \frac{\partial^2}{\partial q^2} - \frac{1}{2}M(t)\omega^2(t)q^2\right) \psi_n(q,t) \\ &= -\frac{\omega_I T}{Mq_-} \left[-\frac{1}{2} \frac{d^2}{d\xi^2} + \frac{1}{2}\xi^2 - \left(n + \frac{1}{2}\right) \right] \varphi_n. \end{split} \tag{A6}$$

This leads to (3.8). It is well known in a time-independent harmonic oscillator that its normalized solution is (3.2).

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