Stokes phase and geometrical phase in a driven two-level system

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The generic two-level model with time-dependent matrix elements becomes soluble in the limit that its diagonal and off-diagonal terms vary along a flat ellipse, encircling the diabolical singular point in the parameter space. The time evolution of the state vector is explicitly obtained, and the condition for its evolution to form a closed circuit in the projective Hilbert space of rays is given as a result of destructive interference at level crossing. The Aharonov-Anandan geometrical phase is shown to be related to the Stokes phase for the Landau-Zener model, which is a natural extension of Berry's phase to nonadiabatic evolutions. [S1050-2947(97)51004-3]

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Since Berry [1] pointed out the existence of a nontrivial phase factor associated with adiabatic evolutions of the state vector in accordance with a cyclic change of parameters contained in the Hamiltonian, a number of works have been devoted to clarifying the meaning of this observation [2,3] and to extending the concept of the *geometrical phase* to a wider class of quantum processes [4–7]. Specifically, Aharonov and Anandan [5] have shown that the assumption of the adiabaticity can be removed if one considers a closed path in the projective Hilbert space of rays instead of those in the parameter space. It is shown that if the state vector returns to its initial value after a time evolution except for a multiplicative phase factor, one can define a geometrical part of this phase in the sense that it depends only on the closed curve in the projective Hilbert space.

One of the prototype models to demonstrate the geometrical phase factor is a spin system in time-dependent magnetic fields [1,5,8,9], or equivalently, a two-level atom driven by a coherent laser field [10]. Aharonov and Anandan presented a few examples of the generalized geometrical phase for spin systems. Suter, Mueller, and Pines [11] performed an experimental verification of Aharonov and Anandan's phase factor by the NMR spin-echo technique. The evolution of the state vector in these examples is essentially a precession of the spin under a static magnetic field, and is trivial as a dynamical problem. Furthermore, the relation with the adiabatic evolution driven by a time-dependent Hamiltonian originally conceived by Berry is not clear. Therefore, it will be worthwhile to have a model that obeys a nontrivial equation of motion driven by a Hamiltonian with explicit time dependence and that is still soluble. In this work, I propose such a model. The model is a two-level system with time-dependent diagonal and off-diagonal matrix elements, which bridges the adiabatic and the diabatic limits continuously. The evolution of the state vector is analytically given in a limiting situation of the orbital shape in the parameter space. The geometrical phase factor for nonadiabatic processes is shown to be related with a phase factor called the Stokes phase, which appears in the theory of second-order differential equations.

Consider a two-level system $|1\rangle$ and $|2\rangle$ driven by the Hamiltonian

$$H(t)=\epsilon(t)(|1\rangle\langle1|-|2\rangle\langle2|)+\Delta(t)(|1\rangle\langle2|+|2\rangle\langle1|),\tag{1}$$

in which the diagonal and the off-diagonal terms are time-dependent real parameters. The adiabatic eigenenergies are degenerate at the diabolical point, $\epsilon=\Delta=0$ in the (ϵ,Δ) plane. Although the following arguments may be advanced for a more general setting, we assume for the sake of definiteness that the point $(\epsilon(t),\Delta(t))$ moves along an ellipse given by $\epsilon(t)=\epsilon_0\cos\omega t$ and $\Delta(t)=\Delta_0\sin\omega t$. The case in which $\Delta=$const has been discussed in a previous paper [12] in connection with the coherent destruction of tunneling [13].

The time evolution of the state vector $\psi(t)$ driven by $i\partial\psi(t)/\partial t=H(t)\psi(t)$, $(\hbar=1$ hereafter) is investigated under the initial condition $\psi(0)=|1\rangle$. Note that the diabatic basis $|1\rangle$ coincides with the adiabatic eigenstate at $t=0$. In the limit of slow variation of the parameter values, $\psi(t)$ traces the upper branch of the adiabatic eigenstates. The adiabatic perturbation theory [14] tells us that the condition for the adiabatic evolution is given by

$$\omega\ll\min\left\{\frac{\Delta_0^2}{\epsilon_0},\frac{\epsilon_0^2}{\Delta_0}\right\},\tag{2}$$

where min{ } means that the smallest should be chosen in the order of magnitude. Then, $\psi(t)$ surely comes back to $|1\rangle$ at $t=2\pi/\omega$, but gains a phase factor $\exp[i\chi^{(a)}]$. Here $\chi^{(a)}$ is decomposed into two parts, $\chi^{(a)}=\chi_d^{(a)}+\chi_g^{(a)}$, in which $\chi_d^{(a)}$ is the dynamical phase given by

$$\chi_d^{(a)}=-\int_0^{2\pi/\omega}\sqrt{\epsilon(t)^2+\Delta(t)^2}dt,\tag{3}$$

and $\chi_g^{(a)}$ is Berry's phase given by $\chi_g^{(a)}=\pi$.

Now we consider another extreme situation that shall be called the limit of impulsive transition. This is characterized by the inequality

$$\Delta_0\ll\epsilon_0.\tag{4}$$

Since the off-diagonal coupling works effectively only for the diagonal energy difference satisfying $\epsilon\lesssim\Delta$ in the order of magnitude, the time evolution of the system in this limit

can be regarded as a successive occurrence of nonadiabatic transitions around the avoided crossing between the adiabatic eigenstates. By choosing the diabatic states $|1\rangle$ and $|2\rangle$ for the basis set, one may also say that the system undergoes successive off-diagonal transitions between $|1\rangle$ and $|2\rangle$ around the level crossings. Hereafter, we adopt the diabatic base for the representation of the state vector. Since the time duration that the system stays in the transition region is estimated to be of order of $\Delta_0/\epsilon_0\omega$ for moderate values of Δ_0, the transition occurs impulsively at crossing times $t_n \equiv (n-\frac{1}{2})\pi/\omega$, $(n=1,2,\dots)$, and the system propagates almost freely between each crossing.

The present author has shown that the time evolution of the two-level system in such a case can well be described by the transfer-matrix formalism [12]. The equation of motion around the crossing time is approximated by that for the Landau-Zener model [15]. At the crossing time t_{2m-1} $(m=1,2,\dots)$, the incoming and outgoing states are connected by the transfer matrix [16]

$$M_1=\begin{pmatrix} \sqrt{q} & -\sqrt{1-q}\,e^{i\phi} \\ \sqrt{1-q}\,e^{-i\phi} & \sqrt{q} \end{pmatrix}, \qquad (5)$$

where the (i,j) component represents the transfer $|j\rangle \rightarrow |i\rangle$. In the above equation, $q\equiv\exp(-2\pi\delta)$, with $\delta\equiv\Delta_0^2/(2\epsilon_0\omega)$ being the adiabaticity parameter. The phase ϕ is the Stokes phase, and is given by

$$\phi=\pi/4+\arg\Gamma(1-i\delta)+\delta(\ln\delta-1), \qquad (6)$$

where $\Gamma(z)$ is the Γ function. The Stokes phase generally originates from the connection of the asymptotic forms of confluent hypergeometric functions, namely, Weber's function in this case [15], at a regular singularity [17]. It also guarantees the single-valued nature of the solution against the rotation of 2π around the singularity in the complex plane. The phase ϕ is a monotonically decreasing function of δ, and takes the following limiting values in the adiabatic $(\delta\rightarrow\infty)$ and the diabatic $(\delta\rightarrow 0)$ limits: $\phi(\delta\rightarrow\infty)=0$ and $\phi(\delta\rightarrow 0)=\pi/4$. At the crossing time t_{2m} $(m=1,2,\dots)$, the transfer matrix is given by $M_2\equiv M_1^*$, where $*$ means the complex conjugate. Note that the transfer matrix depends both on the sign of the off-diagonal matrix element and the way of crossing, whether $|1\rangle$ crosses $|2\rangle$ from the upper side or from the lower side. The outgoing state at t_{2m-1} and the incoming state at t_{2m} is connected by the propagator

$$G_1=\begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}, \qquad (7)$$

where

$$\theta=2\int_0^{\pi/2\omega}\sqrt{\epsilon(t)^2+\Delta(t)^2}\,dt\simeq\frac{2\epsilon_0}{\omega}. \qquad (8)$$

Likewise the propagator from t_{2m} to t_{2m+1} is given by $G_2 \equiv G_1^*$.

Denote the state vector at each half cycle $t=n\pi/\omega$ $(n=0,1,2,\dots)$ as ψ_n. In the representation by a two-component vector, ψ_n is obtained by successive operation of M_i and G_i on $\psi_0\equiv\binom{1}{0}$ as $\psi_1=G_1^{1/2}M_1G_2^{1/2}\psi_0$, $\psi_2=G_2^{1/2}M_2G_1^{1/2}\psi_1$, etc. If one defines a unitary matrix T by

$$T\equiv G_1^{1/2}M_1G_2^{1/2}=\begin{pmatrix} \sqrt{q} & -\sqrt{1-q}\,e^{i(\phi+\theta)} \\ \sqrt{1-q}\,e^{-i(\phi+\theta)} & \sqrt{q} \end{pmatrix}, \qquad (9)$$

ψ_n can be written simply as $\psi_{2m-1}=T(T^*T)^{m-1}\psi_0$, $\psi_{2m}=(T^*T)^m\psi_0$ $(m=1,2,\dots)$, in the impulsive transition limit. Introduce another unitary matrix S defined by

$$S=\begin{pmatrix} \sqrt{1-q}\,e^{-i(\phi+\theta)} & \sqrt{q} \\ -\sqrt{q} & \sqrt{1-q}\,e^{i(\phi+\theta)} \end{pmatrix}. \qquad (10)$$

Then we find

$$T^*T=-S^2 \qquad (11)$$

and

$$S^2=2\cos\xi S-1, \qquad (12)$$

with $\cos\xi\equiv\sqrt{1-q}\cos(\phi+\theta)$. From Eq. (13), we may put $S^n=\alpha_n+\beta_nS$ and derive recursion relations for α_n and β_n as $\alpha_{n+1}=-\beta_n$ and

$$\beta_{n+1}-2\cos\xi\beta_n+\beta_{n-1}=0, \qquad (13)$$

with $\beta_0=0$, $\beta_1=1$. This equation is equivalent to that for a boundary value problem in a one-dimensional tight-binding model, and can be easily solved to yield

$$\beta_n=\frac{\sin n\xi}{\sin\xi}. \qquad (14)$$

Finally, we obtain

$$\psi_{2m-1}=(-1)^{m-1}(\sqrt{q}\beta_{2m-1},\ \sqrt{1-q}\,e^{-i(\phi+\theta)}\beta_{2m-1} \\ -\beta_{2m-2})^T, \qquad (15)$$

$$\psi_{2m}=(-1)^m(\sqrt{1-q}\,e^{-i(\phi+\theta)}\beta_{2m}-\beta_{2m-1},\ -\sqrt{q}\beta_{2m})^T. \qquad (16)$$

The probability P_n that the system exists in $|2\rangle$ at $t=n\pi/\omega$ is given by

$$P_{2m-1}=1-q\left[\frac{\sin[(2m-1)\xi]}{\sin\xi}\right]^2, \qquad (17)$$

$$P_{2m}=q\left[\frac{\sin(2m\xi)}{\sin\xi}\right]^2. \qquad (18)$$

For irrational values of ξ/π, the sequence $\{P_n\}$ distributes uniformly and densely over the interval $[0,1]$. If ξ/π is a rational number, $\{P_n\}$ has a periodic structure, which corresponds to the case of a standing wave in the analogy of the tight-binding model for a linear chain. In particular, the condition for complete return to the initial value after a period of circulation is given by $\cos\xi=0$. This leads to the requirement

$$\phi+\theta=(k+\tfrac{1}{2})\pi,\ \ k=0,1,2,\dots, \qquad (19)$$

which means that the destructive interference between the two transition paths, one through $|1\rangle$ and the other through $|2\rangle$ in the intermediate state, completely suppresses the probability to reach $|2\rangle$ after the second crossing. Equation (19) determines a set of one-dimensional manifolds in the parameter space $(\epsilon_0,\Delta_0,\omega)$. Hereafter we restrict ourselves to one of such manifolds.

From Eq. (16), the state vector in the final state of circulation is given by $\psi_2=|1\rangle$. That is, the state vector returns to its initial value including the phase factor with the dynamical phase being just compensated by the geometrical phase. The dynamical phase χ_d is given by [5]

$$\chi_d = -\int_0^{2\pi/\omega}\langle\psi(t)|H(t)|\psi(t)\rangle dt = -2\theta(1-q) \quad (20)$$

within the impulsive transition approximation. Therefore, the geometrical phase χ_g is given by

$$\chi_g = 2\theta(1-q) \quad (\mathrm{mod}\,2\pi). \quad (21)$$

Equations (19) and (21) connect the geometrical phase with the Stokes phase. In the adiabatic limit $\delta\to\infty$, we find $q\to 0$, $\phi\to 0$ and $\chi_g\to 2\theta=\pi$ $(\mathrm{mod}\,2\pi)$, which recovers Berry's phase. The geometrical phase χ_g changes continuously from 0 to π as the adiabaticity parameter δ changes from 0 to ∞.

The closed curve in the projected Hilbert space of rays for a two-level system is most clearly visualized by a circuit on the two-sphere Σ corresponding to the polarization vector $\vec{p}$ defined for the density matrix [11],

$$\rho = \tfrac{1}{2}(1+\vec{p}\cdot\vec{\sigma}), \quad (22)$$

where $\vec{\sigma}$ is Pauli's spin matrices. Aharonov and Anandan [5] and Suter and co-workers [11] noticed that the geometrical phase $\chi(C)$ is related with the solid angle $\Omega(C)$ subtended by the circuit C on Σ at the origin as

$$\chi(C) = \tfrac{1}{2}\Omega(C). \quad (23)$$

In our model, the locus of the vector $\vec{p}$ is a spherical triangle on Σ. If one represents $\vec{p}$ by the spherical angles (Θ,Φ) as $p_x=\sin\Theta\cos\Phi$, $p_y=\sin\Theta\sin\Phi$, $p_z=\cos\Theta$, the circuit C is given as follows. From $t=0$ to $t=t_1(=\pi/2\omega)$, $\vec{p}$ stays at the north pole $\Theta=0$. At $t=t_1$, it suddenly moves along a meridian to the point (Θ_1,Φ_1), where $\Theta_1=2\cos^{-1}\sqrt{q}$ and $\Phi_1=\phi$. From t_1 to $t_2(=3\pi/\omega)$, it moves along the parallel to (Θ_1,Φ_2) where $\Phi_2=\phi+2\theta$. Then at $t=t_2$, it suddenly goes back to the north pole along the meridian and stays there until $t=2\pi/\omega$. The solid angle subtended at the origin is then $\Omega(C)=2\theta(1-\cos\Theta_1)=4\theta(1-q)$. Thus we find $\chi_g=\Omega(C)/2$ in agreement with the case of Ref. [11]. The geometrical phase is truly geometrical: It depends only on the circuit in the projective Hilbert space but not on the specific Hamiltonian by which the system is driven. As δ increases, satisfying Eq. (19), the area swept by $\vec{p}$ increases, and in the limit $\delta\to\infty$, $\vec{p}$ travels Σ along the great circle with $\Phi=0$ from the north pole to the south pole and goes back to the north pole along the great circle $\Phi=\pi$.

In the present work, I have proposed a soluble model of a driven two-level system, in which the generalized geometri-

cal phase is explicitly calculated for nonadiabatic quantum evolutions. The adiabatic geometrical phase of Berry is recovered as a special case. The only assumption is that the parameters in the Hamiltonian move on a very flat orbital so that the transition is effectively localized near the level crossing. It is remarkable that the geometrical phase, which is a quantity attributed to the global feature of the circuit, is closely related with the Stokes phase, which is a quantity bearing only local information at the level crossing.

Here we have restricted ourselves to a specific model given by Eq. (1) in which the orbital $(\epsilon(t),\Delta(t))$ encircles the singular point. It should be noted that in order to yield a geometrical phase, the orbital need not encircle the singular point. In fact, an analogous analysis can be made for the model in which $\Delta(t)=\Delta_0(\mathrm{const})$ with $\Delta_0\ll\epsilon_0$ [12]. In this case the condition for complete return of the state vector is given in terms of the Stokes phase as

$$\phi+\theta=k\pi, \quad k=1,2,\ldots, \quad (24)$$

where ϕ and θ are defined in the same way as Eqs. (6) and (8) [12]. On the other hand, the geometrical phase is shown to be given by $\chi_g=2\theta(1-q)$. As the adiabaticity increases, the area swept by the polarization vector $\vec{p}$ on Σ enlarges faster than the present case. In the limit of adiabatic evolution, $\vec{p}$ travels only a single half of the great circle connecting the poles along the meridian $\Phi=0$, first downward then upward, so that the geometrical phase approaches 2π instead of π.

If the phase ξ satisfies the condition

$$\xi = \frac{l}{2n}\pi, \quad (25)$$

for integers n and l that obey the restriction $0<l<2n$ and are relatively prime, the system returns to the initial state first after nth cycle. In this case, the density matrix becomes a multivalued function of the parameters $(\epsilon(t),\Delta(t))$. For the process satisfying condition (25), the state vector returns to $\psi_{2n}=(-1)^{n+l}|1\rangle$ after n cycles. The integer n may be called a winding number, and l is an additional quantum number designating the pattern of the evolution. Since the probability that the system exists in the *lower* branch from t_m to t_{m+1} is given by $q[\sin m\xi/\sin\xi]^2$ $(m=1,2,\ldots,2n-1)$, the dynamical phase χ_d is calculated as

$$\chi_d = -\theta - \sum_{m=1}^{2n-1}\{1-2q[\sin m\xi/\sin\xi]^2\}\theta$$

$$= -2n\theta\left(1-\frac{q}{\sin^2\xi}\right). \quad (26)$$

This is an extension of Eq. (20) to the process with winding number n. The geometrical phase χ_g is given by

$$\chi_g = (n+l)\pi + 2n\theta\left(1-\frac{q}{\sin^2\xi}\right). \quad (27)$$

Formula (21) is recovered by setting $n=l=1$ in the above equation.

The experimental observation of the nonadiabatic pro-

cesses and the associated geometrical phase investigated here would be possible, in principle, by using the phase-sensitive technique of magnetic resonance [11] under the time-dependent longitudinal and the transverse magnetic fields. Its optical analog [18] may also be a candidate for the possibility. In fact, experimental observations of the quasi-level-crossing called the optical adiabatic rapid passage induced by resonant laser fields have been done for gas phase [19] as well as for solids [20]. It will be of interest to clarify the role of the quantum phase by using these techniques, although the effect of dephasing [21] should also be considered in realistic situations.

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