Applications of the complex geometric phase for metastable systems

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Garrison and Wright showed that upon undergoing cyclic quantum evolution a metastable state acquires both a geometric phase and a geometric decay probability. This is described by a complex geometric phase associated with the cyclic evolution of two states and is closely related to the two-state formalism developed by Aharonov *et al.* Applications of the complex geometric phase to the Born-Oppenheimer approximation and the Aharonov-Bohm effect are considered. A simple experiment based on the optical properties of absorbing birefringent crystals is proposed. [S1050-2947(96)06112-4]

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In quantum mechanics a state is defined up to an arbitrary phase. However, phase differences have physical meaning. Therefore if a state evolves in such a way that $|\psi(T)\rangle = e^{i\alpha}|\psi(0)\rangle$, the phase $e^{i\alpha}$ can be measured. The remarkable property discovered by Berry in the case of adiabatic evolution [1] and subsequently generalized by Aharonov and Anandan (AA) to arbitrary evolution [2] is that the phase $e^{i\alpha}$ contains not only a dynamical term but also a purely geometric term, the Berry or AA phase, which depends only on the geometry of the circuit described by $|\psi(t)\rangle$ in Hilbert space between $t=0$ and $t=T$. It is the holonomy acquired by $|\psi(t)\rangle$ when it is parallel transported around the circuit [3]. Explicitly it takes the form

$$\phi^{AA} = -i\ln\langle\psi(0)|\psi(T)\rangle + i\int_0^T dt\langle\psi(t)|\partial_t\psi(t)\rangle, \quad (1)$$

where the second term is the subtraction of the dynamical phase.

Berry's and AA's phase have been well verified experimentally in such diverse contexts as optics, NMR, and molecular physics [4–7]. They have also surfaced in a wide variety of theoretical contexts [7]. Berry's phase has been generalized to cyclic evolution of degenerate states [8] and to nonadiabatic evolution [9].

A generalization that has received little attention is Garrison and Wright's (GW) application to metastable states [10]. Garrison and Wright considered a metastable state which undergoes cyclic evolution. They showed that if the metastable system has not decayed during the time T, then its state $|\psi(T)\rangle$ coincides with the original state $|\psi(0)\rangle$ up to a phase, which can as expected be decomposed into a dynamical and a geometrical term. However, a new feature arises in this case, namely, the probability for the metastable state not to decay during the cyclic evolution can also be decomposed into a dynamical and a geometrical factor. This is described by a complex geometric ''phase,'' the real part of which corresponds to the geometric phase and the imaginary part to the geometric decay probability. The complex geometric phase is associated with the cyclic evolution of two states, contrary to the AA phase, which is associated with the cyclic evolution of one state.

Recently Aharonov and co-workers have shown how to describe quantum systems in terms of two states, one evolving towards the future and one evolving towards the past [11–13]. In particular they showed that measured quantities that in the conventional one-state approach are real become complex in the two-state approach. It has also been shown that measurements on metastable systems naturally fit into the two-state formalism [14]. It is therefore natural that the geometric quantity associated with the cyclic evolution of the metastable states is described by the cyclic evolution of two states and that it is complex.

Garrison and Wright (GW) illustrated how the complex geometric phase arises in the case of an excited atom in a cyclically varying laser field. The purpose of this paper is to further analyze the properties of the complex geometric phase and to propose several contexts of theoretical or experimental interest in which the complex geometric phase arises. In the Born-Oppenheimer approximation in the presence of metastable systems it can be realized as a complex vector potential for the slow degrees of freedom. This could have applications when calculating the lifetime and energy levels of excited electronic-vibrational-rotational spectra of molecules. In the Aharonov-Bohm effect it gives rise to topological decay probabilities in addition to the usual topological phase. Finally we suggest a simple experimental scheme in which to verify Garrison and Wright's complex geometric phase, which is based on the optical properties of absorbent birefringent crystals.

Let us first recall Garrison and Wright's derivation of the complex geometric phase. The time evolution of a metastable system is

$$|\psi(t)\rangle = \exp\left(-i\int_0^t dt H_{\text{eff}}\right)|\psi(0)\rangle + (\text{decay products}), \quad (2)$$

where H_{eff} is the effective Hamiltonian, which acts on the metastable state [15]. The most interesting situation arises when there are several coupled metastable states that are nearly degenerate. For a review of some physical systems in which this occurs, see [16]. We shall denote the space of metastable states $\mathcal{H}$. One can then consider that H_{eff} acts only in $\mathcal{H}$. The eigenvalues ω_i of H_{eff} are complex (we shall suppose them nondegenerate). The left and right eigenvectors of H_{eff} ($\langle\phi_i|\omega_i = \langle\phi_i|H_{\text{eff}}$ and $H_{\text{eff}}|\psi_i\rangle = \omega_i|\psi_i\rangle$) each form a nonorthogonal basis of $\mathcal{H}$. They obey the mutual

orthogonality condition $\langle\phi_i|\psi_j\rangle=\delta_{ij}\langle\phi_i|\psi_i\rangle$, which follows from the double equality $\langle\phi_i|H_{\rm eff}|\psi_j\rangle=\omega_i\langle\phi_i|\psi_j\rangle=\omega_j\langle\phi_i|\psi_j\rangle$. Using this orthogonality condition we can express $H_{\rm eff}$ as

$$H_{\rm eff}=\sum_i \omega_i\frac{|\psi_i\rangle\langle\phi_i|}{\langle\phi_i|\psi_i\rangle}. \tag{3}$$

Let us now suppose that $H_{\rm eff}$ is slowly changing with time. The amplitude for the metastable state not to decay is the solution of the effective Schrödinger equation $i\partial_t|\psi\rangle=H_{\rm eff}(t)|\psi\rangle$. We can decompose $|\psi\rangle$ into the basis of instantaneous eigenkets

$$|\psi\rangle=\sum_i a_i(t)\exp\left(-i\int_0^t dt\omega_i(t)\right)|\psi_i(t)\rangle.$$

Inserting this expression into the effective Schrödinger equation and taking the scalar product with $\langle\phi_i|$ yields

$$\partial_t a_i+a_i\frac{\langle\phi_i|\partial_t\psi_i\rangle}{\langle\phi_i|\psi_i\rangle}=-\sum_{j\neq i}a_j\exp\left(-i\int_0^t dt(\omega_j-\omega_i)\right)\times\frac{\langle\phi_i|\partial_t\psi_j\rangle}{\langle\phi_i|\psi_i\rangle}. \tag{4}$$

For a sufficiently slowly varying Hamiltonian the right-hand side of this equation can be neglected (see discussion below). Thus if the initial state $|\psi(0)\rangle$ coincides with the eigenstate $|\psi_i\rangle$, in the adiabatic limit the solution of the effective Schrödinger equation is

$$|\psi(t)\rangle=\exp\left(-i\int^t dt\omega_i\right)\times\exp\left(-\int^t dt\langle\phi_i|\partial_t\psi_i\rangle/\langle\phi_i|\psi_i\rangle\right)|\psi_i(t)\rangle. \tag{5}$$

When $H_{\rm eff}$ has evolved cyclically the second factor is a purely geometric quantity associated with the cyclic evolution of the metastable state:

$$\phi^i_{\rm GW}=i\int_0^T dt\frac{\langle\phi_i|\partial_t\psi_i\rangle}{\langle\phi_i|\psi_i\rangle}=\frac{i}{2}\int_0^T dt\frac{\langle\phi_i|\partial_t\psi_i\rangle-\langle\partial_t\phi_i|\psi_i\rangle}{\langle\phi_i|\psi_i\rangle}+\partial_t\ln\langle\phi_i(t)|\psi_i(t)\rangle. \tag{6}$$

The conditions $|\psi_i(T)\rangle=|\psi_i(0)\rangle$ and $\langle\phi_i(T)|=\langle\phi_i(0)|$ imply that the boundary term in the second equality vanishes. Further manipulation yields an expression for $\phi_{\rm GW}$, which is independent of the choice of phase in the definition of $\langle\phi_i(t)|$ and $|\psi^i(t)\rangle$:

$$\phi^i_{\rm GW}=-\frac{i}{2}\ln\frac{\langle\psi_i(0)|\psi_i(T)\rangle}{\langle\phi_i(T)|\phi_i(0)\rangle}+\frac{i}{2}\int_0^T dt\frac{\langle\phi_i|\partial_t\psi_i\rangle-\langle\partial_t\phi_i|\psi_i\rangle}{\langle\phi_i|\psi_i\rangle}. \tag{7}$$

This expression exhibits the symmetric role of $\langle\phi_i|$ and $|\psi_i\rangle$ and shows explicitly that $\phi^i_{\rm GW}$ is associated only with the cyclic evolution of the two states and not with the structure of the effective Hamiltonian. Thus Eq. (7) is the generalization of geometric phases to systems described by two states [11]. When the two states coincide one recovers the AA phase Eq. (1).

The real part of $\phi^i_{\rm GW}$ is the geometric phase and the imaginary part yields the geometric decay probability. There is, however, an important difference between the real and imaginary parts of $\phi_{\rm GW}$. Indeed the geometric phase $[=\mathrm{Re}(\phi_{\rm GW})]$ is defined only for cyclic evolution. On the other hand, the geometric decay probability $[=\mathrm{Im}(\phi_{\rm GW})]$ is defined even for noncyclic evolution. This is because the decay probability is defined at all times. One verifies that the imaginary part of Eq. (7) is a geometric quantity even for noncyclic evolution since it is independent of the choice of phase for $\langle\phi_i|$ and $|\psi_i\rangle$ and it is independent of the reparametrization of the path. In this paper we shall mostly consider the case of cyclic evolution for which the analogy with Berry's phase is closest.

For cyclic evolution, the integral in Eq. (7) is around a contour, denoted $\mathcal{C}$, in the product, $\mathcal{H}\otimes\mathcal{H}$, of the space of metastable states. It can be reexpressed as the integral of a complex two-form over any surface $\partial\mathcal{C}$ with $\mathcal{C}$ as boundary

$$\phi_{GW}=\int\int_{\partial\mathcal{C}}dx^a\wedge dx^b B_{ab}, \tag{8}$$

$$B_{ab}=\frac{\langle\partial_b\phi|\partial_a\psi\rangle}{\langle\phi|\psi\rangle}-\frac{\langle\partial_b\phi|\psi\rangle\langle\phi|\partial_a\psi\rangle}{\langle\phi|\psi\rangle^2}-(a\leftrightarrow b). \tag{9}$$

Garrison and Wright illustrated this formula in a particular case for which $\phi_{\rm GW}$ could be interpreted as a complex solid angle, in generalization of Berry's result.

Let us return to the condition of validity of the adiabatic approximation in Eq. (4). This is not straightforward because the right-hand side of Eq. (4) contains exponentially growing terms (since the ω_i are complex). However, it was shown in [17] that in the case of Hermitian Hamiltonians the amplitude for nonadiabatic transitions is exponentially small. Since the formal expression for the nonadiabatic transitions is the same in both cases, the adiabatic approximation will be valid provided $\mathrm{Re}(\omega_i-\omega_j)$ is much larger than the other frequencies that appear in this problem.

It is interesting to also consider the opposite limit wherein the time T it takes $H_{\rm eff}$ to change cyclically is much less than $|\omega_i-\omega_j|^{-1}$ (but T must nevertheless be long enough to ensure that the concept of an effective Hamiltonian remains valid at all times). Then $H_{\rm eff}$ can be reexpressed as $H_{\rm eff}=\omega\Sigma_i|\psi_i\rangle\langle\phi_i|/\langle\phi_i|\psi_i\rangle$. In this case the cyclic time evolution is given by the operator

$$\exp\left(-i\int_0^T dtH_{\rm eff}\right)=e^{-i\omega t}\hat{T}\exp\left(i\int_0^T dtA(t)\right)$$

$$A(t)=i\sum_{i,j}|\psi_i\rangle\frac{\langle\phi_i|\partial_t\psi_j\rangle}{\langle\phi_i|\psi_i\rangle}\langle\phi_j|, \tag{10}$$

where $\hat{T}$ is the time ordering operator. $A(t)$ is a ''non-Hermitian non-Abelian gauge potential,'' which generalizes to metastable states the non-Abelian gauge potential found by Wilczek and Zee [8] in the case of cyclic evolution of degenerate states.

We now consider several applications of the complex geometric phase. We first recall that the Berry phase was originally introduced in the context of the Born-Oppenheimer approximation where it appears as a nontrivial vector potential for the slow degrees of freedom [18]. In a similar way one can consider the Born-Oppenheimer approximation for a system composed of rapid but metastable particles coupled to a slow system. The total Hamiltonian for such a system is

$$H_{\text{eff}}=\frac{P^2}{2M}+V(Q)+h_{\text{eff}}(q,Q), \tag{11}$$

where q is the fast degree of freedom and Q is the slow degree of freedom. Let $|\psi_i(q,Q)\rangle$ and $\langle\phi_i(q,Q)|$ be the instantaneous eigenstates of the rapid Hamiltonian $h_{\text{eff}}(q,Q)$. Postulating a wave function of the form $|\Psi\rangle=|\chi_i(Q)\rangle|\psi_i(q,Q)\rangle$, one obtains for $|\chi_i\rangle$ the equation

$$\left[\frac{1}{2M}[P-A_i(Q)]^2+\mathcal{V}_i(Q)\right]|\chi_i\rangle=\Omega_i|\chi_i\rangle, \tag{12}$$

where Ω_i is the complex energy of the eigenstate and

$$\mathcal{V}_i(Q)=V(Q)+\omega_i(Q)+\frac{1}{2M}\left(\frac{\langle\phi_i|\partial_Q^2\psi_i\rangle}{\langle\phi_i|\psi_i\rangle}-\frac{\langle\phi_i|\partial_Q\psi_i\rangle^2}{\langle\phi_i|\psi_i\rangle^2}\right),$$

$$A_i(Q)=-i\frac{\langle\phi_i|\partial_Q\psi_i\rangle}{\langle\phi_i|\psi_i\rangle}. \tag{13}$$

The complex vector potential $A_i(Q)$ that arises in this case could have measurable effects on the lifetimes and energy levels of excited electronic-vibrational-rotational molecular states [7].

Among the most interesting problems that can be analyzed using the concept of geometric phase are the Aharonov-Bohm (AB) [19] and Aharonov-Casher (AC) [20] effects. In this case the phases are purely topological, i.e., they depend only on the winding number of the trajectory. We shall show that in the presence of metastable particles there is also a topological decay probability, i.e., a decay probability that depends only on the winding number of the trajectory. This feature arises because the AB or AC phase becomes complex in the presence of decaying particles.

Let us recall the AC effect (for reasons that will be discussed below, this would be easier to realize experimentally than the AB effect). It consists of a particle with a magnetic moment moving in the presence of a charged line. The charged line is taken along the z axis. The Hamiltonian for the particle is [20]

$$H=\frac{1}{2m}[\mathbf{p}+\mu_z\mathbf{a}(\mathbf{r})]^2+V(\mathbf{r}), \tag{14}$$

where μ_z is the projection of the magnetic moment along the z axis. In the cylindrically symmetric gauge $\mathbf{a}(\mathbf{r})$ takes the form

$$a_\theta=\frac{\rho\theta}{2\pi},\quad a_r=a_z=0, \tag{15}$$

where ρ is the charge per unit length of the charged line and θ is the angle around the z axis in cylindrical coordinates. Consider the amplitude for the particle to go from $P_1=(r_1,\theta_1,z_1)$ to $P_2=(r_2,\theta_2,z_2)$ in time t. We express it using the Feynman path integral and decompose the sum over paths in terms of the winding number of the path:

$$K(P_2,P_1,t)=\int\mathcal{D}(x)e^{iS(x,\mu)}$$

$$=e^{i\mu_z\rho(\theta_2-\theta_1)/2\pi}\sum_n K_n^0(P_2,P_1,t)e^{i\mu_z\rho n}, \tag{16}$$

where

$$K_n^0=\int_{\text{paths with winding number}=n}\mathcal{D}(x)e^{iS(x,\mu=0)} \tag{17}$$

is the contribution of paths with winding number n when $\mu=0$. The factor $e^{i\mu\rho n}$ is the AC phase. It affects interferences between contributions with different winding number.

Let us now turn to the case when the particle with magnetic moment is metastable. Suppose that there are several nearly degenerate metastable states. Then as before there is an effective Hamiltonian $h_{\text{eff}}^{\text{internal}}$ that acts in the space of metastable states. The left and right eigenstates of $h_{\text{eff}}^{\text{internal}}$ will be denoted $\langle\phi_i^{\text{int}}||\psi_i^{\text{int}}\rangle$ and their eigenvalue ω_i. The essential point in the derivation of the complex AC phase is that if the particle is in the eigenstate $|\psi_i^{\text{int}}\rangle$ and if the coupling of the magnetic moment to external systems is sufficiently weak and slowly varying, then the effective value of the magnetic moment of the particle is (the proof is given below, see also [14])

$$\mu^i=\frac{\langle\phi_i^{\text{int}}|\mu|\psi_i^{\text{int}}\rangle}{\langle\phi_i^{\text{int}}|\psi_i^{\text{int}}\rangle}. \tag{18}$$

This expression for μ^i is nontrivial if the magnetic moment operator μ does not commute with $h_{\text{eff}}^{\text{internal}}$ whereupon μ^i can be complex. If the conditions for μ to be effectively given by Eq. (18) are satisfied, the amplitude for the particle to go from P_1 to P_2 and not to decay can be expressed in analogy with Eq. (16) as

$$K(P_2,P_1,t,\text{ no decay})=e^{i\mu_z^i\rho(\theta_2-\theta_1)/2\pi}$$

$$\times\sum_n K_n^0(P_2,P_1,t)e^{i\mu_z^i\rho n}. \tag{19}$$

As before there is a topological phase given by $e^{i\text{Re}(\mu_z^i)\rho n}$. There is also a topological decay probability given by $e^{-\text{Im}(\mu_z^i)\rho n}$, which depends only on the winding number of the path. In addition there is an overall geometric decay probability $e^{-\text{Im}(\mu_z^i)\rho(\theta_2-\theta_1)/2\pi}$, which depends on the angle between P_1 and P_2 but is independent of the details of the path between P_1 and P_2.

We now derive this result in a more rigorous fashion. When the particle is metastable one must add to the Hamiltonian equation (14) the effective Hamiltonian governing the internal state of the particle

$$H_{\rm eff}=\frac{1}{2m}[\mathbf{p}+\mu_z\mathbf{a}(\mathbf{r})]^2+V(\mathbf{r})+h_{\rm eff}^{\rm internal}, \tag{20}$$

with **a** once more given by Eq. (15). Let us postulate a solution of the effective Schrödinger equation of the form $|\Psi_i\rangle=\chi_i(\mathbf{r})|\psi_i^{\rm int}\rangle e^{-i\omega_i t}$. Inserting this ansatz into the effective Schrödinger equation and taking the scalar product with $\langle\phi_i^{\rm int}|$ yields

$$-i\partial_t\chi_i=\left(\frac{1}{2m}(\mathbf{p}-\mu_z^i\mathbf{a})^2+V(\mathbf{r})\right)\chi_i, \tag{21}$$

where we have neglected a term of the form

$$(e^2a^2/4m^2)(\langle\phi_i|\mu_z^2|\psi_i\rangle/\langle\phi_i|\psi_i\rangle-\mu_z^{i2}).$$

One can further verify that nonadiabatic transitions are controlled by terms of the form

$$(\langle\phi_j|\mu_z|\psi_i\rangle/\langle\phi_i|\psi_i\rangle)[(\mathbf{a}\cdot\mathbf{p})/m]e^{-i(\omega_i-\omega_j)t}$$

and

$$(\langle\phi_j|\mu_z^2|\psi_i\rangle/\langle\phi_i|\psi_i\rangle)(a^2/2m)e^{-i(\omega_i-\omega_j)t}.$$

All these terms can be neglected when the particle is sufficiently far from the line of charge (so that **a** is small) and is moving sufficiently slowly (so that **p** is small). It is then legitimate to replace μ by its effective value μ^i. The solution for χ_i is then (in the WKB approximation)

$$\chi_i=e^{-iE_it}\exp\left(i\int^{\mathbf{r}}(\mathbf{p}+\mu_z^i\mathbf{a})\cdot d\mathbf{r}\right) \tag{22}$$

and one obtains a similar expression for the ket $\langle\Phi_i|$ solution of the effective Schrödinger equation $i\partial_t\langle\Phi_i|=\langle\Phi_i|H_{\rm eff}$. To make a connection with the geometric phase, consider the case of cyclic evolution and insert $\langle\Phi_i|$ and $|\Psi_i\rangle$ into Eq. (7) to yield

$$\phi_{\rm GW}=\oint(\mathbf{p}+\mu_z^i\mathbf{a})\cdot d\mathbf{r}=n\mu_z^i\rho+\oint\mathbf{p}\cdot d\mathbf{r}, \tag{23}$$

where n is the winding number of the trajectory.

Several remarks are in order. First, recall that whereas the geometric phase is defined only for cyclic evolution, the geometric decay probability is not. However, the decay probability is topological even for noncyclic evolution since it depends only on the end points of the trajectory and the winding number, not on the details of the trajectory. Second, note that **a** was taken in the cylindrically symmetric gauge. As shown in [21] this is the simplest gauge to use when the magnetic moment operator does not commute with the full Hamiltonian. The analysis in other gauges is possible but more complicated and necessitates the introduction of nonconventional commutation relations. Third, in order to obtain topological decay probabilities in the AB effect it would be necessary to take the solenoid to consist of one metastable particle. This is probably very difficult to realize experimentally. (It is obviously impossible to have an effective complex electric charge since charge is a conserved quantity).

We now consider how $\phi_{\rm GW}$ could be measured in optical experiments. We recall that one of the simplest ways to measure Berry's phase is to pass polarized light through a coiled optical fiber. The cyclic change in propagation direction of the light implies a cyclic change in polarization direction and hence a geometric phase that can be materialized as a rotation of the direction of polarization of the light after exiting from the fiber [4]. A simple generalization of this scheme would be to use an optical fiber made up of absorbing dichroic material. In such media the different polarizations are absorbed at different rates and therefore the polarization eigenstates are in general nonorthogonal [22]. The coils of the fiber will then give rise to a cyclic change in polarization direction and hence to a geometric phase and a geometric attenuation of the beam.

An alternative approach would be to change cyclically the composition of the absorbing dichroic material through which the light is passing. For instance, consider a beam of polarized light that passes through vacuum and two different absorbing dichroic crystals A and B (note that B could consist of the same crystal as A but rotated through an angle θ). If the beam passes successively through vacuum, A, vacuum, B, vacuum then $\phi_{\rm GW}=0$. However, if the sequence is vacuum, A, B, vacuum then the polarization eigenstates describe a nontrivial circuit and $\phi_{\rm GW}\neq 0$. A comparison of the two sequences allows $\phi_{\rm GW}$ to be measured. In this experiment the different interfaces play a similar role to the successive reflections in [5].

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