Extending the quantal adiabatic theorem: Geometry of noncyclic motion

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Abstract

We show that a noncyclic phase of geometric origin has to be included in the approximate adiabatic wave function. The adiabatic noncyclic geometric phase for systems exhibiting a conical intersection as well as for an Aharonov-Bohm situation is worked out in detail. A spin-$\frac{1}{2}$ experiment to measure the adiabatic noncyclic geometric phase is discussed. We also analyze some misconceptions in the literature and textbooks concerning noncyclic geometric phases.

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I. INTRODUCTION

Imagine we slowly modify the state of a quantum system with some external parameters. A paradigmatic example could be a particle with spin in a slowly rotating magnetic field. The adiabatic change could be very large, but it takes place over a long time such that the transition between different energy levels is negligible. What is the approximate form of the adiabatic wave function? This question seemed to be settled since the first treatment of Born and Fock [1] in quantum mechanics that extended previous work of Ehrenfest [2] in classical mechanics and the old quantum theory. Surprisingly, a new insight into the adiabatic theorem had to wait 55 years to Berry’s [3] 1984 paper. Treatments of the adiabatic approximation before Berry’s analysis correctly demonstrated that for a slowly varying Hamiltonian $\hat{H}(t)$ the solution of the Schrödinger equation

$$i\hbar\dot{\Psi} = \hat{H}\Psi$$

for a state vector initially in $|\Psi; 0\rangle = |n; 0\rangle$ is within the adiabatic approximation of the form [4–6]

$$|\Psi; t\rangle = \exp \left( i\alpha_n(t) - \frac{i}{\hbar} \int_0^t dt' E_n(t') \right) |n; t\rangle,$$  \hspace{1cm} (2)

where $|n; t\rangle$ is an instantaneous eigenstate of $\hat{H}(t)$

$$\hat{H}(t)|n; t\rangle = E_n(t)|n; t\rangle.$$ \hspace{1cm} (3)

However, these treatments failed to realize the relevance of the phase $\alpha_n$ as they were more interested in obtaining the conditions of validity of (2) namely that no transition between levels will occur if

$$\hbar \frac{|\langle n; t | \hat{H} | m; t \rangle |}{|E_n(t) - E_m(t)|^2} \ll 1.$$ \hspace{1cm} (4)

Berry showed that if the system is transported around a closed circuit $C_0$ in parameter space in time $T$ by changing the parameters $R$ in the Hamiltonian $\hat{H}(R)$, the final wave function is of the form

$$|\Psi; T\rangle = \exp \left( i\gamma_n[C_0] - \frac{i}{\hbar} \int_0^T dt' E_n(R(t')) \right) |\Psi; 0\rangle$$ \hspace{1cm} (5)

with the geometrical phase change

$$\gamma_n[C_0] = i\oint_{C_0} dR \cdot \langle n; R | \nabla_R | n; R \rangle,$$ \hspace{1cm} (6)

where the instantaneous nondegenerate energy eigenstate $|n; R\rangle$ is singlevalued in a parameter space domain that includes the closed circuit $C_0$. From (6) is clear that $\gamma_n[C_0]$ is independent of how the circuit is traversed provided the traversal is slow enough for the adiabatic approximation to hold. Using Stokes’ theorem the geometric phase in (6) was written by Berry as
\[ \gamma_n[C_0] = -\int_{S_0} dS \cdot V_n(R), \]  
(7)

with

\[ V_n(R) = \text{Im} \sum_{m \neq n} \frac{\langle n; R | (\nabla_R \hat{H}(R)) | m; R \rangle \times \langle m; R | (\nabla_R \hat{H}(R)) | n; R \rangle}{(E_n(R) - E_m(R))^2}. \]

Clearly expression (7) for the geometric phase \( \gamma_n[C_0] \) is independent of the phase choice of \( |n; R\rangle \) and therefore there is no need to choose a singlevalued \( |n; R\rangle \) as in relation (6). This property and the independence of how the path \( C_0 \) is traversed in parameter space are the geometric properties of \( \gamma_n[C_0] \), known as Berry’s geometric phase. This is precisely the relevance of Berry’s result, that \( \gamma_n[C_0] \) is of geometric origin.

Berry’s discovery of the geometric phase for cyclic adiabatic evolution has met several generalizations. Aharonov and Anandan [7] generalized Berry’s phase to nonadiabatic cyclic motion. Samuel and Bhandari [8] obtained the geometric phase for noncyclic cases. Further generalizations have been the purely kinematic approaches of Aitchison and Wanelik [9] and Mukunda and Simon [10]. These works are mostly concerned with the geometric phase of exact solutions of the Schrödinger equation and have introduced a geometrical understanding of quantum theory.

In this paper we are concerned with approximate solutions for quantum adiabatic motion. Treatments of the adiabatic change in quantum mechanics after Berry’s result for cyclic adiabatic evolution stress the necessity of cyclicity [11,12] and even in some cases explicitly state that the phase additional to the dynamical phase \(-\int_0^T dt' E_n(R(t'))/\hbar\) can be eliminated [13,14] in the noncyclic adiabatic case but not in the cyclic one. Is cyclic adiabatic motion so special? Is it necessary for the appearance of the adiabatic geometric phase? It is the purpose of this paper to show that the geometric phase also appears in noncyclic adiabatic motion and that there is nothing special in the cyclic case for the existence of the geometric phase.

We have organized this paper as follows. In Sec. II a derivation of the geometric phase for adiabatic noncyclic change is given. We show that this phase cannot be canceled and that it is geometric. It coincides with Berry’s phase for cyclic evolutions. Secs. III–V discuss examples of noncyclic geometric phases as well as implications for experiments.

II. NONCYCLIC ADIABATIC CHANGE

In this section we show that the correct treatment of noncyclic adiabatic change also needs the inclusion of a phase of geometric origin. This geometric contribution reduces to Berry’s phase for cyclic evolution. We assume the same conditions as in Berry’s derivation of discrete nondegenerate spectrum and Hermitian Hamiltonian. In the noncyclic case, \( R \) traces out an open path \( C \) in parameter space. Under adiabatic evolution the solution of the Schrödinger equation (I) for a state initially in \( |\Psi; 0\rangle = |n; R(0)\rangle \) is approximately

\[ |\Psi; t\rangle = \exp \left( i\alpha_n(t) - \frac{i}{\hbar} \int_0^t dt' E_n(R(t')) \right) |n; R(t)\rangle, \]

where \( |n; R(t)\rangle \) is the nth instantaneous energy eigenstate. Substitution of (I) in Schrödinger’s equation (I) gives the phase \( \alpha_n(t) \) as
\[ \alpha_n(t) - \alpha_n(0) = i \int_0^t dt' \mathbf{\dot{R}}(t') \cdot \langle n; \mathbf{R}(t') | \nabla_{\mathbf{R}} | n; \mathbf{R}(t') \rangle, \] (10)

which is real as the basis \(| n; \mathbf{R}(t) \rangle\) is normalized. Multiplying (9) by \(\langle \Psi; 0 | = \langle n; \mathbf{R}(0) | \) yields

\[ \arg \langle \Psi; 0 | \Psi; t \rangle = \gamma_n[C] - \frac{1}{\hbar} \int_0^t dt' E_n(\mathbf{R}(t')) \] (11)

with \(\gamma_n[C]\) the adiabatic noncyclic phase of the form

\[ \gamma_n[C] = \arg \langle n; \mathbf{R}(0) | n; \mathbf{R}(t) \rangle + i \int_0^t dt' \mathbf{\dot{R}}(t') \cdot \langle n; \mathbf{R}(t') | \nabla_{\mathbf{R}} | n; \mathbf{R}(t') \rangle, \] (12)

which is defined when the eigenvectors \(| n; \mathbf{R}(0) \rangle\) and \(| n; \mathbf{R}(t) \rangle\) are nonorthogonal.

Expression (12) is the general expression for the adiabatic noncyclic geometric phase that only depends on the open path \(C\) in parameter space. Its geometric nature is explained in the following. The adiabatic noncyclic geometric phase in (12) is independent of the phase choice of \(| n; \mathbf{R}(t) \rangle\) as it is invariant under the global phase transformation \(| n; \mathbf{R}(t) \rangle \rightarrow \exp (i \lambda(\mathbf{R}(t))) | n; \mathbf{R}(t) \rangle\). Therefore \(\gamma_n[C]\) cannot be eliminated by a global phase transformation and has to be included in any calculation for adiabatic evolution (the invariance of the geometric phase for other unitary transformations has been discussed in the literature [7, 15–18]). The adiabatic noncyclic geometric phase is also independent of how the path is traversed as any differentiable monotonic transformation \(t \rightarrow \nu(t)\) leaves (12) invariant. An alternative to the expression for the geometric phase in (12) is given by the approach that uses a geodesic closure of the path [8]. The disadvantages of this noncyclic approach for the adiabatic theorem are explained in the Appendix.

Using (11) and (12) for a cyclic evolution we can write the state vector at time \(T\) as in (3) with \(\gamma_n[C_0]\) the adiabatic geometric phase for a cyclic path \(C_0\) writing (12) for the cyclic time \(T\). Obviously, as in the noncyclic case, the adiabatic cyclic geometric phase \(\gamma_n[C_0]\) is globally phase invariant and independent on how the circuit \(C_0\) is traversed. Berry’s result is immediately obtained by making a global phase transformation to a singlevalued basis, for which \(| n; \mathbf{R}(T) \rangle = | n; \mathbf{R}(0) \rangle\), and it can clearly be seen that relation (12) reduces to Berry’s expression (3).

We would like to highlight briefly why the adiabatic noncyclic geometric phase might have been overlooked in the past. First, Berry’s expressions for the geometric phase in (3) and (4) are clearly independent of how the path in parameter space is traversed and are also invariant under global phase transformations. These properties that define the geometric phase are less obvious at first sight in the noncyclic case as discussed above. Secondly, the first treatments and reviews of the geometric phase stressed the theoretical and experimental importance of cyclicity [3, 7, 11, 12, 19]. Thirdly, several incorrect statements have been given in the literature, which might have caused confusion about the significance of the adiabatic noncyclic geometric phase. For example, it has been stated that there is no adiabatic noncyclic geometric phase [13, 14] or that it is given by (11) instead of (12) [20]. Moreover, the nonadiabatic noncyclic treatment of Samuel and Bhandari [8] was very formal and no explicit physical examples were given in their article. The kinematic approach of Aitchison and Wanelik [1] made noncyclic geometric phases more accessible but again no explicit examples were given. In the kinematic study of Mukunda and Simon [10] examples in the
field of optics were given and the adiabatic noncyclic geometric phase in an optical set-up has been correctly calculated by Christian and Shimony [21] using the kinematic approach. We have shown in this section that a phase of geometric origin has to be included in the Schrödinger solution for an adiabatic noncyclic evolution. This adiabatic noncyclic geometric phase cannot be eliminated by a global phase transformation as it is independent of the phase choice of the basis and reduces to Berry’s adiabatic cyclic phase for cyclic times.

III. NONCYCLIC PERSPECTIVE OF THE SIGN CHANGE PROBLEM

It is well-known in molecular physics since the work by Longuet-Higgins and coworkers [22,23] that adiabatically transporting the electronic state around a conical intersection in nuclear configuration space changes the sign of the electronic wave function. Therefore the nuclear wave function must also change sign to make the total product wave function singlevalued. This effect has been observed in the vibrational spectrum of Na$_3$ [24]. We here analyze the sign change problem from a noncyclic perspective. Specifically, consider a two-dimensional subspace of nuclear configuration space in which two electronic states conically intersect at the origin. In a neighborhood of the degenerate point the Hamiltonian can, up to an additive multiple of the unit matrix, be written as a real symmetric $2 \times 2$ matrix [25,26]

$$\hat{H} = R (\sin \Phi \hat{\sigma}_x + \cos \Phi \hat{\sigma}_z),$$

(13)

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the $x-$ and $z-$components of the usual Pauli matrices

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{(14)}$$

and the parameters $(R, \Phi)$, which are here treated as classical, are nuclear polar coordinates. It can be checked that

$$|+; \Phi \rangle = \begin{pmatrix} \cos(\Phi/2) \\ \sin(\Phi/2) \end{pmatrix},$$

$$|-; \Phi \rangle = \begin{pmatrix} -\sin(\Phi/2) \\ \cos(\Phi/2) \end{pmatrix} \quad \text{(15)}$$

are eigenvectors of $\hat{H}$ with the corresponding energy eigenvalues

$$E_{\pm}(R) = \pm R. \quad \text{(16)}$$

Clearly the energies $E_{\pm}(R)$ conically intersect at $R = 0$, as shown in Fig. 1.

Now suppose the nuclear motion is such that $R$ is nonzero and constant but $\Phi$ varies slowly with time, i.e. $|\dot{\Phi}| \ll 4R/\hbar$ from (4). Taking the initial state to be

$$|\Psi; 0 \rangle = |+; \Phi(0) \rangle, \quad \text{(17)}$$

where $|+\rangle$ is given by (15), it follows from (9), (10) and (16) that
\[ |\Psi; t\rangle = \exp \left( \frac{-i}{\hbar} R t \right) |+; \Phi(t)\rangle \] (18)

is a solution of the time dependent Schrödinger equation in the adiabatic approximation. The geometric phase of the solution \(|\Psi; t\rangle\) accumulated during the interval \([0,t]\) can be calculated from (12) using (15)

\[
\gamma_+ [C] = \arg \langle +; \Phi(0) | +; \Phi(t) \rangle + 0 = \arg \cos((\Phi(t) - \Phi(0))/2)
\]

\[
= \begin{cases} 
0 & \text{if } \Phi(0) \leq \Phi(t) < \Phi(0) + \pi \\
\text{undefined} & \text{if } \Phi(t) = \Phi(0) + \pi \\
\pi & \text{if } \Phi(0) + \pi < \Phi(t) \leq \Phi(0) + 2\pi
\end{cases} . \quad (19)
\]

This shows that the adiabatic noncyclic geometric phase is nonzero. It also shows that the sign change of the cyclic electronic wave function, first noticed by Longuet-Higgins and coworkers [22,23], is due to the sign change of the noncyclic geometric phase factor at \(\Phi(t) = \Phi(0) + \pi\).

From the invariance under global phase transformations and independence of how the path is traversed, discussed below (12) in Sec. II, it is clear that the sign change must also follow if we choose an eigenvector which can be complex and/or nondifferentiable at some isolated points along \(C\). It is instructive to demonstrate this explicitly. We introduce, by global phase transformations of \(|+; \Phi(t)\rangle\), two new vectors which are labeled as \(|+; \Phi(t)\rangle'\) and \(|+; \Phi(t)\rangle''\). Take first the complex vector

\[ |+; \Phi(t)\rangle' = \exp (i \Phi(t)/2) |+; \Phi(t)\rangle, \] (20)

which is differentiable and singlevalued in \(\Phi\). We then have

\[ '\langle +; \Phi(t) | \frac{1}{R} \frac{\partial}{\partial \Phi} | +; \Phi(t) \rangle' = \frac{i}{2R} ; \quad (21) \]

and

\[ '\langle +; \Phi(0) | +; \Phi(t) \rangle' = \exp \left( i(\Phi(t) - \Phi(0))/2 \right) \langle +; \Phi(0) | +; \Phi(t) \rangle . \] (22)

Inserting (21) and (22) into (12) we obtain the geometric phase

\[ \gamma_+ [C] = \frac{1}{2}(\Phi(t) - \Phi(0)) + \arg \langle +; \Phi(0) | +; \Phi(t) \rangle - \frac{1}{2} \int_{\Phi(0)}^{\Phi(t)} d\Phi \]

\[ = \arg \langle +; \Phi(0) | +; \Phi(t) \rangle = \gamma_+ [C] . \quad \] (23)

Next let us consider the real vector

\[ |+; \Phi(t)\rangle'' = \exp (-i \arg \langle +; \Phi(0) | +; \Phi(t) \rangle) |+; \Phi(t)\rangle , \] (24)

which is singlevalued but not differentiable everywhere as it has a finite jump at \(\Phi(t) = \Phi(0) + \pi\). We now have

\[
\arg (''\langle +; \Phi(0) | +; \Phi(t) \rangle'') = \begin{cases} 
0 & \text{if } \Phi(t) \neq \Phi(0) + \pi \\
\text{undefined} & \text{if } \Phi(t) = \Phi(0) + \pi
\end{cases} . \quad (25)
\]
and at $\Phi(t) \neq \Phi(0) + \pi$

$$\langle +; \Phi(t) | \left( \frac{1}{R} \frac{\partial}{\partial \Phi} | +; \Phi(t) \right)'' = -i \frac{\partial}{\partial \Phi} \arg \langle +; \Phi(0) | +; \Phi(t) \rangle \rangle.$$ (26)

Inserting (25) and (26) into (12) yields

$$\gamma_+'[C] = 0 + \int_{\Phi(0)}^{\Phi(t)} \frac{\partial}{\partial \Phi} \arg \langle +; \Phi(0) | +; \Phi(t') \rangle d\Phi = \gamma_+'[C].$$ (27)

We have seen in this section that a simple case of degeneracy provides a clear example of the adiabatic noncyclic geometric phase and its properties. It has also been shown that the adiabatic noncyclic geometric phase provides a detailed characterization of the sign change problem. In the particular case chosen here we have shown that the sign change is due to an adiabatic noncyclic geometric phase of value $\pi$ after $\Phi(0) + \pi$.

IV. RELATIONSHIP BETWEEN THE AHA Ronov-Bohm EFFECT AND THE NONCYCLIC GEOMETRIC PHASE

Quantum theory has been given several surprises after it was completed in the early 30s. One of them is precisely the geometric phase. Another surprising result was discovered by Aharonov and Bohm in 1959 [27]. This section concerns the relation between the Aharonov-Bohm effect and the noncyclic geometric phase.

Consider a particle with charge $q$ confined in an impenetrable box transported along a circuit $C$ around a magnetic flux line as shown in Fig. 2. The relative coordinate between the box and a point on the flux line is $R$. An asymmetric shape of the box has been chosen in order to avoid energy degeneracies. The size of the box in Fig. 2 is such that the overlap between the initial wave function and the wave function at any later time is nonvanishing which guarantees that the noncyclic geometric phase is well defined except at isolated $R$—values where these wave functions might be orthogonal.

Suppose $\psi_n(r; R(t))$ is the real-valued energy eigenfunction in absence of magnetic flux associated with the $R$—independent energy $E_n$. Turning on the flux the eigenfunction becomes

$$\varphi_n(r; R(t)) = \exp \left( i \frac{q}{\hbar c} \int_{R(t)}^r dr' \cdot A(r') \right) \psi_n(r; R(t))$$ (28)

and the energy is still $E_n$. In cylindrical coordinates $(r, \theta, z)$ the vector potential reads

$$A = \frac{\Lambda}{2\pi r} e_\theta,$$ (29)

where $\Lambda$ is the flux and $e_\theta$ is the unit vector in the $\theta$—direction. Introducing the dimensionless parameter $\eta = q\Lambda/(2\pi \hbar c)$, the eigenfunction (28) becomes

$$\varphi_n(r; R(t)) = \exp \left( i \eta \int_{R(t)}^r d\theta' \right) \psi_n(r; R(t)),$$ (30)
which has to be singlevalued in $r$ for every $\mathbf{R}(t) = (R \cos \Theta(t), R \sin \Theta(t), Z)$. In the following we analyze the noncyclic geometric phase by dividing the transport of the box into three different cases which correspond to three different intervals of $\Theta(t)$, as shown in Fig. 2. For notational convenience we write the eigenfunctions and the integrals only in terms of $\theta$ and $\Theta$, and restrict $\theta$ to the interval $[0, 2\pi]$.

Case (a). $(0 \leq \Theta(t) \leq 2\pi - \Delta \theta)$ The eigenfunction (30) for this case can be written as

$$\varphi_n(\theta; \Theta(t)) = \begin{cases} 0 & \text{if } 0 \leq \theta \leq \Theta(t) \\ \exp(i\eta(\theta - \Theta(t))) \psi_n(\theta - \Theta(t)) & \text{if } \Theta(t) \leq \theta \leq \Theta(t) + \Delta \theta \\ 0 & \text{if } \Theta(t) + \Delta \theta \leq \theta < 2\pi, \end{cases} \tag{31}$$

where $\Delta \theta$ is the angular length of the box. First we calculate

$$\arg(\varphi_n; 0|\varphi_n; \Theta(t)) = \arg \int_{\Theta(t)}^{\Theta(t) + \Delta\theta} d\theta \exp(-i\eta(\Theta(t))) \psi_n(\theta)\psi_n(\theta - \Theta(t)) = -\eta\Theta(t). \tag{32}$$

Here we have used that $\psi_n$ is real-valued and have chosen $\Theta(0) = 0$. Furthermore we have

$$\langle \varphi_n; \Theta(t)|\nabla_R|\varphi_n; \Theta(t) \rangle = \int_0^{2\pi} d\theta \left( -i\frac{\eta}{R} A(R(t))\psi_n^2(\theta - \Theta(t)) \\
+ \psi_n(\theta - \Theta(t))\nabla_R \psi_n(\theta - \Theta(t)) \right) = -i\frac{\eta}{R} e_\Theta + 0, \tag{33}$$

where the second term on the r.h.s. vanishes as $\psi_n$ is normalized and real-valued. Inserting (32) and (33) into (12) we obtain the noncyclic geometric phase for case (a) as

$$\gamma_n[C] = -\eta\Theta(t) + \int_0^{\Theta(t)} Rd\Theta \frac{\eta}{R} = 0. \tag{34}$$

Case (b). $(2\pi - \Delta \theta \leq \Theta(t) \leq \Delta \theta)$ The eigenfunction for this case that is singlevalued in $r$ is of the form

$$\varphi_n(\theta; \Theta(t)) = \begin{cases} \exp(i\eta(\theta - \Theta(t) + 2\pi)) \psi_n(\theta - \Theta(t) + 2\pi) & \text{if } 0 \leq \theta \leq \Theta(t) + \Delta \theta - 2\pi \\ 0 & \text{if } \Theta(t) + \Delta \theta - 2\pi \leq \theta \leq \Theta(t) \\ \exp(i\eta(\theta - \Theta(t))) \psi_n(\theta - \Theta(t)) & \text{if } \Theta(t) \leq \theta < 2\pi. \end{cases} \tag{35}$$

Using this eigenfunction we find

$$\arg\langle \varphi_n; 0|\varphi_n; \Theta(t) \rangle = -\eta\Theta(t) + \arg \left( \exp(i2\pi\eta) \int_0^{\Theta(t) + \Delta\theta - 2\pi} d\theta \psi_n(\theta)\psi_n(\theta - \Theta(t) + 2\pi) \\
+ \int_{\Theta(t)}^{\Theta(t) + \Delta\theta} d\theta \psi_n(\theta)\psi_n(\theta - \Theta(t)) \right) \tag{36}$$

and the second term in (12) coincides with (33) of case (a). The noncyclic geometric phase is then

$$\gamma[C] = \arg \left( \exp(i2\pi\eta) \int_0^{\Theta(t) + \Delta\theta - 2\pi} d\theta \psi_n(\theta)\psi_n(\theta - \Theta(t) + 2\pi) \\
+ \int_{\Theta(t)}^{\Theta(t) + \Delta\theta} d\theta \psi_n(\theta)\psi_n(\theta - \Theta(t)) \right). \tag{37}$$
Case (c). \((\Theta(t) \geq \Delta \theta)\) The eigenfunction for this case is again given by (35). In fact we can obtain its corresponding noncyclic geometric phase by taking the limit \(\Theta \rightarrow \Delta \theta\) in (37) yielding
\[
\gamma[C] = 2\pi \eta.
\]
Hence the noncyclic geometric phase coincides with the Aharonov-Bohm phase for this \(\Theta\)-interval.

A special case of (c) is the cyclic transport discussed by Berry \cite{3}, and which can also be found in a later addition to Sakurai’s book \cite{28} and in Refs. \cite{29,30,31,32,33}. Note however that the noncyclic transport shows a richer relation between the geometric phase and the Aharonov-Bohm effect. That is, the noncyclic geometric phase interpolates smoothly between 0 (case (a)) and the Aharonov-Bohm value \(2\pi \eta\) (case (c)) as shown by (37). It is in principle possible to experimentally verify this from the interference in the overlapping regions between a box transported along \(C\) and another one not transported as they both would have the same dynamical phase.

V. NONCYCLIC NEUTRON POLARIZATION EXPERIMENT

The geometric phase for adiabatic cyclic evolutions has been observed for various physical systems such as neutrons \cite{34} and photons \cite{35}. Is it also possible to experimentally verify the noncyclic geometric phase? A claim that this has been done appeared in a paper by Weinfurter and Badurek \cite{36}, but it has recently been pointed out \cite{37} that the phase they observed is not of geometric origin. Correct theoretical proposals of how to observe the noncyclic geometric phase have been put forward \cite{21,37,38}. Here we give an elementary demonstration of how the adiabatic noncyclic geometric phase can be measured.

Consider a neutron beam subject to a homogeneous magnetic field with constant magnitude \(B\). Its direction, given by the unit vector \(\mathbf{e}\), varies slowly. Denoting the magnetic moment of the neutrons by \(\mu\), the spin-Hamiltonian reads
\[
\hat{H} = -\mu B \mathbf{e}(t) \cdot \hat{\sigma},
\]
where \(\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)\) are the Pauli matrices \cite{14}. Writing the unit vector \(\mathbf{e}(t)\) in spherical coordinates
\[
\mathbf{e}(t) = (\sin \Theta(t) \cos \Phi(t), \sin \Theta(t) \sin \Phi(t), \cos \Theta(t))
\]
the instantaneous eigenstates of (39) can be expressed as
\[
|+; \mathbf{e}(t)\rangle = \exp(-i\Phi(t)/2) \cos(\Theta(t)/2)|+; \mathbf{e}_z\rangle + \exp(i\Phi(t)/2) \sin(\Theta(t)/2)|-; \mathbf{e}_z\rangle
\]
\[
|-; \mathbf{e}(t)\rangle = -\exp(-i\Phi(t)/2) \sin(\Theta(t)/2)|+; \mathbf{e}_z\rangle + \exp(i\Phi(t)/2) \cos(\Theta(t)/2)|-; \mathbf{e}_z\rangle,
\]
with the corresponding energies
\[
E_{\pm}(B) = \mp \mu B \equiv \mp \hbar \omega_B.
\]
We see that the energies conically intersect at \(B = 0\) in three-dimensional space spanned by the spherical coordinates \((B, \Theta, \Phi)\). If the magnetic field traces out a curve \(C\) starting at \(\mathbf{e}(0)\) and ending at \(\mathbf{e}(t)\), the noncyclic geometric phase for the eigenstates \((\mathbf{e})\) becomes
\[ \gamma_{\pm}[C] = \mp \arg \{ \exp(-i(\Phi(t) - \Phi(0))/2) \cos(\Theta(t)/2) \cos(\Theta(0)/2) \]
\[ + \exp(i(\Phi(t) - \Phi(0))/2) \sin(\Theta(t)/2) \sin(\Theta(0)/2) \} \mp \frac{1}{2} \int_0^t dt' \hat{\Phi}(t') \cos(\Theta(t')) \]
\[ \equiv \mp f(e(0), e(t)) \mp \frac{1}{2} \int_0^t dt' \hat{\Phi}(t') \cos(\Theta(t')) \equiv \pm \gamma[C]. \quad (43) \]

In particular it is straightforward to check that for \( \Theta(t) = \Theta(0) = \pi/2 \), (43) reduces, up to an integer multiple of 2\( \pi \), to the geometric phase discussed for the sign change problem in Sec. III.

Let us discuss how the geometric phase \( \gamma[C] \) can be measured in a spin-polarization experiment. The idea is to analyze the polarization vector \( P = \langle \Psi | \hat{\sigma}_z | \Psi \rangle \) of a neutron beam in the pure state \( |\Psi\rangle\langle \Psi| \), which has acquired a noncyclic geometric phase. Let us concentrate on the \( z \)-component \( P_z \) of \( P \). To observe \( P_z \) one could for example split the beam using a Stern-Gerlach field in the \( z \)-direction. Suppose \( |\Psi\rangle = c_+ |+; e_z \rangle + c_- |--; e_z \rangle \) and using that \( I_\pm \propto |c_\pm|^2 \), where \( I_\pm \) are the intensities of the two emergent sub-beams, we then obtain the normalized experimental \( z \)-polarization
\[ P_z^{exp} = \frac{1 - I_-/I_+}{1 + I_-/I_+}. \quad (44) \]

We now derive the corresponding theoretical expression for \( P_z \) in the geometric phase experiment. Suppose the neutrons are prepared in the pure state \( |+; e_z \rangle \langle +; e_z| \), so that the initial polarization in the \( z \)-direction \( P_z(0) \) equals unity. Assume \( e \) is taken, during the time interval \([0,t]\), from \( e(0) = (\sin \Theta(0), 0, \cos \Theta(0)) \) to \( e(t) = (\sin \Theta(t) \cos \Phi(t), \sin \Theta(t) \sin \Phi(t), \cos \Theta(t)) \). Expressing \( |\Psi; 0\rangle = |+; e_z \rangle \) in terms of \( |\pm; e(0)\rangle \) using (46) yields
\[ |\Psi; 0\rangle = \cos(\Theta(0)/2)|+; e(0)\rangle - \sin(\Theta(0)/2)|--; e(0)\rangle, \quad (45) \]
and it follows that in the adiabatic approximation the final state vector is
\[ |\Psi; t\rangle = \exp (i\omega_B t + \alpha_+(t)) \cos(\Theta(0)/2)|+; e(t)\rangle \]
\[ - \exp (-i\omega_B t + \alpha_-(t)) \sin(\Theta(0)/2)|--; e(t)\rangle, \quad (46) \]
where \( \alpha_\pm(t) \) are given by (46) for the state vectors \( |\pm; e(t)\rangle \). From (46) and the relations
\[ \langle \pm; e(t)| \hat{\sigma}_z |\pm; e(t)\rangle = \pm \cos \Theta(t) \]
\[ \langle \pm; e(t)| \hat{\sigma}_z |\mp; e(t)\rangle = - \sin \Theta(t) \]
(47)
we obtain
\[ P_z(t) = \cos \Theta(0) \cos \Theta(t) - \sin \Theta(0) \sin \Theta(t) \cos(2f(e(0), e(t))) + 2\omega_B t + \gamma_+[C] - \gamma_-[C], \]
(48)
where \( \gamma_+[C] - \gamma_-[C] = 2\gamma[C] \) according to (33). So keeping \( B, t, e(0) \) and \( e(t) \) fixed for a given initial pure state and varying the shape of \( C \), the adiabatic noncyclic geometric phase alone causes \( P_z(t) \) to vary. Thus by observing \( P_z \) for different \( C \)'s, \( \gamma[C] \) can be verified up to an additive integer multiple of \( \pi \). By repeating the experiment for different times \( t \) but for the same path \( C \) it is furthermore possible to check the indifference of \( \gamma[C] \) on how the path \( C \) is traversed. Similarly, the global phase invariance of the adiabatic noncyclic geometric phase can be verified by checking that \( \gamma[C] \) is independent of \( B \).
VI. CONCLUSIONS

We have shown that cyclicity is not a necessary condition for the existence of a geometric phase in adiabatic evolution. A noncyclic phase of geometric origin has to be included in the approximate adiabatic wave function. This phase has been shown to be independent of how the path is traversed in parameter space and of the phase of the instantaneous energy eigenstate $|n; R(t)\rangle$. This adiabatic noncyclic geometric phase has been frequently overlooked in the literature and reasons for this have been analyzed here. The adiabatic noncyclic geometric phase has been shown to be nonzero by explicit calculations for the sign-change problem and a noncyclic Aharonov-Bohm set-up. Moreover these two examples show that the noncyclic geometric phase gives a deeper physical insight than considering only the cyclic times. We have also discussed a spin-$\frac{1}{2}$ experiment to measure the adiabatic noncyclic geometric phase and that can be used to check its properties.

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APPENDIX

In this Appendix we compare the approach taken in this paper and an approach based on the geodesic closure of the path. Although both methods are numerically equivalent the latter is shown to have two disadvantages: (a) calculations of the geometric phase are much easier in the approach of this paper, and most importantly for the adiabatic theorem, (b) the geodesic closure will in general lie outside the adiabatic manifold.

It was demonstrated by Samuel and Bhandari [8] that for a nonadiabatic noncyclic evolution the geometric phase can be written as

\[
\gamma_{SB} = \oint_{C + C_{g-c} + C_v} A = \int_{S_{g-c}} dA,
\]

(A.1)

where, as shown in Fig. 3, \( C \) is the open path in Hilbert space \( \mathcal{H} \), \( C_{g-c} \) the horizontal lift of the shortest geodesic joining the initial and final points of the projection of \( C \) on ray space \( \mathcal{P} \), i.e. the space where Hilbert space vectors differing only in phase are identified, and \( C_v \) the vertical path in the phase direction. The quantity \( A \) is given by

\[
A = \text{Im}\langle \phi | d\phi \rangle
\]

(A.2)

with

\[
|\phi; t\rangle = |\Psi; t\rangle \exp\left(\frac{i}{\hbar} \int_0^t dt' \langle \Psi; t' | \hat{H}(t') | \Psi; t' \rangle\right)
\]

(A.3)

and \( |\Psi; t\rangle \) is the Schrödinger solution for the Hamiltonian operator \( \hat{H}(t) \). \( S_{g-c} \) is the surface inside the projection on \( \mathcal{P} \) of the closed Hilbert space curve \( C + C_{g-c} + C_v \), and we have used Stokes’ theorem for the last equality in (A.1). Moreover these authors demonstrated that this phase is equal to the Pancharatnam phase \( \beta \) [39], i.e.

\[
\gamma_{SB} = \beta = \arg\langle \phi; 0 | \phi; t \rangle.
\]

(A.4)

Using this last equality it is straightforward to show that expression (12) for the noncyclic adiabatic phase is numerically equal to the Samuel-Bhandari phase (A.1) for adiabatic evolution. That is, by choosing the global phase for the adiabatic eigenvector \( |n; R(t)\rangle \) such that

\[
\text{Im}\langle n; R(t) | \nabla_R | n; R(t) \rangle = 0,
\]

(A.5)

then (12) reduces to (A.4).

However the use of the geodesic approach has clear disadvantages. On the practical side the evaluation of \( \gamma_{SB} \) in (A.1) needs the extra calculation of the geodesic. More fundamental for the adiabatic theorem is the fact that in general the geodesic lies outside the adiabatic manifold. In this general case the surface \( S_{g-c} \) in (A.1) cannot be represented in the space of slow parameters \( R \). In the most favorable case, when the slow parameter space covers the whole ray space, Stokes’ theorem can be used directly on parameter space. An example of this is of two-level systems discussed in Sec. V, for which also holds that the parameter space metric and the ray space metric are the same [40]. Therefore Berry’s result for cyclic adiabatic evolution in two-level systems, \( \gamma_{\pm}[C_0] = \mp \Omega/2 \), with \( \Omega \) the solid angle enclosed
by the closed path $C_0$, generalizes in the noncyclic case to $\gamma_{\pm}[C] = \mp \Omega_{g-c}/2$, with $\Omega_{g-c}$ the solid angle defined by the closed path $C + C_{g-c}$, where $C_{g-c}$ is the shortest geodesic in parameter space connecting the end-points of $C$.

In the following we illustrate this result for two particular examples. First consider the case when $\Theta = \pi/2$, i.e. the sign change case, for which (43) becomes

$$\gamma_{\pm}[C] = \mp \arg\cos((\Phi(t) - \Phi(0))/2)
= \mp \begin{cases} 0 & \text{if } \Phi(0) \leq \Phi(t) < \Phi(0) + \pi \\ \text{undefined} & \text{if } \Phi(t) = \Phi(0) + \pi \\ \pi & \text{if } \Phi(0) + \pi < \Phi(t) \leq \Phi(0) + 2\pi \end{cases} = \mp \frac{1}{2}\Omega_{g-c} \quad (A.6)$$

as shown in Fig. 4. Note that when $\Phi(t) = \Phi(0) + \pi$ there are infinitely many geodesics connecting the end-points and all of them give different values of the geometric phase which is then undefined. Another interesting example is given in Fig. 5 for which (43) can be checked to give the solid angle result

$$\gamma_{\pm}[C] = \mp \frac{\pi}{4} = \mp \frac{1}{2}\Omega_{g-c}. \quad (A.7)$$
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FIGURE CAPTIONS

Fig. 1. Two electronic potential energy surfaces $E_{\pm}(R)$ which conically intersect at the origin $R = 0$ in nuclear configuration space.

Fig. 2. A charged particle confined in an impenetrable box by the potential $V$ and transported along $C$ around a magnetic flux line. The box is situated at $R$ and the particle is described by the coordinate $r$. An asymmetric shape has been chosen and the size of the box is such that the overlap between the initial wave function and the wave function at any later time $t$ is nonvanishing. The box at the initial time is plotted with thin line. We have divided the transport of the box into three $\Theta$-intervals: (a) $0 \leq \Theta(t) \leq 2\pi - \Delta \theta$, (b) $2\pi - \Delta \theta \leq \Theta(t) \leq \Delta \theta$ and (c) $\Theta(t) \geq \Delta \theta$, with $\Delta \theta$ the angular length of the boxes.

Fig. 3. Illustration of the geodesic closure approach. $C$ is the open path in Hilbert space $\mathcal{H}$, $C_{g-c}$ the horizontal lift of the shortest geodesic joining the initial and final points of the projection of $C$ on ray space $\mathcal{P}$, $C_v$ the vertical path in the phase direction, and $S_{g-c}$ the surface inside the projection on $\mathcal{P}$ of the closed Hilbert space curve $C + C_{g-c} + C_v$.

Fig. 4. Noncyclic sign change from the geodesic closure perspective. The noncyclic geometric phase is equal to the solid angle defined by the path $C$ and its shortest geodesic join (indicated by dashed line). There are three cases: (a) $\Phi(0) \leq \Phi(t) < \Phi(0) + \pi$ with $\gamma_{\pm}[C] = \mp \Omega_{g-c}/2 = 0$, (b) $\Phi(t) = \Phi(0) + \pi$ which has an infinite number of geodesic closures making $\gamma_{\pm}[C]$ undefined, and (c) $\Phi(0) + \pi < \Phi(t) \leq \Phi(0) + 2\pi$ with $\gamma_{\pm}[C] = \mp \Omega_{g-c}/2 = \mp \pi$.

Fig. 5. Case for which an open path together with its shortest geodesic closure encloses one fourth of the upper hemisphere. The adiabatic noncyclic geometric phase is $\gamma_{\pm} = \mp \Omega_{g-c}/2 = \mp \pi/4$. 

16
Figure 1.
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