Contribution of adiabatic phases to noncyclic evolution

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We show that the difference of adiabatic phases, that are basis-dependent, in noncyclic evolution of non-degenerate quantum systems have to be taken into account to give the correct interference result in the calculation of physical quantities in states that are a superposition of instantaneous eigenstates of energy. To verify the contribution of those adiabatic phases in the interference phenomena, we consider the spin-$1/2$ model coupled to a precessing external magnetic field. In the model, the adiabatic phase increases in time up to reach the difference of the Berry's phases of the model when the external magnetic field completes a period.

Keywords: Berry's phase, adiabatic phase, noncyclic adiabatic evolution, spin-1/2 model

In 1928 Born and Fock[1] proofed the Adiabatic Theorem. In a quantum system with non-degenerate energy spectrum, this theorem says that if the system at $t = 0$ is an eigenstate of energy with quantum numbers $\{n\}$, along an adiabatic evolution it continues to be in an eigenstate of energy at time t with the same initial quantum numbers $\{n\}$. As a consequence of this theorem, the vector state of the quantum system acquires an extra phase besides the dynamical phase. This extra phase is actually named geometric phase. Before the important work by MV Berry in 1984[2] with cyclic adiabatic hamiltonian, this extra phase was realized to be dependent on the choice of the basis of instantaneous eigenstates of energy. This extra phase was considered non-physical since it could be absorbed in the choice of the states in the instantaneous basis.[3].

In Ref. [2], MV Berry showed that the adiabatic phase acquired by the instantaneous eigenstates of energy, after a closed evolution in the classical parameter space, is physical due to its independence to the chosen basis to describe the state vector at each instant. Since the publication of the Ref. [2], the study of Berry's phase has followed very interesting and broad directions. More recently, the geometric phases have been proposed as a prototype for a quantum bit (qubit)[4–7]. In 1988 Samuel and Bhandari[8] generalized the geometric phase to noncyclic evolution. Many others interesting papers appear to discuss those physical phases in noncyclic evolution in the classical parameter space[9–11]. Experimental verification to the presence of those noncyclic geometric phases have been realized[12].

The interference effect is a keystone in the linearity of the Quantum Mechanics. In the present letter we address to the question of the effect of the adiabatic evolution on the phases in quantum systems leaves a physical trace in measurable quantities associated to the noncyclic evolution of states described by a superposition of instantaneous eigenstates of energy. The same question was proposed in the nice Ref. [9], but differently from them we do not look for a physical noncyclic geometric phase.

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Let us consider a time-dependent hamiltonian $\mathbf{H}(t)$ that evolves adiabatically. Following Ref. [2], we leave open the possibility that this time dependence comes from a set of classical parameters that we call $\vec{R}(t)$ ($\vec{R}(t) \equiv (X_1(t), X_2(t), \cdots, X_m(t))$), but we also include the possibility that the hamiltonian can have an explicit time dependence. As a matter of simplification, we assume that the spectrum of eigenvalues of $\mathbf{H}(t)$ is non-degenerate.

Let $\{|\varphi_j;t\rangle, j = 1,2,\cdots\}$ be an instantaneous basis of orthonormalized eigenstates of the energy

$$\mathbf{H}(t)|\varphi_j;t\rangle = E_j(t)|\varphi_j;t\rangle, \tag{1}$$

where $\langle\varphi_l;t|\varphi_j;t\rangle = \delta_{lj}$ and $l, j = 1,2,\cdots$.

We assume that the initial vector state is a superposition of M eigenstates of energy at $t = 0$,

$$|\psi(0)\rangle = \sum_{j=1}^{M} a_j\,|\varphi_j;0\rangle, \tag{2}$$

with $M > 1$ and $\sum_{j=1}^{M} |a_j|^2 = 1$.

Applying the Adiabatic Theorem[1, 3] to the Schrödinger eq. of the adiabatic evolution of the initial vector state (2), it gives,

$$|\psi(t)\rangle = \sum_{j=1}^{M} a_j\, e^{i\gamma_j(t)}\, e^{-\frac{it}{\hbar}\langle E_j(t)\rangle}\,|\varphi_j;t\rangle, \tag{3a}$$

where $\langle E_j(t)\rangle$ is the average energy during the interval of time t,

$$\langle E_j(t)\rangle \equiv \frac{1}{t}\int_0^t dt'\, E_j(t') \tag{3b}$$

and $\gamma_j(t) \in \mathbb{R}$ is the adiabatic phase,

$$\gamma_j(t) = i\int_0^t dt'\,\langle\varphi_j;t'|\left(\frac{d}{dt'}|\varphi_j;t'\rangle\right). \tag{3c}$$

It is well known that the adiabatic phase (3c) is non-physical.

An obvious physical quantity to calculate from the vector state (3a) is the density of probability to find the particle at

position $\vec{x}$ at any instant t,

$$|\psi(\vec{x},t)|^2 = \sum_{j=1}^{M} |a_j|^2 |\varphi_j(\vec{x};t)|^2 + \sum_{\substack{j,l=1 \\ j\neq l}}^{M} a_j a_l^* e^{i[\gamma_j(t)-\gamma_l(t)]}\ e^{-\frac{it}{\hbar}\left[\langle E_j(t)\rangle - \langle E_l(t)\rangle\right]}\ \varphi_j(\vec{x};t)\varphi_l^*(\vec{x};t), \tag{4}$$

where $\psi(\vec{x},t) = (\vec{x}|\psi(t)\rangle$ and $\varphi_j(\vec{x};t) = (\vec{x}|\varphi_j;t\rangle$.

The interference phenomenon comes from the terms on the second sum on the r.h.s. of eq.(4). Each interference term depends only on the difference of adiabatic phases (3c).

Let $\{|\Phi_j;t\rangle,\ j = 1,2,\cdots\}$ be another basis of instantaneous eigenstates of energy,

$$|\Phi_j;t\rangle = e^{i\alpha_j(t)}\ |\varphi_j;t\rangle, \qquad j = 1,2,\cdots \tag{5}$$

and $\alpha_j(t) \in \mathbb{R}$ and its time-dependence comes through $\vec{R}(t)$ and/or an explicit time dependence. The initial state (2) is rewritten in this basis as

$$|\psi(0)\rangle = \sum_{j=1}^{M} \tilde{a}_j |\Phi_j;0\rangle. \tag{6a}$$

Therefore

$$\tilde{a}_j = a_j e^{-i\alpha_j(0)}. \tag{6b}$$

Written in the new basis, $|\psi(t)\rangle$ becomes

$$|\psi(t)\rangle = \sum_{j=1}^{M} \tilde{a}_j e^{i\tilde{\gamma}_j(t)}\ e^{-\frac{it}{\hbar}\langle E_j(t)\rangle}\ |\Phi_j;t\rangle, \tag{7}$$

where the relation between the adiabatic phases $\gamma_j(t)$ and $\tilde{\gamma}_j(t)$ is

$$\tilde{\gamma}_j(t) = \gamma_j(t) - \alpha_j(t) + \alpha_j(0), \qquad j = 1,2,\cdots,M. \tag{8}$$

The density of probability written in the new basis is,

$$|\psi(\vec{x},t)|^2 = \sum_{j=1}^{M} |\tilde{a}_j|^2 |\Phi_j(\vec{x};t)|^2 + \sum_{\substack{j,l=1 \\ j\neq l}}^{M} \tilde{a}_j \tilde{a}_l^* e^{i[\tilde{\gamma}_j(t)-\tilde{\gamma}_l(t)]}\ e^{-\frac{it}{\hbar}\left[\langle E_j(t)\rangle - \langle E_l(t)\rangle\right]}\ \Phi_j(\vec{x};t)\Phi_l^*(\vec{x};t). \tag{9}$$

From the eqs. (5), (6b) and (8), we obtain

$$\tilde{a}_j \tilde{a}_l^* e^{i[\tilde{\gamma}_j(t)-\tilde{\gamma}_l(t)]}\ \Phi_j(\vec{x};t)\Phi_l^*(\vec{x};t) = a_j a_l^* e^{i[\gamma_j(t)-\gamma_l(t)]}\ \varphi_j(\vec{x};t)\varphi_l^*(\vec{x};t), \tag{10}$$

$l, j = 1,2,\cdots,M$. In eq.(10) we include the terms $l = j$. Result (10) tells us that each term in the two sums on the r.h.s. of eq.(4) is independent of the basis of the instantaneous eigenvectors of energy that we use to do the calculation.

Certainly, the result (10) can be recast in terms of a geometric phase along a closed path, showing that the phase difference $\gamma_j(t) - \gamma_l(t)$ is gauge invariant at any instant t[13]. However, our main point is calling attention to the fact that in order to obtain the correct result for $|\psi(t)|^2$ one has to take into account the non-physical adiabatical phase (3a), that is non-physical, when we use a basis of instantaneous eigenstates of energy that are not paralell transported.

To generalize the conclusions derived from result (10) we consider $\mathbf{O}$ to be an hermitian operator associated to a physical quantity. The time-evolution of the average of this operator in the initial state (2) is

$$o(t) = \langle\psi(t)|\mathbf{O}|\psi(t)\rangle = \sum_{j=1}^{M} |a_j|^2 \langle\varphi_j;t|\mathbf{O}|\varphi_j;t\rangle + \sum_{\substack{j,l=1 \\ j\neq l}}^{M} a_j a_l^* e^{i[\gamma_j(t)-\gamma_l(t)]}\ e^{-\frac{it}{\hbar}\left[\langle E_j(t)\rangle - \langle E_l(t)\rangle\right]} \langle\varphi_j;t|\mathbf{O}|\varphi_l;t\rangle. \tag{11}$$

Following the same steps as we did to proof that the terms that contribute to the density probability is basis-independent, we show that the same is true for each term in the two sums on the r.h.s. of eq.(11).

Therefore if we use a basis of instantaneous eigenstates of energy, that is not of parallel transported states, to describe the adiabatic evolution of a vector state that initially is in a superposition of eigenstates of energy at $t = 0$, the non-physical adiabatic phases (3a) have to be taken into account to give the correct interference terms when we calculate physical quantities.

To exemplify the importance to take into account the adiabatic phases (3c) to obtain the correct result in physical quantities, we consider the soluble model of the spin-$1/2$ in the presence of an external classical magnetic field. This field precesses around a z-direction with constant angular frequency ω_0. This model was discussed by Berry in Ref. [2] and by García de Polavieja and Sjöqvist in Ref.[9]. Being a soluble model we can verify the result obtained in the adiabatic regime by applying the adiabatic approximation directly in the exact result[14].

The hamiltonian of a spin-$1/2$ in the presence of an external classical magnetic field $\vec{B}(t)$ is[14]

$$\mathbf{H}(t) = \frac{\mu\hbar}{2}\vec{B}(t)\cdot\vec{\sigma}, \tag{12a}$$

where

$$\vec{B}(t) = (B\sin(\theta)\cos(\omega_0 t), B\sin(\theta)\sin(\omega_0 t), B\cos(\theta)), \tag{12b}$$

with $B \equiv |\vec{B}|$ and θ is the angle between the external magnetic field and the z-direction. The σ_i, $i \in \{x,y,z\}$ are the Pauli matrices, $\mu = g\mu_B$, where μ_B is the Bohr magneton and g is the Landé's factor.

In Ref.[14] we obtain the two eigenvectors of hamiltonian (12a) and their respective eigenvalues,

$$|\phi_1;t\rangle = -\sin(\frac{\theta}{2})|\uparrow\rangle + \cos(\frac{\theta}{2})e^{i\omega_0 t}|\downarrow\rangle \quad \Rightarrow \quad E_1 = -\frac{\mu\hbar B}{2}, \tag{13a}$$

$$|\phi_2;t\rangle = \cos(\frac{\theta}{2})|\uparrow\rangle + \sin(\frac{\theta}{2})e^{i\omega_0 t}|\downarrow\rangle \quad \Rightarrow \quad E_2 = \frac{\mu\hbar B}{2}. \tag{13b}$$

We denote the eigenvector of σ_z with eigenvalue +1 (-1) to be $|\uparrow\rangle$ ($|\downarrow\rangle$).

We choose the initial vector state of the spin-$1/2$ system to be,

$$|\psi(0)\rangle = a_1|\phi_1;0\rangle + a_2|\phi_2;0\rangle \tag{14}$$

and $|a_1|^2 + |a_2|^2 = 1$. For simplicity we take a_1 and $a_2 \in \mathbb{R}$.

From eq.(3a), the adiabatic evolution of the previous initial state is

$$|\psi(t)\rangle = e^{i\gamma_1(t)}\, e^{-\frac{itE_1}{\hbar}} \left[a_1|\phi_1;t\rangle + a_2\, e^{i\alpha[\gamma_2(t)-\gamma_1(t)]}\, e^{-\frac{it}{\hbar}[E_2-E_1]}\, |\phi_2;t\rangle\right]. \tag{15}$$

The previous equation is similar to eq.(46) of Ref.[9].

From a direct calculation of phase (3c), we obtain: $\gamma_1(t) = -\frac{(1+\cos(\theta))\omega_0 t}{2}$ and $\gamma_2(t) = -\frac{(1-\cos(\theta))\omega_0 t}{2}$.

In eq.(15) we include the tracer α to verify if the difference of adiabatic phases contribute to physical quantities. At the end of the calculation we take $\alpha = 1$.

The expectation value of the operator $\mathbf{s}_z$ in the state $|\psi(t)\rangle$ is

$$\langle\psi(t)|\mathbf{s}_z|\psi(t)\rangle = \frac{\hbar}{2}\cos(\theta)[a_2^2 - a_1^2] - 4a_1a_2\hbar\sin(\theta)\cos[(\mu B - \alpha\omega_0\cos(\theta))t]. \tag{16}$$

From what we discussed in the first part of this letter, result (16) is physical. We verify that the adiabatic phases (3c) contribute to the second term on the r.h.s. of expression (16) with a phase that increases in time up to reach the difference of Berry's phases when the $t = \frac{2\pi}{\omega_0}$.

In Ref. [14] we have the exact dynamics of the initial vector (14). Using the exact time dependence of the $|\psi(t)\rangle$ we calculate the expectation value of the operator $\mathbf{s}_z$ and implement in it the adiabatic approximation. This approximated result coincides with expression (16) with $\alpha = 1$.

In conclusion, we show that although the adiabatic phase (3c) is non-physical, the phase differences do contribute to physical quantities during the adiabatic evolution of a non-cyclic quantum system if the vector state is a superposition of instantaneous eigenstates of energy.

The result of each interference term on the r.h.s. of eq.(11) is independent of a particular choice of basis of the instantaneous energy eigenstates. In order to verify the consequences of an adiabatic variation of the hamiltonian on the motion of the quantum system driven by it, we do not need to define a noncyclic geometric phase, as it has been done in the literature.

In order to show the importance of the contribution of this phase difference of adiabatic nature, we calculate the expectation value of the operator $\mathbf{s}_z$ of a spin-$1/2$ model coupled to an external magnetic field that precesses around a fixed direction. We verify that the adiabatic approximation of $\langle\psi(t)|\mathbf{s}_z|\psi(t)\rangle$, derived from its exact expression, only coincides with the calculation of the adiabatic evolution of this operator if the difference of the adiabatic phases (3c) is included in the dynamics of the instantaneous eigenstates (13a) and (13b).

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