Nonadiabatic Berry's phase for a quantum system with a dynamical semisimple Lie group

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The nonadiabatic Berry's phase is investigated for a quantum system with a dynamical semisimple Lie group within the framework of the generalized cranking approach. An expression for nonadiabatic Berry's phase is given, which indicates that the nonadiabatic Berry's phase is related to the expectation value of Cartan operators along the cranking direction in group space, and that it depends on (i) the geometry of the group space, (ii) the time evolution ray generated by the Hamiltonian (i.e., by the dynamics) in some irreducible representation Hilbert space, and (iii) the cranking rate. The expression also provides a simple algorithm for calculating the nonadiabatic Berry's phase. The general formalism is illustrated by examples of SU(2) dynamic group.

The adiabatic Berry's phase[1] has been exploited extensively in a great number of theoretical and experimental articles,[2] and much knowledge and deep insights have been obtained in this respect. However, although the nonadiabatic Berry's phase has been addressed by Berry[3] and several other authors,[4] we do not have the same level of insight and knowledge as for the adiabatic phase. Since the nonadiabatic Berry's phase is related to the dynamical effect on the adiabatic-geometric Berry's phase, its study depends on specific dynamics, i.e., the structure of the Hamiltonian. Thus investigation of the nonadiabatic Berry's phase is more difficult. From our previous studies, we found that the study of nonadiabaticity may become easier if a quantum system possesses a dynamical group. In our previous papers, three types of systems are investigated: A photon propagating in an optical helix,[5] a spin particle in a rotating magnetic field,[6] and a rotating deformed nucleus.[7] For all the three systems, the relevant dynamical group is the SU(2) group, and the problems are solved by the cranking method, developed in nuclear physics.[8] Berry's phase is obtained analytically if the Hamiltonian is a linear function of SU(2) generators, and can be calculated straightforwardly, even though the Hamiltonian is nonlinear in the generators. It is found that for the SU(2) dynamical group, Berry's phase is related to the expectation value of spin, and the nonadiabatic effect on Berry's phase manifests itself as spin alignment. In this article, we generalize the above-noted studies to a quantum system that possesses a dynamical semisimple Lie group and exploit physical-geometrical aspects of the nonadiabatic Berry's phase.

Consider a quantum system whose Hamiltonian is a function of generators of a semisimple Lie group G,

$$\mathcal{H}_0=\mathcal{H}_0(X_\mu)=\mathcal{H}_0(H_i,E_\alpha)\ , \tag{1}$$

where the generators $\{X_\mu\}$ or $\{H_i,E_\alpha\}$ in the Cartan form obey standard commutator relations[9]

$$[H_i,H_j]=0,\quad i,j=1,2,\ldots,1 \tag{2a}$$

$$[H_i,E_\alpha]=\alpha_i E_\alpha,\quad \alpha=1,2,\ldots,n-1\ , \tag{2b}$$

$$[E_\alpha,E_{-\alpha}]=\alpha^i H_i\ , \tag{2c}$$

$$[E_\alpha,E_\beta]=N_{\alpha\beta}E_{\alpha+\beta}\quad \text{if } \alpha+\beta\neq 0\ , \tag{2d}$$

where $\{H_i\}$ is the Cartan subalgebra, $\{E_\alpha,E_{-\alpha}\}$ are raising and lowering operators, l the rank of the group, and n the order of the group.

First consider the simplest case where the Hamiltonian is a linear function of the generators. Generally,

$$\mathcal{H}_0=\epsilon\boldsymbol{\beta}\cdot\mathbf{X}=\epsilon\sum_\mu \beta_\mu X_\mu=\epsilon\left[\sum_\alpha \beta_\alpha E_\alpha+\sum_i \beta_i H_i\right]\ , \tag{3a}$$

where ϵ is an energy constant and $\boldsymbol{\beta}$ is a vector in group parameter space,

$$\boldsymbol{\beta}=\{\beta_\mu\}=\{\beta_\alpha,\beta_i\}\ . \tag{3b}$$

$\mathcal{H}_0$ can be rewritten as

$$\mathcal{H}_0=\epsilon\exp\left[-\sum_\alpha(z_\alpha E_\alpha-z_\alpha^* E_{-\alpha})\right]\mathbf{a}\cdot\mathbf{H}\times\exp\left[+\sum_\alpha(z_\alpha E_\alpha-z_\alpha^* E_{-\alpha})\right]\ , \tag{4}$$

where

$$\mathbf{a}\cdot\mathbf{H}=\sum_i a_i H_i,\quad \sum_i a_i^2=1,\quad \sum_\alpha|\beta_\alpha|^2+\sum_i\beta_i^2=1\ , \tag{5}$$

and a_i and $z_\alpha(z_\alpha^*)$ are functions of β_μ. Suppose $|m\rangle$ are eigenvectors of $\mathbf{H}$,

$$\mathbf{H}|m\rangle=\mathbf{m}|m\rangle,\quad \mathbf{m}=\{m_i|i=1,\ldots,l\}\ . \tag{6}$$

Now we crank the system through a periodic time-dependent unitary transformation. The Hamiltonian of the system then becomes time dependent,

$$\mathcal{H}(t)=\exp(-i\mathbf{n}\cdot\mathbf{H}\omega t)\mathcal{H}_0\exp(i\mathbf{n}\cdot\mathbf{H}\omega t)$$
$$=\epsilon[\boldsymbol{\beta}_{\rm I}(t)\cdot\mathbf{E}+\boldsymbol{\beta}_{\rm II}\cdot\mathbf{H}] , \quad (7)$$

where

$$\boldsymbol{\beta}_{\rm I}(t)=\{\beta_\alpha\exp(-i\mathbf{n}\cdot\boldsymbol{\alpha}\omega t)\},\quad \boldsymbol{\beta}_{\rm II}=\{\beta_i\} , \quad (8)$$

with

$$\mathbf{n}\cdot\boldsymbol{\alpha}=\sum_i n_i\alpha_i=\pm\text{integer} . \quad (9)$$

Since $\mathbf{b}\cdot\mathbf{X}$ can be considered to be a Cartan operator or a combination of Cartan operators, $\exp(-i\mathbf{n}\cdot\mathbf{H}\omega t)$ is a general periodic time-dependent transformation in the group space. Thus the cranked Hamiltonian (7) is a general form.

The equation of motion for the cranked system is

$$i\frac{\partial\psi(t)}{\partial t}=\mathcal{H}(t)\psi(t) . \quad (10)$$

We turn to the intrinsic frame through a unitary transformation,

$$\psi(t)=\exp(-i\mathbf{n}\cdot\mathbf{H}\omega t)\eta(t) . \quad (11)$$

Equation of motion for $\eta(t)$ is

$$i\frac{\partial\eta(t)}{\partial t}=\mathcal{H}(\omega)\eta(t) , \quad (12)$$

where Routhian operator $\mathcal{H}(\omega)$ is defined as

$$\mathcal{H}(\omega)=\mathcal{H}_0-\omega\mathbf{n}\cdot\mathbf{H}$$
$$=\epsilon\left[\sum_\alpha\beta_\alpha E_\alpha+\sum_i\left[\beta_i-\frac{\omega}{\epsilon}n_i\right]H_i\right]$$
$$=\bar{\epsilon}(\bar{\boldsymbol{\beta}}_{\rm I}\cdot\mathbf{E}+\bar{\boldsymbol{\beta}}_{\rm II}\cdot\mathbf{H}) , \quad (13a)$$

which can be rewritten as

$$\mathcal{H}(\omega)=\bar{\epsilon}\exp\left[-\sum_\alpha(\bar{z}_\alpha E_\alpha-\bar{z}^*_\alpha E_{-\alpha})\right]\mathbf{a}\cdot\mathbf{H}\exp\left[\sum_\alpha(\bar{z}_\alpha E_\alpha-\bar{z}^*_\alpha E_{-\alpha})\right] , \quad (13b)$$

where a_i, $\bar{z}_\alpha$, and $\bar{z}^*_\alpha$ are functions of $\bar{\beta}_\mu$, and the renormalized parameters are

$$\bar{\epsilon}=\epsilon\gamma , \quad (14)$$

$$\bar{\beta}_\alpha=\beta_\alpha/\gamma,\quad \bar{\beta}_i=\left[\beta_i-\frac{\omega}{\epsilon}n_i\right]\Big/\gamma , \quad (15a)$$

$$\gamma=\left[1-2\frac{\omega}{\epsilon}\sum_i\beta_i n_i+\left[\frac{\omega}{\epsilon}\right]^2\sum_i n_i^2\right]^{1/2} . \quad (15b)$$

The solutions of Eqs. (10) and (12) are

$$\eta(t)=\exp[-i\mathcal{H}(\omega)t]\eta(0) , \quad (16)$$

$$\psi(t)=U(t)\psi(0) . \quad (17)$$

Where the evolution operator is

$$U(t)=\exp(-i\mathbf{n}\cdot\mathbf{H}\omega t)\exp[-i\mathcal{H}(\omega)t] . \quad (18)$$

Let us consider the eigenequations of $\mathcal{H}_0$ and $\mathcal{H}(\omega)$,

$$\mathcal{H}_0\varphi_m=\epsilon_m\varphi_m , \quad (19)$$

$$\mathcal{H}(\omega)\eta_m=E_m\eta_m , \quad (20)$$

with the solutions

$$\epsilon_m=\epsilon\mathbf{a}\cdot\mathbf{m}=\epsilon\sum_i a_i m_i , \quad (21a)$$

$$\varphi_m=\exp\left[-\sum_\alpha(z_\alpha E_\alpha-z^*_\alpha E_{-\alpha})\right]|m\rangle , \quad (21b)$$

and

$$E_m=\bar{\epsilon}\mathbf{a}\cdot\mathbf{m}=\bar{\epsilon}\sum_i a_i m_i , \quad (22a)$$

$$\eta_m=\exp\left[-\sum_\alpha(\bar{z}_\alpha E_\alpha-\bar{z}^*_\alpha E_{-\alpha})\right]|m\rangle . \quad (22b)$$

Consider solutions in one period T ($T=2\pi/\omega$). The evolution operator in one period is

$$U(T)=\exp(-i\mathbf{n}\cdot\mathbf{H}2\pi)\exp[-i\mathcal{H}(\omega)T] . \quad (23)$$

Since

$$\exp(-i\mathbf{n}\cdot\mathbf{H}2\pi)\mathcal{H}(\omega)\exp(i\mathbf{n}\cdot\mathbf{H}2\pi)=\mathcal{H}(\omega) , \quad (24)$$

$U(T)$ and $\mathcal{H}(\omega)$ commute and have common eigenvectors, i.e.,

$$U(T)\eta_m=\exp(-i\phi_m)\eta_m , \quad (25)$$

where the total phase ϕ_m will be given later.

Consider cyclic or recurrent solutions whose initial states are eigenstates of $\mathcal{H}(\omega)$,

$$\psi_m(0)=\eta_m . \quad (26)$$

After one period,

$$\psi_m(T)=\exp(-i\mathbf{n}\cdot\mathbf{H}2\pi)\exp[-i\mathcal{H}(\omega)T]\eta_m$$
$$=\exp(-iE_mT-i2\pi\mathbf{n}\cdot\mathbf{m})\psi_m(0) . \quad (27)$$

The total phase is

$$\phi_m=E_mT+2\pi\mathbf{n}\cdot\mathbf{m} . \quad (28)$$

The expectation value of $\mathcal{H}(t)$ is

$$\begin{aligned}\varepsilon_m(t) &= \langle \psi_m(t)|\mathcal{H}(t)|\psi_m(t)\rangle \\ &= \langle \eta_m|\mathcal{H}_0|\eta_m\rangle \\ &= E_m(\omega)+\omega\langle \eta_m|\mathbf{n}\cdot\mathbf{H}|\eta_m\rangle \\ &= E_m(\omega)+\omega\mathbf{n}\cdot\langle \mathbf{m}\rangle \ ,\end{aligned} \tag{29}$$

where

$$\langle \mathbf{m}\rangle = \langle \eta_m|\mathbf{H}|\eta_m\rangle \ . \tag{30}$$

From Eq. (29) we obtain the dynamical phase

$$\phi_m^d = \int_0^T \varepsilon_m(t)dt = E_m(\omega)T + 2\pi\mathbf{n}\cdot\langle \mathbf{m}\rangle \ , \tag{31}$$

and Berry's phase

$$\begin{aligned}\phi_m^B &= -(\phi_m - \phi_m^d) \\ &= -2\pi\mathbf{n}\cdot\mathbf{m}(1-\mathbf{n}\cdot\langle \mathbf{m}\rangle/\mathbf{n}\cdot\mathbf{m}) \\ &= -2\pi\mathbf{n}\cdot\mathbf{m}(1-\langle \eta_m|\mathbf{n}\cdot\mathbf{H}|\eta_m\rangle/\mathbf{n}\cdot\mathbf{m}) \ .\end{aligned} \tag{32}$$

Equation (32) indicates that Berry's phase is related to the expectation value of Cartan operators along the cranking $\mathbf{n}$ direction and depends on (i) the geometry of the group space where the vectors $\mathbf{n}$ and $\mathbf{m}$ reside, (ii) the ray or η_m generated by the Hamiltonian (dynamics), and (iii) the cranking rate ω. The expression (32) also provides an algorithm to calculate the nonadiabatic Berry's phase, since, given an irreducible representation of the dynamical group, the calculation of eigenvectors η_m and expectation value $\langle \eta_m|\mathbf{n}\cdot\mathbf{H}|\eta_m\rangle$ is straightforward.

Now consider general cases where the Hamiltonian is a nonlinear function of the group generators,

$$\mathcal{H}_0 = \mathcal{H}_0(\beta_\alpha E_\alpha, \beta_i H_i) \ . \tag{33}$$

After cranking, the Hamiltonian becomes

$$\mathcal{H}(t) = \mathcal{H}_0(\beta_\alpha(t) E_\alpha, \beta_i H_i) \ . \tag{34}$$

The expression (32) of Berry's phase is also applicable for the nonlinear case. However, the eigensolutions of $\mathcal{H}(\omega)$ should be obtained by numerical calculation, although it is straightforward.

In what follows we give examples to illustrate the above general formalism. Consider the SU(2) dynamical group, which, as we mentioned before, is of practical and theoretical interest. For the linear case, the Hamiltonian is assumed to be[6]

$$\mathcal{H}_0 = \mathbf{\Omega}\cdot\mathbf{J} = \Omega\exp[-\theta(J_+ - J_-)]J_z\exp[\theta(J_+ - J_-)] \ , \tag{35}$$

which describes a spin particle in magnetic field, where

$$\mathbf{a}\cdot\mathbf{H} = J_z \ , \tag{36a}$$

$$\mathbf{\Omega} = \Omega(\sin\theta, 0, \cos\theta) \ . \tag{36b}$$

The cranked Hamiltonian is

$$\mathcal{H}(t) = \exp(-iJ_z\omega t)\mathcal{H}_0\exp(iJ_z\omega t) = \mathbf{\Omega}(t)\cdot\mathbf{J} \ , \tag{37a}$$

$$\mathbf{\Omega}(t) = \Omega(\sin\theta\cos\omega t, \sin\theta\sin\omega t, \cos\theta) \ , \tag{37b}$$

which indicates that the magnetic field is in precession along the z axis with frequency ω. The Routhian operator and its eigensolutions are

$$\begin{aligned}\mathcal{H}(\omega) &= \mathcal{H}_0 - \omega J_z = \bar{\mathbf{\Omega}}\cdot\mathbf{J} \\ &= \bar{\Omega}\exp[-\bar{\theta}(J_+ - J_-)]J_z\exp[+\bar{\theta}(J_+ - J_-)] \ ,\end{aligned} \tag{38a}$$

$$\bar{\mathbf{\Omega}} = \bar{\Omega}(\sin\bar{\theta}, 0, \cos\bar{\theta}) \ , \tag{38b}$$

$$\eta_m = \exp(-i\bar{\theta}J_y)|m\rangle \ , \tag{38c}$$

$$E_m = m\bar{\Omega} \ , \tag{38d}$$

$$\bar{\Omega} = \Omega\gamma, \quad \gamma = \left[1 - 2\frac{\omega}{\Omega}\cos\theta + \left[\frac{\omega}{\Omega}\right]^2\right]^{1/2} \ . \tag{38e}$$

Berry's phase is

$$\phi_m^B = -2m\pi(1-\langle \eta_m|J_z|\eta_m\rangle/m) \tag{39a}$$

$$= -2m\pi(1-\cos\bar{\theta}) \ , \tag{39b}$$

where

$$\cos\bar{\theta} = (\cos\theta - \omega/\Omega)/\gamma \ . \tag{39c}$$

For the nonlinear case, the Hamiltonian is assumed

$$\mathcal{H}_0 = (\mathbf{\Omega}\cdot\mathbf{J})^2 \tag{40a}$$

and

$$\mathcal{H}(t) = [\mathbf{\Omega}(t)\cdot\mathbf{J}]^2 \ , \tag{40b}$$

which are used to describe nuclear quadrupole resonances.[10] The Berry's phase takes the same expression (39a). However, the eigensolutions of $\mathcal{H}(\omega)$ should be calculated numerically.

In conclusion, we have generalized the investigation of the nonadiabatic Berry's phase of a quantum system with the SU(2) dynamic group to a quantum system with any dynamic semisimple Lie group within the framework of the cranking approach. The nonadiabatic Berry's phase is given in terms of the expectation value of the Cartan operators, which provides a simple algorithm to calculate the nonadiabatic Berry's phase and gives Berry's phase a physical-geometric explanation, since the expectation value of Cartan operators in a quantum system has both physical and geometric meanings. The illustrations of the SU(2) examples indicate that the above formalism is useful.

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