Dynamical Meaning of Quantum Adiabatic Phase: The Case of a Noncanonical System

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A dynamical meaning is given for the phase Γ recently found in a quantum adiabatic process. A noncanonical system, specifically a spin system coupled with a proper intrinsic system, is considered by use of a path integral in a SU(2) coherent-state representation. It is shown that Γ appears as an addition of topological nature to the conventional action function, which leads to a novel form of the semiclassical quantization rule including the phase Γ.

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Following an early implication in chemical physics,[1,2] a remarkable phenomenon was recently discovered in the general context of the quantum adiabatic theorem[3]: During an excursion along a closed loop C in the external parameter space the adiabatic deformation of the wave function gives an extra phase in addition to the usual dynamical phase,

$$\psi_n(T)=\exp[i\Gamma_n(C)]\exp[-(i/\hbar)\int E_n(R_t)dt]|n(R_T)\rangle .$$

This phase $\Gamma_n(C)$ (which we call the "adiabatic phase" after Berry[3]) was shown to reflect a singular nature of the degeneracy of adiabatic levels.[2,3] Further, this phase was shown to be nothing but the "holonomy" constructed from the vector bundle of the parametrized wave function,[4] which leads to a connection with the quantized Hall effect.[5] The non-Abelian extension of the phase Γ has also been studied.[6]

In spite of such remarkable features of the adiabatic phase in the general context of nonrelativistic quantum mechanics, the work in this area so far has been mainly concerned with the static aspect only, that is, the case in which the motion in the external parameter space is fixed from the outset. Thus it would be highly desirable to develop a dynamical argument such that one can deal with the case where the external space itself is a dynamical object. In the following we shall give a simple but nontrivial answer to this problem. This viewpoint has previously been pursued by Mead and Truhlar[1] using the Schrödinger equation. However, the argument based on the Schrödinger equation is of an essentially local nature. So in order to clarify the nonintegrable nature of the adiabatic phase, we adopt here the path-integral formulation which provides us with a global description of quantum mechanics. The first step in this approach was made earlier[7] for the case where the external system is described by canonical variables. In this Letter, as a further step, we consider the systems which can be treated by use of so-called coherent states. Specifically, we consider a spin interacting with a proper intrinsic system.

Effective action by path integral.—Consider two interacting systems which are described by variables $\hat{q}$ and $\hat{S}$ which we conventionally call "internal" and "collective" variables, respectively. The noncanonical system we consider is a spin system with $\hat{S}$ given by an SU(2) Lie algebra $\{\hat{S}_i, i=1,2,3\}$ with the commutation relation $[\hat{S}_i,\hat{S}_j]=i\epsilon_{ijk}\hat{S}_k$. We write the Hamiltonian as $\hat{H}=\hat{H}_0(\hat{S})+\hat{h}(\hat{q},\hat{S})$, where $\hat{H}_0$ is the collective Hamiltonian and $\hat{h}$ is the internal Hamiltonian which includes the coupling with collective variables. Let us consider the trace of an evolution operator $K(T)=\mathrm{Tr}[\exp(-i\hat{H}T/\hbar)]$, which we shall express in terms of a path integral. For this purpose we adopt the SU(2) generalized coherent state [SU(2)-CS] as the basis Hilbert space.[8] In short, SU(2)-CS is defined as $|Z\rangle=(1+|Z|^2)^{-S}\exp[Z\hat{S}_+]|0\rangle$, where $|0\rangle=|S,S_3=-S\rangle$ is the initial vector satisfying $\hat{S}_-|0\rangle=0$ with S the magnitude of the spin and Z a complex coordinate of the parameter space. The characteristic property for $|Z\rangle$ is the "partition of unity," $\int|Z\rangle d\mu(Z)\langle Z|=1$ with $d\mu(Z)=\mathrm{const}\times(1+|Z|^2)^{-2}dZ\wedge dZ^*$ the invariant measure which becomes a measure of a two-dimensional sphere $d\mu=\mathrm{const}\times\sin\theta\, d\theta\wedge d\phi$ if we use a stereographic projection $Z=\tan(\theta/2)e^{-i\phi}$. In this representation, the trace function is written as

$$K(T)=\sum_n\int\langle n(Z_0),Z_0|\exp(-i\hat{H}T/\hbar)|n(Z_0),Z_0\rangle\, d\mu(Z_0). \tag{1}$$

In Eq. (1), one naturally picks up the transition amplitude for the quantum process starting from the initial state of product form $|n(Z_0),Z_0\rangle$ $[\equiv |n(Z_0)\rangle \times |Z_0\rangle]$ and returning to the same state, where $|n(Z_0)\rangle$ denotes a complete set of the internal system at the variable $Z=Z_0$. Using time discretization together with the partition of unity,[9] we get the path-integral expression for (1),[7,10]

$$K(T)=\sum_n\int T_{nn}(C)\exp[(i/\hbar)S_0(C)]\prod_t d\mu(Z_t). \tag{2}$$

Here $S_0(C)$ is the action function for the collective motion along the loop C in Z space,

$$S_0(C)=\int_0^T\langle Z(t)|i\hbar\,\partial/\partial t-\hat{H}_0|Z(t)\rangle\,dt.$$

$T_{nn}(C)$ is just the internal transition amplitude,

$$T_{nn}(C)=\lim_{N\to\infty}\langle n(Z_0)|\prod_{k=1}^{N}\exp[-(i/\hbar)\hat{h}(Z_k^*,Z_{k-1};\hat{q})]|n(Z_0)\rangle \quad [\hat{h}(Z_k^*,Z_{k-1};\hat{q})\equiv\langle Z_k|\hat{h}|Z_{k-1}\rangle],$$

i.e., the time-ordered product. $T_{nn}(C)$ is also written as $T_{nn}(C)=\langle n(Z_0)|n(T)\rangle$, where $|n(T)\rangle$ is a solution of the following time-dependent Schrödinger equation:

$$i\hbar\,\partial/\partial t|n(t)\rangle=\hat{h}(Z^*(t),Z(t);\hat{q})|n(t)\rangle$$

with the initial condition $|n(0)\rangle=|n(Z_0)\rangle$. Here, the time dependence of $\hat{h}$ enters through a closed loop $\{Z(t)\}$ with a period T.

With the above prescription, we turn to the case of the adiabatic motion of the collective variable $Z(t)$ and use the adiabatic theorem. This theorem asserts that *during the motion along the loop C the state $|n(t)\rangle$ remains at the same adiabatic level denoted by $|n(Z(t))\rangle$ with an adiabatic energy λ_n*. Thus, $T_{nn}(C)$ becomes

$$T_{nn}(C)=\exp[-(i/\hbar)\int\lambda_n(Z(t))\,dt]\langle n(Z_0)|n(Z(T))\rangle_C,$$

where

$$\langle n(Z_0)|n(Z(T))\rangle_C\equiv\lim_{N\to\infty}\prod_{k=1}^{N}\langle n(Z_k)|n(Z_{k-1})\rangle,$$

which just gives a finite connection along the loop C. Following the same procedure as in Ref. 7, we finally obtain

$$T_{nn}(C)=\exp\left[-(i/\hbar)\int_0^T\lambda_n(Z(t))\,dt\right]\exp[i\Gamma_n(C)],$$

with

$$\Gamma_n(C)=\oint\omega\equiv i\oint[\langle n|\partial/\partial Z|n\rangle\,dZ+\langle n|\partial/\partial Z^*|n\rangle\,dZ^*]. \tag{3}$$

Equation (3) gives an expression for the adiabatic phase extended to the case in which the external system is described by spin variables.[11] Thus we arrive at the effective path integral associated with the adiabatic change of the (noncanonical) collective variable Z,

$$K^{\text{eff}}(T)=\sum_n\int\exp\{(i/\hbar)[S_n^{\text{ad}}(C)+\hbar\Gamma_n(C)]\}\prod_t d\mu(Z_t), \tag{4}$$

where S_n^{ad} $[\equiv S_0-\int\lambda_n(Z_t)\,dt]$ is the adiabatic action function.[12] From (4) we get the natural explanation that the phase $\Gamma_n(C)$ appears as an action of topological nature[4] which is to be added to the usual dynamical action function.

Semiclassical quantization rule.—We now address a dynamical consequence of the phase Γ, which is most directly examined by evaluation of the energy spectra. The energy spectra are rapidly estimated by the semiclassical quantization condition which is derived by use of the effective propagator (4). Consider the Fourier transform of $K^{\text{eff}}(T)$,[13]

$$K(E)=\int_0^\infty K^{\text{eff}}(T)\,e^{iET/\hbar}\,dT, \tag{5}$$

where we are concerned with a specific adiabatic level (and we drop the label n). First, the semiclassical limit of $K^{\text{eff}}(T)$ is obtained with the aid of the method of stationary phase in the lowest order:

$$K^{\text{sc}}(T)\sim\sum_{\text{p.o.}}\exp\{(i/\hbar)[S^{\text{ad}}(C)+\hbar\Gamma(C)]\}, \tag{6}$$

where $\sum_{\text{p.o.}}$ indicates the sum over periodic orbits C which are determined by the extremum condition $\delta(S^{\text{ad}}+\hbar\Gamma)=0$.[14] Next, substituting (6) into (5) and evaluating the integral over T by the method of stationary phase, we get

$$K^{\text{sc}}(E)\sim\sum_{\text{p.o.}}\exp[(i/\hbar)W^{\text{ad}}(E)+i\Gamma(C)].$$

Here $W^{ad}(E) = S^{ad} + ET$ (action integral) and $T(E)$ is determined by the extremum condition $\partial/\partial T(S^{ad} + ET) = 0$, which yields the energy surface $\mathcal{H}_{ad} = \mathcal{H}_0 + \lambda = E$. Since the spin system is known to reduce to a one-dimensional (generalized) Hamiltonian system,[9] the energy surface suffices to determine *one (and only one)* basic periodic orbit C with the basic period $T(E)$. Then $\sum_{p.o.}$ turns out to be the contribution from the multiple traversals of the basic orbit, i.e., if we put $W^{ad} \to mW^{ad}$ and $\Gamma \to m\Gamma$ for m-time traversals and sum over m, $K^{sc}(E)$ becomes

$$K^{sc}(E) = \sum_{m=1}^{\infty} \exp\{(i/\hbar)m[W^{ad}(E) + \hbar\Gamma(C)]\} = \exp[i\tilde{W}(E)/\hbar]\{1 - \exp[i\tilde{W}(E)/\hbar]\}^{-1}, \tag{7}$$

with $\tilde{W}(E) = W^{ad}(E) + \hbar\Gamma(C)$. From the pole of (7), we get the semiclassical quantization condition explicitly,[15]

$$iS\oint(Z^*dZ - ZdZ^*)/(1+|Z|^2) = S\int \sin\theta\, d\theta \wedge d\phi = (n - \Gamma/2\pi)2\pi, \quad n = \text{integer}. \tag{8}$$

This gives the energy spectra for the motion of the spin system including the effect of Γ.[16]

Simple model calculations.—Here we shall demonstrate the effect of Γ by the use of the following specific model. We consider a simplified version of a particle-plus-rotor model which is familiar in the theory of nuclear structure.[17] This model consists of a rigid rotor representing collective rotations and an internal single-particle Hamiltonian

$$\hat{H} = \hat{H}_{sp} + \sum_{k=1}^{3} (\hat{I}_k - \hat{j}_k)^2/(2\mathcal{J}_k).$$

Here, $\hat{I}_k$ and $\hat{j}_k$ denote total and single-particle angular momenta in the body-fixed frame and $\mathcal{J}_k$ is a moment of inertia of the rotor. Specifically we are concerned with an axially symmetric case, $\mathcal{J}_1 = \mathcal{J}_2$. We make a further simplification for $\hat{H}_{sp}$, that is we consider only two single-particle levels with quantum numbers ($j = \frac{3}{2}$, $j_3 = \frac{3}{2}, \frac{1}{2}$) and retain the Coriolis term $\hat{H}_{cor} = -\sum_k \hat{I}_k\hat{j}_k/\mathcal{J}_k$ as particle-rotor coupling. The reduced Hamiltonian is given by

$$\hat{H} = [S(S+1)/2\mathcal{J}_1] + \tfrac{1}{2}[(1/\mathcal{J}_3) - (1/\mathcal{J}_1)]\hat{S}_3^2 + \tfrac{1}{2}\begin{bmatrix} \epsilon - 3\hat{S}_3/\mathcal{J}_3, & -\sqrt{3}\hat{S}_+/\mathcal{J}_1 \\ -\sqrt{3}\hat{S}_-/\mathcal{J}_1, & -\epsilon - \hat{S}_3/\mathcal{J}_3 \end{bmatrix},$$

where ϵ is a single-particle level spacing.[18] The adiabatic levels are evaluated as

$$\lambda_{\pm} = -S\cos\theta/\mathcal{J}_3 \pm \tfrac{1}{2}[(\epsilon + S\cos\theta/\mathcal{J}_3)^2 + (3/\mathcal{J}_1^2)S^2\sin^2(\theta)]^{1/2},$$

from which we can see that two levels cross each other at $S = |\epsilon\mathcal{J}_3|$, $\theta = 0$ or π. In this model the basic orbit is a circle (see Fig. 1) and the adiabatic phase is easily calculated as $\Gamma_{\pm} = \mp\pi[1 - (S\cos\theta/\mathcal{J}_3 + \epsilon)/\Delta\lambda]$ with $\Delta\lambda = (\lambda_+ - \lambda_-)/2$. Then the semiclassical quantization condition (8) becomes, for an upper adiabatic level λ_+, $S\cos\theta + \Gamma_+/2\pi = \text{integer}$. In Fig. 2, the semiclassical eigenvalues are plotted versus the magnitude of angular momenta S. The eigenvalues calculated without Γ are also plotted for comparison, as are the exact ones which are obtained by the diagonalizing of $\hat{H}$. We can see improvements due to the inclusion of Γ. In order to demonstrate the effect of Γ more clear-

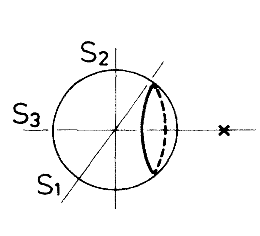

FIG. 1. A basic orbit (thick line) in S space is the intersection of the equienergy surface $\mathcal{H}_{ad} = E$ and a sphere (thin line). The cross denotes the level-crossing point $S_1 = S_2 = 0$, $S_3 = \epsilon I_3$ for the case $\epsilon < 0$.

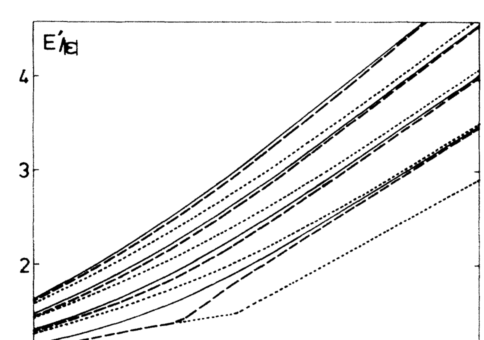

FIG. 2. Several energy eigenvalues $E' = E - \{S(S+1)/2\mathcal{J}_1 + S^2(1/\mathcal{J}_3 - 1/\mathcal{J}_1)/2\}$ plotted vs S for upper adiabatic levels. Solid lines denote exact values. Dashed and dotted lines denote semiclassical results with and without Γ, respectively. The parameters are set as follows: $|\epsilon|\mathcal{J}_1 = |\epsilon|\mathcal{J}_2 = 68.1\hbar^2$, and $|\epsilon|\mathcal{J}_3 = 82.5\hbar^2$, $\epsilon = -3.3$ MeV. The arrow indicates the crossing point $S_c = |\epsilon\mathcal{J}_3|$.

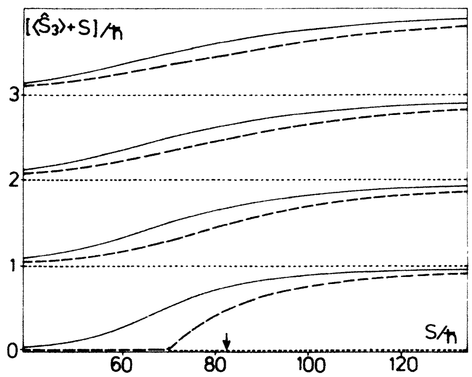

FIG. 3. Expectation values $\langle \hat{S}_3 \rangle + S$ plotted vs S for eigenstates whose eigenvalues are shown in Fig. 2. Solid lines denote exact results. Dashed and dotted lines denote semiclassical results with and without Γ, respectively. The arrow indicates the crossing point $S_c = |\epsilon \mathcal{J}_3|$.

ly, we evaluate the expectation value of $\hat{S}_3$ versus S, Fig. 3. From this figure, we can see that by inclusion of Γ, $\langle \hat{S}_3 \rangle + S$ increases by just one unit as S passes through the crossing point $S_c = |\epsilon \mathcal{J}_3|$, which is essential for reproduction of exact results. This feature corresponds to the quantum-mechanical consequence that the mixing ratio of S_3 components in energy eigenstates changes drastically before and after the crossing point. By considering the effect of Γ, we can properly describe this transition within the semiclassical scheme.

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[1]C. A. Mead and D. G. Truhlar, J. Chem. Phys. **70**, 2284 (1979); C. A. Mead, Chem. Phys. **49**, 23, 33 (1980).

[2]H. C. Longuet-Higgins, Proc. Roy. Soc. London, Ser. A **344**, 147 (1975); A. J. Stone, Proc. Roy. Soc. London, Ser. A **351**, 141 (1976).

[3]M. V. Berry, Proc. Roy. Soc. London, Ser. A **392**, 45 (1984), and J. Phys. A **18**, 15 (1985).

[4]B. Simon, Phys. Rev. Lett. **51**, 2167 (1983).

[5]D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).

[6]F. Wilczek and A. Zee, Phys. Rev. Lett. **52**, 2111 (1984).

[7]H. Kuratsuji and S. Iida, Prog. Theor. Phys. **74**, 439 (1985), and Phys. Lett. **111A**, 220 (1985).

[8]J. R. Klauder, J. Math. Phys. **4**, 1055, 1058 (1963); R. Gilmore, Ann. Phys. (N.Y.) **74**, 391 (1972).

[9]H. Kuratsuji and T. Suzuki, J. Math. Phys. **21**, 472 (1980); J. R. Klauder, Phys. Rev. D **19**, 2349 (1979).

[10]P. Pechukas, Phys. Rev. **181**, 174 (1969).

[11]As was demonstrated by Berry and Stone (see Refs. 2 and 3), the phase $\Gamma_n(C)$ reflects the structure of level crossing occurring in the internal system; $\Gamma_n(C)$ yields the "magnetic flux" emerging from the degenerate point which is regarded as an "effective Dirac pole" and leads to the famous topological quantization condition [see P. A. M. Dirac, Proc. Roy. Soc. London, Ser. A **133**, 60 (1931)]. These known facts are easily shown to be reproduced for the present noncanonical system, the detail of which is omitted here.

[12]It may be formally straightforward to extend the above formulation to the case of many-dimensional ($n \geq 2$) collective motions in the generalized phase space for which we simply apply the more general type coherent state instead of SU(2)-CS (see Ref. 8).

[13]M. C. Gutzwiller, J. Math. Phys. **12**, 343 (1971); W. H. Miller, J. Chem. Phys. **63**, 996 (1975).

[14]Hamilton's equations of motion are modified by inclusion of Γ in the extremum condition; however, for one-dimensional cases the periodic orbits are still determined by $\mathscr{H}_{\text{ad}} = \text{const}$.

[15]The more precise form of formula (8) includes the Maslov indices (see Ref. 13).

[16]A formula similar to (8) has been derived by Wilkinson concerning the Bloch electrons in magnetic field [M. Wilkinson, J. Phys. A **17**, 3459 (1984)].

[17]J. Krumlinde and Z. Szymanski, Ann. Phys. (N.Y.) **79**, 201 (1973).

[18]Angular momenta in a body-fixed frame satisfy commutation relations $[\hat{I}_i, \hat{I}_j] = -i\epsilon_{ijk}\hat{I}_k$. Then, we relate $\hat{I}$ with $\hat{S}$ as $\hat{I}_1 = \hat{S}_1$, $\hat{I}_2 = -\hat{S}_2$, and $\hat{I}_3 = \hat{S}_3$.