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# Effective Action for Adiabatic Process

## —— *Dynamical Meaning of Berry and Simon's Phase* ——

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By applying the path integral method to two interacting systems, it is shown that the specific phase $\Gamma$ appearing in the quantum adiabatic process recently found by Berry and Simon is obtained as an additive action to the conventional dynamical action function. This scheme naturally gives a dynamical meaning to Berry and Simon's topological phase, which leads to a novel form of semiclassical quantization rule including the phase $\Gamma$.

Following an early implication in molecular physics,[1] Berry[2] recently discovered a rather unexpected phenomenon on quantum adiabatic theorem: During an excursion along a closed loop $C$ in the external parameter space the adiabatic change of a wave function gains an extra phase in addition to the conventional dynamical phase; $\psi_n(T) = \exp[i\Gamma_n(C)]\exp[-i/\hbar\int_0^T E_n(R(t))\,dt]|n(R(T))\rangle$. Here Berry demonstrated that the phase $\Gamma(C)$ reflects a peculiar structure associated with the level-crossing which is inherent to the global geometric nature of the external parameter space. Subsequently Simon[3] gave this specific phase a topological meaning that it is nothing but the "holonomy" constructed from the vector bundle of parametrized wave functions and discussed a connection with the quantized Hall effect.[4] The topological concept such as vector bundle or connection has now become familiar in gauge field theory.[5] However it is rather surprising that the topological concept appears even in the usual non-relativistic quantum mechanics.

Although Berry and Simon's phase (B-S phase) has such an appealing feature, it is still concerned with the static aspect only, i.e., time development of external parameter space is given from the outset. Actually, the parameter space itself can be regarded as a dynamical object. For example, in the Born-Oppenheimer theory, the internuclear distance, which is frozen in the adiabatic process, should be regarded as a dynamical variable. Thus we are forced to inquire a dynamical meaning to Berry and Simon's topological phase. The purpose of this paper is to put forward an answer to this question. A similar dynamical argument was suggested by Mead and Truhlar[1] before Berry and Simon; they showed that this specific phase acquires a meaning of the effective vector potential in the Schrödinger equation for the nuclear motion in molecular collisions. However, the argument based on the Schrödinger equation is of essentially local nature and does not seem to be appropriate for describing the global character of this non-integrable phase. In order to push the global aspect forward, we adopt the path integral formulation for the bound state problem of interacting two systems. In this formulation, the B-S phase naturally arises as an additional action to the conventional action function

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induced by adiabatic process. Simultaneously this topological action is shown to modify the semiclassical quantization rule for the motion of the external system.

*Effective action by path integral*: Consider two interacting systems, which are described by the variables conventionally called "internal" and "collective" coordinates; $q$ and $X$ respectively. We adopt a Hamiltonian $\hat{H}=\hat{h}(q, X)+\hat{H}_0(P, X)$, where the internal Hamiltonian $\hat{h}$ is assumed to depend on $X$ and not on its conjugate momentum $P$. Let us consider the trace of the evolution operator $K(T)=\mathrm{Tr}[\exp(-i\hat{H}T/\hbar)]$, which is written as

$$K(T)=\sum_n \int \langle n(X_0), X_0|\exp[-i\hat{H}T/\hbar]|n(X_0), X_0\rangle d\mu(X_0). \tag{1}$$

In Eq. (1) one naturally picks up the transition amplitude for the quantum process starting from the initial state of product form $|n(X_0), X_0\rangle(\equiv|n(X_0)\rangle\otimes|X_0\rangle)$ and returning via closed loops $C$ to the same state, where $|X_0\rangle$ denotes the eigenstate of $\hat{X}$ and $|n(X_0)\rangle$ is the eigenstate of $\hat{h}(q, X_0)$ at $X=X_0$ with eigenvalue $E_n(X_0)$. Then, with the aid of the time-discretization together with the completeness relation holding for $X$, we get

$$\begin{aligned}&\langle n(X_0), X_0|\exp[-i\hat{H}T/\hbar]|n(X_0), X_0\rangle\\ &\quad=\int\prod_{k=1}^{N-1} d\mu(X_k)\langle n(X_0), X_0|\exp[-i\hat{H}\varepsilon/\hbar]|X_{N-1}\rangle\cdots\langle X_1|\exp[-i\hat{H}\varepsilon/\hbar]|n(X_0), X_0\rangle\end{aligned} \tag{2}$$

with $\varepsilon=T/N$. Further noting the relation for $\varepsilon\approx 0$,

$$\begin{aligned}\langle X_k|\exp[-i\hat{H}\varepsilon/\hbar]|X_{k-1}\rangle&\simeq\langle X_k|\exp[-i\hat{H}_0\varepsilon/\hbar]|X_{k-1}\rangle\exp[-i\hat{h}(X_k)\varepsilon/\hbar]\\ &=\int dP_k\exp[(iP_k(X_k-X_{k-1})-iH_0(X_k, P_k)\varepsilon)/\hbar]\exp[-i\hat{h}(X_k)\varepsilon/\hbar],\end{aligned} \tag{3}$$

Eq. (1) can be expressed as

$$K(T)=\sum_n \int T_{nn}(C)\exp\left[\frac{i}{\hbar}S_0(C)\right]\prod_t d\mu(X_t, P_t) \tag{4}$$

with $S_0(C)(\equiv\int(P\dot{X}-H_0)\,dt)$ the action for the collective motion along closed loops $C$. $T_{nn}(C)$ is just the internal transition amplitude and given by

$$T_{nn}(C)=\langle n(X_0)|\exp[-i\hat{h}(N)\varepsilon/\hbar]\cdots\exp[-i\hat{h}(1)\varepsilon/\hbar]|n(X_0)\rangle, \tag{5}$$

i.e., the time ordered product, where $\hat{h}(k)$ denotes the internal Hamiltonian at the point $X=X_k$ on the loop $C$.[6] Namely, if we denote $|\phi_n(T)\rangle$ as a solution of the time-dependent Schrödinger equation; $(i\hbar\partial/\partial t-\hat{h}(q, X_t))|\phi_n(t)\rangle=0$ with the boundary condition $|\phi_n(0)\rangle=|n(X_0)\rangle$, $T_{nn}(C)$ is written as $T_{nn}(C)=\langle n(X_0)|\phi_n(T)\rangle$.

Under the above prescription we turn to the case of the adiabatic motion where the period $T$ is large. By inserting the completeness relation holding for the internal state on each point of external variables $X_k$; $\sum_{m_k}|m_k\rangle\langle m_k|=1$, Eq. (5) is written as

$$T_{nn}(C)=\sum_{m_1}\cdots\sum_{m_{N-1}}\langle n(X_0)|\exp[-i\hat{h}(N)\varepsilon/\hbar]|m_{N-1}\rangle$$

$$\cdots\langle m_k|\exp[-i\hat{h}(k)\varepsilon/\hbar]|m_{k-1}\rangle\cdots\langle m_1|\exp[-i\hat{h}(1)\varepsilon/\hbar]|n(X_0)\rangle. \tag{6}$$

In the adiabatic approximation, we pick up the quantum transition only between the states with the same quantum number $n$; $\langle n_k|\exp(-i\hat{h}(k)\varepsilon/\hbar)|n_{k-1}\rangle$. Then using the relation $\hat{h}(k)|n_k\rangle=E_n(k)|n_k\rangle$ ($E_n(k)$ is an energy of an adiabatic level $n$ at $X=X_k$), we obtain $T_{nn}(C)=\exp[-i/\hbar\int_0^T E_n(X_t)\,dt]\langle n(X_0)|n(X_T)\rangle_C$. Here the overlap function $\langle n(X_0)|n(X_T)\rangle_C$ is given as an infinite product:

$$\langle n(X_0)|n(X_T)\rangle_C=\lim_{N\to\infty}\prod_{k=1}^{N}\langle n(X_k)|n(X_{k-1})\rangle, \tag{7}$$

where we adopt a phase convention $|n(X_0)\rangle=|n(X_T)\rangle$. This overlap function naturally involves the history of the excursion in the $X$-space which is indicated by the suffix $C$. Each factor $\langle n(X_k)|n(X_{k-1})\rangle$ in (7) defines a "connection" between two infinitesimally separated points $X_{k-1}$ and $X_k$, hence Eq. (7) gives a finite connection along circuit $C$ given by a set of division points $\{X_k\}$.[7] Thus, by using the approximate relation

$$\langle n(X_k)|n(X_{k-1})\rangle\simeq 1-\langle n|\partial/\partial X_i|n\rangle\Delta X_i\approx\exp[i\omega],$$

Eq.(7) is written as

$$\langle n(X_0)|n(X_T)\rangle_C=\exp[i\Gamma_n(C)] \tag{8}$$

with

$$\Gamma_n(C)=\oint_C\omega=\oint\langle n|i\partial/\partial X_k|n\rangle dX_k\,. \tag{9}$$

Equation (9) is essentially the same as the phase obtained by Berry.*) However the present derivation is quite different from Berry's and somewhat similar to Simon's[3] which is based upon the holonomy of vector bundle over $X$-space. Thus we arrive at the effective path integral associated with the adiabatic change of the external dynamical variable $X$,

$$K^{\text{eff}}(T)=\sum_n\int\exp\left[\frac{i}{\hbar}(S_n^{ad}+\hbar\Gamma_n(C))\right]\prod_t d\mu(X_t,P_t), \tag{10}$$

where $S_n^{ad}(\equiv S_0-\int_0^T E_n(X_t)\,dt)$ is the adiabatic action function. From (10) we get a natural explanation that the phase $\Gamma_n(C)$ *appears as a topological action function which is to be added to the usual dynamical action.* This is a first consequence of the paper. If we note $\omega=A_i\dot{X}_i$ dt with $A_i=\langle n|i\partial/\partial X_i|n\rangle$, the effective action in (10) can be regarded as the action function for a system in the effective "gauge field" described by the "vector potential" $A_i$. This result was already obtained by Mead and Truhlar[1] by using the Schrödinger equation which was described by only usual canonical variables $(X,P)$. However, the present path integral formulation is applicable to more general external systems which are described by non-canonical variables, e.g., spin variables.[8),9)]

*Level-crossing structure revisited*: Here we examine a specific model Hamiltonian revealing the topological meaning of the phase $\Gamma$; consider the following internal Hamiltonian:

*) Here, it is noted that in the present procedure the closed loop $C$ is naturally introduced as a consequence of the trace formula, whereas in Ref. 2) it is presupposed from the outset.

$$\hat{h}(X)=\begin{pmatrix} z & x+iy \\ x-iy & -z \end{pmatrix}, \qquad X=(x,y,z)\,. \tag{11}$$

Although this model already has been studied by Berry,[2] we treat it in a different way by adopting the "coherent-state" representation,[9] which may reserve an applicability to more complicated Hamiltonians. Using two-component Pauli spinor we write the eigenvector of (11) as $|\xi\rangle=\cos(\theta/2)|-1/2\rangle+\sin(\theta/2)e^{i\phi}|1/2\rangle={}^t(\sin(\theta/2)e^{i\phi},\cos(\theta/2))\equiv{}^t(a,b)$, which is given as the $SU(2)$ (spin) coherent-state

$$|\xi\rangle=(1+|\xi|^2)^{-1/2}\exp[\xi\hat{S}_+]|-1/2\rangle \tag{12}$$

with $\xi=\tan(\theta/2)e^{i\phi}$. The eigenvalues of (11) are calculated as

$$\lambda_\pm=\pm\sqrt{x^2+y^2+z^2}\,, \tag{13}$$

which show a remarkable feature that two levels $\lambda_+$ and $\lambda_-$ cross at $X=0$, namely, the origin $X=0$ becomes a singular-point of cone type. In the following we take the lower level $\lambda_-$, for which the corresponding eigenvector is given by

$$a/b=\tan(\theta/2)e^{i\phi}=-(x+iy)/(\sqrt{x^2+y^2+z^2}+z)\,, \tag{14}$$

which yields $\phi=\beta$ and $\theta=-\alpha$, where $\alpha$ and $\beta$ are the polar angle defined by $x=r\sin\alpha\cdot\cos\beta$, $y=r\sin\alpha\sin\beta$, $z=r\cos\alpha$. $\Gamma(C)$ is thus evaluated as

$$\Gamma(C)=\oint\frac{1}{2i}\frac{(\xi^*\nabla\xi-\text{c.c.})}{1+|\xi|^2}dX=\frac{1}{2}\oint(1-\cos\alpha)\nabla\beta dX\,, \tag{15}$$

which is written as $\oint A\,dX$, where the vector potential becomes

$$A_x=(\cos\alpha-1)\frac{\sin\beta}{r\sin\alpha},\quad A_y=(1-\cos\alpha)\frac{\cos\beta}{r\sin\alpha} \tag{16}$$

and $A_z=0$. The striking point is that the negative $z$-axis (i.e., $\alpha=\pi$) forms a *singular line* on which $A$ diverges.[10] This suggests that the "Dirac pole" is located at the origin as was pointed out by Berry, but the present result gives an explicit form of the specific singular nature. The phase $\Gamma$ is converted into the surface integral by Stokes' theorem; $\Gamma(C)=\int_S d\omega=\frac{1}{2}\int_S\sin\alpha d\alpha\wedge d\beta$, which is just the solid angle suspended by the closed loop $C$. Here we note that the present path integral formalism naturally allows the "topological quantization" analogous to the Dirac quantization which is familiar in gauge theory. Consider a sphere $S^2$ and divide it by $C$ into two hemispheres $S$ and $\tilde{S}$. We can choose two different gauges such that $\omega$ is singular-free on hemispheres $S$ or $\tilde{S}$, respectively. Then, the topological part of the propagator $K^{\text{eff}}(T)$ can be expressed in two ways according to these two choices, and the consistency condition asserts these two expressions should coincide. Namely, the relation

$$\exp\left[i\oint_C\omega\right]=\exp\left[i\int_S d\omega\right]=\exp\left[-i\int_{\tilde{S}}d\omega\right] \tag{17}$$

should hold, which leads to the quantization condition $\int_S d\omega+\int_{\tilde{S}}d\omega=\int_{S^2}d\omega=2\pi\times(\text{integer})$.

Finally we give a remark on a generalization to $n\times n$ matrix Hamiltonian; it may be simply achieved by replacing the eigenstate of form (12) by the $SU(n)$ coherent-state[9]

where the parameter space becomes the complex projective space $U(n)/U(n-1)\times U(1)$ the point of which is coordinated by $n$-dimensional complex vector $\boldsymbol{\xi}=(\xi_1, \cdots, \xi_n)$ and the resultant phase yields

$$\Gamma(C)=\frac{i}{2}\oint_C\sum_{\mu,i}\left(\frac{\partial \log F}{\partial \xi_\mu}\frac{\partial \xi_\mu}{\partial X_i}-\text{c.c.}\right)dX_i \tag{18}$$

with $F(\equiv 1+\xi^\dagger\xi)$ being the overlap function of the coherent state. There may also occur the singularity due to level crossing leading to the general form of the topological quantization.

*Semiclassical quantization rule*: Now we address a question how one can look at the effect of the topological phase. The most direct way for this is to examine the energy spectra. The energy spectra is rapidly estimated by the semiclassical quantization rule[11] which is derived from the effective propagator (10). Consider the Fourier transform of $K^{\text{eff}}(T)$; $K(E)=i\int_0^\infty K^{\text{eff}}(T)\exp[iET/\hbar]dT$, where we restrict ourselves to a specific adiabatic level $n$. Firstly the semiclassical limit of $K^{\text{eff}}(T)$ is approximated by the method of stationary phase,

$$K^{\text{sc}}(T)\sim\sum_{P\cdot O}\exp\left[\frac{i}{\hbar}S^{ad}(C)+i\Gamma(C)-i\frac{\pi}{2}\alpha(C)\right], \tag{19}$$

where $\alpha(C)$ denotes the so-called Keller-Maslov index and $\sum_{P\cdot O}$ indicates the sum over periodic orbits. Next, taking the Fourier transform of (19) and evaluating the integral over $T$ by the method of stationary phase, then we get

$$K^{\text{sc}}(E)\sim\sum_{P\cdot O}\exp\left[\frac{i}{\hbar}W^{ad}(E)+i\Gamma(C)-i\frac{\pi}{2}\alpha(C)\right], \tag{20}$$

where $W^{ad}(E)=S^{ad}+ET$ (action integral) and $T(E)$ is determined by the stationary phase condition $\partial/\partial T(S^{ad}+ET)=0$. Here, we restrict ourselves to the case that there appear a finite number of isolated closed orbits for each value of the energy. For this case, a semi-classical quantization condition can be written down explicitly. Namely, taking account of the contribution from the multiple traversals of basic orbits, i.e., putting $W^{ad}\to m\cdot W^{ad}$, $\alpha\to m\cdot\alpha$ and $\Gamma\to m\cdot\Gamma$ for $m$-times traversals and summing over $m$, $K^{\text{sc}}(E)$ turns out to be

$$K^{\text{sc}}(E)\sim\sum_{P\cdot O}\exp[i\tilde{W}/\hbar]\cdot\{1-\exp[i\tilde{W}/\hbar]\}^{-1} \tag{21}$$

with $\tilde{W}(E)=W^{ad}(E)+\hbar\Gamma(C)-\hbar\alpha/2\cdot\pi$. From the pole of (21) we get the formula*)

$$W^{ad}(E)=\oint \boldsymbol{P}d\boldsymbol{X}=\left(n+\frac{\alpha}{4}-\frac{\Gamma}{2\pi}\right)2\pi\hbar\,. \tag{22}$$

This gives the energy spectrum for the collective motion including the effect of the topological phase $\Gamma$.** Equation (22) is the second main consequence of this paper.

We examine the above formula for a simple case. Consider the internal Hamiltonian

*) The more precise form of formula (22) includes stability exponents (see Ref. 11)).

**) A similar formula has been recently presented by Wilkinson[12] in the course of investigating the band structure of Bloch electrons in the magnetic field, which is, however, concerned with a rather specific problem. On the other hand, our formula is derived on the general framework of the adiabatic theorem.

of type (11). The level-crossing (singular point) is just located at $x=y=z=0$. Further, we restrict collective periodic orbits to circular motions around the $z$-axis with a radius $\rho$, namely collective motions occur in the plane $z=\eta=$const. Assuming that the collective Hamiltonian has a rotational symmetry, $\hat{H}_0$ expressed in the polar coordinate is essentially a function of $\hat{p}_\phi=i/\hbar\partial/\partial\phi$ alone. Then, the total Hamiltonian considered is given by

$$\hat{H}=\hat{H}_0(\hat{P}_\phi)+\begin{pmatrix}\eta & \rho e^{i\phi}\\ \rho e^{-i\phi} & -\eta\end{pmatrix}. \tag{23}$$

The B-S phase is $\Gamma_\pm(C)=\mp\pi(1-\eta/e_\pm)$ for the internal upper (lower) state where $e_\pm=\pm\sqrt{\rho^2+\eta^2}$ denotes an internal energy eigenvalue. From Eq. (22), the semiclassical quantization condition becomes

$$\frac{1}{2\pi}\oint_C P_\phi d\phi=P_\phi(E_\pm)=\left(m-\frac{\Gamma_\pm}{2\pi}\right)\hbar, \tag{24}$$

where $p_\phi(E)$ is defined as an inverse relation of $H_{\text{eff}}(P_\phi)=E$. Semiclassical energy eigenvalues are calculated as

$$\begin{aligned}E_\pm^{sc}&=H_0\left(P_\phi=m\hbar-\frac{\hbar}{2\pi}\Gamma_\pm\right)+e_\pm\\&=H_0(P_\phi=m\hbar)+e_\pm\pm\frac{\hbar}{2}\frac{dH_0}{dP_\phi}\bigg|_{P_\phi=m\hbar}-\frac{\hbar}{2}\frac{\eta}{e_\pm}\frac{dH_0}{dP_\phi}\bigg|_{P_\phi=m\hbar}+O(\hbar^2).\end{aligned} \tag{25}$$

In the present case, $\hat{H}$ can easily be diagonalized and we get exact energy eigenvalues as

$$\begin{aligned}E_\pm&=\frac{1}{2}[H_0(P_\phi=m\hbar)+H_0(P_\phi=(m\pm1)\hbar)\\&\quad\pm\sqrt{\{H_0(P_\phi=m\hbar)-H_0(P_\phi=(m\pm1)\hbar)\pm2\eta\}^2+4\rho^2}\\&=H_0(P_\phi=m\hbar)\pm\sqrt{\rho^2+\eta^2}\pm\frac{\hbar}{2}\frac{dH_0}{dP_\phi}\bigg|_{P_\phi=m\hbar}\mp\frac{\hbar}{2}\frac{\eta}{\sqrt{\rho^2+\eta^2}}\frac{dH_0}{dP_\phi}\bigg|_{P_\phi=m\hbar}+O(\hbar^2).\end{aligned} \tag{26}$$

In Eq. (25), the first and the second term represent the unperturved eigenvalue of collective Hamiltonian $\hat{H}_0$ and a conventional adiabatic potential which is constant $e_\pm$ in the present case, respectively. The third and fourth terms come from the B-S phase $\Gamma_\pm(C)$. In comparison with Eq. (26), we can see that this modification of the quantization rule reproduces the exact result up to $\hbar$-order. Since higher-order terms than $\hbar$ are beyond a semiclassical approximation, eigenvalues (25) can be regarded to be exact within a semiclassical treatment in spite of adiabatic approximation. In addition to the above, Eq. (24) shows that the angular momentum quantization is modified by the existence of the level-crossing. This phenomenon is very analogous to angular momentum quantization in the presence of magnetic flux generated by a solenoid.[13] Following an analogy with this, Eq. (24) suggests that due to the elimination of internal degrees of freedom the level-crossing produces an "effective spin" for an external dynamical system, which is a sort not to be locally described but only describable by a global aspect of the internal level structure.

*Final remarks*: The appearance of the topological additive term in the action function

may be regarded as a rather universal phenomenon whenever one deals with interacting dynamical systems in the adiabatic approximation. This viewpoint may shed a light on a wide class of theoretical problems. For example, the "anomaly" in gauge field theory may be naturally understood within the present scheme, which would indeed await a further investigation.

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### References

1) C. A. Mead and D. G. Truhlar, J. Chem. Phys. **70** (1979), 2284.
2) M. V. Berry, Proc. Roy. Soc. **A392** (1984), 45.
3) B. Simon, Phys. Rev. Lett. **51** (1983), 2167.
4) D. J. Thouless, M. Kohmoto, M. P. Nightingale and M. den Nijs, Phys. Rev. Lett. **49** (1982), 405.
5) See, e.g., R. Jackiw, Lecture at Les Houches, July, 1983.
6) P. Pechukas, Phys. Rev. **181** (1969), 174.
7) H. Kuratsuji and T. Hatsuda, in *Proceedings of 13-th International Colloquium in Group Theoretical Method in Physics,* Univ. of Maryland, May 1984, ed. W. W. Zachary (World Scientific), p. 238.
8) H. Kuratsuji and T. Suzuki, J. Math. Phys. **21** (1980), 472.
9) R. Gilmore, Ann. of Phys. **74** (1972), 391.
J. R. Klauder, J. Math. Phys. **4** (1963), 1055, 1058.
10) P. A. M. Dirac, Proc. Roy. Soc. **A133** (1931), 60.
11) See, e.g., M. C. Gutzwiller, J. Math. Phys. **12** (1971), 343.
W. H. Miller, J. Chem. Phys. **63** (1975), 996.
12) M. Wilkinson, J. of Phys. **A17** (1984), 3459.
13) F. Wilczek, Phys. Rev. Lett. **48** (1982), 1144.

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