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Non-Abelian Induced Topological Action for Slowly Changing Quantum System and Non-Adiabatic Corrections[1]

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Abstract

The induced topological action relevant to the non-Abelian Berry's phase factor (NABPF) is derived by combining the high-order adiabatic approximation (HOAA) method with Kuratsuji and Iida's adiabatic path integral formulation. The non-adiabatic corrections for the transition amplitude are thereby obtained and the corresponding graphic representations are defined for convenience in the calculation. The gauge invariant properties and the dynamical implications of the non-Abelian induced topological action are also analyzed in detail. Finally, some explicit calculations for a model of physics are carried out as examples.

I. Introduction

In order to throw a deep light on the dynamic implication of the Abelian Berry's phase factor (ABPF)[1] and the origin of anomaly in gauge theory, Neimi, Semenoff[2], Kuratsuji and Iida[3] applied a path integral formulation to a quantum system with two sets of variables, a fast one ("internal" coordinates) and a slow one ("collective" coordinates). They observed that, when the fast part of the Hamiltonian of the system has non-degenerate instantaneous spectra, the adiabatic effective action governing the slow variables includes the ABPF as an additional topological term. This topological term would be regarded as a "Wess-Zumino" term in some generalized senses[4]. It is easy to see that the effective Hamiltonian corresponding to this effective action is just what obtained by the generalized Born-Oppenheimer approximation[5]. Then, a generalization of this path integral formulation naturally rises for the cases that the fast part of the Hamiltonian has degenerate eigenstates in this paper. For the case with degeneracy, Wilczek and Zee have made a generalization of ABPF, which is called non-Abelian Berry's phase factor (NABPF)[6]. They also recognized that the NABPF can induce a non-Abelian gauge structure just as the ABPF can induce an Abelian one-U(1) induced gauge structure. While the discussions concerning the NABPF and the induced gauge structure were carried out, the relevant observable effects have been pointed out by different authors[7].

In this paper we will discuss how the NABPF appears in the effective action as an additional topological term, what properties the induced topological action possesses and what the higher-order corrections are when the adiabatic conditions do not hold. All the discussions are based on a generalization of an adiabatic path integral formulation given by Kuratsuji and Iida and a combination of the high order adiabatic approximation method (HOAA-method)

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suggested by one (C.P. SUN) of the authors[8] with Wu's adiabatic Dyson expansion (ADE) for HOAA[9]. The graphic representation of the higher-order non-adiabatic corrections is also defined for convenience. With a model relating to the nuclear quadrupole resonance (NQR) as an example, some explicit calculations are finally done in this paper.

II. Quasi-Adiabatic Path Integration for Degenerate Case and Graphic Representation

Let $\hat{H} = \hat{H}_0[R,\ P] + \hat{h}[R,\ r]$ be the Hamiltonian of a quantum system where R and r represent the slow variable and fast variable respectively. The Hamiltonian $\hat{h}[R,\ r]$ of the fast part depends only on the slow coordinates R and not on their conjugate momentum P. We also assume that there is not accident degeneracy of $\hat{h}[R,\ r]$, i.e. the degenerate instantaneous eigenstates $|\,n,\ \alpha[R]\,\rangle$ $(\alpha = 1,\ 2,\ \cdots,\ d_n)$ with the eigenvalues $E_n[R]$ transform as an irreducible representation $\Gamma^{[n]}$ of a continuously-varying symmetry group $G[R]$. At each instant, $\hat{h}[R,\ r]$ has different symmetry group $G[R(t)]$, but $G[R(t)]$ is always an isomorphism of a fixed group G[6]. Now, we consider a matrix element $K(t,\ t_0)_{n\alpha,m\beta} = \langle n,\ \alpha[R(t)]|K(t,t_0)|m\beta[R(t_0)]\,\rangle$ of the evolution operator $K(t,\ t_0) = \exp[-i\hat{H}\cdot(t-t_0)]$, where we have taken $\hbar = 1$ and defined the following expressions $|\,n,\ \alpha,\ R(t)\,\rangle = |\,n\alpha(t)\,\rangle \otimes |R(t)\,\rangle$ and $|\,n\alpha(t)\,\rangle \equiv |\,n\alpha[R(t)]\,\rangle$ in terms of the eigenstate $|R(t)\,\rangle$ of the coordinate operator R such that $R|R(t)\,\rangle = R(t)|R(t)\,\rangle$. Following a procedure similar to that in Ref. [3], we obtain for the matrix element a path integral expression

$$K(t,\ t_0)_{n\alpha,m\beta} = \int [dR]\cdot U(R;\ t,\ t_0)_{n\alpha,m\beta}\cdot \exp[iS_0[R;\ t,\ t_0]]\,, \tag{1}$$

where $S_0 \equiv S_0[R;\ t,\ t_0] = \int_{t_0}^{t}(P\cdot\dot{R} - \hat{H}_0[R,\ P])dt'$ is the action associated with $\hat{H}_0$ and

$$U(R;\ t,\ t_0)_{n\alpha,m\beta} = \langle\, n\alpha[R(t)]|\mathcal{P}\exp\Big[-i\int_{t_0}^{t}\hat{h}[R(t')]dt'\Big]|m\beta[R(t_0)]\rangle\,. \tag{2}$$

It should be noticed that the evolution matrix $U = U(t,t_0) \equiv U(R;t,t_0)$ of the fast part appearing in Eq. (1) satisfies the Schrödinger equation

$$i\frac{\partial}{\partial t}U(t,\ t_0) = \hat{h}[R(t)]U(t,\ t_0)\,; \qquad U(t_0,\ t_0) = I\,. \tag{3}$$

By combining the original HOAA method with Wu's ADE formulation for HOAA, we obtain a series of solutions of Eq. (3) (for the details of derivation see Appendix)

$$\begin{aligned}
U(t,\ t_0) &= \sum_{k=0}^{\infty} U^{[k]}(t,\ t_0)\,,\\
U^{[0]}(t,\ t_0) &= \sum_{n}\sum_{\alpha,\beta=1}^{dn} W(n;\ t,\ t_0)_{\alpha\beta}\exp\Big[-i\int_{t_0}^{t}E_n[R(t')]dt'\Big]|n,\alpha[R(t)]\rangle\langle n\beta[R(t_0)]|\,,\\
U^{[1]}(t,\ t_0) &= -\sum_{n}\sum_{m\neq n}\sum_{\alpha,\beta=1}^{dn}\sum_{\gamma,\delta=1}^{dm}\int_{t_0}^{t}W(n;\ t,\ \tau)_{\alpha\beta}A(n,\ m,\ \tau)_{\beta\gamma}\\
&\qquad\times e^{i\omega_{nm}(\tau)}e^{-i\int_{t_0}^{t}E_n(R(t'))dt'}W(n,\ \tau,\ t_0)_{\gamma\delta}|n\alpha[R(t)]\rangle\langle m\delta[R(t_0)]|\,,\\
&\cdots\\
U^{[l]}(t,\ t_0) &= (-1)^l\sum_{n} e^{-i\int_{t_0}^{t}E_n(t')dt'}\sum_{n_{l-1}\neq n}\ \sum_{n_{l-2}\neq n_{l-1}}\cdots\sum_{n_1\neq n_2}\ \sum_{n_0\neq n_1}
\end{aligned} \tag{4}$$

$$\times\int_{t_0}^{t}d\tau_{l-1}\int_{t_0}^{\tau_{l-1}}d\tau_{l-2}\cdots\int_{t_0}^{\tau_2}d\tau_1\int_{t_0}^{\tau_1}d\tau_0\Big\{W(n;\,t,\,\tau_{l-1})A(n,\,n_{l-1},\,\tau_{l-1})$$
$$\times\exp\left[i\omega_{nn_{l-1}}(\tau_{l-1})\right]\prod_{k=l-1}^{1}\left[W(n_k,\,\tau_k,\,\tau_{k-1})A(n_k,\,n_{k-1},\,\tau_{k-1})\right.$$
$$\left.\times\exp\left[i\omega_{n_kn_{k-1}}(\tau_{k-1})\right]W(n_0\tau_0t_0)\Big\}_{\alpha\beta}|n,\,\alpha[R(t)]\rangle\langle n_0,\,\beta[R(t_0)]|\right|,$$

where $\omega_{nm}(t)=\int_{t_0}^{t}(E_n[R(t')]-E_m[R(t')])dt'$, $A(m,\,n,\,t)$ is a $d_n\times d_m$ matrix with its elements

$$A(m,\,n,\,t)_{\alpha\beta}=\begin{cases}\left\langle n\alpha[R]\,\Big|\,\dfrac{\partial}{\partial t}\,\Big|\,n\beta[R]\right\rangle\equiv A(n)_{\alpha\beta}\,, & m=n\,;\\ \dfrac{\langle n\alpha[R]|(d/dt)\hat{h}[R(t)]|m\beta[R]\rangle}{[E_m[R]-E_n[R]]}\,, & m\neq n\end{cases}\tag{5}$$

and the path-order integration

$$W(n,\,t,\,t_0)=\mathcal{P}\exp\Big[-\int_{R(t_0)}^{R(t)}\mathcal{A}(n)\Big]\equiv\mathcal{P}\exp\Big[-\int_{t_0}^{t}A(n,\,t')dt'\Big]\tag{6}$$

is just the NABPF with a matrix-value induced gauge potential one-form $\mathcal{A}(n)\equiv\mathcal{A}(n,\,R)$;

$$\mathcal{A}(n)_{\alpha\beta}=\langle n\alpha[R]|d|n\beta[R]\rangle\,,\qquad \alpha,\,\beta=1,\,2,\,\cdots d_n\,,\tag{7}$$

where d is the exterior differential operator on the manifold $\mu:\{R\}$. Substituting Eq. (4) into Eq. (1), we obtain

$$K(t,\,t_0)=\sum_{l=0}^{\infty}K^{[l]}(t,\,t_0)\,,$$

$$K^{[0]}(t,\,t_0)_{n\alpha,m\beta}=\int[dR]W(n;\,t,\,t_0)_{\alpha\beta}\exp\Big[iS_0-i\int_{t_0}^{t}E_n[R(t')]dt'\Big]\delta_{mn}\,,\tag{8a}$$

$$K^{[1]}(t,t_0)_{n\alpha,m\beta}=\int[dR]\Big\{\int_{t_0}^{t}d\tau W(n;t,\tau)A(n,m,\tau)e^{i\omega_{nm}(\tau)}W(m;\tau,t_0)\Big\}_{\alpha,\beta}\times\exp\Big[iS_0-i\int_{t_0}^{t}E_n[R(t')]dt'\Big](1-\delta_{mn})\,,\tag{8b}$$

...

$$K^{[l]}(t,\,t_0)_{n\alpha,m\beta}=\int[dR]\exp\Big[iS_0-i\int_{t_0}^{t}E_n[R(t')]dt'\Big]\cdot\tilde{U}^{[l]}(t,\,t_0)_{n\alpha,m\beta}\,,\tag{8c}$$

where

$$\begin{aligned}\tilde{U}^{[l]}(m,\,n,\,t,\,t_0)_{\alpha\beta}&=\exp\Big[i\int_{t_0}^{t}E_n[R(t')]dt'\Big]\langle n\alpha[R(t)]|U^{[l]}(t,\,t_0)|m\beta[R(t_0)]\rangle\\&=(-1)^l\sum_{n_{l-1}\neq n}\;\sum_{n_{l-2}\neq n_{l-1}}\cdots\sum_{n_2\neq n_3}\;\sum_{n_1\neq n_2}\int_{t_0}^{t}d\tau_{l-1}\int_{t_0}^{\tau_{l-1}}d\tau_{l-2}\cdots\\&\quad\times\int_{t_0}^{\tau_2}d\tau_1\int_{t_0}^{\tau_1}d\tau_0\Big\{W(n,\,t,\,\tau_{l-1})A(n,\,n_{l-1},\,\tau_{l-1})e^{i\omega_{nn_{l-1}}(\tau_{l-1})}\\&\quad\times\prod_{k=l-1}^{1}\left[W(n_k,\,\tau_k,\,\tau_{k-1})A(n_k,\,n_{k-1},\,\tau_{k-1})e^{i\omega_{n_kn_{k-1}}(\tau_{k-1})}\right]\\&\quad\times W(m,\,\tau_0,\,t_0)\Big\}_{\alpha,\beta}\,,\qquad n_0=m.\end{aligned}\tag{9}$$

For convenience in practical calculation, the graphic representation of the high-order correction term is defined as shown in Fig. 1.

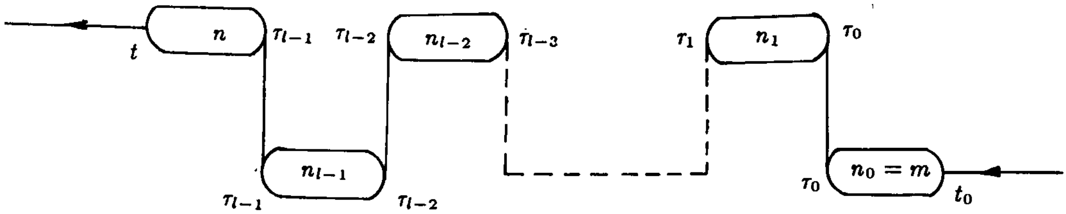

Fig. 1. A graphic representation of high-order correction $U^{[l]}(m, n, t, t_0)$.

In the above diagram, the loop with indices $(t_{k-1}, n_{k-1}, t_{k-2})$ represents the NABPF $W(n_{k-1}, t_{k-1}, t_{k-2})$ while the straight line with end point indices (n_k, t_{k-1}, n_{k-1}) represents the "propagator"

$$\tilde{A}(n_k, n_{k-1}, \tau_{k-1}) = A(n_k, n_{k-1}, \tau_{k-1}) \exp\left[i\omega_{n_k n_{k-1}}(\tau_{k-1})\right] \tag{10}$$

from state $|n_{k-1}\alpha(\tau_{k-1})\rangle$ to state $|n_k\beta(\tau_k)\rangle$. The limited sum of $n_{k-1} \neq n_k$ is implied by the assignment that the indices n_{k-1} and n_k do not lie the same horizontal line. In comparison with the oscillation of the factor $\exp\left[-i\int_0^t (E_n - E_m)[R(t')]dt'\right]$, if $\langle n\alpha(t)|\frac{\partial}{\partial t}|m\beta(t)\rangle$ $(m \neq n)$ changes slowly enough, then the adiabatic conditions

$$\frac{|\langle n\alpha[R]|\frac{\partial}{\partial R_\mu}|m\beta[R]\rangle \cdot \dot{R}_\mu|}{|E_n[R] - E_m[R]|} \ll 1 \tag{11}$$

hold, and so that we can neglect all the terms $K^{[l]}(t, t_0)$ $(l \geq 1)$, obtaining the first transition amplitude $K^{[0]}(t, t_0)$ corresponding to a diagram of graphic representation with one loop. When the conditions do not hold, we need to calculate the higher-order approximation corrections according to the graphic representations with many loops.

III. Induced Topological Action and Its Gauge Invariance

When the adiabatic conditions (11) hold, we have $U(T)_{n\alpha,n\beta} \simeq U^{[0]}(T, 0)_{n\alpha,n\beta}$ with $U^{[0]}(T, 0)_{n\alpha,n\beta} = \exp\left[-i\int_0^T E_n[R(t')]dt'\right] W(n, T)_{\alpha,\beta}$, where we have taken $t = T$, $t_0 = 0$ and defined $f(t, 0) = f(t)$ for any function $f(t, t')$. If the system is subjected to a cycle evolution, i.e., $R(t)$ is a function with period T, $W(n, T)$ is a loop phase factor[10] $W(n, T) \equiv W_n[C] = \mathcal{P}\exp\left[-\oint \mathcal{A}(n, R)\right]$, and $C : \{R(t)|R(0) = R(T)\}$. In this case, the transition amplitude from $|R(0)\rangle$ to $|R(T)\rangle$ is[3]

$$\begin{aligned} Z(T) &= \sum_n \int [dR]\ \mathrm{Tr}\,(W_n[C]) \exp\left[iS_0^{(T)} - i\int_0^T E_n[R(t')]dt'\right] \\ &= \mathrm{Tr}\left\{\sum_n \int [dR] \mathcal{P}\exp\left\{i\int_0^T [\mathcal{L}_0(\dot{R}, R) - E_n[R(t)] + iA_\mu[R]\dot{R}_\mu] dt\right\}\right\}, \end{aligned} \tag{12}$$

where $\mathcal{L}_0(\dot{R}, R) = P\dot{R} - \hat{H}_0(P, R)$, $S_0^{(T)} = \int_0^T \mathcal{L}_0(\dot{R}, R)dt$ and $A_\mu[R(t)]_{\alpha\beta} = \langle n\alpha[R]|\frac{\partial}{\partial R_\mu}|n\beta[R]\rangle$. In the presence of an external source $J(t)$ that can be regarded as an external force acting on the coordinate, the "generating function"

$$Z(T)_J = \sum_n \int [dR]\ \mathrm{Tr}\left\{\mathcal{P}\exp\left[i\int_0^T (\mathcal{L}_0(\dot{R}, R) - E_n[R(t)] + iA_\mu\dot{R}_\mu + J(t)R)\right]\right\} \tag{13}$$

sufficiently describes the whole dynamics of the slow variables in the adiabatic situations. We observe from Eq. (12) that, associated with the induced effective action

$$S_{\rm eff}(T) = S_0(T) - \int_0^T E_n[R(t')]dt' + \ln(W_n[C])\,, \tag{14}$$

the matrix-value effective Lagrangian is

$$\mathcal{L}_{\rm eff} = \mathcal{L}_0(\dot{R},\, R) - E_n[R] + iA_\mu[R]\dot{R}_\mu\,, \tag{15}$$

which corresponds to the effective Hamiltonian

$$H_{\rm eff} = \hat{H}_0(-i\nabla_\mu + A_\mu,\, R) + E_n[R]\,. \tag{16}$$

Especially, when $\hat{H}_0(P,\, R)$ is taken to be a concrete form $\hat{H}_0 = -\frac{1}{2M}\nabla^2 + V(R)$, we have

$$\hat{H}_{\rm eff} = -\frac{1}{2M}(\nabla_\mu - iA_\mu)^2 + V(R) + E_n[R]\,. \tag{17}$$

Therefore, the non-Abelian "Wess-Zumino" term $\ln W_n[C]$ resulting from the NABPF provides the motion of the slow variables R with a background vector field A_μ and a scalar field $E_n(R)$. This fact shows the possible dynamic effects of the NABPF. However, the eigenequation of $\hat{h}(R,\, r)$ allows a local unitary freedom in determining an eigenstate $|n\alpha[R]\rangle$, i.e., its unitary transformation

$$|n\alpha[R]\rangle' = \Omega_n[R]|n\alpha[R]\rangle = \sum_{\beta=1}^{dn}\Omega_n[R]_{\beta\alpha}|n\beta[R]\rangle \tag{18}$$

by a local unitary matrix $\Omega_n[R]$ is still an eigenstate with the same eigenvalue. This unitary transformation (17) results in gauge transformations of induced gauge potential one-form $\mathcal{A}(n) = \mathcal{A}(n, R)$ and its corresponding field strength two–form $\mathcal{F}(n, R) = d\mathcal{A}(n) + \mathcal{A}(n)\wedge\mathcal{A}(n)$, i.e.

$$\begin{aligned}\mathcal{A}(n,\, R) &\to \mathcal{A}'(n,\, R) = \Omega_n[R]^+\mathcal{A}(n,\, R)\Omega_n[R] + \Omega_n^+[R]d\Omega_n[R]\,,\\ \mathcal{F}(n,\, R) &\to \mathcal{F}'(n,\, R) = \Omega_n[R]^+\mathcal{F}(n,\, R)\Omega_n[R]\,.\end{aligned} \tag{19}$$

We can prove that for a cycle evolution, $Z(T)$ and $Z(T)_J$ are invariant under the gauge transformation (18), i.e. $Z(T)$ and $Z(T)_J$ are independent of the choice of the basis $|n\alpha[R]\rangle$. In fact, we first notice that the NABPF $W(n;\, t,\, t_0)$ satisfies a one-form equation

$$dW(n,\, t,\, t_0) + \mathcal{A}(n,\, R)W(n,\, t,\, t_0) = 0\,, \qquad W(n,\, t_0,\, t_0) = I\,. \tag{20}$$

Using Eq. (19), we can directly verify that the $d_n \times d_n$ matrix

$$\widetilde{W}(n,t,t_0) = \Omega_n^+[R(t)]W(n,t,t_0)\Omega_n[R(t_0)]$$

satisfies a similar one-form equation

$$d\widetilde{W}(n,t,t_0) + \mathcal{A}'(n,R)\widetilde{W}(n,t,t_0)\,, \qquad \widetilde{W}(n,t_0,t_0) = I\,. \tag{21}$$

which has a formal solution

$$\widetilde{W}(n,\, t,\, t_0) = \mathcal{P}\exp\Big[-\int_{R(0)}^{R(T)}\mathcal{A}'(n,\, R)\Big]\,. \tag{22}$$

It follows from Eqs. (21) and (22) that

$$\mathcal{P}\exp\Big[-\int_{R(0)}^{R(T)}\mathcal{A}'(n,\, R)\Big] = \Omega_n^+[R(T)]\mathcal{P}\exp\Big[-\int_{R(0)}^{R(T)}\mathcal{A}(n,\, R)\Big]\Omega_n[R(0)]\,.$$

For a cycle evolution, $\Omega_n^+[R(T)] = \Omega_n^+[R(0)]$ such that $\mathrm{Tr}\,\widetilde{W}(n,\, T) = \mathrm{Tr}\,W(n,\, T)$. Thus, as we claimed, $Z(T)$ and $Z(T)_J$ do not depend on the choice of the basis $|n\alpha[R]\rangle$.

Considering the way of transformation of $A(n, m, t)$

$$A(n, m, t) \rightarrow A'(n, m, t) = \Omega_n^+[R]A(n, m, t)\Omega_m[R] \tag{23}$$

under the gauge transformation (19), we easily observe the invariance of high-order correction calculation. This is just what we expected.

IV. Some Explicit Calculations for a Model Relating to NQR and Kramers Molecule

In this section, with a model relating to the NQR and the Kramers molecule with double degeneracy, we do some explicit calculations about path integration of the transition amplitude. The similar problems have been discussed in the contexts of Born-Oppenheimer approximation by Moody, Shapere, Wilczek and Jackiw[5], and the usual adiabatic approximation or HOAA by Segert, Zee and one of the present authors (C.P. SUN)[6,7], but a different context — the path integral formulation is concerned here.

The Hamiltonian for the model is

$$\hat{H} = \frac{\hat{p}_z^2}{2M} + \omega_0(z)(\vec{n}(z)\cdot\hat{\vec{J}})^2 \equiv -\frac{1}{2M}\frac{d^2}{dz^2} + \hat{h}[\vec{n}(z)], \tag{24}$$

where $\vec{n}(z) = (\sin\theta(z)\cos\phi(z), \sin\theta(z)\sin\phi(z), \cos\theta(z))$ is a unit vector parametrized by the spatial coordinate z. For a given instantaneous value of z, the Hamiltonian $\hat{h}(\vec{n})$ of the fast part has doubly degenerate eigenvalues

$$E_{|m|}(z) = m^2\omega_0(z), \qquad m = j, j-1\cdots, -j, \tag{25a}$$

and the corresponding eigenstates

$$|jm(\vec{n})\rangle = \exp[-i\hat{J}_z\phi(z)]\exp[-iJ_z\theta(z)]|j, m\rangle, \tag{25b}$$

where $|j, m\rangle$ is a standard angular momentum state. With the two-dimensional eigen-space $V_{(\vec{n})}^{[m]}$: $\{|j, \pm m(\vec{n})\rangle\}$ as a fiber and the sphere S^2 : $\{\vec{n} \in R^3||\vec{n}| = 1\}$ as a basis manifold, we define a non-trivial fiber bundle: F_m : $\{(\vec{n}, V_{(\vec{n})}^{[m]})|\vec{n} \in S^2\}$, whose structure group is U(2). According to Refs. [6] and [7], the structure has a reduction to the Abelian group U(1) in the case with $m \neq \frac{1}{2}$. Therefore, we only consider a more complicate case, $m = \frac{1}{2}$. Denoting $|j, \frac{1}{2}(\vec{n})\rangle$ and $|j, -\frac{1}{2}(\vec{n})\rangle$ respectively by $||m| = \frac{1}{2}, \alpha = 1(\vec{n})\rangle$ and $||m| = \frac{1}{2}, \alpha = 2(\vec{n})\rangle$, we have the potential one-form[7]

$$\mathcal{A}(\tfrac{1}{2}, z) = -\frac{1}{2}\Big\{\Big[\cos\theta(z)\sigma_3 - \Big(j+\frac{1}{2}\Big)\sin\theta(z)\sigma_1\Big]d\phi(z) + \Big(j+\frac{1}{2}\Big)\sigma_2 d\theta(z)\Big\}. \tag{26}$$

The induced topological action

$$Z_{\frac{1}{2}}(T) = \int[dz]\mathcal{P}\exp\Big[i\int_0^T\Big(\frac{1}{2}M\dot{z}^2 - E_{1/2}(z) + A_3(z)\dot{z}\Big)dt\Big] \tag{27}$$

corresponds to the matrix-value effective Hamiltonian

$$\begin{aligned}\hat{H}_{\text{eff}} &= \frac{-1}{2M}\Big(\frac{d}{dz} - iA(\tfrac{1}{2})_3\Big)^2 + \frac{1}{4}\omega_0(z)\\ &= \frac{-1}{2M}\begin{bmatrix}\frac{d}{dz} - \frac{1}{2}\phi'(z)\cos\theta(z), & \mathcal{B}_1\\ \mathcal{B}_2 & \frac{d}{dz} + \frac{1}{2}\phi'(z)\cos\theta(z)\end{bmatrix}^2 + \frac{1}{4}\omega_0(Z),\end{aligned} \tag{28}$$

$$\phi'(z) = \frac{d}{dz}\phi(z), \qquad \theta'(z) = \frac{d}{dz}\theta(z),$$

where $\mathcal{B}_1 = \frac{1}{2}(j+\frac{1}{2})[-i\theta'(z)+\sin\theta(z)\phi'(z)]$, and $\mathcal{B}_2 = \frac{1}{2}(j+\frac{1}{2})[i\theta'(z)+\sin\theta(z)\phi'(z)]$. The similar result has been given by Moody *et al.* and Jackiw[5] from Born-Oppenheimer approximation.

In the following two cases the NABPF $W(\frac{1}{2},t,t_0) = \mathcal{P}\exp[-\int_0^t \mathcal{A}(\frac{1}{2},n)]$ can be integrated out.

Case 1: θ=constant:

$$W(\tfrac{1}{2},t,t_0) = \frac{1}{\lambda}\begin{bmatrix}\Delta_1, & \Delta_2\\ \Delta_3, & \Delta_4\end{bmatrix}, \tag{29}$$

where $\Delta_1 = i\cos\theta\sin\Gamma(t,t_0) - \lambda\cos\Gamma(t,t_0)$, $\Delta_2 = -i(j+\frac{1}{2})\sin\theta\sin\Gamma(t,t_0)$, $\Delta_3 = -i(j+\frac{1}{2})\sin\theta\sin\Gamma(t,t_0)$, $\Delta_4 = -i\cos\theta\sin\Gamma(t,t_0) - \lambda\cos\Gamma(t,t_0)$, $\lambda = [(j+\frac{1}{2})^2\sin^2\theta+\cos^2\theta]^{1/2}$ and $\Gamma(t,t_0) = \frac{\lambda}{2}\int_{t_0}^t \dot{\Phi}[z(t')]dt'$.

Case 2: $\phi = 0$:

$$W(\tfrac{1}{2},t,t_0) = \exp\Big[\frac{i}{2}\Big(j+\frac{1}{2}\Big)\sigma_2\int_{t_0}^t \dot{\theta}[z(t')]dt'\Big] = \begin{bmatrix}\cos\alpha(t,t_0), & -\sin\alpha(t,t_0)\\ \sin\alpha(t,t_0), & \cos\alpha(t,t_0)\end{bmatrix}, \tag{30}$$

where

$$\alpha(t,t_0) = \frac{1}{2}\Big(j+\frac{1}{2}\Big)\int_{t_0}^t \dot{\theta}[z(t')]dt'.$$

Then, we have

$$Z(T) = 2\cos\Big[\frac{1}{2}k\Big(j+\frac{1}{2}\Big)(\theta(T)-\theta(0))\Big]\int[dz]\exp\Big[i\int_0^T\Big(\frac{1}{2}M\dot{z}^2-\frac{1}{4}\omega_0(z(t))\Big)dt\Big], \tag{31a}$$

$$Z(T)_J = 2\cos\Big[\frac{1}{2}k\Big(j+\frac{1}{2}\Big)(\theta(T)-\theta(0))\Big]\exp\Big[-i\int_0^T\frac{1}{4}\omega_0\Big(\frac{\delta}{\delta J}\Big)\Big]Z_0(J), \tag{31b}$$

$$\begin{aligned}Z_0(J) = \Big[\frac{M}{2\pi Ti}\Big]^{1/2}\exp\Big\{\frac{i}{2}M[z(T)-z(0)]^2T^{-1} + \Big(iT^{-1}z(0)\int_0^T J(t')(T-t')dt'\\ +iT^{-1}z(T)\int_0^T J(t')t'd\tau\Big) - \frac{1}{M^2T}\int_0^T d\tau'\int_0^{\tau'} d\tau(T-\tau')\tau J(\tau)J(\tau'),\end{aligned} \tag{31c}$$

where $k = \begin{cases}0 & \text{for case 1},\\ \lambda & \text{for case 2}.\end{cases}$ Especially, when $\omega_0(z)/4 = \varepsilon_0+\beta z$, we have

$$Z'(T) = -\beta(z(0)+z(T))\cos\Big[\frac{1}{2}k\Big(j+\frac{1}{2}\Big)(\theta(T)-\theta(0))\Big]\sqrt{\frac{iMT}{2\pi}}\exp\Big[\frac{i}{2}M\frac{(z(T)-z(0))^2}{T}\Big].$$

Now, we calculate the non-adiabatic corrections corresponding to the diagrams with two loops and three loops respectively as shown in Figs. 2a and 2b. Here, we only discuss case 2 because case 1 can be studied in the same way.

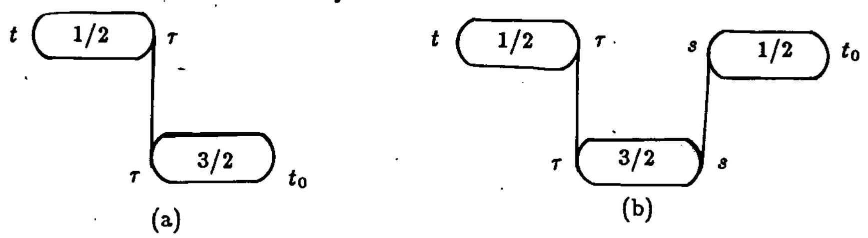

Fig. 2. The non-adiabatic corrections for two loops and three loops.

By direct calculation, we obtain

$$\widetilde{U}^{[1]}\left(\tfrac{1}{2}, \tfrac{1}{2}, t, t_0\right) = 0, \tag{32a}$$

$$\begin{aligned}\widetilde{U}^{[1]}\left(\tfrac{1}{2}, \tfrac{3}{2}, t, t_0\right) &= \int_{t_0}^{t} d\tau W\left(\tfrac{1}{2}, t, \tau\right) \exp\left[-2i\int_{t_0}^{\tau} \omega_0(z(t'))dt'\right] A\left(\tfrac{1}{2}, \tfrac{3}{2}, \tau\right) W\left(\tfrac{3}{2}, \tau, t_0\right) \\ &= i\frac{\sqrt{3}}{2}\int_{t_0}^{t} d\tau \left\{\dot{\theta}(z(\tau)) \exp\left[-2i\int_{t_0}^{\tau} \omega_0(z(t')dt'\right] \begin{bmatrix} \Delta_5, & \Delta_6 \\ -\Delta_6, & \Delta_5 \end{bmatrix}\right\}\end{aligned} \tag{32b}$$

with $\Delta_5 = \cos[\theta(t) - \theta(\tau)]$, $\Delta_6 = \sin[\theta(t) - \theta(\tau)]$ and

$$\begin{aligned}\widetilde{U}^{[2]}\left(\tfrac{1}{2}, \tfrac{1}{2}, t, t_0\right) &= \frac{3}{4}\int_{t_0}^{t} d\tau \int_{t_0}^{\tau} ds \dot{\theta}(z(\tau))\dot{\theta}(z(s)) \exp\left[2i\int_{s}^{\tau} \omega(z(t'))dt'\right] \\ &\times \begin{bmatrix} \cos\Omega(t,\tau,s,t_0), & \sin\Omega(t,\tau,s,t_0) \\ -\sin\Omega(t,\tau,s,t_0), & \cos\Omega(t,\tau,s,t_0) \end{bmatrix},\end{aligned} \tag{32c}$$

where we have considered

$$\begin{aligned}&A\left(\tfrac{3}{2}, \tfrac{1}{2}, t\right) = -A\left(\tfrac{1}{2}, \tfrac{3}{2}, t\right) = -\frac{1}{2}\sqrt{3}\sigma_3\dot{\theta}(z(t)), \\ &A\left(\tfrac{3}{2}, \tfrac{3}{2}, t\right) = 0, \qquad A\left(\tfrac{1}{2}, \tfrac{1}{2}, t\right) = -i\dot{\theta}\sigma_2,\end{aligned} \tag{33}$$

and defined $\Omega(t, \tau, s, t_0) = \theta(t) - \theta(\tau) + \theta(s) - \theta(t_0)$. It immediately follows from Eqs. (32c) and (8c) that the transition amplitude from state $|\frac{1}{2}\beta(R(t_0))\rangle$ to state $|\frac{1}{2}\alpha(R(t))\rangle$ is $f_{\frac{1}{2}}(\beta \to \alpha) = K^{[0]}(t,t_0)_{\frac{1}{2}\alpha,\frac{1}{2}\beta} + K^{[2]}(t,t_0)_{\frac{1}{2}\alpha,\frac{1}{2}\beta}$, e.g.

$$f_{\frac{1}{2}}(1 \to 1) = \int [dz] \exp\left[iS_0 - \frac{1}{4}\int_{t_0}^{t} \omega_0(z)dt'\right]\left\{\cos\theta(z) + \frac{3}{4}\int_{t_0}^{t} d\tau \int_{t_0}^{\tau} ds \cos\Omega(t,\tau,s,t_0)\right\}.$$

Finally, it should be pointed out that the matrix $\widetilde{U}^{[1]}(\frac{1}{2}, \frac{3}{2}, t, t_0)$ only contributes the transition between states $|n\alpha(t_0)\rangle$ and $|m\beta(t)\rangle$ $(m \neq n)$ other than that between states $|n\alpha(t_0)\rangle$ and $|n\beta(t)\rangle$.

V. Two Remarks

1). Considering that the effective Hamiltonians (16) and (17) can be derived by the Born-Oppenheimer approximation, we naturally expect that the higher-order corrections obtained in this paper are achieved by the generalized Born-Oppenheimer approximation method proposed by two of the authors (SUN and GE)[5] for non-degenerate cases. This will require some further works based on Ref. [5]. 2). Because the slow variables R or their functions such as $n(z)$ usually form a manifold, we can not use a single coordinate system to cover the whole manifold, several coordinate charts are needed for the problem and some interesting geometrical phenomena such as the path-phase factor[10]. These discussions will be prepared for publication.

Appendix: New Formulation of the HOAA Method

In this appendix, a new formulation of the original HOAA method[8] is derived by associating it with Wu's work[9]. The new formulation is convenient for concrete calculations. Let

$$|\psi(t)\rangle = \sum_{n}\sum_{\alpha=1}^{dn} C_{n\alpha}(t) \exp\left[-i\int_{t_0}^{t} E_n(\tau)d\tau\right] |n\alpha[R(\tau)]\rangle \tag{A1}$$

be a solution of the Schrödinger equation $i\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{h}[R(t)]|\psi(t)\rangle$. Then,

$$\dot{C}_n(t) + A(n,\, t)C_n(t) = -\sum_{m\neq n} \exp[i\omega_{nm}(t)]A(n,\, m,\, t)C_m(t)\,, \quad n = 1,\, 2\cdots\,, \tag{A2}$$

where we have defined

$$C_n(t) = (C_{n1}(t),\, C_{n2}(t),\, \cdots,\, C_{nd_n}(t))^T\,. \tag{A3}$$

According to Refs. [8] and [9], we can regard the terms on the right-hand side of Eq. (A2) as perturbations so long as parameter R changes slowly enough. Using the perturbation theory of the linear differential equation, we obtain

$$\begin{cases} C_n(t) = \sum\limits_{l=0}^{\infty} C_n^{[l]}(t)\,, \\ \dot{C}_n^{[0]}(t) + A_n(t)C_n^{[0]}(t) = 0\,, \\ C_{n\alpha}^{[0]}(t_0) = \langle n\alpha[R(t_0)]|\psi(0)\rangle\,, \\ \dot{C}_n^{[l]}(t) + A_n(t)C_n^{[l]}(t) = -\sum\limits_{m\neq n} \exp[i\omega_{nm}(t)]A(n,m,t)C_m^{[l-1]}(t)\,, \\ C_n^{[l]}(t_0) = 0\,, \qquad l \geq 1\,, \qquad n = 1,\, 2\,\cdots\,. \end{cases} \tag{A4}$$

The above equations have formal solutions

$$\begin{cases} C_n^{[0]}(t) = W(n,\, t,\, t_0)C_n^{[0]}(t_0)\,, \\ C_n^{[l]}(t) = -\sum\limits_{m\neq n} \int_{t_0}^{t} d\tau\, W(n,\, t,\, \tau)e^{i\omega_{nm}(\tau)} \cdot A(n,\, m,\, \tau)C_m^{[l-1]}(\tau) \\ \quad = (-1)^l \sum\limits_{n_{l-1}\neq n}\ \sum\limits_{n_{l-2}\neq n_{l-1}} \cdots \sum\limits_{n_1\neq n_2}\ \sum\limits_{n_0\neq n_1} \int_{t_0}^{t} d\tau_{l-1} \int_{t_0}^{\tau_{l-1}} d\tau_{l-2} \cdots \\ \quad \times\int_{t_0}^{\tau_2} d\tau_1 \int_{t_0}^{\tau_1} d\tau_0 W(n,t,\tau_{l-1})A(n,n_{l-1},\tau_{l-1}) \exp\left[i\omega_{nn_{l-1}}(\tau_{l-1})\right] \\ \quad \times \prod\limits_{k=l-1}^{1} \left\{W(n_k,\, \tau_k,\, \tau_{k-1})A(n_k,\, n_{k-1},\, \tau_{k-1}) \exp\left[i\omega_{n_k n_{k-1}}(\tau_{k-1})\right]\right\} \\ \quad \times W(n_0,\, \tau_0,\, t_0)C_{n_0}^{[0]}(t_0)\,. \end{cases} \tag{A5}$$

Substituting Eq. (A4) into Eq. (A1), we have

$$|\psi^{[0]}(t)\rangle = \Big\{\sum_{n_0}\ \sum_{\alpha_0,\beta_0=1}^{d_{n_0}} \exp\Big[-i\int_{t_0}^{t} E_{n_0}[R(t')]dt'\Big]W(n_0,\, t,\, t_0)_{\alpha_0\beta_0}$$
$$\times|n_0\alpha_0[R(t)]|\rangle\langle n_0\beta_0[R(t_0)]||\Big\}|\psi(0)\rangle\,,$$

$$|\psi^{[1]}(t)\rangle = \Big\{\sum_{n_1}\ \sum_{n_0\neq n_1}\ \sum_{\beta_1=1}^{dn_1}\ \sum_{\alpha_0,\beta_0=1}^{dn_0} \exp\Big[-i\int_{t_0}^{t} E_{n_1}[R(t')]dt'\Big]\int_{t_0}^{t} W(n_1,\, t,\, t_1)_{\alpha_1\beta_1}$$
$$\times A(n_1,\, n_0,\, t_1)_{\beta_1\alpha_0} \exp\left[i\omega_{n_1n_0}(t_1)\right]W(n_0,\, t_1,\, t_0)_{\alpha_0\beta_0}dt_1$$
$$\times|n_1\alpha_1[R(t)]|\rangle\langle n_0\beta_0[R(t_0)]||\Big\}|\psi(0)\rangle\,,$$

$$\cdots \tag{A6}$$

$$|\psi^{[l]}(t)\rangle = (-1)^l \Big\{ \sum_n e^{-i\int_{t_0}^t E_n(t')dt'} \cdot \sum_{n_{l-1}\neq n} \sum_{n_{l-2}\neq n_{l-1}} \cdots \sum_{n_1\neq n_2} \sum_{n_0\neq n_1}$$
$$\times \int_{t_0}^{t} d\tau_{l-1} \int_{t_0}^{\tau_{l-1}} d\tau_{l-2} \cdots \int_{t_0}^{\tau_2} d\tau_1 \int_{t_0}^{\tau_1} d\tau_0 \Big(W(n;\, t,\, \tau_{l-1}) A(n,\, n_{l-1},\, \tau_{l-1})$$
$$\times \exp\left[i\omega_{nn_{l-1}}(\tau_{l-1})\right] \prod_{k=l-1}^{1} \{ W(n_k,\, \tau_k,\, \tau_{k-1}) A(n_k,\, n_{k-1},\, \tau_{k-1})$$
$$\times \exp\left[i\omega_{n_k n_{k-1}}(\tau_{k-1})\right] \} W(n_0,\, \tau_0,\, t_0) \Big)_{\alpha\beta} |n\alpha[R(t)]\rangle\langle n_0\beta[R(t_0)]| \Big\} |\psi(0)\rangle ,$$
$$l = 1,\, 2,\, 3,\, \cdots .$$

By considering

$$|\psi(t)\rangle = U(t,\, t_0)|\psi(0)\rangle , \qquad U(t,\, t_0) = \sum_{l=0}^{\infty} U^{[l]}(t,\, t_0) ,$$
$$|\psi^{[l]}(t)\rangle = U^{[l]}(t,\, t_0)|\psi(0)\rangle , \tag{A7}$$

the formulas in Eq. (4) can easily be obtained from the above equations.

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