

Adiabatic approximation in the second quantized formulation

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Recently there have been some controversies about the criterion of the adiabatic approximation. It is shown that an approximate diagonalization of the effective Hamiltonian in the second quantized formulation gives rise to a reliable and unambiguous criterion of the adiabatic approximation. This is illustrated for the model of Marzlin and Sanders [Phys. Rev. Lett. **93**, 160408 (2004)] and a model related to the geometric phase which can be exactly diagonalized in the present sense.

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I. INTRODUCTION

Recently there have been some controversies about the criterion of the adiabatic approximation [1], which was triggered by an interesting model of Marzlin and Sanders [2]. This model gives rise to an apparently nonsensical result on the basis of a series of logical steps which appear to be justified on the basis of the conventional wisdom of the adiabatic approximation.

We here recapitulate the analysis in [2]. They start with the evolution operator

$$U(t) = T^* \exp \left[-\frac{i}{\hbar} \int_0^t dt \hat{H}(t) \right] \quad (1.1)$$

and define the object

$$\bar{\psi}_n(t) = U(t)^\dagger v_n(0) \quad (1.2)$$

where $\hat{H}(t)v_n(t) = E_n(t)v_n(t)$. This object satisfies the exact relation

$$\begin{aligned} i\hbar \partial_t \bar{\psi}_n(t) &= -U(t)^\dagger \hat{H}(t) v_n(0) \\ &= -U(t)^\dagger \hat{H}(t) U(t) U(t)^\dagger v_n(0) \\ &= -U(t)^\dagger \hat{H}(t) U(t) \bar{\psi}_n(t). \end{aligned} \quad (1.3)$$

They then introduce the quantity

$$\phi_n(t) = \exp \left[\frac{i}{\hbar} \int_0^t dt E_n(t) \right] v_n(0) \quad (1.4)$$

which satisfies the relation

$$\begin{aligned} i\hbar \partial_t \phi_n(t) &= -E_n(t) \phi_n(t) \\ &= -E_n(t) U(t)^\dagger U(t) \exp \left[\frac{i}{\hbar} \int_0^t dt E_n(t) \right] v_n(0) \\ &\simeq -U(t)^\dagger \hat{H}(t) U(t) \exp \left[\frac{i}{\hbar} \int_0^t dt E_n(t) \right] v_n(0) \\ &= -U(t)^\dagger \hat{H}(t) U(t) \phi_n(t) \end{aligned} \quad (1.5)$$

where we used the conventional adiabatic approximation (diagonal dominance) for the Hamiltonian $\hat{H}(t)$ in the sense [3,4]

$$\begin{aligned} U(t)v_n(0) &= \sum_m v_m(t) v_m^\dagger(t) U(t)v_n(0) \\ &\simeq v_n(t) \exp \left\{ -\frac{i}{\hbar} \int_0^t dt [E_n(t) - v_n^\dagger(t) i\hbar \partial_t v_n(t)] \right\} \end{aligned} \quad (1.6)$$

and thus $\hat{H}(t)U(t)v_n(0) \simeq E_n(t)U(t)v_n(0)$, namely, the state $v_n(0)$ which is the eigenstate of $\hat{H}(0)$ with the eigenvalue $E_n(0)$ at $t=0$ remains the eigenstate of $\hat{H}(t)$ with eigenvalue $E_n(t)$ for the time development defined by $U(t)v_n(0)$.

On the basis of the relation (1.5), one may attempt to identify [2]

$$\bar{\psi}_n(t)_{\text{adiabatic}} = \phi_n(t). \quad (1.7)$$

The authors of [2] then showed on the basis of the identification (1.7) and by using (1.6)

$$\begin{aligned} v_n^\dagger(0)v_n(0) &= v_n^\dagger(0)U(t)U(t)^\dagger v_n(0) = v_n^\dagger(0)U(t)\bar{\psi}_n(t) \\ &\simeq v_n^\dagger(0)U(t)\phi_n(t) \\ &\simeq v_n^\dagger(0)v_n(t) \exp \left[i \int_0^t dt v_n^\dagger(t) i\hbar \partial_t v_n(t) \right] \neq 1 \end{aligned} \quad (1.8)$$

which they argued is false. We shall analyze this problem in detail in Sec. III.

Since the publication of the paper by Marzlin and Sanders [2], many papers which attempted to clarify the problem appeared [5–20]. Some of these papers presented a general and more precise criterion of the adiabatic approximation in the first quantization scheme. But it appears that a more precise criterion means more involved conditions and thus the basic simplicity is generally lost.

The purpose of the present paper is to show that a field theoretical technique, namely, the second quantization technique, gives a simple, reliable, and unambiguous formulation of the adiabatic approximation. The adiabatic approximation is defined as an approximate diagonalization of the effective Hamiltonian in the second quantized approach, and thus it is equally applicable to the operator formulation and to the path integral formulation [21,22]. In

the second quantized formulation, contrary to the first quantized formulation, we start with an exact formulation and apply the adiabatic approximation later and thus the adiabatic geometric phase appears from an approximate diagonalization of the effective Hamiltonian. The adiabatic geometric phase is a part of the effective Hamiltonian and thus dynamical, and it is topologically trivial [21]. This aspect is quite different from the first quantized treatment where the adiabatic geometric phase is usually treated separately from the approximate diagonalization of the Hamiltonian.

The second quantized approach has been applied to the analyses of all the geometric phases, namely, the adiabatic [21], nonadiabatic [23], and mixed state geometric phases [24], though no adiabatic approximation is involved in the last two examples. A salient feature is that an exact hidden local symmetry appears in the Schrödinger equation in this formulation [22] and the associated holonomy controls all the known geometric phases [24]. In particular, the non-adiabatic phase is treated without using the notion of the projective Hilbert space whose consistency with the superposition principle is not obvious [23].

In the present paper, we first briefly summarize the second quantized formulation of the adiabatic approximation and then apply the formulation to the model of Marzlin and Sanders [2] and to a model related to the geometric phase which can be exactly diagonalized in the present sense.

II. SECOND QUANTIZED FORMULATION

We summarize a second quantized formulation of the adiabatic approximation [21,22]. We expand the field variable in the second quantization

$$\hat{\psi}(t) = \sum_n \hat{b}_n(t) v_n(t, \vec{x}) \quad (2.1)$$

by using a specific basis set defined by

$$\hat{H}(t) v_n(t, \vec{x}) = E_n(t) v_n(t, \vec{x}). \quad (2.2)$$

When one uses the above expansion in the action

$$\begin{aligned} S &= \int_0^T dt \int d^3x \left[\hat{\psi}^*(t, \vec{x}) i\hbar \frac{\partial}{\partial t} \hat{\psi}(t, \vec{x}) \right. \\ &\quad \left. - \hat{\psi}^*(t, \vec{x}) \hat{H}(t) \hat{\psi}(t, \vec{x}) \right] \\ &= \int_0^T dt \left\{ \sum_n \hat{b}_n^\dagger(t) i\hbar \partial_t \hat{b}_n(t) - \hat{H}_{\text{eff}}(t) \right\} \end{aligned} \quad (2.3)$$

one obtains the effective Hamiltonian

$$\begin{aligned} \hat{H}_{\text{eff}}(t) &= \sum_{n,m} \hat{b}_n^\dagger(t) \int d^3x [v_n^\dagger(t, \vec{x}) \hat{H}(t) v_m(t, \vec{x}) \\ &\quad - v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_m(t, \vec{x})] \hat{b}_m(t) \\ &= \sum_{n,m} \hat{b}_n^\dagger(t) \left[E_n(t) \delta_{nm} \right. \\ &\quad \left. - \int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_m(t, \vec{x}) \right] \hat{b}_m(t) \end{aligned} \quad (2.4)$$

with the quantized operators satisfying the equal-time commutators $[\hat{b}_n(t), \hat{b}_m^\dagger(t)]_\mp = \delta_{n,m}$, but the Bose or Fermi statistics are not important in our application.

The exact Schrödinger probability amplitude with $\psi_n(0, \vec{x}) = v_n(0, \vec{x})$ is defined by [by noting $i\hbar \partial_t \hat{\psi}(t, \vec{x}) = \hat{H}(t) \hat{\psi}(t, \vec{x})$]

$$\begin{aligned} \psi_n(t, \vec{x}) &= \langle 0 | \hat{\psi}(t, \vec{x}) \hat{b}_n^\dagger(0) | 0 \rangle \\ &= \sum_m v_m(t, \vec{x}) \langle m | T^* \exp \left\{ -\frac{i}{\hbar} \int_0^t \hat{\mathcal{H}}_{\text{eff}}(t) dt \right\} | n \rangle \end{aligned} \quad (2.5)$$

which is equal to the amplitude in the first quantization

$$\begin{aligned} \psi_n(t, \vec{x}) &= \langle \vec{x} | T^* \exp \left\{ -\frac{i}{\hbar} \int_0^t \hat{H}(t) dt \right\} | n(0) \rangle \\ &= \sum_m v_m(t, \vec{x}) \langle m(t) | T^* \exp \left\{ -\frac{i}{\hbar} \int_0^t \hat{H}(t) dt \right\} | n(0) \rangle \end{aligned} \quad (2.6)$$

if one notes the equality [21,22]

$$\begin{aligned} \langle m | T^* \exp \left\{ -\frac{i}{\hbar} \int_0^t \hat{\mathcal{H}}_{\text{eff}}(t) dt \right\} | n \rangle \\ = \langle m(t) | T^* \exp \left\{ -\frac{i}{\hbar} \int_0^t \hat{H}(t) dt \right\} | n(0) \rangle \end{aligned} \quad (2.7)$$

where the state $|m\rangle$ on the left-hand side is defined by $\hat{b}_m^\dagger(0)|0\rangle$ and the state on the right-hand side is defined by $\langle \vec{x} | m(t) \rangle = v_m(t, \vec{x})$, respectively, and the Schrödinger picture $\hat{\mathcal{H}}_{\text{eff}}(t)$ is defined by setting all $\hat{b}_n(t) \rightarrow \hat{b}_n(0)$ in $\hat{H}_{\text{eff}}(t)$. The symbol T^* stands for the time ordering. A salient feature of the second quantization is that the general “geometric terms” $\int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_m(t, \vec{x})$ automatically appear in the *exact* $\hat{\mathcal{H}}_{\text{eff}}(t)$.

The adiabaticity means that the probability amplitude starting with $v_n(0, \vec{x})$ at $t = 0$ stays in the state $v_n(t, \vec{x})$ for any later time [1]. This is equivalent to the statement that $\hat{\mathcal{H}}_{\text{eff}}(t)$ is diagonal for each time t . The adiabatic approximation in the second quantization is thus defined by the diagonal dominance in $\hat{\mathcal{H}}_{\text{eff}}(t)$ which is ensured if any difference of the diagonal elements is much bigger than off-diagonal elements, namely,

$$|v_n^\dagger(t) i\hbar \partial_t v_{m'}(t)| \ll \left| (E_n(t) - \int d^3x v_n^\dagger(t) i\hbar \partial_t v_n(t)) - (E_m(t) - \int d^3x v_m^\dagger(t) i\hbar \partial_t v_m(t)) \right| \quad (2.8)$$

and

$$|v_n^\dagger(t) i\hbar \partial_t v_{m'}(t)| \ll \left| E_n(t) - \int d^3x v_n^\dagger(t) i\hbar \partial_t v_n(t) \right| \quad (2.9)$$

for any $n \neq m$ and $n' \neq m'$. In this case one can approximately diagonalize the above effective Hamiltonian

$$\hat{\mathcal{H}}_{\text{eff}}(t) \simeq \sum_n \hat{b}_n^\dagger(0) \left[E_n(t) \delta_{nm} - \int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_n(t, \vec{x}) \right] \hat{b}_n(0) \quad (2.10)$$

and thus the Schrödinger probability amplitude is approximately given by [3]

$$\psi_n(t, \vec{x}) \simeq v_n(t, \vec{x}) \exp \left\{ -\frac{i}{\hbar} \int_0^t dt \left[E_n(t) - \int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_n(t, \vec{x}) \right] \right\} \quad (2.11)$$

with $\psi_n(0, \vec{x}) = v_n(0, \vec{x})$. This statement is accurate for a finite number of degrees of freedom with $n = 1$ to N , and when $N \rightarrow \infty$ one needs to estimate carefully an infinite sum of small off-diagonal elements. The condition (2.8) ensures that the transition between different eigenstates is small and the condition (2.9) ensures that the diagonal element represents the total phase such as in (2.11) accurately. In most cases, the condition (2.9) is trivially satisfied since one can adjust the origin of the energy eigenvalue at will by adding a constant. This adjustment of the energy eigenvalue does not influence the geometric phase since all the geometric phases are defined as the holonomy of the basis vectors [24], for example,

$$\tilde{v}_n(0, \vec{x})^\dagger \tilde{v}_n(T, \vec{x}) = v_n(0, \vec{x})^\dagger v_n(T, \vec{x}) \exp \left\{ \frac{i}{\hbar} \int_0^T dt \int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_n(t, \vec{x}) \right\}, \quad (2.12)$$

in (2.11) for a cyclic evolution with $v_n(0, \vec{x}) = v_n(T, \vec{x})$. Here we defined

$$\tilde{v}_n(t, \vec{x}) = v_n(t, \vec{x}) \exp \left\{ \frac{i}{\hbar} \int_0^t dt \int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_n(t, \vec{x}) \right\} \quad (2.13)$$

which satisfies the parallel transport condition $\int d^3x \tilde{v}_n(t, \vec{x})^\dagger \partial_t \tilde{v}_n(t, \vec{x}) = 0$.

We emphasize that this diagonal dominance or approximate diagonalization of the effective Hamiltonian is a

precise restatement of the *conventional* idea of the adiabatic approximation.

In passing, we note an exact local (i.e., time-dependent) symmetry [22]

$$v_n(t, \vec{x}) \rightarrow v'_n(t, \vec{x}) = e^{i\alpha_n(t)} v_n(t, \vec{x}), \\ \hat{b}_n(t) \rightarrow \hat{b}'_n(t) = e^{-i\alpha_n(t)} \hat{b}_n(t), \quad n = 1, 2, 3, \dots, \quad (2.14)$$

in the operator $\hat{\psi}(t, \vec{x})$ in (2.1), which arises from an arbitrariness in the choice of the coordinates in the functional space. Under this local symmetry the Schrödinger amplitude $\psi_n(t, \vec{x}) = \langle 0 | \hat{\psi}(t, \vec{x}) \hat{b}_n^\dagger(0) | 0 \rangle$ is transformed as $\psi'_n(t, \vec{x}) = e^{i\alpha_n(0)} \psi_n(t, \vec{x})$ for any t , which corresponds to the ray representation. We thus find an enormous exact local symmetry behind the ray representation, and this local symmetry is responsible for the holonomy appearing in all the geometric phases [24].

III. APPLICATIONS OF THE FORMULATION

A. Model of Marzlin and Sanders

We now analyze the model introduced by Marzlin and Sanders [2] which is defined by the Hamiltonian [see Eq. (1.3)]

$$\hat{H} = -U(t)^\dagger \hat{H}(t) U(t) \quad (3.1)$$

in the second quantized formulation of the adiabatic approximation. We expand the field variable as

$$\hat{\psi}(t) = \sum_n \hat{b}_n(t) \bar{v}_n(t) \quad (3.2)$$

where $\bar{v}_n(t)$ is defined by

$$\bar{v}_n(t) = U(t)^\dagger v_n(t). \quad (3.3)$$

The basis vectors $\{v_n(t)\}$ are defined for $\hat{H}(t)$ by $\hat{H}(t)v_n(t) = E_n(t)v_n(t)$, and thus the basis set $\{\bar{v}_n(t)\}$ satisfies

$$\hat{H} \bar{v}_n(t) = -U(t)^\dagger \hat{H}(t) U(t) \bar{v}_n(t) = -E_n(t) \bar{v}_n(t). \quad (3.4)$$

In this section, we consider the problem where the spatial coordinates $\vec{x}$ do not appear explicitly [2]. We then have the effective Hamiltonian in the second quantized formulation

$$\hat{H}_{\text{eff}}(t) = \sum_{n,m} \hat{b}_n^\dagger(t) [\bar{v}_n^\dagger(t) \hat{H} \bar{v}_m(t) - \bar{v}_n^\dagger(t) i\hbar \partial_t \bar{v}_m(t)] \hat{b}_m(t) \\ = \sum_{n,m} \hat{b}_n^\dagger(t) [-E_n \delta_{n,m} - \bar{v}_n^\dagger(t) i\hbar \partial_t \bar{v}_m(t)] \hat{b}_m(t). \quad (3.5)$$

The off-diagonal terms in the geometric terms are evaluated as

$$\begin{aligned}
\bar{v}_m^\dagger(t) i \partial_t \bar{v}_n(t) &= \bar{v}_m^\dagger(t) \left[-\frac{1}{\hbar} U(t)^\dagger \hat{H}(t) v_n(t) \right. \\
&\quad \left. + U(t)^\dagger i \partial_t v_n(t) \right] \\
&= -\frac{1}{\hbar} v_m^\dagger(t) E_n(t) v_n(t) + v_m^\dagger(t) i \partial_t v_n(t) \\
&= v_m^\dagger(t) i \partial_t v_n(t) \quad (3.6)
\end{aligned}$$

for $m \neq n$. Thus the eigenvalues (up to signature) and the off-diagonal terms in the geometric terms agree with those of the original system specified by $\hat{H}(t)$, for which we assume the validity of the adiabatic approximation: Namely, we assume that not only the *naïve* criterion of the adiabatic approximation for the original system specified by $\hat{H}$

$$|v_{n'}^\dagger(t) i \hbar \partial_t v_{m'}(t)| \ll |E_n(t) - E_m(t)| \quad (3.7)$$

but also the precise conditions (2.8) and (2.9) are always satisfied for any $n \neq m$ and $n' \neq m'$. In the present problem defined by $\hat{H}$, the naïve criterion (3.7) is satisfied and thus one might expect that the adiabatic approximation may be valid in the present problem also.

We now examine the diagonal elements of the geometric terms

$$\begin{aligned}
\bar{v}_n^\dagger(t) i \hbar \partial_t \bar{v}_n(t) &= \bar{v}_n^\dagger(t) [-U(t)^\dagger \hat{H}(t) v_n(t) \\
&\quad + U(t)^\dagger i \hbar \partial_t v_n(t)] \\
&= -v_n^\dagger(t) E_n(t) v_n(t) + v_n^\dagger(t) i \hbar \partial_t v_n(t) \\
&= -E_n(t) + v_n^\dagger(t) i \hbar \partial_t v_n(t). \quad (3.8)
\end{aligned}$$

The above effective Hamiltonian (3.5) is thus rewritten as

$$\begin{aligned}
\hat{H}_{\text{eff}}(t) &= \sum_{n,m} \hat{b}_n^\dagger(t) \left[-E_n(t) \delta_{nm} + E_n(t) \delta_{nm} \right. \\
&\quad \left. - v_n^\dagger(t) i \hbar \frac{\partial}{\partial t} v_m(t) \right] \hat{b}_m(t) \\
&= \sum_{n,m} \hat{b}_n^\dagger(t) \left[-v_n^\dagger(t) i \hbar \frac{\partial}{\partial t} v_m(t) \right] \hat{b}_m(t). \quad (3.9)
\end{aligned}$$

The system introduced in [2] is quite peculiar. This system contains only the “small” elements in the effective Hamiltonian and thus we have no reliable diagonal dominance, i.e., no reliable adiabatic approximation for $\hat{H}(t)$ in the conventional sense. The crucial property of the present problem is that the condition (2.8) for the system specified by $\hat{H}$

$$\begin{aligned}
|\bar{v}_{n'}^\dagger(t) i \hbar \partial_t \bar{v}_{m'}(t)| &\ll |(-E_n(t) - \bar{v}_n^\dagger(t) i \hbar \partial_t \bar{v}_n(t)) \\
&\quad - (-E_m(t) - \bar{v}_m^\dagger(t) i \hbar \partial_t \bar{v}_m(t))| \quad (3.10)
\end{aligned}$$

for any $n \neq m$ and $n' \neq m'$ is not satisfied.

If it happens that

$$\begin{aligned}
|\bar{v}_{n'}^\dagger(t) i \hbar \partial_t \bar{v}_{m'}(t)| &\ll |v_n^\dagger(t) i \hbar \partial_t v_n(t) - v_m^\dagger(t) i \hbar \partial_t v_m(t)|, \\
|\bar{v}_{n'}^\dagger(t) i \hbar \partial_t \bar{v}_{m'}(t)| &\ll |v_n^\dagger(t) i \hbar \partial_t v_n(t)| \quad (3.11)
\end{aligned}$$

for any $n \neq m$ and $n' \neq m'$ in (3.9), however, one can define a reliable adiabatic approximation for the above $\hat{H}_{\text{eff}}(t)$. The second condition in (3.11) corresponds to (2.9). We thus examine the possibility (3.11). In this case we have from (2.5)

$$\begin{aligned}
\bar{\psi}_n(t) &= \sum_m \bar{v}_m(t) \langle m | T^* \exp \left[-\frac{i}{\hbar} \int_0^t dt \hat{\mathcal{H}}_{\text{eff}}(t) \right] | n \rangle \simeq \bar{v}_n(t) \exp \left\{ \frac{i}{\hbar} \int_0^t dt v_n^\dagger(t) i \hbar \partial_t v_n(t) \right\} \\
&= \sum_m v_m(0) v_m(0)^\dagger U(t)^\dagger v_n(t) \exp \left\{ \frac{i}{\hbar} \int_0^t dt v_n^\dagger(t) i \hbar \partial_t v_n(t) \right\} \\
&\simeq v_n(0) \exp \left\{ \frac{i}{\hbar} \int_0^t dt [E_n(t) - v_n^\dagger(t) i \hbar \partial_t v_n(t)] \right\} \exp \left\{ \frac{i}{\hbar} \int_0^t dt v_n^\dagger(t) i \hbar \partial_t v_n(t) \right\} = v_n(0) \exp \left\{ \frac{i}{\hbar} \int_0^t dt E_n(t) \right\} \quad (3.12)
\end{aligned}$$

where we used the adiabatic approximation (diagonal dominance) for the original system specified by $\hat{H}(t)$

$$\begin{aligned}
v_m^\dagger(0) U(t)^\dagger v_n(t) &= (v_n(t)^\dagger U(t) v_m(0))^* \\
&\simeq \exp \left\{ \frac{i}{\hbar} \int_0^t dt [E_n(t) \right. \\
&\quad \left. - v_n^\dagger(t) i \hbar \partial_t v_n(t)] \right\} \delta_{n,m}. \quad (3.13)
\end{aligned}$$

We thus recover the result (1.7) in (3.12) under the conditions (3.11).

The conditions (3.11) imply that

$$\partial_t v_n(t) = \sum_m v_m(t) (v_m^\dagger(t) \partial_t v_n(t)) \simeq v_n(t) (v_n^\dagger(t) \partial_t v_n(t)) \quad (3.14)$$

which in turn implies

$$\partial_t \left[v_n(t) \exp \left\{ i \int_0^t dt v_n^\dagger(t) i \hbar \partial_t v_n(t) \right\} \right] \simeq 0, \quad (3.15)$$

namely,

$$v_n(0) \simeq v_n(t) \exp\left\{i \int_0^t dt v_n^\dagger(t) i \partial_t v_n(t)\right\} \quad (3.16)$$

and thus the relation (1.8) is *not* false under the conditions (3.11). Equation (3.16) implies that the geometric phase or holonomy is trivial for a periodic system $v_n(0) = v_n(T)$ with a period T .

In the generic case where the conditions (3.11) are not satisfied, we have the exact amplitude

$$\begin{aligned} \bar{\psi}_n(t) &= \sum_m \bar{v}_m(t) \langle m | T^* \exp\left[-\frac{i}{\hbar} \int_0^t dt \hat{\mathcal{H}}_{\text{eff}}(t)\right] | n \rangle \\ &= \sum_m \bar{v}_m(t) \bar{v}_m^\dagger(t) T^* \exp\left[-\frac{i}{\hbar} \int_0^t dt \hat{H}(t)\right] v_n(0) \\ &= T^* \exp\left[\frac{i}{\hbar} \int_0^t dt U(t)^\dagger \hat{H}(t) U(t)\right] v_n(0) \\ &= U(t)^\dagger v_n(0) \end{aligned} \quad (3.17)$$

but no reliable adiabatic approximation for the dynamics specified by $\hat{H}$. The last equality in (3.17), which is a result of (1.3), is directly confirmed by defining $f(t) = T^* \exp\left[\frac{i}{\hbar} \int_0^t dt U(t)^\dagger \hat{H}(t) U(t)\right]$ and then $U(t)f'(t) = (i/\hbar)\hat{H}(t)U(t)f(t) = -U'(t)f(t)$, namely, $U(t)f(t) = \text{const} = 1$.

One may attempt to rewrite the amplitude (3.17) as

$$\begin{aligned} \bar{\psi}_n(t) &= \sum_{k,m} v_k(0) \langle v_k^\dagger(0) | U(t)^\dagger | v_m(t) \rangle v_m^\dagger(t) v_n(0) \\ &\simeq \sum_m v_m(0) \exp\left\{\frac{i}{\hbar} \int_0^t dt [E_m(t) \right. \\ &\quad \left. - v_m^\dagger(t) i \hbar \partial_t v_m(t)]\right\} v_m^\dagger(t) v_n(0) \end{aligned} \quad (3.18)$$

where we used the diagonal dominance (3.13) for the system specified by $\hat{H}(t)$, but no further reliable approximation. If the system has a period T in the sense $\hat{H}(T) = \hat{H}(0)$, however, one has a simpler expression after one cycle by using $v_n(0) = v_n(T)$ and $v_m^\dagger(T) v_n(0) = v_m^\dagger(T) v_n(T) = \delta_{m,n}$ in (3.18)

$$\begin{aligned} \bar{\psi}_n(T) &\simeq v_n(0) \exp\left\{\frac{i}{\hbar} \int_0^T dt [E_n(t) - v_n^\dagger(t) i \hbar \partial_t v_n(t)]\right\} \\ &= v_n(T) \exp\left\{\frac{i}{\hbar} \int_0^T dt [E_n(t) - v_n^\dagger(t) i \hbar \partial_t v_n(t)]\right\} \end{aligned} \quad (3.19)$$

which has the same form as the conventional adiabatic approximation for the system specified by $\hat{H}(t)$, except for the reversed signature in the exponential. This result (3.19) is consistent with (3.12) for $t = T$ if one recalls that (3.12) is valid only under the condition (3.16). It is important that the basis vectors $v_n(t)$ are defined for $\hat{H}(t)$ and not for $\hat{\tilde{H}}(t)$, and thus (3.19) is not called an adiabatic approximation for the dynamics defined by $\hat{\tilde{H}}(t)$.

Second model of Marzlin and Sanders

We here briefly comment on the second ‘‘counterexample’’ in [2]. They consider a two-level system with exact time evolution defined by

$$U(t) = \exp\{-i\omega_0 \mathbf{n}(t) \cdot \boldsymbol{\sigma}\} \quad (3.20)$$

with

$$\mathbf{n}(t) = (\cos(2\pi t/\tau), \sin(2\pi t/\tau), 0) \quad (3.21)$$

and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denoting the Pauli matrices. Although it is not clearly stated in [2], it is natural to understand the above evolution operator standing for

$$U(t_2, t_1) = \exp\{-i\omega_0(t_2 - t_1)\mathbf{n}(t_2 - t_1) \cdot \boldsymbol{\sigma}\}. \quad (3.22)$$

One can then confirm that the above operator does not satisfy the basic composition law of quantum mechanics

$$U(t_3, t_1) = U(t_3, t_2)U(t_2, t_1) \quad (3.23)$$

except for the time-independent $\mathbf{n}(t)$. Since their operator $U(t)$ does not depend on the intermediate time, the condition (3.23) implies

$$U(2t) = U(t)U(t) \quad (3.24)$$

if one chooses $t_3 - t_2 = t_2 - t_1 = t$. This relation is satisfied only for the time-independent $\mathbf{n}(t)$. The second model in [2] does not constitute a meaningful counterexample of the adiabatic approximation.

One may instead start with their Hamiltonian [2]

$$\hat{H}(t) = \mathbf{R}(t) \cdot \boldsymbol{\sigma} \quad (3.25)$$

where

$$\begin{aligned} R_x(t) &\equiv |R(t)| \sin\Theta(t) \cos\varphi(t) \\ &= \omega_0 \cos(\omega t) - \frac{1}{2}\omega \sin(\omega t) \sin(2\omega_0 t), \\ R_y(t) &\equiv |R(t)| \sin\Theta(t) \sin\varphi(t) \\ &= \omega_0 \sin(\omega t) + \frac{1}{2}\omega \cos(\omega t) \sin(2\omega_0 t), \\ R_z(t) &\equiv |R(t)| \cos\Theta(t) = \omega \sin^2(\omega_0 t) \end{aligned} \quad (3.26)$$

with $\omega = 2\pi/\tau$ and

$$|R(t)| = \sqrt{\omega_0^2 + \omega^2 \sin^2(\omega_0 t)}, \quad (3.27)$$

without asking where it came from. [If the composition law (3.23) is satisfied, one can define the Hamiltonian by $U(t_2 + \Delta t, t_2) = \exp\{-i\hat{H}(t_2)\Delta t\}$, namely, the generator of infinitesimal time development. Since the composition law is not satisfied by the present example, the Hamiltonian thus defined does not agree with (3.25) except for the time-independent $\mathbf{n}(t)$.]

One can then construct the instantaneous eigenvectors

$$v_+(R) = \begin{pmatrix} \cos\frac{\Theta}{2} e^{-i\varphi} \\ \sin\frac{\Theta}{2} \end{pmatrix}, \quad v_-(R) = \begin{pmatrix} \sin\frac{\Theta}{2} e^{-i\varphi} \\ -\cos\frac{\Theta}{2} \end{pmatrix} \quad (3.28)$$

as

$$\hat{H}(t)v_{\pm}(R) = \pm |R(t)|v_{\pm}(R). \quad (3.29)$$

By denoting m and n to run over $\pm$, we define $v_m^\dagger(R)i\frac{\partial}{\partial t}v_n(R) = \langle m|i\frac{\partial}{\partial t}|n\rangle$ and then

$$\begin{aligned} \langle +|i\frac{\partial}{\partial t}|+\rangle &= \frac{(1 + \cos\Theta)}{2} \dot{\varphi}, \\ \langle +|i\frac{\partial}{\partial t}|-\rangle &= \frac{\sin\Theta}{2} \dot{\varphi} + \frac{i}{2} \dot{\Theta} = \left(\langle -|i\frac{\partial}{\partial t}|+\rangle \right)^*, \\ \langle -|i\frac{\partial}{\partial t}|-\rangle &= \frac{1 - \cos\Theta}{2} \dot{\varphi}. \end{aligned} \quad (3.30)$$

When one expands $\hat{\psi}(t)$ as

$$\hat{\psi}(t) = \sum_n \hat{b}_n(t)v_n(t), \quad (3.31)$$

the exact second quantized effective Hamiltonian (2.4) is given by

$$\begin{aligned} \hat{H}_{\text{eff}}(t) &= |R(t)|\hat{b}_+^\dagger \hat{b}_+ - |R(t)|\hat{b}_-^\dagger \hat{b}_- \\ &\quad - \hbar \sum_{m,n} \hat{b}_m^\dagger \langle m|i\frac{\partial}{\partial t}|n\rangle \hat{b}_n. \end{aligned} \quad (3.32)$$

One can confirm that the diagonal dominance (or conventional adiabatic approximation) perfectly works for

$$\omega_0 = 2n\omega \gg \omega \quad (3.33)$$

with an integer n , which is the assumption made in [2]. One may note $|R(t)| \simeq \omega_0$, $0 \leq \cos\Theta(t) \ll 1$, $\dot{\Theta}(t) \sim \omega$, and $\dot{\varphi}(t) \sim \omega$ in (3.26).

One can also confirm that the evolution operator defined in (2.7)

$$\begin{aligned} \langle m|T^* \exp\left\{-\frac{i}{\hbar} \int_0^t \hat{\mathcal{H}}_{\text{eff}}(t) dt\right\}|n\rangle \\ = \langle m(t)|T^* \exp\left\{-\frac{i}{\hbar} \int_0^t \hat{H}(t) dt\right\}|n(0)\rangle \end{aligned} \quad (3.34)$$

satisfies the basic composition law (3.23).

B. Exactly solvable model

We next study the model described by

$$\hat{H}(t) = -\mu\hbar\vec{B}(t)\vec{\sigma} \quad (3.35)$$

where $\vec{\sigma}$ stands for Pauli matrices and

$$\vec{B}(t) = B(\sin\theta \cos\varphi(t), \sin\theta \sin\varphi(t), \cos\theta). \quad (3.36)$$

Here we assume $\varphi(t) = \omega t$ with constant ω , B , and θ . This

model has been studied by various authors in the past by using the adiabatic approximation [3,4], but to our knowledge, an exact treatment was first given in Ref. [23]. We here present the essence of the analysis with additional comments from the point of view of the adiabatic approximation.

We have the effective Hamiltonian in (2.4)

$$\begin{aligned} \hat{H}_{\text{eff}}(t) &= \left[-\mu\hbar B - \frac{(1 + \cos\theta)}{2} \hbar\omega \right] \hat{b}_+^\dagger \hat{b}_+ \\ &\quad + \left[\mu\hbar B - \frac{1 - \cos\theta}{2} \hbar\omega \right] \hat{b}_-^\dagger \hat{b}_- \\ &\quad - \frac{\sin\theta}{2} \hbar\omega [\hat{b}_+^\dagger \hat{b}_- + \hat{b}_-^\dagger \hat{b}_+] \end{aligned} \quad (3.37)$$

with

$$v_+(t) = \begin{pmatrix} \cos\frac{1}{2}\theta e^{-i\varphi(t)} \\ \sin\frac{1}{2}\theta \end{pmatrix}, \quad v_-(t) = \begin{pmatrix} \sin\frac{1}{2}\theta e^{-i\varphi(t)} \\ -\cos\frac{1}{2}\theta \end{pmatrix} \quad (3.38)$$

which satisfy $\hat{H}(t)v_{\pm}(t) = \mp \mu\hbar B v_{\pm}(t)$ and the relations

$$\begin{aligned} v_+^\dagger(t)i\frac{\partial}{\partial t}v_+(t) &= \frac{(1 + \cos\theta)}{2} \omega, \\ v_+^\dagger(t)i\frac{\partial}{\partial t}v_-(t) &= \frac{\sin\theta}{2} \omega = v_-^\dagger(t)i\frac{\partial}{\partial t}v_+(t), \\ v_-^\dagger(t)i\frac{\partial}{\partial t}v_-(t) &= \frac{1 - \cos\theta}{2} \omega. \end{aligned} \quad (3.39)$$

We next perform a unitary transformation

$$\begin{pmatrix} \hat{b}_+(t) \\ \hat{b}_-(t) \end{pmatrix} = \begin{pmatrix} \cos\frac{1}{2}\alpha & -\sin\frac{1}{2}\alpha \\ \sin\frac{1}{2}\alpha & \cos\frac{1}{2}\alpha \end{pmatrix} \begin{pmatrix} \hat{c}_+(t) \\ \hat{c}_-(t) \end{pmatrix} \equiv U^T \begin{pmatrix} \hat{c}_+(t) \\ \hat{c}_-(t) \end{pmatrix} \quad (3.40)$$

where U^T stands for the transpose of U . The eigenfunctions are transformed to

$$\begin{pmatrix} w_+(t) \\ w_-(t) \end{pmatrix} = \begin{pmatrix} \cos\frac{1}{2}\alpha & \sin\frac{1}{2}\alpha \\ -\sin\frac{1}{2}\alpha & \cos\frac{1}{2}\alpha \end{pmatrix} \begin{pmatrix} v_+(t) \\ v_-(t) \end{pmatrix} \quad (3.41)$$

or explicitly

$$\begin{aligned} w_+(t) &= \begin{pmatrix} \cos\frac{1}{2}(\theta - \alpha) e^{-i\varphi(t)} \\ \sin\frac{1}{2}(\theta - \alpha) \end{pmatrix}, \\ w_-(t) &= \begin{pmatrix} \sin\frac{1}{2}(\theta - \alpha) e^{-i\varphi(t)} \\ -\cos\frac{1}{2}(\theta - \alpha) \end{pmatrix}. \end{aligned} \quad (3.42)$$

The field variable $\hat{\psi}(t, \vec{x})$ in the second quantization is given by

$$\hat{\psi}(t, \vec{x}) = \sum_{n=\pm} \hat{b}_n(t)v_n(t) = \sum_{n=\pm} \hat{c}_n(t)w_n(t). \quad (3.43)$$

We also have

$$\begin{aligned} w_{\pm}^{\dagger}(t)\hat{H}w_{\pm}(t) &= \mp\mu\hbar B\cos\alpha \\ w_{\pm}^{\dagger}(t)i\hbar\partial_t w_{\pm}(t) &= \frac{\hbar\omega}{2}(1\pm\cos(\theta-\alpha)). \end{aligned} \quad (3.44)$$

If one chooses the constant parameter α in (3.40) as

$$\tan\alpha = \frac{\hbar\omega\sin\theta}{2\mu\hbar B + \hbar\omega\cos\theta} \quad (3.45)$$

or equivalently $2\mu\hbar B\sin\alpha = \hbar\omega\sin(\theta-\alpha)$, one obtains a diagonal effective Hamiltonian

$$\begin{aligned} \hat{H}_{\text{eff}}(t) &= \hat{c}_{+}^{\dagger}(t)\left[-\mu\hbar B\cos\alpha - \frac{\hbar\omega}{2}(1+\cos(\theta-\alpha))\right]\hat{c}_{+}(t) \\ &\quad + \hat{c}_{-}^{\dagger}(t)\left[+\mu\hbar B\cos\alpha - \frac{\hbar\omega}{2}(1-\cos(\theta-\alpha))\right]\hat{c}_{-}(t) \\ &= \sum_{n=\pm} \hat{c}_n^{\dagger}(t)[w_n^{\dagger}(t)\hat{H}w_n(t) - w_n^{\dagger}(t)i\hbar\partial_t w_n(t)]\hat{c}_n(t). \end{aligned} \quad (3.46)$$

The above unitary transformation is time-independent and thus the effective Hamiltonian is not changed $\hat{H}_{\text{eff}}(b_{\pm}^{\dagger}(t), b_{\pm}(t)) = \hat{H}_{\text{eff}}(c_{\pm}^{\dagger}(t), c_{\pm}(t))$.

We thus have the *exact* Schrödinger amplitudes in (2.5)

$$\begin{aligned} \psi_{\pm}(t) &= w_{\pm}(t)\exp\left\{-\frac{i}{\hbar}\left[\mp\mu\hbar B\cos\alpha - \frac{\hbar\omega}{2}(1\pm\cos(\theta-\alpha))\right]t\right\} \\ &= w_{\pm}(t)\exp\left\{-\frac{i}{\hbar}\int_0^t dt[w_{\pm}^{\dagger}(t)\hat{H}w_{\pm}(t) - w_{\pm}^{\dagger}(t)i\hbar\partial_t w_{\pm}(t)]\right\} \end{aligned} \quad (3.47)$$

which satisfy the Schrödinger equation

$$i\hbar\partial_t\psi_{\pm}(t) = \hat{H}(t)\psi_{\pm}(t) \quad (3.48)$$

with the Hamiltonian in (3.35). This equation is directly confirmed for (3.47). The amplitudes in (3.47) are periodic with period $T = \frac{2\pi}{\omega}$ up to a phase, and they are exact and thus valid in a nonadiabatic sense also. From the viewpoint of the diagonalization of the Hamiltonian, we have not completely diagonalized the starting Hamiltonian (3.35) since $w_{\pm}(t)$ carry certain time dependence.

The separation of the “dynamical phase” (the first term in the exponential) and the geometric phase (the second term in the exponential) in (3.47), both of which arise from the effective Hamiltonian, is achieved by varying the parameters in the Hamiltonian, namely, B and ω in the present case. The formula (3.47), however, shows that both the “dynamical phase” and the geometric phase depend on these parameters in a nontrivial way.

We examine two extreme limits:

- (i) For the *adiabatic* limit $\hbar\omega/(\hbar\mu B) \ll 1$, which ensures the diagonal dominance in (3.37), we have from (3.45)

$$\alpha \simeq [\hbar\omega/2\hbar\mu B]\sin\theta. \quad (3.49)$$

If one sets $\alpha = 0$ approximately in the exact solution of the Schrödinger equation (3.47), one recovers the ordinary Berry phase [3]

$$\begin{aligned} \psi_{\pm}(T) &\simeq \exp\{i\pi(1\pm\cos\theta)\} \\ &\quad \times \exp\left\{\pm\frac{i}{\hbar}\int_0^T dt\mu\hbar B\right\}v_{\pm}(T) \end{aligned} \quad (3.50)$$

with $v_{\pm}$ defined in (3.38). The phase factor $\exp\{i\pi(1\pm\cos\theta)\}$ is known to be similar to the phase induced by a magnetic monopole located at the origin of the parameter space.

- (ii) For the other limit, namely, *nonadiabatic* limit $\hbar\mu B/(\hbar\omega) \ll 1$, we have from (3.45)

$$\theta - \alpha \simeq [2\hbar\mu B/\hbar\omega]\sin\theta \quad (3.51)$$

and if one sets $\alpha = \theta$ approximately in the exact solution (3.47), one obtains the trivial geometric phase

$$\psi_{\pm}(T) \simeq w_{\pm}(T)\exp\left\{\pm\frac{i}{\hbar}\int_0^T dt[\mu\hbar B\cos\theta]\right\} \quad (3.52)$$

with

$$w_{+}(t) = \begin{pmatrix} e^{-i\varphi(t)} \\ 0 \end{pmatrix}, \quad w_{-}(t) = \begin{pmatrix} 0 \\ -1 \end{pmatrix}. \quad (3.53)$$

This shows that the monopolelike singularity is smoothly connected to the trivial phase inside the exact solution of the Schrödinger equation, and thus the geometric phase is *topologically trivial* [21].

This example shows that the second quantized formulation is useful not only in formulating a reliable adiabatic approximation but also in allowing an exact treatment in some cases.

IV. CONCLUSION

It has been shown that the adiabatic approximation in the second quantized formulation [21,22] in the sense of an approximate diagonalization of the effective Hamiltonian provides a reliable criterion of the adiabatic approximation. The validity of the approximate diagonal dominance depends on the conditions (2.8) and (2.9). The model of Marzlin and Sanders [2] reminded us of the importance of the crucial conditions (2.8) and (2.9); the appearance of the combination $E_n(t) - \int d^3x v_n^{\dagger}(t, \vec{x})i\hbar\partial_t v_n(t, \vec{x})$ in the

conditions implies that the geometric phase $\int d^3x v_n^\dagger(t, \vec{x}) i\hbar \partial_t v_n(t, \vec{x})$ is in fact a part of the energy eigenvalue.

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