Geometric phases for mixed states and decoherence

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Abstract

The gauge invariance of geometric phases for mixed states is analyzed by using the hidden local gauge symmetry which arises from the arbitrariness of the choice of the basis set defining the coordinates in the functional space. This approach gives a reformulation of the past results of adiabatic, non-adiabatic and mixed state geometric phases. The geometric phases are identified uniquely as the holonomy associated with the hidden local gauge symmetry which is an exact symmetry of the Schrödinger equation. The purification and its inverse in the description of de-coherent mixed states are consistent with the hidden local gauge symmetry. A salient feature of the present formulation is that the total phase and visibility in the mixed state, which are directly observable in the interference experiment, are manifestly gauge invariant.

1 Introduction

The phase is a fundamental notion in quantum mechanics\cite{1, 2}, and the study of geometric phases is an attempt to understand quantum mechanics better. The notion of gauge symmetry or equivalence class plays a basic role in the analysis of geometric phases\cite{3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18}, but its origin in the theory without gauge fields was not clear. It has been recently shown that the gauge symmetry without gauge fields is identified with the hidden local gauge symmetry inherent in the second quantization, namely, the arbitrariness of the phase choice of coordinates in the functional space \cite{19, 20}. To be specific, one has the expansion of the field operator

\[ \hat{\psi}(t, \vec{x}) = \sum_n \hat{b}_n(t) v_n(t, \vec{x}) \]  

(1.1)
which is invariant under the simultaneous transformations, $\hat{b}_n(t) \rightarrow e^{-i\alpha_n(t)}\hat{b}_n(t)$ and $v_n(t, \vec{x}) \rightarrow e^{i\alpha_n(0)}v_n(t, \vec{x})$. For the generic case, we thus have the local symmetry $U = U(1) \times U(1) \times U(1)\ldots$, and in the presence of the degeneracy of basis vectors we have $U = U(n_1) \times U(n_2) \times U(n_3)\ldots \ [19]$. Any formulation should preserve this exact symmetry, and the basic observation is that the Schrödinger amplitude with $\psi_n(0, \vec{x}) = v_n(0, \vec{x})$ is transformed under this symmetry as $\psi_n(t, \vec{x}) \rightarrow e^{i\alpha_n(0)}\psi_n(t, \vec{x})$ independently of $t$ and thus the Schrödinger equation is invariant under this symmetry. It has been shown that both of the adiabatic$^{[19]}$ and non-adiabatic$^{[21]}$ phases are uniquely specified as the holonomy associated with this symmetry, and the adiabatic and non-adiabatic phases are treated on a completely equal footing. This formulation emphasizes that the geometric phases arise from the holonomy of the basis vectors rather than from the holonomy of the Schrödinger amplitudes. The basic aspects of the hidden local symmetry are summarized in Appendix A.

The definitions of geometric phases in mixed states have been proposed by several authors$^{[22,23]}$, and it appears that the direct connection of the geometric phase with the geometrical picture of the motion of the polarization vector, for example, is lost. The gauge symmetries and associated holonomy in the geometric phases for mixed states have also been discussed$^{[22,23,24,25,26]}$, but the quantities invariant under the gauge symmetries discussed so far are non-linear (to be precise, not bi-linear) in the Schrödinger amplitudes, and the total phase and visibility which are directly observable in the interference experiment$^{[23]}$ are not invariant under the gauge symmetries discussed so far.

In the present paper, we analyze the gauge invariance of geometric phases for mixed states from the point of view of the hidden gauge symmetry explained above for pure states. We discuss the geometric phases for mixed states proposed in$^{[23]}$, which are direct generalizations of geometric phases in pure states. The geometric phases thus defined are known to be an intrinsic property of the mixed states without referring to the ancilla subsystem$^{[24,25]}$. On the other hand, the geometric phases proposed in$^{[22]}$ are based on the “purification” and crucially depend on the ancilla part$^{[24,25]}$; these geometric phases may have some implications in quantum information, for example, but we forgo their analysis. Our basic observation is that an exact treatment of the Schrödinger equation automatically contains all the geometric phases which are uniquely identified as the holonomy associated with the hidden local symmetry, without going through an analysis of the projective Hilbert space. More importantly, the total phase and visibility which are directly observable in the interference experiment$^{[23]}$ are manifestly invariant under the hidden local gauge symmetry.
2 Geometric phases in mixed states

2.1 Conventional formulation

In the conventional formulation of geometric phases it is customary to classify the geometric phases into adiabatic and non-adiabatic ones. In connection with the geometric phase for mixed states, we first briefly summarize the customary analysis of non-adiabatic phase which starts with \[9\]

\[
\nonumber i\hbar \partial_t \psi(t, \vec{x}) = \dot{H}(t)\psi(t, \vec{x}), \quad \int d^3 x \psi^\dagger(t, \vec{x})\psi(t, \vec{x}) = 1 \quad (2.1)
\]

and the cyclic evolution is defined by

\[
\psi(T, \vec{x}) = e^{i\phi}\psi(0, \vec{x}) \quad (2.2)
\]

with a constant \(\phi\).

The equivalence class of state vectors, i.e., “projective Hilbert space”, is defined by \[9, 12\]

\[
\{e^{i\alpha(t)}\psi(t, \vec{x})\}, \quad (2.3)
\]

and we have an equivalence class of Hamiltonians

\[
\{\dot{H}(t) - \hbar \partial \alpha(t)\} \quad (2.4)
\]

with an arbitrary function \(\alpha(t)\) to maintain the Schrödinger equation. The total phase of the cyclic evolution is given by

\[
\phi_T = \arg\psi^\dagger(0, \vec{x})\psi(T, \vec{x}) = \arg\psi^\dagger(0, \vec{x})U(t)\psi(0, \vec{x}) \quad (2.5)
\]

with

\[
U(t) = T^* \exp\left[-\frac{i}{\hbar} \int_0^t \dot{H}(t) dt\right] \quad (2.6)
\]

where \(T^*\) stands for the time ordering operation. Note that the total phase is not invariant under the equivalence class (2.3). One may then define the “dynamical phase” by

\[
\phi_D = -\frac{1}{\hbar} \int_0^T dt \int d^3 x \psi^\dagger(t, \vec{x})\dot{H}(t)\psi(t, \vec{x}) = -i \int_0^T dt \int d^3 x \psi^\dagger(t, \vec{x})\partial_t \psi(t, \vec{x}). \quad (2.7)
\]
The non-adiabatic phase defined by the difference of $\phi_T$ and $\phi_D$

\[ \phi_G = \arg \psi \dagger (0, \vec{x}) \psi (T, \vec{x}) + \frac{1}{\hbar} \int_0^T dt \int d^3 x \psi \dagger (t, \vec{x}) \hat{H} (t) \psi (t, \vec{x}) \]

\[ = \arg \psi \dagger (0, \vec{x}) \mathcal{U} (t) \psi (0, \vec{x}) + i \int_0^T dt \int d^3 x \psi \dagger (0, \vec{x}) \mathcal{U} (t) \dot{\mathcal{U}} (t) \psi (0, \vec{x}) \]  

(2.8)

is invariant under the equivalence class (2.3) and (2.4). This is customarily called the gauge invariance condition of non-adiabatic phase.

By using the equivalence class, one may choose a representative $\bar{\psi} (t, \vec{x}) = e^{i \alpha (t)} \psi (t, \vec{x})$ to satisfy the parallel transport condition

\[ i \int d^3 x \bar{\psi} \dagger (t, \vec{x}) \partial_t \bar{\psi} (t, \vec{x}) = i \int d^3 x \psi \dagger (t, \vec{x}) \partial_t \psi (t, \vec{x}) - \partial_t \alpha (t) = 0 \]  

(2.9)

namely,

\[ \bar{\psi} (t, \vec{x}) = \exp \left[ i \int_0^t dt \int d^3 x \psi \dagger (t, \vec{x}) \partial_t \psi (t, \vec{x}) \right] \psi (t, \vec{x}). \]  

(2.10)

For this $\bar{\psi} (t, \vec{x})$, which is non-linear in the Schrödinger amplitude, the non-adiabatic phase for the pure state is given by

\[ \phi_G = \arg \bar{\psi} \dagger (0, \vec{x}) \bar{\psi} (T, \vec{x}) = \arg \left\{ \psi \dagger (0, \vec{x}) \exp \left[ i \int_0^T dt \int d^3 x \psi \dagger (t, \vec{x}) i \partial_t \psi (t, \vec{x}) \right] \psi (T, \vec{x}) \right\}. \]  

(2.11)

This quantity is confirmed to be invariant under the gauge transformation, and $\phi_G$ stands for the holonomy of the vector $\bar{\psi} (t, \vec{x})$ for cyclic evolution.

In the case of the mixed state described by the density matrix $\rho (t) = \mathcal{U} (t) \rho (0) \mathcal{U} (t) \dagger$, the interference pattern is given by

\[ I \propto 1 + |\text{Tr} \mathcal{U} (T) \rho (0)| \cos \left[ \chi - \arg \text{Tr} \mathcal{U} (T) \rho (0) \right] \]  

(2.12)

where $\chi$ stands for the variable $U (1)$ phase in one of the interference beams. The total phase of the mixed state is thus given by

\[ \gamma_T = \arg \text{Tr} \mathcal{U} (T) \rho (0). \]  

(2.13)

In a basis where the density matrix is written as

\[ \rho (0) = \sum_{k=1}^N \omega_k \langle k | k \rangle \]  

(2.14)
the total phase is written as
\[ \gamma_T = \sum_{k=1}^{N} \omega_k \text{arg}[(k|U(T)|k)]. \] (2.15)

The parallel transport condition for a mixed state is imposed by requiring that \( \text{Tr} \rho(t) U(t + dt) U(t)\dagger \) be real and positive which in turn leads to
\[ \text{Tr} \rho(t) \dot{U}(t) U(t)\dagger = \text{Tr} \rho(0) U(t)\dagger \dot{U}(t) = 0 \] (2.16)

or equivalently
\[ \sum_{k=1}^{N} \omega_k \langle k|U(t)\dagger \dot{U}(t)|k \rangle = 0. \] (2.17)

Under this condition, the “dynamical phase” defined by
\[ \gamma_D = -\frac{1}{\hbar} \int_0^T dt \text{Tr}[\rho(t) \dot{H}(t)] = -i \int_0^T dt \text{Tr}[\rho(0) U(t)\dagger \dot{U}(t)] \] (2.18)

vanishes identically. It has also been asserted [23] that the condition (2.16) or (2.17) while necessary, is not sufficient. Instead, the stronger conditions [27]
\[ \langle k|U(t)\dagger \dot{U}(t)|k \rangle = 0, \quad k = 1, 2, \ldots N \] (2.19)

have been proposed; all the constituent pure states in the mixed state are required to be parallel transported independently.

To understand the prescription (2.19), it is convenient to analyze the N-state density matrix in the diagonal basis. On may then consider the transformation [26]
\[ U(t) \rightarrow U'(t) = U(t) \sum_k e^{i\theta_k(t)} |k\rangle \langle k| \] (2.20)

then the orbit of the density matrix remains unchanged
\[ \rho(0) \rightarrow \rho'(t) = U'(t)\rho(0) U'(t)\dagger = U(t)\rho(0) U(t)\dagger = \rho(t). \] (2.21)

The total phase is then transformed as
\[ \gamma_T \rightarrow \gamma'_T = \text{arg}\{\text{Tr}[\rho(0) U'(T)]\} = \text{arg}\{\sum_k \omega_k \langle k|U(T)|k \rangle e^{i\theta_k(T)}\} \] (2.22)
while the “dynamical phase” is transformed as

\[
\gamma_D \rightarrow \gamma'_D = -i \int_0^T dt \text{Tr}[\rho(0)U'(t)^\dagger \dot{U}'(t)]
\]

\[
= -i \int_0^T dt \text{Tr}[\rho(0)U(t)^\dagger \dot{U}(t)] + \sum_k \omega_k (\theta_k(T) - \theta_k(0)).
\]  

(2.23)

The simple subtraction of the "dynamical phase" from the total phase does not give a result invariant under the above transformation for the general non-degenerate mixed state.

To alleviate this gauge non-invariance, a manifestly gauge invariant expression

\[
\gamma_G[U] = \text{arg}\left\{ \sum_k \omega_k \langle k|U(T)|k\rangle \exp\left\{ i \int_0^T dt \langle k|U(t)^\dagger \dot{U}(t)|k\rangle \right\} \right\}
\]

(2.24)

has been proposed \[26\]. When the stronger condition (2.19) is imposed, this expression of \(\gamma_G[U]\) agrees with the total phase.

We note that the expression for \(\gamma_G[U]\) (2.24) is written as

\[
\gamma_G[U] = \text{arg}\left\{ \sum_k \omega_k [\psi_k^\dagger(0)\psi_k(T) \exp\left\{ i \int_0^T dt \psi_k^\dagger(t) i\partial_t \psi_k(t) \right\}] \right\}
\]

(2.25)

in terms of the Schrödinger amplitudes defined by \(\psi_k(t) = U(t)|k\rangle\) which satisfy

\[
i\hbar \partial_t \psi_k(t) = \hat{H}(t)\psi_k(t), \quad k = 1 \sim N.
\]  

(2.26)

The formula for \(\gamma_G[U]\), which is non-linear (to be precise, not bi-linear) in the Schrödinger amplitudes, is thus a direct generalization of (2.11) for a pure state, and it is invariant under the transformation (2.20), namely, the equivalence class

\[
\{ e^{i\theta_k(t)}\psi_k(t) \}, \quad k = 1 \sim N.
\]  

(2.27)

Note that \(\gamma_G[U]\) is also written as

\[
\gamma_G[U] = \text{arg}\left\{ \sum_k \omega_k [\psi_k^\dagger(0)\psi_k(T) \exp\left\{ \frac{i}{\hbar} \int_0^T dt \psi_k^\dagger(t) \hat{H}(t)\psi_k(t) \right\}] \right\}
\]

(2.28)

and thus one implicitly assumes the equivalence class of Hamiltonians

\[
\{ \hat{H}(t) - \hbar \partial_t \theta_k(t) \}, \quad k = 1 \sim N
\]  

(2.29)
for each state $\psi_k(t)$ separately corresponding to (2.27).

The stronger condition (2.19) is written as

$$
\psi_k^\dagger(t) i\hbar \partial_t \psi_k(t) = \psi_k^\dagger(t) \hat{H}(t) \psi_k(t) = 0, \quad k = 1 \sim N.
$$

(2.30)

The Schrödinger equation (2.26) is, however, not maintained under the gauge transformation (2.27) except for the case

$$
\partial_t \theta_1(t) = ... = \partial_t \theta_N(t).
$$

(2.31)

For this special case, the modified Schrödinger equation

$$
i\hbar \partial_t \psi'_k(t) = \hat{H}'(t) \psi'_k(t), \quad k = 1 \sim N
$$

(2.32)

with $\psi'_k(t) = e^{i\theta_k(t)} \psi_k(t)$ and the $k$-independent $\hat{H}'(t) = \hat{H}(t) - \hbar \partial_t \theta_k(t)$ is satisfied. All the pure states in the density matrix in quantum statistical mechanics, for example, are specified by a single Hamiltonian, and thus the expression of the partition function $\text{Tr} e^{-\beta \hat{H}}$ is valid. One may impose the same constraint on the density matrix in the present case also, and thus the condition (2.31); the universal Hamiltonian for all the pure states and the gauge invariance requirement (2.27) are not compatible. The interpretation of the geometric phase (2.25) as the holonomy associated with the gauge transformation (2.27), which is a direct generalization of (2.11), is not compatible with the universal Hamiltonian. It is also significant that the physical observable (2.12) which is expressed in terms of the total phase and visibility $|\text{Tr} [\rho(0) \mathcal{U}(T)]|$ is not gauge invariant as is shown in (2.22).

### 2.2 A new formulation

We start with a given hermitian Hamiltonian $\hat{H}(t)$ and thus given $\mathcal{U}(t) = T^* \exp[-i/\hbar \int_0^t \hat{H}(t) dt]$ in (2.6). We employ a diagonal form of the density matrix

$$
\rho(0) = \sum_k \omega_k |k\rangle \langle k|, \quad \langle k|l\rangle = \delta_{k,l}
$$

(2.33)

and observe that

$$
\psi'_k(t) = \delta_{k,l}
$$

(2.34)

for $\psi_k(t) = \mathcal{U}(t) |k\rangle$ in (2.26). We then have the total phases for pure states $\psi_k(t)$ as

$$
\phi_k(t) = \text{arg} \psi'_k(0) \psi_k(t).
$$

(2.35)
The complete set of basis vectors \( \{ v_k(t) \} \) in Appendix A may then be chosen as

\[
v_k(t) = e^{-i\phi_k(t)}\psi_k(t), \quad v_k^\dagger(t)v_l(t) = \delta_{k,l}. \tag{2.36}
\]

Note that

\[
v_k^\dagger(0)v_k(t) = \text{real and positive} \quad (2.37)
\]

in the present definition.

In the general \( \vec{x} \)-dependent case, we define the Schrödinger amplitudes by

\[
\psi_k(t,\vec{x}) = \langle \vec{x}|U(t)|k \rangle = \int d^3 y \langle \vec{x}|U(t)|\vec{y} \rangle v_k(0,\vec{y}) \tag{2.38}
\]

and \( v_k(t,\vec{x}) = e^{-i\phi_k(t)}\psi_k(t,\vec{x}) \). We can also write the Schrödinger amplitudes as

\[
\psi_k(t,\vec{x}) = v_k(\vec{x},t)
\]

\[
\times \exp\left\{ -\frac{i}{\hbar} \int_0^t \left[ \int d^3 x v_k^\dagger(\vec{x},t)\hat{H}(t)v_k(\vec{x},t) - \langle k|ih\frac{\partial}{\partial t}|k \rangle \right] \right\}
\]

with

\[
\langle k|ih\frac{\partial}{\partial t}|k \rangle \equiv \int d^3 x v_k^\dagger(\vec{x},t)ih\frac{\partial}{\partial t}v_k(\vec{x},t). \tag{2.40}
\]

The Schrödinger amplitudes in (2.39) are non-linear in the basis vectors, but the non-linearity of the probability amplitudes in the basis vectors is common in field theory. The existence of a hidden local symmetry in \( \psi_k(t,\vec{x}) \) becomes clear in the second quantized formulation, where the field operator is expanded by using the basis vectors in (2.36)

\[
\hat{\psi}(t,\vec{x}) = \sum_k \hat{b}_k(t)v_k(t,\vec{x}) \tag{2.41}
\]

and the effective Hamiltonian in (A.4) is given by

\[
\hat{H}_{\text{eff}}(t) = \sum_n \hat{b}_n^\dagger(t)[\int d^3 x v_n^\dagger(\vec{x},t)\hat{H}(t)v_n(\vec{x},t)
\]

\[
-\langle n|ih\frac{\partial}{\partial t}|n \rangle|\hat{b}_n(t) \tag{2.42}
\]

which is diagonal. The operator \( \hat{\psi}(t,\vec{x}) \) is invariant under the hidden local gauge symmetry

\[
v_k(\vec{x},t) \to e^{i\alpha_k(t)}v_k(\vec{x},t), \quad \hat{b}_k(t) \to e^{-i\alpha_k(t)}\hat{b}_k(t) \tag{2.43}
\]
with a general function $\alpha_k(t)$. Any formulation should preserve this exact symmetry. The Schrödinger amplitude $\psi_k(t, \vec{x})$ in (2.39) is transformed under the hidden local symmetry as

$$\psi_k(t, \vec{x}) \rightarrow e^{i\alpha_k(0)}\psi_k(t, \vec{x})$$

(2.44)

independently of $t$ and thus the Schrödinger equation with a fixed Hamiltonian is invariant under the hidden local symmetry. This property is clearly seen in the general expression (A.6) in Appendix. The difference between the equivalence class (2.27) and the present hidden local gauge symmetry is obvious. From the point of view of the hidden local symmetry, the condition (2.37) is realized by a specific choice of the hidden local gauge.

The quantity $\text{Tr}U(T)\rho(0)$ appearing in (2.12) is then written as

$$\text{Tr}U(T)\rho(0) = \sum_k \omega_k \psi_k^\dagger(0, \vec{x})\psi_k(T, \vec{x})$$

$$= \sum_k \omega_k v_k^\dagger(0, \vec{x})v_k(T, \vec{x}) \exp\left\{\frac{i}{\hbar} \int_0^T dt d^3x [v_k^\dagger(t, \vec{x})i\hbar \partial_t v_k(t, \vec{x})$$

$$-v_k^\dagger(t, \vec{x})\hat{H}(t)v_k(t, \vec{x})]\right\}$$

(2.45)

by using the density matrix $\rho(0) = \sum_k \omega_k \psi_k(0, \vec{x})\psi_k^\dagger(0, \vec{x})$. This quantity is manifestly invariant under the hidden local symmetry with a fixed Hamiltonian, and thus not only the total phase (2.15) but also the visibility $|\text{Tr}U(T)\rho(0)|$ in (2.12) are invariant. This expression of $\text{Tr}U(T)\rho(0)$ contains the holonomy

$$\bar{v}_k^\dagger(0, \vec{x})\bar{v}_k(T, \vec{x})$$

(2.46)

for

$$\bar{v}_k(t, \vec{x}) = v_k(t, \vec{x}) \exp\left\{\frac{i}{\hbar} \int_0^t dt \langle k |i\hbar \partial_t |k\rangle\right\}.$$  

(2.47)

This holonomy is fixed by the hidden local symmetry. If one considers $\bar{v}_k(t, \vec{x}) = e^{i\alpha_k(t)}v_k(t, \vec{x})$ by using the hidden local symmetry, the parallel transport condition

$$\int d^3x \bar{v}_k^\dagger(t, \vec{x})i\hbar \partial_t \bar{v}_k(t, \vec{x}) = 0$$

(2.48)

fixes $\alpha_k(t)$ as in (2.47).

If all the pure states perform cyclic evolution with the same period $T$, one can choose the hidden local gauge such that

$$v_k^\dagger(0, \vec{x})v_k(T, \vec{x}) = \text{real and positive}$$

(2.49)
for all $k$, and the exponential factor in (2.45) exhibits the entire geometrical phase together with the “dynamical phase” $(1/\hbar) \int_0^T dt d^3x v_k^\dagger(t, \vec{x}) \hat{H}(t)v_k(t, \vec{x})$ of each pure state. In the case of the cyclic evolution, one can use the formula (2.45) for the spatial interference pattern analogous to the Aharonov-Bohm phase. In practice, the cyclic evolution of all the pure states $\psi_k(t)$ with a period $T$ may be rather exceptional. For a generic case, we need to define the total phase for non-cyclic evolution \cite{12} as the phase of

$$\text{Tr} \mathcal{U}(T) \rho(0) = \sum_k \omega_k \int d^3x v_k^\dagger(0, \vec{x}) \psi_k(T, \vec{x})$$

$$= \sum_k \omega_k \int d^3x v_k^\dagger(0, \vec{x})v_k(T, \vec{x})$$

$$\times \exp\left\{ \frac{i}{\hbar} \int_0^T dt d^3x [v_k^\dagger(t, \vec{x})i\hbar \partial_t v_k(t, \vec{x}) - v_k^\dagger(t, \vec{x}) \hat{H}(t)v_k(t, \vec{x})] \right\}.$$ 

where we included the integration over the spatial coordinates $\vec{x}$ in the trace by following the analysis in \cite{19}. Note that (2.37), which is realized by a suitable choice of the hidden local gauge, is written in the present notation as $\int d^3x v_k^\dagger(0, \vec{x})v_k(t, \vec{x}) = \text{real and positive.}$

A salient feature of the present formulation is that the total phase and visibility in (2.45) or (2.50), which are the direct observables in the interference experiment \cite{23}, are gauge invariant, and the geometric phase arises from the holonomy of the basis vectors rather than from the Schrödinger amplitudes. The Schrödinger equation is invariant under the hidden local symmetry with a fixed Hamiltonian. The parallel transport condition on the Schrödinger amplitudes constrains the Hamiltonian as in (2.30), whereas the parallel transport of the basis vectors is realized without any constraint on the Hamiltonian as in (2.47). In the present formulation, the geometric phase is analyzed on the basis of a given general Hamiltonian instead of imposing constraints on the Hamiltonian, which is in accord with the original idea of the non-adiabatic phase \cite{9,12}. For some applications in quantum information \cite{28,29,30,31,32}, for example, one may be interested in the inverse, namely, in finding a Hamiltonian which reproduces a given density matrix \cite{33}. In such a case, one may impose the condition (2.30) also. In any case, if the stronger condition (2.30) happens to be satisfied for a specific Hamiltonian, our formula for the total phase gives the geometric phase which is the same as in the past formulation.
3 Example: Spin polarization

We analyze a simple example described by a time dependent Hamiltonian
\[ \hat{H} = -\mu \hbar \vec{B}(t) \vec{\sigma}, \]
\[ \vec{B}(t) = B(\sin \theta \cos \varphi(t), \sin \theta \sin \varphi(t), \cos \theta) \quad (3.1) \]
where \( \varphi(t) = \omega t \) with constant \( \omega, B \) and \( \theta \). The effective Hamiltonian in (A.4) then becomes
\[ \hat{H}_{\text{eff}}(t) = \left[ -\mu \hbar B - \frac{(1 + \cos \theta)}{2} \hbar \omega \hat{b}_+^\dagger \hat{b}_+ + [\mu \hbar B - \frac{1 - \cos \theta}{2} \hbar \omega] \hat{b}_-^\dagger \hat{b}_- \right. \]
\[ \left. - \frac{\sin \theta}{2} \hbar \omega [\hat{b}_+^\dagger \hat{b}_- + \hat{b}_-^\dagger \hat{b}_+] \right] \quad (3.2) \]
if one uses the basis set
\[ v_+(t) = \begin{pmatrix} \cos \frac{1}{2} \theta e^{-i\varphi(t)} \\ \sin \frac{1}{2} \theta \end{pmatrix}, \quad v_-(t) = \begin{pmatrix} \sin \frac{1}{2} \theta e^{-i\varphi(t)} \\ -\cos \frac{1}{2} \theta \end{pmatrix} \quad (3.3) \]
which satisfy \( \hat{H}(t)v_+(t) = \mp \mu \hbar B v_+(t) \) and the relations
\[ v^+_i(t) i \frac{\partial}{\partial t} v_+(t) = \frac{(1 + \cos \theta)}{2} \hbar \omega \]
\[ v^+_i(t) i \frac{\partial}{\partial t} v_-(t) = \frac{\sin \theta}{2} \hbar \omega v_+(t) \]
\[ v^-_i(t) i \frac{\partial}{\partial t} v_-(t) = \frac{1 - \cos \theta}{2} \hbar \omega. \quad (3.4) \]
The above effective Hamiltonian (3.2) is not diagonal, and thus quantum state mixing takes place if one uses the basis set \( v_\pm(t) \). We thus perform a unitary transformation
\[ \begin{pmatrix} \hat{b}_+ \quad \hat{b}_- \end{pmatrix} = \begin{pmatrix} \cos \frac{1}{2} \alpha & -\sin \frac{1}{2} \alpha \\ \sin \frac{1}{2} \alpha & \cos \frac{1}{2} \alpha \end{pmatrix} \begin{pmatrix} \hat{c}_+ \quad \hat{c}_- \end{pmatrix} \]
\[ \equiv U^T \begin{pmatrix} \hat{c}_+ \quad \hat{c}_- \end{pmatrix} \quad (3.5) \]
where \( U^T \) stands for the transpose of \( U \). The eigenfunctions are transformed to
\[ \begin{pmatrix} w_+ \quad w_- \end{pmatrix} = U \begin{pmatrix} v_+ \quad v_- \end{pmatrix} \]
\[ = \begin{pmatrix} \cos \frac{1}{2} \alpha & -\sin \frac{1}{2} \alpha \\ -\sin \frac{1}{2} \alpha & \cos \frac{1}{2} \alpha \end{pmatrix} \begin{pmatrix} v_+ \quad v_- \end{pmatrix} \quad (3.6) \]
or explicitly
\[
    w_+(t) = \left( \frac{\cos \frac{1}{2}(\theta - \alpha)e^{-i\psi(t)}}{\sin \frac{1}{2}(\theta - \alpha)} \right), \quad w_-(t) = \left( \frac{\sin \frac{1}{2}(\theta - \alpha)e^{-i\psi(t)}}{-\cos \frac{1}{2}(\theta - \alpha)} \right). \quad (3.7)
\]

The field variable \( \hat{\psi}(t, \vec{x}) \) in second quantization is given by
\[
    \hat{\psi}(t, \vec{x}) = \sum_{n=\pm} \hat{b}_n(t) v_n(t)
\]
\[
    = \sum_{n=\pm} \hat{c}_n(t) w_n(t) \quad (3.8)
\]

which is invariant under the hidden local symmetry
\[
    w_n(t) \rightarrow e^{i\alpha} w_n(t), \quad \hat{c}_n(t) \rightarrow e^{-i\alpha} \hat{c}_n(t). \quad (3.9)
\]

We also have
\[
    w_\pm(t) \hat{H} w_\pm(t) = \mp \mu \hbar H \cos \alpha
\]
\[
    w_\pm(t) \hbar \partial_t w_\pm(t) = \frac{\hbar \omega}{2} (1 \pm \cos(\theta - \alpha)). \quad (3.10)
\]

If one chooses the parameter \( \alpha \) in (3.5) as
\[
    \tan \alpha = \frac{\hbar \omega \sin \theta}{2 \mu \hbar B + \hbar \omega \cos \theta} \quad (3.11)
\]

or equivalently \( 2 \mu \hbar B \sin \alpha = \hbar \omega \sin(\theta - \alpha) \), one obtains a diagonal effective Hamiltonian \[21\]
\[
    \hat{H}_{\text{eff}}(t) = \sum_{n=\pm} \hat{c}_n^\dagger \left[ \mp \mu \hbar B \cos \alpha - \frac{\hbar \omega}{2} (1 \pm \cos(\theta - \alpha)) \right] \hat{c}_n
\]
\[
    = \sum_{n=\pm} \hat{c}_n^\dagger \left[ w_\pm(t) \hat{H} w_\pm(t) - w_\pm(t) \hbar \partial_t w_\pm(t) \right] \hat{c}_n \quad (3.12)
\]

and thus the quantum state mixing is avoided. 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 have the Schrödinger amplitudes with initial conditions \( \psi_\pm(0) = w_\pm(0) \) as (see (A.7) in Appendix)
\[
    \psi_\pm(t) = w_\pm(t) \exp \left\{ -\frac{i}{\hbar} \left[ \mp \mu \hbar B \cos \alpha - \frac{\hbar \omega}{2} (1 \pm \cos(\theta - \alpha)) \right] t \right\}
\]
\[
    = w_\pm(t) \exp \left\{ -\frac{i}{\hbar} \int_0^t dt [w_\pm(t) \hat{H} w_\pm(t) - w_\pm(t) \hbar \partial_t w_\pm(t)] \right\} \quad (3.13)
\]
These expressions are periodic with a period $T = \frac{2\pi}{\omega}$ up to a phase by noting $w_\pm(0) = w_\pm(T)$, and they are exact. From the point of view of the diagonalization of the Hamiltonian, we have not completely diagonalized the Hamiltonian since $w_\pm(t)$ carry certain time-dependence. These formulas $\psi_\pm(t)$ are invariant under the hidden local symmetry (3.9) up to a constant phase factor, $\psi_\pm(t) \rightarrow e^{ia\pm(\theta)}\psi_\pm(t)$, and the geometric phase is identified by means of the analysis of hidden local symmetry as the phase of

$$\exp\left\{-\frac{i}{\hbar} \int_0^T dt [ - w_\pm(t) i \hbar \partial_t w_\mp(t) ] \right\} = \exp\left\{-i\pi (1 \mp \cos(\theta - \alpha)) \right\}$$

(3.14)

up to $2n\pi$.

One can measure $\psi_+^\dagger(0)\psi_+(T)$, for example, which is manifestly invariant under the hidden local symmetry by the interference in

$$\frac{1}{2} |\psi_+(T) + \psi_+(0)|^2 = |\psi_+(0)|^2 + \text{Re} \psi_+^\dagger(0)\psi_+(T)$$

$$= 1 + \cos[(\mu B \cos \alpha)T - \frac{1}{2} \Omega_+]$$

(3.15)

where

$$\Omega_+ = 2\pi [1 - \cos(\theta - \alpha)]$$

(3.16)

stands for the solid angle subtended by $w_+^\dagger(t)\vec{\sigma}w_+(t)$ by noting

$$w_+^\dagger(t)\vec{\sigma}w_+(t) = (\sin(\theta - \alpha) \cos \varphi, \sin(\theta - \alpha) \sin \varphi, \cos(\theta - \alpha))$$

$$= -w_-^\dagger(t)\vec{\sigma}w_-(t).$$

(3.17)

The separation of the non-adiabatic phase $\frac{1}{2} \Omega_+$ and the “dynamical phase” $(\mu B \cos \alpha)T$ in (3.15) is achieved by varying the parameters in the Hamiltonian, namely, $B$, $\omega$ and $\theta$. In passing, we note that the non-adiabatic phase $\frac{1}{2} \Omega_+$ in (3.16) (or non-adiabatic phase in general) is topologically trivial [21] and thus the stability argument on the basis of topology is not used.

To define the basis set to represent any state $|k\rangle$ of the initial density matrix
\[ \rho(0) = \sum |k\rangle \langle k| \text{ in } (2.33), \text{ one may define linear combinations} \]

\[
\Psi_+(t) = \cos \frac{\Theta}{2} \psi_+(t) + \sin \frac{\Theta}{2} \psi_-(t) \\
= \tilde{w}_+(t) \exp \left\{ - \frac{i}{\hbar} \left[ -2\mu B \cos \alpha - \frac{\hbar \omega}{2} (1 + \cos(\theta - \alpha)) \right] t \right\} \\
= \tilde{w}_+(t) \exp \left\{ - \frac{i}{\hbar} \int_0^t dt \left[ \tilde{w}^\dagger_+(t) \hat{H} \tilde{w}_+(t) - \tilde{w}^\dagger_+(t) i\hbar \partial_t \tilde{w}_+(t) \right] \right\}, \\
\Psi_-(t) = - \sin \frac{\Theta}{2} \psi_+(t) + \cos \frac{\Theta}{2} \psi_-(t) \\
= \tilde{w}_-(t) \exp \left\{ - \frac{i}{\hbar} \left[ -2\mu B \cos \alpha + \frac{\hbar \omega}{2} (1 - \cos(\theta - \alpha)) \right] t \right\} \\
= \tilde{w}_-(t) \exp \left\{ - \frac{i}{\hbar} \int_0^t dt \left[ \tilde{w}^\dagger_-(t) \hat{H} \tilde{w}^\dagger_-(t) - \tilde{w}^\dagger_-(t) i\hbar \partial_t \tilde{w}^\dagger_-(t) \right] \right\} \quad (3.18)
\]

where

\[
\tilde{w}_+(t) = \cos \frac{\Theta}{2} w_+(t) + \sin \frac{\Theta}{2} w_-(t) \exp \left\{ - \frac{i}{\hbar} \left[ 2\mu B \cos \alpha + \hbar \omega \cos(\theta - \alpha) \right] t \right\}, \\
\tilde{w}_-(t) = - \sin \frac{\Theta}{2} w_+(t) \exp \left\{ \frac{i}{\hbar} \left[ 2\mu B \cos \alpha + \hbar \omega \cos(\theta - \alpha) \right] t \right\} + \cos \frac{\Theta}{2} \tilde{w}_-(t) \quad (3.19)
\]

These \( \Psi_\pm(t) \) satisfy the Schrödinger equation, and one can represent any initial state \( |k\rangle \) by choosing \( \Theta \) suitably. The basis vectors \( \tilde{w}_\pm(t) \) satisfy \( \tilde{w}^\dagger_\pm(t) \tilde{w}_\mp(t) = \delta_{n,m} \) and

\[
\tilde{w}^\dagger_\pm(t) \hat{H} \tilde{w}_\pm(t) = \mp \mu B \left[ \cos \alpha \cos \Theta - \sin \alpha \sin \Theta \cos \beta(t) \right], \\
\tilde{w}^\dagger_\pm(t) i\hbar \partial_t \tilde{w}_\pm(t) = \pm \mu B \left[ \cos \alpha \left( 1 - \cos \Theta \right) + \sin \alpha \sin \Theta \cos \beta(t) \right] \\
+ \frac{\hbar \omega}{2} \left( 1 \pm \cos(\theta - \alpha) \right) \quad (3.20)
\]

where \( \beta(t) = \left[ 2\mu B \cos \alpha + \omega \cos(\theta - \alpha) \right] t \).

The basis set \( \tilde{w}_\pm(t) \) are not periodic in general, and they are periodic with a period \( T \) only when

\[
T \omega = 2\pi n, \\
T \left[ 2\mu B \cos \alpha + \omega \cos(\theta - \alpha) \right] = 2\pi m \quad (3.21)
\]

with two integers \( n \) and \( m \). Related to this property, the geometric phase for a pure state \( \Psi_+(t) \), for example,

\[
\Psi_+^\dagger(0) \Psi_+(T) = \tilde{w}^\dagger_+(0) \tilde{w}_+(T) \\
\times \exp \left\{ - \frac{i}{\hbar} \int_0^T dt \left[ \tilde{w}^\dagger_+(t) \hat{H} \tilde{w}_+(t) - \tilde{w}^\dagger_+(t) i\hbar \partial_t \tilde{w}_+(t) \right] \right\} \quad (3.22)
\]
arises not only from the phase factor, \textit{i.e.}, the second term on the exponential but also from the pre-factor $\tilde{w}_+(0)\tilde{w}_+(T)$ for a general $T$ which does not satisfy (3.21). One may utilize the hidden local gauge symmetry $\tilde{w}_+(t) \to e^{i\tilde{\alpha}(t)}\tilde{w}_+(t)$, under which the quantity (3.22) is invariant, to make the pre-factor $\tilde{w}_+(0)\tilde{w}_+(T)$ real and positive, and then only the phase factor on the exponential contributes to the geometric phase.

3.1 Mixed states

We study a specific density matrix defined by a pure state in (3.18)

$$\rho(t) = |\Psi_+(t)\rangle\langle\Psi_+(t)|$$ (3.23)

which is not cyclic in general. The density matrix for a mixed state may be defined by

$$\rho_{mix}(t) = \cos^2 \Theta |\psi_+(0)\rangle\langle\psi_+(T)| + \sin^2 \Theta |\psi_-(0)\rangle\langle\psi_-(T)|$$ (3.24)

by assuming the de-coherence of $\psi_\pm(t)$, and $\rho_{mix}(t)$ is cyclic with a period $T$.

The total phase may be defined as the phase of

$$\text{Tr}\{T^* e^{-\frac{i}{\hbar} \int_0^T dt\hat{H}(t)\rho_{mix}(0)}\}$$

$$= \cos^2 \Theta |\psi_+(0)\rangle\langle\psi_+(T)| + \sin^2 \Theta |\psi_-(0)\rangle\langle\psi_-(T)|$$ (3.25)

$$= \cos^2 \Theta \tilde{w}_+(0)w_+(T) \exp\{-\frac{i}{\hbar} \int_0^T dt[w^\dagger_+(t)\hat{H}w_+(t) - w^\dagger_+(t)i\hbar\partial_tw_+(t)]\}
+ \sin^2 \Theta \tilde{w}_-(0)w_-(T) \exp\{-\frac{i}{\hbar} \int_0^T dt[w^\dagger_-(t)\hat{H}w_-(t) - w^\dagger_-(t)i\hbar\partial_tw_-(t)]\}$$

which is manifestly invariant under the hidden local symmetry $w_\pm(t) \to e^{i\alpha(t)}w_\pm(t)$ and one can uniquely identify the geometric phase for each pure state $\psi_\pm(t)$. In the present case, one can in principle distinguish the geometric phase from the “dynamical phase” contained in the total phase by varying the parameters $T = 2\pi/\omega$, $B$, $\theta$ and the angle $\Theta$. See also [29, 30, 31]. Note that we can in principle separate the geometric phase and the “dynamical phase” by varying the parameters $T = 2\pi/\omega$, $B$ and $\theta$ for pure states $\psi_\pm(t)$ as in (3.15).

As a special example, one may choose $\alpha = \pi/2$ in (3.11), namely

$$2\mu\hbar B + \hbar\omega \cos \theta = 0.$$ (3.26)
Then $w_\pm^\dagger(t) \hat{H}(t) w_\pm(t) = 0$ in (3.10), and only the geometric phases remain in (3.25),

$$\text{Tr}\{T^* e^{-\frac{i}{\hbar} \int_0^T dt \hat{H}(t)} \rho_{\text{mix}}(0)\} = \cos \frac{\Theta}{2} e^{-i\pi(1+\cos(\theta-\alpha))} + \sin^2 \frac{\Theta}{2} e^{-i\pi(1-\cos(\theta-\alpha))}$$

by using (3.14) and the periodicity $w_\pm(T) = w_\pm(0)$. One also has

$$\psi_\pm^\dagger(t) \hat{H}(t) \psi_\pm(t) = 0$$

and thus the parallel transport condition (2.30) in the conventional formulation is realized by a suitable choice of the Hamiltonian instead of the gauge transformation (2.27). This choice of parameters corresponds to an explicit example in [33].

In the example discussed here, the explicit form of basis vectors $w_\pm(t)$ in (3.7) was defined by a diagonalization of the effective Hamiltonian which is a natural generalization of the analysis of adiabatic phase, instead of the construction discussed in Section 2.2. The periodicity condition $w_\pm(T) = w_\pm(0)$ with $T = 2\pi/\omega$ severely constrains the possible initial state $|k\rangle$ of $\rho(0) = \sum_k \omega_k |k\rangle \langle k|$ in (2.33). For generic states $|k\rangle$ one may use the basis vectors $\tilde{w}_\pm(t)$ in (3.19). The basis vectors $\tilde{w}_\pm(t)$ generally agree with the basis vectors $v_k(t)$ in (2.36) up to hidden local gauge symmetry.

4 Discussion

The mixed state generally appears as a result of de-coherence in the actual experimental situation. A precise description of de-coherent processes in quantum mechanics is involved. Operationally, one may reduce a pure state to a mixed state by random phase approximation, for example. A more elegant procedure is the purification and its inverse, namely, reduction. See, for example, Ref. [22]. The basic idea of the reduction starts with a normalized pure (entangled) state

$$\psi(t) = \sum_{n,m} a_{n,m} |\psi_n(t)\rangle |\phi_m(t)\rangle$$

and a density matrix for the pure state

$$\rho(t) = |\psi(t)\rangle \langle \psi(t)|.$$  \hspace{1cm} (4.2)

One then takes a partial trace over the states $|\phi_m(t)\rangle$ and obtains a density matrix for a mixed state

$$\rho_{\text{mix}}(t) = \text{Tr}_\phi \{\rho(t)\} = \sum_{n,l} \omega_{n,l} |\psi_n(t)\rangle \langle \psi_l(t)|$$

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where

$$\omega_{n,l} \equiv \sum_m a_{n,m}a^*_{l,m}. \tag{4.4}$$

If the dimension of the states \(\{|\psi_n(t)\rangle\}\) is \(N\), one may choose the dimension of the states \(\{|\phi_m(t)\rangle\}\) to be equal to or larger than \(N\). One then has more than \(N^2\) free parameters \(a_{n,m}\) which are naively sufficient to describe \(N^2\) parameters \(\omega_{n,l}\). The purification is the inverse of the above procedure and corresponds to a construction of a pure state starting with a mixed state, though the purification is not unique.

The time development of the pure state is given by

$$i\hbar\partial_t\psi(t) = [\hat{H} + \hat{\tilde{H}}]\psi(t) \tag{4.5}$$

where \(\hat{H}\) acts on the states \(\{|\psi_n(t)\rangle\}\) and \(\hat{\tilde{H}}\) on the states \(\{|\phi_m(t)\rangle\}\). The pure state (4.1) is transformed under the equivalence class \(\{e^{i\theta_k(t)}\psi_k(t)\}\) in (2.27) as

$$\psi(t) \rightarrow \psi'(t) = \sum_{n,m} a_{n,m}e^{i\theta_n(t)}|\psi_n(t)\rangle|\phi_m(t)\rangle \tag{4.6}$$

and thus the Schrödinger equation is not maintained. To satisfy the Schrödinger equation one needs to consider an equivalence class of Hamiltonians

$$\{\hat{H} - \hbar\partial_t\theta_k(t)\} \tag{4.7}$$

for each state \(|\psi_n(t)\rangle\) separately. To maintain the universal Hamiltonian for all the states contained in (4.5) only a limited set of gauge transformations (2.31) is allowed. As a consequence, one cannot achieve the parallel transport for all the states (2.30) by means of the gauge transformation, which implies that the geometric phase (2.25) is not interpreted as the holonomy associated with (2.27) if one wants to maintain the universal Hamiltonian. The limited set of gauge transformations (2.31) can achieve only (2.17). (This property is related to the general incompatibility of the equivalence class (2.27) with the superposition principle such as (4.1), as analyzed in [21].) When one adopts the diagonal form of the density matrix (2.14) it is manifestly invariant under the equivalence class as in (2.21), but one needs to use a transformed Hamiltonian to define the physical total phase in (2.22). The invariance of the density matrix does not necessarily imply the gauge invariance of physical observables.

The hidden local gauge symmetry discussed in the present paper transforms the state vectors as

$$\{|\psi_n(t)\rangle\} \rightarrow \{e^{i\alpha_n(0)}|\psi_n(t)\rangle\} \tag{4.8}$$
and thus the pure state (4.1)

$$\psi(t) \rightarrow \psi'(t) = \sum_{n,m} a_{n,m} e^{i\alpha_n(0)} |\psi_n(t)\rangle |\phi_m(t)\rangle.$$  \hspace{1cm} (4.9)

The hidden local symmetry thus maps one allowed solution of the Schrödinger equation to another allowed solution with a fixed Hamiltonian, although the pure state itself is changed. But the diagonal density matrix and the physically observable interference in the present application are kept invariant under this transformation as in (2.45) or (2.50).

In conclusion, we have illustrated the advantage of the use of the hidden local gauge symmetry, which is clearly recognized in the second quantization, in the analyses of geometric phases both for pure and mixed states. As for other applications of the second quantized formulation, it has been shown elsewhere \cite{34} that the geometric phase and the quantum anomaly, which have been long considered to be closely related, have in fact little to do with each other.

A Hidden local gauge symmetry

In this appendix, for the sake of completeness, we recapitulate the basic idea of hidden local gauge symmetry. We start with the generic hermitian Hamiltonian $\hat{H} = \hat{H}(\hat{p}, \hat{x}, X(t))$ for a single particle theory in the background variable $X(t) = (X_1(t), X_2(t), \ldots)$. We then define a complete set of (time-dependent) eigenfunctions

$$\int d^3x v^\dagger_n(\vec{x}, t)v_m(\vec{x}, t) = \delta_{n,m}, \hspace{1cm} (A.1)$$

which are arbitrary at this moment. We take the time $T$ as a period of the variable $X(t)$ and the basis set $\{v_n(t, \vec{x})\}$ in the analysis of geometric phases, unless stated otherwise.

We then expand the field variable $\hat{\psi}(t, \vec{x})$ in the notation of second quantization as

$$\hat{\psi}(t, \vec{x}) = \sum_n \hat{b}_n(t) v_n(\vec{x}, t). \hspace{1cm} (A.2)$$

By using the above expansion in the action

$$S = \int dt d^3x \{\hat{\psi}^\dagger i\hbar \partial_t \hat{\psi} - \hat{\psi}^\dagger \hat{H} \hat{\psi}\} \hspace{1cm} (A.3)$$

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we obtain the effective Hamiltonian (depending on Bose or Fermi statistics)

\[ \hat{H}_{\text{eff}}(t) = \sum_{n,m} \hat{b}_n^\dagger(t) \int d^3x v_n^\dagger(\vec{x}, t) \hat{H} v_m(\vec{x}, t) - \langle n| i\hbar \frac{\partial}{\partial t} |m \rangle \hat{b}_m(t) \] (A.4)

with \([\hat{b}_n(t), \hat{b}_m^\dagger(t)] = \delta_{n,m}\). The second term in the effective Hamiltonian is defined by

\[ \int d^3x v_n^\dagger(\vec{x}, t) i\hbar \frac{\partial}{\partial t} v_m(\vec{x}, t) \equiv \langle n| i\hbar \frac{\partial}{\partial t} |m \rangle. \] (A.5)

The probability amplitude which satisfies the Schrödinger equation with \(\psi_n(\vec{x}, 0) = v_n(\vec{x}; 0)\) is given by

\[ \psi_n(\vec{x}, t) = \langle 0| \hat{\psi}(t, \vec{x}) \hat{b}_n^\dagger(0)|0 \rangle \] (A.6)

since \(i\hbar \partial_t \hat{\psi} = \hat{H} \hat{\psi}\) in the present problem. When one defines the Schrödinger picture \(\hat{\mathcal{H}}_{\text{eff}}(t)\) by replacing all \(\hat{b}_n(t)\) by \(\hat{b}_n(0)\) in the above \(\hat{H}_{\text{eff}}(t)\), one can write \[19, 20\]

\[ \psi_n(\vec{x}, t) = \sum_m v_m(\vec{x}, t) \times \langle m| T^* \exp\{ -\frac{i}{\hbar} \int_0^T \hat{\mathcal{H}}_{\text{eff}}(t) dt \}|n \rangle \] (A.7)

where \(T^*\) stands for the time ordering operation, and the state vectors in the second quantization are defined by \(|n \rangle = \hat{b}_n^\dagger(0)|0 \rangle\). This formula is exact.

Our formulation contains an exact hidden local gauge symmetry which keeps the field variable \(\hat{\psi}(t, \vec{x})\) invariant

\[ v_n(\vec{x}, t) \rightarrow v'_n(\vec{x}, t) = e^{i\alpha_n(t)} v_n(\vec{x}, t), \]
\[ \hat{b}_n(t) \rightarrow \hat{b}'_n(t) = e^{-i\alpha_n(t)} \hat{b}_n(t), \quad n = 1, 2, 3, \ldots, \] (A.8)

where the gauge parameter \(\alpha_n(t)\) is a general function of \(t\). This gauge symmetry (or substitution rule) states the fact that the choice of coordinates in the functional space is arbitrary and this symmetry by itself does not give any conservation law. This symmetry is exact under a rather mild condition that the basis set (A.1) is not singular, and consequently the physical observables should always respect this symmetry.

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Our next observation is that \( \psi_n(\vec{x}, t) \) is transformed under the hidden local gauge symmetry (A.8) as

\[
\psi'_n(\vec{x}, t) = e^{i\alpha_n(0)}\psi_n(\vec{x}, t)
\]

independently of the value of \( t \). This transformation is derived by using the exact representation (A.6) or (A.7), and it implies that \( \psi_n(\vec{x}, t) \) is a physical object since \( \psi_n(\vec{x}, t) \) stays in the same ray \([1, 2]\) under an arbitrary hidden local gauge transformation.

A.1 Adiabatic phase

We choose the specific basis set \([5]\)

\[
\hat{H}(\hbar \frac{\partial}{\partial \vec{x}}, \vec{x}, X(t))v_n(\vec{x}, t) = \mathcal{E}_n(X(t))v_n(\vec{x}, t),
\]

and by assuming the dominance of diagonal elements in (A.7) in the adiabatic approximation, we have

\[
\psi_n(\vec{x}, t) \approx v_n(\vec{x}, t) \exp\left\{-\frac{i}{\hbar} \int_0^t \left[ \mathcal{E}_n(X(t)) - \langle n|i\hbar \frac{\partial}{\partial t}|n\rangle \right] dt \right\}.
\]

which is confirmed to be invariant under the hidden local symmetry up to a constant phase. The product

\[
\psi_n(\vec{x}, 0)\psi_n(\vec{x}, T)
\]

\[
= v_n(0, \vec{x})\psi_n(T, \vec{x})
\]

\[
\times \exp\left\{-\frac{i}{\hbar} \int_0^T \left[ \mathcal{E}_n(X(t)) - \langle n|i\hbar \frac{\partial}{\partial t}|n\rangle \right] dt \right\}.
\]

is thus manifestly invariant under the hidden local symmetry. By choosing the hidden local gauge such that \( v_n(T, \vec{x}) = v_n(0, \vec{x}) \), the pre-factor \( v_n(0, \vec{x})^\dagger v_n(T, \vec{x}) \) becomes real and positive, and the phase factor in (A.12) defines a physical quantity uniquely. After this gauge fixing, the phase in (A.12) is still invariant under residual gauge transformations satisfying the periodic boundary condition \( \alpha_n(0) = \alpha_n(T) \).
A.2 Non-adiabatic phase

We start with the basic assumptions [9, 12]

\[ i\hbar \partial_t \psi(t, \vec{x}) = \hat{H}(t)\psi(t, \vec{x}), \quad \int d^3x \psi^\dagger(t, \vec{x}) \psi(t, \vec{x}) = 1, \]

\[ \psi(t, \vec{x}) = e^{i\phi(t)} \tilde{\psi}(t, \vec{x}), \quad \tilde{\psi}(T, \vec{x}) = \tilde{\psi}(0, \vec{x}), \]

\[ \phi(T) = \phi, \quad \phi(0) = 0. \]  \hspace{1cm} (A.13)

We now choose the first element of the complete orthonormal set \{v_n(t, \vec{x})\} in (A.1) such that

\[ v_1(t, \vec{x}) = \tilde{\psi}(t, \vec{x}), \]  \hspace{1cm} (A.14)

which is possible since \{v_m(t, \vec{x})\} is an arbitrary complete orthonormal set. The amplitude \psi_1(t, \vec{x}) in (A.7) satisfies the Schrödinger equation and

\[ \psi_1(0, \vec{x}) = v_1(0, \vec{x}) = \psi(0, \vec{x}). \]  \hspace{1cm} (A.15)

We thus have [21]

\[ \psi(t, \vec{x}) = \psi_1(t, \vec{x}) \]

\[ = v_1(t, \vec{x}) \exp\left\{ -\frac{i}{\hbar} \int_0^t dt \int d^3x v_1^\dagger(t, \vec{x}) \hat{H} v_1(t, \vec{x}) \right\} \]

\[ \quad - \int_0^t dt \int d^3x v_1^\dagger(t, \vec{x}) i\hbar \partial_t v_1(t, \vec{x}) \} \right\} \]  \hspace{1cm} (A.16)

where the last structure is fixed by noting \psi(t, \vec{x}) = v_1(t, \vec{x})e^{i\phi(t)} by assumption (A.13), namely, by the assumption that only the diagonal component survives for \psi_1(t, \vec{x}) in (A.7).

The amplitude \psi(t, \vec{x}) is invariant under the hidden local symmetry \psi_1(t, \vec{x}) \rightarrow e^{i\alpha_1(t)}v_1(t, \vec{x}) up to a constant phase, \psi(t, \vec{x}) \rightarrow e^{i\alpha_1(0)}\psi(t, \vec{x}). The quantity

\[ \psi^\dagger(0, \vec{x})\psi(T, \vec{x}) \]

\[ = v_1^\dagger(0, \vec{x})v_1(T, \vec{x}) \exp\left\{ -\frac{i}{\hbar} \int_0^T dt \int d^3x v_1^\dagger(t, \vec{x}) \hat{H} v_1(t, \vec{x}) \right\} \]

\[ \quad - \int_0^T dt \int d^3x v_1^\dagger(t, \vec{x}) i\hbar \partial_t v_1(t, \vec{x}) \} \]  \hspace{1cm} (A.17)

is thus manifestly invariant under the hidden local symmetry with a fixed Hamiltonian. If one chooses the gauge such that \psi_1(0, \vec{x}) = v_1(T, \vec{x}) as in our starting
construction (A.1), the exponential factor in (A.17) extracts the entire phase from the gauge invariant quantity and, in particular, the non-adiabatic phase \([9]\) is given by

\[
\beta = \oint dt \int d^3x v_1^\dagger(t, \vec{x}) i\hbar \partial_t v_1(t, \vec{x}).
\] (A.18)

It is clear that the geometric term in (A.17) is determined uniquely by the hidden local symmetry in (A.8) without referring to any explicit form of the Hamiltonian. The basis set \(\{v_n(t, \vec{x})\}\) specify the coordinates in the functional space, and they do not satisfy the Schrödinger equation nor are the eigenvectors of \(\hat{H}\) in general.

References


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