On adiabatic evolution for a general time-dependent quantum system

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Abstract

The unitary operator corresponding to the classical canonical transformation that connects a general closed system to an open system under adiabatic conditions is found. The quantum invariant operator of the adiabatic open system is derived from the unitary transformation of the quantum Hamiltonian of the closed system. On the basis of these results, we investigate the evolution of the general quantum adiabatic system and construct a revised adiabatic theorem. The adiabatic theorem developed here exactly reduces to the well-known Berry adiabatic theorem when the control parameter of an adiabatic system is constant in time.
1. INTRODUCTION

Although quantum states of a closed conserved system are given as solutions of the Schrödinger equation, there is no general method to derive quantum states of an open quantum system that is affected by an external environment\([1, 2]\). However, an open quantum system that deviates slightly from a closed system may satisfy the adiabatic condition and, consequently, we can regard the Schrödinger solutions as the corresponding quantum states of the system. A well-known method to treat this problem is Berry’s adiabatic theorem, which states that “the quantum states of an adiabatic open quantum system are proportional to the eigenstates of its Hamiltonian”\([2–4]\). Active searches for Berry’s phase have been undertaken on account of its importance in various fields of theoretical physics such as Aharonov Bohm oscillations\([8]\), quantum dots\([9]\), quantum Hall effect\([10]\) and geometric phase gate\([11]\).

Here, we obtained the unitary operator that connects quantum states of an open quantum system that depends on time-varying external parameters with those of a conserved system. We demonstrate that the quantum states of an adiabatic open quantum system can be derived from those of a conserved system.

Though the invariant operator of an adiabatic open quantum system can be found from a straightforward evaluation, it is also possible to evaluate this operator via a unitary transformation of the Hamiltonian of a conserved system. From this we want to demonstrate that the quantum states of an adiabatic open quantum system are proportional to the eigenstates of the invariant operator of the system. Among various types of invariant operators for a quantum system, the quadratic invariant operator is the same as the Hamiltonian when the control parameter does not vary with time. Thus, we can view this concept as an extended version of Berry’s adiabatic theorem.

2. A QUANTUM SYSTEM WITH TIME-DEPENDENT EXTERNAL PARAMETER

We first consider a linear classical transformation given as

\[
\begin{align*}
q(t) &= e^{\alpha(t)}Q(t) - \beta(t), \\
p(t) &= e^{-\alpha(t)}P(t) + m\dot{\alpha}(t)e^{\alpha(t)}Q(t),
\end{align*}
\]

(1)
or

\[
\begin{aligned}
Q(t) &= e^{-\alpha(t)}[q(t) + \beta(t)], \\
P(t) &= e^{\alpha(t)}p(t) - m\dot{\alpha}(t)e^{\alpha(t)}[q(t) + \beta(t)],
\end{aligned}
\]

(2)

where \(\alpha(t)\) and \(\beta(t)\) are real functions of \(t\) and are differentiable with respect to \(t\). From now on, for simplicity, we do not explicitly display the time-variable dependence for the time functions \(\alpha, \beta, \) etc. except for some special cases. In Eqs. (1) and (2), \(q\) and \(p\) are canonical variables of the system whose Hamiltonian is given in the form

\[
H_1(q, p) = \frac{p^2}{2m} + V(q, R_0),
\]

(3)

where \(R_0\) is an external parameter at \(t = 0\). If the transformation of Eqs. (1) and (2) is canonical, \(Q\) and \(P\) are canonical variables of the system described by the following Hamiltonian \([12, 13]\):

\[
H_2(Q, P, t) = \frac{e^{-2\alpha}}{2m}P^2 + \frac{m}{2}(\dot{\alpha}^2 + \ddot{\alpha})e^{2\alpha}Q^2 + \dot{\beta}e^{-\alpha}P + m\dot{\alpha}\dot{\beta}e^\alpha Q + V(e^{\alpha}Q - \beta, R_0).
\]

(4)

Let us assume, in the spirit of a canonical transformation, that the system of the Hamiltonian of Eq. (4) is physically changed from that of Eq. (3) by environmental influences of an external driving force and/or dissipative frictional force. Here, we consider only the case of \(\alpha(0) = 0, \beta(0) = 0, \alpha(t) \approx 0, \beta(t) \approx 0\) and \(\dot{\alpha}, \dot{\beta} \ll \dot{q}\), so that the change of the system associated with the canonical transformation of Eq. (1) [or Eq. (2)] is adiabatic. If this condition is satisfied, Eq. (1) [or Eq. (2)] is the classical adiabatic relation.

Now, we would like to find the unitary transformation corresponding to the canonical transformation of Eq. (1) [or Eq. (2)]. The quantum Hamiltonians \(\hat{H}_1\) and \(\hat{H}_2\) corresponding to the classical Hamiltonians \(H_1\) and \(H_2\) can be obtained through the replacement of canonical variables by their corresponding quantum operators from Eqs. (3) and (4), respectively. Since the \(\hat{H}_1\) system is closed, its quantum state, \(|\psi\rangle\), can be obtained from the Schrödinger equation,

\[
\text{i}\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H}_1 |\psi\rangle.
\]

(5)

Since the \(\hat{H}_2\) system depends on time, there is no general method to derive the exact quantum states of the system. However, under the adiabatic condition, we can assert that the quantum
state of the system, \( |\Psi\rangle \), obeys the Schrödinger equation,

\[
i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H}_2 |\Psi\rangle.\tag{6}
\]

Let us find an unitary operator \( \hat{U} \) that connects the two quantum states associated with the \( \hat{H}_1 \) and \( \hat{H}_2 \) systems \[13–15\]:

\[
|\Psi\rangle = \hat{U} |\psi\rangle.\tag{7}
\]

From Eq. (7), we obtain a differential equation for the operator from Eqs. (5) and (6) as

\[
i\hbar \frac{\partial}{\partial t} \hat{U} = \hat{H}_2 \hat{U} - \hat{U} \hat{H}_1
\]

\[
= \left( -\frac{\dot{\alpha}}{2}(\dot{\hat{q}}\hat{p} + \dot{\hat{p}}\hat{q}) + \beta e^{-\alpha} \hat{p} + m\dot{\hat{q}} + \frac{m}{2} \dot{\alpha} e^{2\alpha} \hat{q}^2 \right) \hat{U}.\tag{8}
\]

We assume that \( \hat{U} \) gives the following relations for \( \hat{q} \) and \( \hat{p} \):

\[
\begin{cases}
\hat{U}\hat{q}\hat{U}^\dagger = e^{\alpha}\hat{q} - \beta, \\
\hat{U}\hat{p}\hat{U}^\dagger = e^{-\alpha}\hat{p} + m\dot{\alpha} e^{\alpha} \hat{q}.
\end{cases}\tag{9}
\]

This, in fact, corresponds to the classical canonical transformation given in Eq. (1). From straightforward algebra, the operator \( \hat{U} \) satisfying Eqs. (8) and (9) is obtained in the form

\[
\hat{U} = \exp \left[ -\frac{i}{2\hbar} m\dot{\alpha} e^{2\alpha} \hat{q}^2 \right] \exp \left[ \frac{i}{2\hbar} \alpha (\dot{\hat{q}}\hat{p} + \dot{\hat{p}}\hat{q}) \right] \exp \left[ -\frac{i}{\hbar} \beta \hat{p} \right].\tag{10}
\]

By inserting Eq. (10) into Eq. (7), the relation of \( n \)-th quantum state between both systems in \( x \)-space is calculated as

\[
\Psi_n(x, t) = \hat{U}\psi_n(x, t) = e^{\alpha/2} \exp \left[ -\frac{i}{2\hbar} m\dot{\alpha} e^{2\alpha} x^2 \right] \psi_n(e^{\alpha} x - \beta, t).\tag{11}
\]

This is a Schrödinger solution of Eq. (6) but not the eigenfunction of the Hamiltonian \( \hat{H}_2 \). Equation (11) tells us that \( n \)-th quantum state of a system is transformed to that of only another system by \( \hat{U} \). That is, Eq. (11) is an adiabatic change of the quantum state of the \( \hat{H}_1 \) system.

If an operator \( \hat{I}(\hat{q}, \hat{p}, t) \) satisfies the Liouville-von Neumann equation,

\[
\frac{d\hat{I}}{dt} = \frac{\partial \hat{I}}{\partial t} + \frac{1}{i\hbar} [\hat{I}, \hat{H}_2] = 0,\tag{12}
\]
\( \hat{I}(\hat{q}, \hat{p}, t) \) is then an invariant operator of the system \[ 16 \]. Generally, there are innumerable invariant operators satisfying Eq. \[ 12 \] in a system. Substituting Eq. \[ 6 \] into Eq. \[ 12 \], the invariant operator quadratic in both \( \hat{q} \) and \( \hat{p} \) is obtained as

\[
\hat{I}(\hat{q}, \hat{p}, t) = e^{-\alpha \hat{p}^2} + \frac{m\alpha^2 e^{2\alpha \hat{q}^2}}{2} + \frac{\dot{\alpha}}{2} (\hat{q}\hat{p} + \hat{p}\hat{q}) + V(e^\alpha \hat{q} - \beta, R_0). \tag{13}
\]

From Eq. \[ 12 \], we see that \( \hat{I}(\hat{q}, \hat{p}, t) \) does not commute with \( \hat{H}_2 \). This implies that the eigenstates of \( \hat{I}(\hat{q}, \hat{p}, t) \) are different from those of \( \hat{H}_2 \) for the time-dependent Hamiltonian system. We also see that Eq. \[ 13 \] is obtained from the unitary transformation of \( \hat{H}_1 \), i.e.,

\[
\hat{I}(\hat{q}, \hat{p}, t) = \hat{U} \hat{H}_1 \hat{U}^\dagger. \tag{14}
\]

Let us denote the eigenvalues and eigenfunctions of \( \hat{I}(\hat{q}, \hat{p}, t) \) as \( \lambda_n \) and \( |\phi_n(t)\rangle \), respectively:

\[
\hat{I}(\hat{q}, \hat{p}, t)|\phi_n(t)\rangle = \hat{U} \hat{H}_1 \hat{U}^\dagger |\phi_n(t)\rangle = \lambda_n |\phi_n(t)\rangle. \tag{15}
\]

If we consider that \( \hat{I}(\hat{q}, \hat{p}, t) \) as Hermitian, \( \lambda_n \) is a real constant. Since \( \hat{U} \) is a unitary operator and \( \hat{H}_1 \) does not depend on time, the eigenvalues and eigenfunctions of \( \hat{H}_1 \) should satisfy

\[
\hat{H}_1 \hat{U}^\dagger |\phi_n(t)\rangle = \lambda_n \hat{U}^\dagger |\phi_n(t)\rangle = \lambda_n |\psi_n(t)\rangle. \tag{16}
\]

From Eqs. \[ 5 \], \[ 7 \] and \[ 16 \], we see that

\[
|\Psi_n(t)\rangle = \hat{U}|\psi_n(t)\rangle = e^{-\frac{i}{\hbar} \lambda_n t} |\phi_n(t)\rangle. \tag{17}
\]

In \( x \)-space, Eq. \[ 17 \] can be rewritten as

\[
\Psi_n(x, t) = e^{-\frac{i}{\hbar} \lambda_n t} \phi_n(x, t) = \hat{U}\psi_n(x, t) = \exp \left[ -\frac{i}{2\hbar} m\alpha e^{2\alpha x^2} \right] e^{\alpha/2} \psi_n(e^\alpha x - \beta, t). \tag{18}
\]

The Schrödinger solution \( \Psi_n(x, t) \) of the \( \hat{H}_2 \) system is not an eigenfunction of \( \hat{H}_2 \), but rather an eigenfunction of the invariant operator \( \hat{I}(\hat{q}, \hat{p}, t) \) of \( \hat{H}_2 \) system.

3. **EXTENDED ADIABATIC THEOREM**

Berry’s adiabatic theorem states that the quantum state \( |\Psi_n(R(0), t)\rangle \) of the \( \hat{H}_2(R(0)) \) system is proportional to the \( n \)-th eigenket \( |\Phi_n(R(0))\rangle(t) \) of the Hamiltonian \( \hat{H}_2(R(0)) \), which is
dependent on the external parameter $R(0)$. Specifically,

$$|\Psi_n(R(0), t)\rangle = e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} e^{i\gamma_n(t)} |\Phi_n(R(0))\rangle,$$

(19)

where $E_n(t)$ and $|\Phi_n(t)\rangle$ are eigenvalues and eigenkets of the Hamiltonian $\hat{H}_2$, respectively,

$$\hat{H}_2 |\Phi_n(t)\rangle = E_n(t) |\Phi_n(t)\rangle,$$

(20)

and Berry’s phase $\gamma_n(t)$ is determined by

$$\gamma_n(t) = i \int_{R(0)}^{R(t)} \langle \Phi_n(R')| (t') |\nabla_R \Phi_n(R')| (t') \rangle dt'.$$

(21)

Here, $|\Psi_n(R(0), t)\rangle$ is not the solution of the Schrödinger equation (6). If we replace $|\phi_n(t)\rangle$ by $|\Phi_n(t)\rangle$ from Eq. (17), $|\Psi_n(t)\rangle$ can no longer be Schrödinger solution because $\hat{H}_2$ is dependent on time. Only in the case that the eigenstate $\Phi_n(t)$ of Hamiltonian is the same as the eigenstate of the invariant operator, Eq. (19) is valid as a Schrödinger solution.

To better understand the above theory, let us give an example. We choose $\hat{H}_1$ as the Hamiltonian of the quantum simple harmonic oscillator and $\hat{H}_2$ as that of the quantum driven harmonic oscillator:

$$\hat{H}_1 = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2 \hat{x}^2,$$

(22)

and

$$\hat{H}_2 = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2 \hat{x}^2 - \hat{x} R(t).$$

(23)

Recall that Eq. (18) enables us to obtain the Schrödinger solution of $\hat{H}_2$ system, provided that the Schrödinger solution of $\hat{H}_1$ system is known. Since we can easily identify the Schrödinger solution of $\hat{H}_1$ system in this case, we have the Schrödinger solution of the driven harmonic oscillator as

$$\Psi_n(x, t) = \frac{x_0^{-1/2}}{\pi^{1/4} \sqrt{2^n}} e^{-\left(\frac{\text{Im} a_p(t)}{x_0}\right)^2} e^{-i(n+1/2)\omega t} e^{-\frac{1}{2x_0^2} (x - a_p(t))^2} \tilde{H}_n \left(\frac{x - a_p(t)}{x_0}\right),$$

(24)

where $x_0 = \sqrt{\hbar/(m\omega)}$ and

$$a_p(t) = \frac{i}{m\omega} \int_0^t ds R(s) e^{-i\omega(t-s)}.$$

(25)
We also obtain, straightforwardly, the eigenfunctions and eigenvalues of \( \hat{H}_2 \) in the form

\[
\Phi_n(R(t))(x,t) = \frac{x_0^{-1/2}}{\pi^{1/4} \sqrt{2^n n!}} e^{-\frac{1}{2x_0^2} \left[ (x-R(t)) \right]^2} H_n \left( \frac{x-R(t)}{(m\omega^2)} \right), \tag{26}
\]

\[
E_n(t) = \hbar \left( n + \frac{1}{2} \right) - \frac{R^2(t)}{2m\omega^2}. \tag{27}
\]

From a rigorous evaluation using Eq. (26), we have

\[
|\nabla_R \Phi_n(R(t))(t)\rangle = |\Phi_n(R(t))-1(t)\rangle. \tag{28}
\]

This implies that \( \gamma_n(t) = 0 \), and from this we know that Eq. (19) holds only for \( \hat{H}_2(R(0)) \) system.

Equation (24) is not proportional to Eq. (26), i.e., the function \( \Psi_n(R(t))(x,t) \) in Berry’s adiabatic theorem is not the Schrödinger solution of the quantum driven harmonic oscillator. Berry’s adiabatic theorem should be extended in regard to our research as follows: “The quantum state, \( |\Psi_n(t)\rangle \) of the \( \hat{H}_2 \) system is proportional to the \( n \)-th eigenfunction of the invariant operator, \( \hat{I}(q,p,t) \), of \( \hat{H}_2 \) system, but not to the eigenket \( |\Phi_n(R(t)),t\rangle \) of Hamiltonian \( \hat{H}_2(t) \).” This revised theorem includes Berry’s original adiabatic theorem, because \( \hat{H}_2(R(0)) \) itself is an invariant operator when \( R(t) = R(0) \).

4. CONCLUSION

Here, we have derived a unitary operator that corresponds to a classical canonical transformation connecting an adiabatic open system, that is affected by external circumstances, to a conserved system. Because the canonical transformation that connects a general conserved system with its corresponding adiabatic open system can be regarded as a general treatment of adiabatic change classically, the derivation of quantum states using a unitary transformation corresponding to adiabatic change is a general treatment of a quantum adiabatic open system. Thus, the results derived here are the counterparts of the classical results. If Eq. (11), which is a canonical transformation, has another form, the adiabatic condition cannot be satisfied classically. In this case, the connection fulfilled by the unitary operator corresponding to the canonical transformation does not always give the same quantum state, but can be different.
from the former one. Thus, the adiabatic theorem related to the connection of quantum states does not hold.

Though it is impossible to understand classically the quantum systems that have no classical counterpart, like spin systems, we can derive relevant quantum states for adiabatic quantum systems from the eigenstates of a quantum invariant operator. In Eq. (1), any type of canonical conjugate for \( q(t) \) is acceptable provided it has the form \( p(t) + g(q, t) \). In other words, there are innumerable Hamiltonians that give the same classical solution, and each Hamiltonian has its particular canonical momentum. The reason is that the canonical momenta cannot be distinguished from the classical equations of motion, whereas we can distinguish different positions. The fact that there exist many different canonical momenta corresponding to a single classical canonical position tells us that there are numerous quantum mechanical systems corresponding to a classical solution. In other words, the canonical momenta are distinguishable from a quantum mechanical viewpoint. The development of the theory presented here is possible for any type of canonical momentum.

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