Effect of inter-subsystem couplings on the evolution of composite systems

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The effect of inter-subsystem coupling on the adiabaticity of composite systems and that of its subsystems is investigated. Similar to the adiabatic evolution defined for pure states, non-transitional evolution for mixed states is introduced; conditions for the non-transitional evolution are derived and discussed. An example that describes two coupled qubits is presented to detail the general presentation. The effects due to non-adiabatic evolution on the geometric phase are also presented and discussed.

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The study on the adiabaticity of quantal system may be traced back to the mid 1980s, when Berry [1] conceived that a quantal system in an eigenstate, adiabatically transport round a circuit by varying parameters \( \vec{R} \) in its Hamiltonian \( H(\vec{R}) \), will acquire a geometric phase in addition to the familiar dynamical phase factor. Since then geometric phase became an interesting subject and has been extensively studied [2, 3, 4] and generalized to non-adiabatic evolution [5], mixed states [6, 7, 8], and open systems [9]. The geometric phase of a composite system in particular has attracted a lot of attention for its possible applications in quantum information processing, where the whole set of universal quantum gates are achieved based on the Abelian and/or non-Abelian geometric operations [10, 11, 12, 13, 14]. In view of the geometric computation, the adiabaticity of the composite system is of course an important issue, because it would determine how well the system follows the loops. Nevertheless, thorough studies aimed to address this issue, in particular for a composite system with inter-subsystem coupling, are still few and certainly not exhaustive [13].

On the other hand, the geometric phase for mixed states is a new subject and much remains to be understood. Uhlmann [10] was the first to address this issue and later Sjöqvist et al. formulated it from the viewpoint of quantum interferometry [11]. This formulation is available when the system undergoes an unitary evolution. For subsystems that compose a composite system with non-zero inter-subsystem couplings, however, the evolution of each subsystem is not unitary in general. This problem was explored in a recent paper [12] for a very rare situation when both the composite system and its subsystems evolve adiabatically, but how the subsystems may evolve while the composite system transport adiabatically (or non-adiabatically) remains an open question.

In this paper, we will address these issues by investigating the adiabaticity of a composite system that consists of two coupled spin-\( \frac{1}{2} \) subsystems or a pair of quantum bit. We analyze the case where one of the spin-\( \frac{1}{2} \) is driven by a precessing magnetic field, a case of relevance to Nuclear Magnetic Resonance(NMR) quantum computation [13] as well as to the test of mixed state geometric phases [14]. We calculate and analyze the effects of spin-spin couplings on the adiabaticity of the composite system and its counterpart of the subsystems, four different kinds of time evolution are clarified and illustrated, conditions for those evolutions are presented and discussed.

Let a composite system be govern by the Hamiltonian

\[
H = H_1 + H_2 + H_{12},
\]

where \( H_i (i=1,2) \) denote the free Hamiltonian of subsystem \( i \) and \( H_{12} \) stands for the interaction between them. We suppose that the Hamiltonian \( H \) is changed by varying parameters \( \vec{R} = (X,Y,...) \) on which it depends. Then the excursion of the system between times \( t = 0 \) and \( t = T \) can be pictured as transport round a closed path \( \vec{R}(t) \) in parameter space with Hamiltonian \( H(\vec{R}(t)) \) and such that \( \vec{R}(T) = \vec{R}(0) \). At any instant, the natural basis consists of the eigenstates \( |\phi(\vec{R})\rangle \) of \( H(\vec{R}) \) for \( \vec{R} = \vec{R}(t) \), that satisfy \( H(\vec{R})|\phi_n(\vec{R})\rangle = E_n(\vec{R})|\phi_n(\vec{R})\rangle \), with energies \( E_n(\vec{R}) \). If \( H(\vec{R}) \) is altered slowly such that

\[
\left| \frac{\langle \phi_n(\vec{R}) | \frac{\partial}{\partial \vec{R}} | \phi_m(\vec{R}) \rangle}{E_n(\vec{R}) - E_m(\vec{R})} \right| << 1,
\]

it follows from the adiabatic theorem that at any instant the system will be in an eigenstate of the instantaneous Hamiltonian. In particular, if the Hamiltonian is returned to its original form, the composite system will return to its original state, apart from a phase factor. Eq. 2 is the well known condition for the adiabatic theorem to hold.

We next develop a generalization for the subsystems, going back to the original adiabatic scenario in which the system returns to its original state, but now taking mixed states into account instead of pure states. To this end, we first of all define non-transitional evolution for mixed states [14], this definition is non-trivial in particular for subsystems that have no effective Hamiltonian available for it [15]. Let a state \( \rho(t) \) of the subsystem (say, subsystem 1) be written in the diagonal form of

\[
\rho(t) = \sum_i p_i(t) |E_i(t)\rangle \langle E_i(t)|,
\]

\( p_i(t) \) depends on time via \( \vec{R}(t) \) and we would write the time-dependence of \( \vec{R}(t) \) explicitly. It is clear that \( p_i(t) \) gives the probability of
the subsystem in state $|E_i(t)\rangle$. This form of writing is called the spectral representation, while $p_i(t)$ denotes the eigenvalues and $|E_i(t)\rangle$ the corresponding eigenvectors of $\rho(t)$. One special case is that $p_i(t)$ (for any $i$) are time-independent, this is a rare situation which implies no transitions among the eigenstates of $\rho(t)$ when the composite system experiences transport along the parameter loops. The subsystem in this state with time-independent coefficients $p_i(t)$, i.e., $p_i(t) = p_i(0)$ independent of the varying parameters, is defined to undergo non-transitional evolution, and the corresponding eigenstates $|E_i(t)\rangle$ will be called non-transitional eigenstates. Obviously the non-transitional evolution would return to the adiabatic evolution when the states $|E_i(t)\rangle$ are the eigenstates of the subsystem’s Hamiltonian (if any available). Moreover this definition is meaningful even if there is no Hamiltonian available for the subsystem, a general situation for coupled multi-particle systems. Thus the definition could find broad use instead of the adiabatic evolution for pure states in composite systems. Now we will drive a condition for the subsystem to undergo this non-transitional evolution. For the composite system governed by Hamiltonian Eq. 1, a state $|\psi(t)\rangle$ may be decomposed into Schmidt form

$$|\psi(t)\rangle = \sum_i \sqrt{p_i(t)} e^{-i \int_0^t H_{ii}(t')dt'} |E_i(t)\rangle_1 |e_i(t)\rangle_2,$$

with $H_{ij}(t) = \langle E_i(t)|H|e_j(t)\rangle_2 \langle e_j(t)|_2$ and $|e_j(t)\rangle_2 \equiv |e_j(t)\rangle_2 \otimes |E_j(t)\rangle_1$. The reduced density matrix for the subsystem $1$ follows straightforwardly from Eq. 3 that $p_i(t) = \text{Tr}_2(|\psi(t)\rangle\langle\psi(t)|) = \sum_j p_j(t)|E_i(t)\rangle_2 \langle E_j(t)|_1$. To find the condition of the non-transitional evolution is now equivalent to finding conditions for $p_i(t)$ in Eq. 3 to be time-independent. In units with $\hbar = 1$, $|\psi(t)\rangle$ satisfies

$$i \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle,$$

where here and hereafter time-dependence are understood where not written explicitly and $|E_i(t)\rangle \langle e_i(t)|$ denotes states for subsystem $1$ ($2$) where suffix omitted. We would like to note that $|E_i(t)|\langle e_i(t)|$ are not the instantaneous eigenstates of $H$ in general, so under the action of $H$ transitions among those states would occur. As you will see, the condition for the non-transitional evolution would be equivalent to negligible ratios of the transition amplitude to the respective energy spacing. The derivative equation for $p_i(t)$ follows from Eq. 4 that,

$$i \sqrt{p_j} \langle E_j|H_{ij} |\psi(t)\rangle + \sqrt{p_j} \langle e_j|\dot{e}_j\rangle - \sum_{k \neq j} \sqrt{p_k} \exp(-i \int_0^t (H_{kk} - H_{j})dt') H_{jk} \psi = 0. \quad (5)$$

The simplest approximation is to neglect the off-diagonal elements on the grounds that

$$\left| \frac{H_{jk}}{H_{jj} - H_{kk}} \right| << 1, \quad (6)$$

having this approximation, Eq. 4 yields

$$\sqrt{p_j}(t) = \sqrt{p_j(0)} e^{i(\gamma_{1j} + \gamma_{2j})}, \quad (7)$$

where $\gamma_{1j} = \int_0^t \langle E_j|H|\psi(t)\rangle d\tau$, and $\gamma_{2j} = \int_0^t \langle e_j|\dot{e}_j\rangle d\tau$. We may rewrite $|E_j(t)\rangle \langle e_j(t)|$ to be $e^{i\gamma_j}|E_j(t)\rangle \langle e_j(t)|$ such that $p_j(t) = p_j(0)$. Usually, $|E_j(t)|\langle e_j(t)|$ are not the instantaneous eigenstates of the Hamiltonian $H$, so $H_{jk}$ represent the transition amplitude between states $|E_j(t)|\langle e_j(t)|$ and $|E_k(t)|\langle e_k(t)|$. Condition Eq. 5 indicates that for non-transitional evolutions, transitions induced by $H$ among $|E_j(t)|\langle e_j(t)|$ should be small with respect to the energy spacing between the two. Conditions 6 and 7 together imply that there might be four different kinds of evolution for the composite system, as follows. (a) Adiabatic evolution: The composite system undergoes an adiabatic evolution while its subsystems follow non-transitional evolutions, this means that the composite system would follow one of its instantaneous eigenstates while its subsystem evolve along the non-transitional eigenstates. (b) Quasi-adiabatic evolution 1: The composite system undergoes an adiabatic evolution while its subsystems do not; (c) Quasi-adiabatic evolution 2: The composite system evolve non-adiabatically while its subsystems follow non-transitional evolutions. (d) Non-adiabatic evolution: The composite system evolve non-adiabatically, while its subsystems undergo out of non-transitional evolutions.

It is worthwhile to mention that the condition/criterion for non-transitional evolution given by Eq. 6 is also valid for the system with a mixed state under unitary evolutions, this can be understood as follows. Write the state (density matrix) of the composite system in a spectral representation

$$\rho(t) = \sum_\alpha \lambda_\alpha |\psi_\alpha(t)\rangle \langle \psi_\alpha(t)|,$$

$|\psi_\alpha(t)\rangle$ would obey the Schrödinger equation and has the same form of decomposition as Eq. 3 but with $\sqrt{p_j}(t)$ instead of $\sqrt{p_j}(t)$. The von Neumann equation $i\hbar \frac{\partial}{\partial t} \rho = [H, \rho]$ then yields the same equation as in Eq. 5 but with $\sqrt{p_j} = \sum_\alpha p_j^{(a)} \lambda_\alpha$. $\sum_\alpha p_j^{(a)} \lambda_\alpha$ represents the population of the subsystem $1$ in state $|E_j(t)\rangle$, non-transitional evolution that requires $p_j$ constant would result in the same condition as in Eq. 6, indeed for a closed system the transitions among the eigenstates of the subsystem’s density matrix are only induced by the system Hamiltonian, for open systems, however, this is not the case, since the bath which couples to the whole system may lead to population transfer among those states. To this respect, in addition to the condition Eq. 6, criteria

$$\frac{|\langle E_k|\langle e_k|\Gamma_\alpha(e_j)|E_j|\rangle|}{H_{jj} - H_{kk}} << 1 \quad (9)$$

is required to be satisfied in order to ensure the non-transitional evolutions for open systems, where $\Gamma_\alpha$ represent the agents (operators) of the whole system coupled
to a bath. This is the reason why the non-transitional condition should be different from each other for an open system and for a closed system, and this is also an explanation for closed systems, regardless of in a pure state or a mixed state, hold the same criteria for non-transitional evolutions.

As an example, we consider two qubits \( S_k(k = 1, 2) \) as represented by a pair of spin-\( \frac{1}{2} \) particles, coupled through a uniaxial exchange interaction in the z-direction. One of the qubits (say, qubit 1) is driven by a time-dependent magnetic field \( \vec{B}(t) = B_0 \hat{n}(t) \) with the unit vector \( \hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \), the Hamiltonian of this system reads (\( \hbar = 1 \))

\[
H(t) = 4JS_1^z \otimes S_2^z + \mu \vec{B}(t) \cdot \vec{S}_1
\]  

(10)

\[
\begin{align*}
|\phi_{1,2}(t)\rangle &= \frac{1}{\sqrt{M_{1,2}}} (\sin \theta e^{-i\phi} |\downarrow\rangle + (g + \cos \theta + \mathcal{E}_{1,2}) |\uparrow\rangle), \\
|\phi_{3,4}(t)\rangle &= \frac{1}{\sqrt{M_{3,4}}} (\sin \theta e^{-i\phi} |\downarrow\rangle + (\cos \theta + \mathcal{E}_{3,4} - g) |\uparrow\rangle),
\end{align*}
\]

(11)

and

\[
\mathcal{E}_{1,2} = \pm \sqrt{(g^2 + 1) + 2g \cos \theta},
\]

\[
\mathcal{E}_{3,4} = \pm \sqrt{(g^2 + 1) - 2g \cos \theta},
\]

where \( g = \frac{2J}{\mu B_0} \) denotes the rescaled exchange interaction constant, \( M_j \) the renormalization constant and \( |\uparrow\downarrow\rangle = |\uparrow\rangle_1 \otimes |\downarrow\rangle_2 \) and the others likely. For a simplest case where the exchange interaction \( g = 0 \), the eigenvalues are reduced to \( \mathcal{E}_+ = \pm 1 \), with corresponding instantaneous eigenstates \( |\phi_+(t)\rangle = (\cos \frac{\theta}{2} |\uparrow\rangle + \sin \frac{\theta}{2} e^{-i\phi} |\downarrow\rangle) \otimes |\uparrow\rangle \) (or \( \otimes |\downarrow\rangle \)), \( |\phi_-(t)\rangle = (\sin \frac{\theta}{2} |\uparrow\rangle + \cos \frac{\theta}{2} e^{-i\phi} |\downarrow\rangle) \otimes |\uparrow\rangle \) (or \( \otimes |\downarrow\rangle \)). Suppose the external magnetic fields precess with time-independent azimuthal angles \( \theta \) and a constant precessing frequency \( \omega \), i.e., \( \phi = \omega t \), the adiabatic evolution for the composite system requires \( |\langle \phi_+ |\phi_-(t)\rangle/(\mathcal{E}_+ - \mathcal{E}_-)| << 1 \), that is (in units of \( \mu B_0/2 \)) \( \omega << \frac{1}{\sin \theta} \). Obviously, in this limit the two spin-\( \frac{1}{2} \) particles remain uncoupled and the adiabatic condition is exactly the one for the driven particles 1. From the aspect of non-transitional evolution, no constraints on \( \omega \) could be made, because of there is no coupling between the two qubits and each qubit would remain in pure states if the initial states are pure. So, for a composite system without inter-subsystem couplings, the evolutions would fall in regime (a) or (c), i.e., the composite system might undergo an adiabatic or non-adiabatic evolution, while its subsystems evolve along the non-transitional states certainly.

Now we turn to study the case with inter-subsystem couplings. For the composite system, to make the adiabatic theorem valid, it should be satisfied that \( (i, j = 1, ..., 4, i \neq j) \)

\[
\begin{align*}
\Gamma_{ij} &\equiv \frac{|\langle \phi_i |\phi_j\rangle|}{\mathcal{E}_i - \mathcal{E}_j} = \frac{1}{\sqrt{M_i M_j}} \frac{\omega \sin^2 \theta}{\mathcal{E}_i - \mathcal{E}_j} << 1, i, j = 1, 2 \quad \text{or} \quad i, j = 3, 4, \\
\Gamma_{ij} &= 0, \text{others.}
\end{align*}
\]

(13)

This condition follows straightforwardly from Eq.(2) by assuming the azimuthal angle \( \theta \) time-independent and \( \phi = \omega t \). Clearly, the eigenenergies \( \mathcal{E}_i \) and the renormalization constant \( M_i \) are independent of \( \omega \), so \( \Gamma_{ij} \) increase linearly with \( \omega \), i.e., slowly precessing magnetic fields would benefit the adiabatic evolution. The dependence of \( \Gamma_{ij} \) \( (i, j = 1, 2 \text{ or } 3, 4) \) on \( g \) and \( \theta \) was illustrated in figure 1. A common feature of these fig-
The Schrödinger equation $i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle$ yields (with $\Omega_{jk}(t) = \int_0^t \mathcal{E}_k(\tau) - \mathcal{E}_j(\tau) d\tau$)

$$\dot{c}_j(t) + (\langle \phi_j(t)|\dot{\phi}_j(t)\rangle)c_j(t)
= -\sum_{k\neq j} e^{i\Omega_{jk}(t)}(\langle \phi_j(t)|\phi_k(t)\rangle)c_k(t),$$

(16)

the Berry’s phase is just a follow up of this equation by ignoring its right-hand side, further consideration would treat the terms in the right-hand side as perturbations. Up to the first order in $|\langle \phi(t)|\dot{\phi}(t)\rangle|$, the usual perturbation theory give

$$c_n(t) \approx e^{i\gamma_n(t)},$$
$$c_j(t) \approx \frac{e^{i\Omega_{jn}(t)} + i\gamma_n(t)\langle \phi_j(t)|\dot{\phi}_n(t)\rangle}{\mathcal{E}_j - \mathcal{E}_n}.$$  

(17)

with $\gamma_n(t) = i\int_0^t \langle \phi_n(t)|\dot{\phi}_n(t)\rangle d\tau$, the Berry phase pertaining to instantaneous eigenstate $|\phi_n(t)\rangle$. Eqs. (14) and (17) together yield the geometric phase

$$\phi_g = \arg[e^{i\gamma_n(T)} + \sum_{m\neq n} c_m(T)].$$

(18)

To get this expression, all terms equal or smaller than $\Gamma_{mn}^2$ have been ignored. It is clear that the main correction caused by the non-adiabatic evolution to the geometric phase come from terms $\sum_{m\neq n} c_m(T)$, that may be expressed up to first order in $\Gamma_{mn}$ as

$$\phi_g = \gamma_n(T) + \sum_{m\neq n} \Gamma_{mn}[\Omega_{nm}(T) + \gamma_m(T) + \arg\langle \phi_n(T)|\dot{\phi}_m(T)\rangle],$$

(19)

with $\Gamma_{mn} \to 0$ the geometric phases approach the Berry phases $\gamma_n(T)$ as expected. We may divide the correction due to the non-adiabatic evolution to the geometric phase into two kinds, the first is the population transfer among the instantaneous eigenstates, this contribution appears in the correction as $\sum_{m\neq n} \Gamma_{mn}[\Omega_{nm}(T) + \arg\langle \phi_n(T)|\dot{\phi}_m(T)\rangle]$, while the second that exhibit the geometric feature of the transited eigenstates scales as $\sum_{m\neq n} \Gamma_{mn}\gamma_m(T)$. We would like to note that only $\Gamma_{12}$ and $\Gamma_{34}$ are not zero in the example Eq. (11), but the representation Eq. (18) is quite general for quantum systems.

It is not difficult to show from Eq. (14) that the transport of the subsystems is always non-transitional in this situation. For example, suppose the composite system undergo an adiabatic evolution in the instantaneous eigenstate $|\phi_n(t)\rangle(n = 1, 2)$, the reduced density matrix of the subsystem 1 reads...
with $\rho_{+,-} = 0, 1$. Clearly, $\rho_{\pm}$ are time-independent. This point will be changed when the spin-spin coupling takes the form of $(J\sigma^+_i \sigma^-_j + h.c.)$, the instantaneous eigenstates in this situation are entangled states of the two particles, the diagonal elements of the reduced density matrix $\rho_1$ is $\theta$-dependent as Ref. [14] shown, and the slowly varying $\theta$ can make the composite system an adiabatic evolution meanwhile make the subsystems out of non-transitional evolution.

Some remarks on the non-transitional evolutions are now in order. For subsystems with an available Hamiltonian, the concept of non-transitional evolution covers the concept of adiabatic evolution, this can be understood as follows. Write an initial state (generally mixed) $\rho_0 = \sum_{i,j} \rho_{ij} |\Phi_i(0)\rangle \langle \Phi_j(0)|, (i,j = 1,...,4)$, adiabatic evolution yields $\rho_1(t) = \sum_{i,j} \rho_{ij} |\Phi_i(t)\rangle \langle \Phi_j(t)|, (i,j = 1,...,4)$. Diagonalizing $\rho(t)$, we can get non-negative and time-independent eigenvalues since $\rho_{ij} = \rho'_{ij}$, this means that the usual adiabatic evolution must fall in the regime of the non-transitional evolution, but the inverse could not be proven correct.

In conclusion, the evolution of composite systems and its subsystems has been studied. By the definition of non-transitional evolution, four different kinds of evolution were identified and illustrated via the coupled two-qubit system. The non-transitional evolution would find its use in formulating evolution of composite systems, in particular for subsystems that have no Hamiltonian available.

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\[ \rho_1(t) = \frac{1}{M_n} \left( \frac{(g + \cos \theta + \mathcal{E}_n)^2}{\sin \theta (g + \mathcal{E}_n + \cos \theta)} e^{-i\phi} \right) = \rho_+ |\rho_+\rangle \langle \rho_+ | + \rho_- |\rho_-\rangle \langle \rho_- | \]

\[ \sin \theta (g + \mathcal{E}_n + \cos \theta) e^{i\phi} \]

\[ \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{12}^* & \rho_{22} \end{pmatrix} \]