Nonadiabatic Transition Probabilities in the Presence of Strong Dissipation

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Strong dissipative effects on the nonadiabatic transition for the two level system are studied. We focus on a strong dissipation for the diabatic states, and derive the exact transition probability making use of the effective master equation. We consider the case where the external field is swept from not only a negative large value but also from the resonant field, and the exact transition probabilities in these cases are derived.

§1. Introduction

The well-known Landau and Zener (LZ) transition probability plays a crucial role in quantum dynamical changes of states in physics and chemistry. There the energy gap and the sweeping velocity of the external field are key ingredients. Although the LZ transition probability is given in the two-level system, it is approximately applicable to a multi-level system where the avoided level crossings are effectively well described by only localized two levels. Hence it is adopted in the analyses of many experiments which treat time dependent phenomena, such as collision of particles, optics, and magnetic phenomena.

On the other hand, the effect of dissipation cannot be neglected since real experiments are always exposed to thermal environment. Inevitable deviation of transition probability from the one of pure quantum case becomes significant in real experiments such as the adiabatic rapid passage with phonon couplings, the nonadiabatic transitions in localized centers in solids, and nonadiabatic magnetization process in molecular magnets such as Mn_{12} and Fe_{8}. Such thermal noise effect for the two-level was first studied by perturbation approach, and the effective transition probability was derived in the extreme case of strong damping dissipation. Ao and Rammer carried out first principle calculation to investigate temperature dependence of the transition probability of the two-level system with phonon reservoir. Especially they found some compensation effect that the transition probability for zero temperature becomes the same value as the Landau-Zener probability.

In this paper, we study strong dissipation effect for another nonadiabatic situation. That is, we study unfamiliar but realizable case that the field is swept from resonant field (zero field) to large positive field. We used an effective master equation instead of the perturbation approach adopted in previous studies. We show that the effective master equation approach is very convenient for deriving the transition probability in the strong damping limit. Using this approach we reproduce Kayanuma’s formula in the two-level system when the external field is reversed from...
a large negative value to a large positive value. We next consider the case that the field is swept from resonant field and derive the exact transition probability. As a result the exact relations between these cases are found.

§ 2. Transition probability

For two-level system, the transition probabilities in the strong damping case have been studied by several authors using perturbation approach. Here we alternatively adopt the different approach, deriving the effective master equation which simplifies derivations of transition probabilities for the case. In this paper, the following two situations are studied. That is, we first consider the familiar situation that the external field is reversed from $-\infty$ to $\infty$. In this case, we demonstrate that Kayanuma’s transition probability $P_{\text{SD}}^{+\to-}$ is reproduced easily using the effective master equation. We second consider somewhat unfamiliar but realizable situation that the external field is swept from 0 to $\infty$ when initially a diabatic state is occupied.

The model we shall consider in this section is described as,

$$
\mathcal{H}_{\text{tot}}(t) = \mathcal{H}(t) + \xi(t)\sigma^z,
$$

(2.1)

$$
\mathcal{H}(t) = -v t \frac{1}{2} \sigma^z + \Gamma \frac{1}{2} \sigma^x,
$$

(2.2)

where $\sigma^\alpha$ is the $\alpha (= x, y, z)$ component of the Pauli matrix and $\xi(t)$ is the white gaussian noise which satisfies $\langle \xi(t')\xi(t) \rangle = \gamma \delta(t-t')$. $v$ is the sweeping velocity. The diabatic states correspond to the down state $|1\rangle$ and up state $|2\rangle$ which satisfy $\sigma^z|1\rangle = -|1\rangle$ and $\sigma^z|2\rangle = |2\rangle$, respectively. $\Gamma$ is the transverse field which is responsible for the tunneling between the diabatic states. Here we take only $\sigma^z$ as the operator on which the noise acts. We define the variables as $c_1 = \rho_{11} - \rho_{22}$, $c_2 = \rho_{12}$ and $c_3 = \rho_{21}$, for the density matrix $\{\rho_{ij}\}$, and the master equation concretely reads as,

$$
\dot{c}_1 = -i\Gamma(c_3 - c_2),
$$

(2.3)

$$
\dot{c}_2 = (-ivt - \gamma)c_2 + \frac{i\Gamma}{2} c_1,
$$

(2.4)

$$
\dot{c}_3 = (ivt - \gamma)c_3 - \frac{i\Gamma}{2} c_1.
$$

(2.5)

Here we focus on the strong damping (SD) limit, $\gamma \to \infty$. The variable $c_2(t)$ is then formally solved from Eq. (2.4), and can be expanded using the partial integral;

$$
c_2(t) = c_2(t_0) + \frac{i\Gamma}{2} e^{-ivt^2/2+\gamma t} \int_{t_0}^{t} du e^{ivu^2/2+\gamma u} c_1(u)
$$

$$
= c_2(t_0) + \frac{i\Gamma}{2} e^{-ivt^2/2-\gamma t} \left[ e^{ivu^2/2+\gamma u} \frac{c_1(u)}{ivu + \gamma} \right]_{t_0}^{t}
$$

$$
- \frac{\Gamma}{2v} \int_{t_0}^{t} du e^{ivu^2/2+\gamma u} \frac{d}{du} \left( \frac{c_1(u)}{ivu + \gamma} \right) \sim c_2(t_0) + \frac{i\Gamma}{2} \frac{c_1(t)}{ivt + \gamma}.
$$

(2.6)

Here we used the fact that the term $e^{-\gamma(t-t_0)}$ is negligible due to large $\gamma$, and we
neglected the higher order terms of \((i\nu t + \gamma)^{-1}\). In the case of \(c_1(t_0) = 1\), \(c_2(t_0) = c_3(t_0) = 0\), \(c_2(t)\) and \(c_3(t)\) are approximated as,

\[
c_2(t) = \frac{i\Gamma}{2} \frac{c_1(t)}{i\nu t + \gamma} \quad \text{and} \quad c_3(t) = -\frac{i\Gamma}{2} \frac{c_1(t)}{-i\nu t + \gamma}.
\] (2.7)

These relations yield the effective master equation by substituting the relations (2.7) into Eq. (2.3);

\[
\dot{c}_1(t) = \frac{\Gamma^2}{2i\nu} \left\{ \frac{1}{t + i\gamma/v} - \frac{1}{t - i\gamma/v} \right\} c_1(t).
\] (2.8)

We consider the first problem, i.e. \(t_0 = -\infty\). In this case, we can readily integrate the master equation (2.8) to get,

\[
c_1(\infty) = \exp \left( -\frac{\pi\Gamma^2}{v} \right).
\] (2.9)

We now consider the tunneling probability from the state \(|1\rangle\) at \(t = -\infty\) to the state \(|2\rangle\) at \(t = \infty\). This corresponds to the value of \(\rho_{22}(\infty)\). By using the conservation of probability \(\text{Tr}\rho = 1\), this transition probability \(P_{\text{SD}}^{-+}(\equiv \rho_{22}(\infty))\) is obtained,

\[
P_{\text{SD}}^{-+} = \frac{1}{2} \left( 1 - \exp \left( -\frac{\pi\Gamma^2}{v} \right) \right).
\] (2.10)

This is nothing but Kayanuma’s transition probability.\(^{17}\) In the same manner, for the second case where the field is swept from resonant field, i.e., \(t_0 = 0\), the transition probability \(P_{\text{SD}}^{0+}\) is readily calculated as,

\[
P_{\text{SD}}^{0+} = \frac{1}{2} \left( 1 - \exp \left( -\frac{\pi\Gamma^2}{2v} \right) \right).
\] (2.11)

We have numerically confirmed the validity of these probabilities (2.10) and (2.11).

The variable \(c_1(t)\) is directly connected with the magnetization \(M(t) = \text{Tr} \sigma^z \rho(t)\). We obtain the magnetization process solving (2.8) as,

\[
M^{-+}(t) = -\exp \left[ \frac{\Gamma^2}{v} \arctan \left( \frac{\gamma}{\nu} \right) \right],
\] (2.12)

\[
M^{0+}(t) = -\exp \left[ \frac{\Gamma^2}{v} \arctan \left( \frac{\gamma}{\nu} \right) - \frac{\pi}{2} \right],
\] (2.13)

where the function \(y = \arctan x\) is defined in the region of \(x \in [-\infty, \infty]\) and \(y \in [-\pi, 0]\). This shows that the magnetization process depends on the noise strength \(\gamma\), whereas final magnetization does not. This was also numerically confirmed.

\(^{17}\) This approximation should be justified under the condition that the transition time in the pure quantum case is much larger than the dissipation time scale \(1/\gamma\).
§3. Relation between $P_{SD}$ and $P_{LZ}$

We discuss the exact relation of the transition probabilities for pure quantum case and in strong damping case. When the field is reversed from large negative value without dissipation, the transition probability is denoted by $P_{LZ}^{-+}$. Here the subscript ‘LZ’ means that it is the pure quantum case. In the case of the field swept from the resonant point without dissipation, the transition probability is written as $P_{SD}^{0+}$. The transition probability in each case is written as follows,

$$P_{SD}^{-+} = \frac{1}{2} \left( 1 - \exp \left( -\frac{\pi v}{2} \right) \right), \quad P_{LZ}^{-+} = 1 - \exp \left( -\frac{\pi v}{4} \right),$$

$$P_{SD}^{0+} = \frac{1}{2} \left( 1 - \exp \left( -\frac{\pi v}{4} \right) \right), \quad P_{LZ}^{0+} = \frac{1}{2} \left( 1 - \exp \left( -\frac{\pi v}{8} \right) \right).$$

These exact probabilities satisfy the following relations,

$$P_{SD}^{-+} \leq P_{LZ}^{-+},$$

$$P_{SD}^{0+} \geq P_{LZ}^{0+}.$$  \hspace{1cm} (3.1)

The inequality (3.2) means that the dissipation reduces tunneling that the state remains in the ground state. This means that the thermal excitation from ground state to the excited state represses such adiabatic transition. Thus the inequality (3.2) is easily understood. On the other hand, the inequality (3.3) indicates the opposite property. The initial state $\psi(0) = |1\rangle$ is the superposition between the ground state $|G(0)\rangle$ and the excited state $|E(0)\rangle$,

$$\psi(0) = \frac{1}{2} (|G(0)\rangle + |E(0)\rangle).$$  \hspace{1cm} (3.4)

In case of almost adiabatic evolution in the pure quantum case, $v \ll 1$, the state of the system almost follows such superposition at $t$,

$$\psi(t) \sim \frac{1}{2} \left( e^{i\phi_1(t)} |G(t)\rangle + e^{i\phi_2(t)} |E(t)\rangle \right),$$

with the dynamical phases $e^{i\phi_1(t)}$ and $e^{i\phi_2(t)}$. Since $|G(t)\rangle \to |2\rangle$, $|E(t)\rangle \to |1\rangle$ in the limit of $t \to \infty$, the maximum value of transition probability is $\frac{1}{2}$ in the pure quantum evolution. When the strong dissipation exists, the noise also induces such uniform distribution, because the dissipation we now consider can be regarded as thermal effects with very high temperature. As a result the tunneling probability is larger in presence of the dissipation. We expect these characteristic relations (3.2) and (3.3) will be verified in real experiments.

§4. Discussion

The effective master equation approach is quite useful because the differential equation of system’s variable becomes very simple. This approach will be applicable in the other systems whose exact transition probabilities can be analytically enumerated in the pure quantum case. We consider the two cases where the external field is
swept from large negative field and from zero field. Both situations are easily realized in real experiments. We hope that the exact relation (3.2) and (3.3) is confirmed in real experiments using classical optical system\(^4\) and Cooper pair,\(^{20}\) and so on.

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