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Initial-Slip Term Effects on the Dissipation-Induced Transition of a Simple Harmonic Oscillator *

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We investigate the effects of the initial-slip term by studying the dissipation-induced transition probabilities between any two eigenstates of a simple harmonic oscillator. The general analytical expressions for the transition probabilities are obtained, then the special cases of transition probabilities ignoring the Brownian motion from the ground state to the first few excited states are discussed. It is found that the initial-slip term not only makes the forbidden transitions between states of different parity possible but also lifts the initial value of the transition probabilities.

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The physics of dissipative quantum systems[1−10] has attracted much attention in the past decades, especially after the pioneering work of Calderia and Legget (CL) on the quantum tunneling of a macroscopic variable.[2−4] The well developed methodology to describe the dynamics of the dissipative system is the generalized Langevin equations (GLE).[10] The usual way to derive the GLE is through the so-called system plus bath approach, i.e., putting the system S into an environment simulated by a bath R of N harmonic oscillators interacting with the system through certain coupling. The whole system $S+R$ is treated as one conservative system, the GLE is obtained by eliminating the variables of the bath R from its corresponding Heisenberg equations or the canonical equations in the classical level. Consequently, the coupling of a system to its environment leads to two effects that occur for classical as well as quantum systems: dissipation and fluctuations of the system degree of freedom which manifest itself for example as Brownian motion.

The exact GLE so derived[4,11] will have both the friction and fluctuation force, plus an additional term, i.e. the so-called initial-slip term (IST).[1,10,12] In the context of classical statistical mechanics, the origin of the IST as perhaps first pointed out by Bez[13] was due to the decoupled initial conditions (DIC), i.e., the system and the bath are assumed not to interact initially. Bez showed that if the system is assumed to be initially in thermal equilibrium with the bath, then no such term appears and the correct GLE can be derived. Later, this point has also been noticed by Cortés *et al.*[14] for both classical and quantum systems. Upon noticing the role of IST,[13−15] it has been argued[10] that the IST is an artefact and simply dropped. However, as noted in Ref. [15], this way of treating the IST is not satisfactory since the recipe to circumvent the problem caused by the use of DIC is only clearly formulated in the semiclassical limit. In the quantum regime the remedy is not clear. Nevertheless, the DICs are widely used especially in path integral approaches.[16,17]

On the other hand, some dynamical problems can also be treated conveniently via the use of an effective Hamiltonian. For instance, the Hamiltonian of quantum damped harmonic oscillator (QDHO)[18,19] is a typical effective Hamiltonian for the model of a harmonic oscillator coupling linearly to the bath, i.e., the model of quantum Brownian motion (QBM).[20−30] However, unlike the GLE, the equation of the motion from the effective Hamiltonian will have solely the friction force, neither the fluctuation force nor the IST will appear. The connection between the effective Hamiltonian and the system plus bath approach has been shown by Yu and Sun (YS).[31,32] For the model of QBM, they obtained the effective Hamiltonian using the system plus bath approach and the exact solution for the wave function of the system plus the bath, while the IST was simply dropped in their derivation.

In this Letter, we consider the model of a QBM here since it is analytically tractable. Taking the effects of the IST into account, we calculate the transition probabilities from one stationary state of a simple harmonic oscillator to another due to the perturbative effect of dissipation. Actually, this type of problem has been studied by several groups using different methods for various purposes. However, in those previous studies the IST either has never been touched upon[33−38] or has been simply ignored.[31,32,39] Consequently, it is unclear whether the IST will have any effects on the transition probabilities or not. In the present work, using the wave function obtained by YS, the general analytical expressions for the transition probabilities are calculated. We then discuss the special case of transition from ground to the first few excited states, and show the effects of IST on the transition probabilities which have never been reported in prior works.

Let us begin by giving a brief introduction to the

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IST. Considering the CL model,[2,3] a system S of a simple one-dimensional harmonic oscillator described by the following Hamiltonian

$$\hat{H}_{\rm s} = \frac{\hat{p}^2}{2M} + \frac{1}{2}M\omega_0^2 q^2, \tag{1}$$

where M is the mass, and ω_0 the frequency. Adopting the DIC, namely when time $t < 0$, the system is assumed at its nth eigenstate

$$\Phi_n^{\rm SHO}(x) = \langle x|n\rangle = N_n e^{-\frac{1}{2}\alpha_0^2 x^2} H_n(\alpha_0 x), \tag{2}$$

where the normalization constant $N_n = (\frac{\alpha_0}{\sqrt{\pi}2^n n!})^{\frac{1}{2}}$, $\alpha_0 = \sqrt{\frac{M\omega_0}{\hbar}}$ and $H_n(z)$ is the usual Hermite polynomial. We assume that the system is moved into an environment of a bath at $t = 0$. The bath B consists of N harmonic oscillators B_i that has mass m_i, coordinates x_i and frequency ω_i. The Hamiltonian of the composite system of S and B is[2,3]

$$\hat{H} = \frac{\hat{p}^2}{2M} + \frac{1}{2}M(\omega_0^2 + \Delta\omega^2)q^2 - q\sum_j c_j x_j + \sum_j (\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 x_j^2), \tag{3}$$

where $\Delta\omega^2$ is the coupling induced renormalization of the frequency. The Heinsenberg equation of motion is

$$M\ddot{q} = -M(\omega_0^2 + \Delta\omega^2)q + \sum_j c_j x_j, \tag{4}$$

$$m_j\ddot{x_j} = -m_j\omega_j^2 x_j + c_j q, \ (j = 1, 2, \ldots, N). \tag{5}$$

Assuming that the bath is Ohmic, and eliminating the variables of the bath R from its corresponding Heisenberg equations results in the GLE for the system[31,32]

$$\ddot{q} + \eta\dot{q} + \omega_0^2 q = f_{\rm s}(t) + f_i(t), \tag{6}$$

where

$$f_{\rm s}(t) = \sum_{j=1}^{N}\frac{c_j}{M}\Big[x_{j0}\cos(\omega_j t) + \frac{\dot{x}_{j0}\sin(\omega_j t)}{\omega_j}\Big], \tag{7}$$

is the Brownian motion driving force, and

$$f_i(t) = -\eta q(0)\delta(t), \tag{8}$$

the IST, which is simply dropped in many previous investigations such as in the method of YS.[31,32]

Notice that if the IST is taken into account, the YS method will still be applicable except that the system wave function $\psi(Q,t)$ with $Q = q - \xi$ describes the motion of the physical variable q eliminating the Brownian motion part ξ, and will evolve according to a new effective Hamiltonian[31,39,40]

$$\hat{H}_Q = e^{-\eta t}\frac{\hat{P}^2}{2M} + \frac{1}{2}M\omega_0^2 e^{\eta t}Q^2 - e^{\eta t}f_I(t)Q, \tag{9}$$

where $\hat{P}$ is the corresponding conjugate momentum for Q, $f_I(t) = Mf_i(t)$, and the last term of this Hamiltonian is due to the IST. For a general time-dependent external force $f_{\rm ext}(t)$, this effective Hamiltonian describes a damped driven harmonic oscillator (DDHO).[36] Notice that here the physical variable $q = Q + \xi$ fluctuates about Q, since ξ describes the Brownian motion, this is a dissipative effect due to the bath.

Next we use the above Hamiltonian of Eq. (9) to calculate the dissipation-induced transition probabilities. We first focus on the evolution of the wave function for the dissipative system. Employing Feynman's path integral method,[16,17] we have

$$\psi_n(q,t) = \int_{-\infty}^{\infty} K(q,t;q_0,0)\,\Phi_n^{\rm SHO}(q_0)dq_0, \tag{10}$$

where the propagator for a DDHO[19,36] is

$$K(q,t;q_0,0) = F(t)e^{\frac{iM}{2\hbar}(\tilde{a}q^2 + \tilde{b}q_0^2 + 2\tilde{c}qq_0 + 2\tilde{d}q + 2\tilde{e}q_0 - \tilde{f})}, \tag{11}$$

with $F(t) = (\frac{M\omega e^{\frac{\eta t}{2}}}{2\pi i\hbar\sin\omega t})^{\frac{1}{2}}$, and the time-dependent coefficients

$$\begin{aligned}
&\tilde{a}(t) = \Big(-\frac{\eta}{2} + \omega\cot\omega t\Big)e^{\eta t},\ \tilde{b}(t) = \Big(\frac{\eta}{2} + \omega\cot\omega t\Big),\\
&\tilde{c}(t) = \frac{-\omega e^{\frac{\eta t}{2}}}{\sin\omega t},\ \tilde{d}(t) = \frac{e^{\frac{\eta t}{2}}\int_0^t d\tau f_I(\tau)e^{\frac{\eta\tau}{2}}\sin\omega\tau}{M\sin\omega t},\\
&\tilde{e}(t) = \frac{\int_0^t d\tau f_I(\tau)e^{\frac{\eta\tau}{2}}\sin\omega(t-\tau)}{M\sin\omega t},\\
&\tilde{f}(t) = \frac{2\int_0^t d\tau f_I(\tau)e^{\frac{\eta\tau}{2}}\int_0^\tau ds f_I(s)e^{\frac{\eta s}{2}}\sin\omega(t-\tau)\sin\omega s}{M^2\omega\sin\omega t},
\end{aligned} \tag{12}$$

with $\omega = \sqrt{\omega_0^2 - \frac{\eta^2}{4}}$. Inserting Eq. (8) into Eq. (12) yields

$$\tilde{d}(t) = 0,\ \tilde{e}(t) = -\eta q(0),\ \tilde{f}(t) = 0. \tag{13}$$

Combining Eqs. (11)–(13) with Eq. (10), one obtains

$$\begin{aligned}
\psi_n(q,t) = &\frac{N_n e^{\frac{1}{4}\eta t}}{(|\zeta(t)\sin\omega t|)^{\frac{1}{2}}}\\
&\cdot e^{-i(n+\frac{1}{2})\arccot[\frac{\omega}{\omega_0}(\frac{\eta}{2\omega} + \cot\omega t)]}\\
&\cdot e^{-A_1 q^2 - A_2 q - A_3}H_n(Dq + E),
\end{aligned} \tag{14}$$

where

$$A_1 = \frac{\alpha^2 e^{\eta t}}{2}\Big[\frac{\zeta(t)}{|\zeta(t)|^2\sin^2\omega t} - i\Big(\cot\omega t - \frac{\eta}{2\omega}\Big)\Big], \tag{15}$$

$$A_2 = \frac{M\eta q(0)e^{\eta t/2}}{\hbar\sin\omega t\zeta^*(t)},\ A_3 = \frac{M\eta^2 q^2(0)}{2\hbar\omega\zeta^*(t)}, \tag{16}$$

$$D = \frac{\alpha_0 e^{\frac{\eta t}{2}}}{|\zeta(t)\sin\omega t|},\ E = \frac{D}{\omega}\Big(\eta q(0)\sin\omega t e^{-\frac{\eta t}{2}}\Big), \tag{17}$$

with $\zeta(t) = \frac{\omega_0}{\omega} + i(\frac{\eta}{2\omega} + \cot\omega t)$ and $\alpha = \sqrt{\frac{m\omega}{\hbar}}$.

It is obvious that the transition probabilities from the nth to the mth excited state is

$$\mathcal{P}(n\to m)=\frac{1}{\sqrt{2\pi}\sigma_\xi(T,t)}\int_{-\infty}^{\infty}|\mathcal{A}_{nm}(\xi)|^2 e^{-\frac{\xi^2}{2\sigma_\xi^2}}d\xi, \quad (18)$$

where $\mathcal{A}_{nm}(\xi)$ is the ξ-dependent transition amplitude

$$\mathcal{A}_{nm}(\xi)=\int_{-\infty}^{\infty}\Phi_m^{\rm SHO}(x)\psi_n(x-\xi,t)dx. \quad (19)$$

Note that ξ is the contribution of the bath to the Brownian motion which obeys the Gaussian distribution with width $\sigma_\xi^2(T,t)$; for more details see Refs. [31,32]. The integral on the right-hand side of Eq. (19) can be evaluated by using the generating function method.[19] Combining Eqs. (2), (14), (19) and (18), we finally obtain

$$\begin{aligned}\mathcal{P}(n\to m)=&\frac{N_m^2N_n^2e^{\frac{1}{2}\eta t}}{|\frac{\alpha_0^2}{2}+A_1||\zeta(t)\sin\omega t|}\Big(\frac{\pi}{2\sigma_\xi^2}\Big)^{\frac{1}{2}}\\ &\cdot\sum_{p=0}^{\min(m,n)}\sum_{i=0}^{[\frac{(m-p)}{2}]}\sum_{k=0}^{[\frac{(n-p)}{2}]}\\ &\cdot\sum_{p'=0}^{\min(m,n)}\sum_{i'=0}^{[\frac{(m-p)}{2}]}\sum_{k'=0}^{[\frac{(n-p)}{2}]}\\ &\times\int_{-\infty}^{\infty}d\xi e^{-\frac{\tilde\beta}{2}\xi^2+(B_2+B_2^*)\xi+(B_3+B_3^*)}\\ &\cdot D_{p,i,k}^{mn}(\xi,t)[D_{p',i',k'}^{mn}(\xi,t)]^*, \end{aligned}\quad (20)$$

where $[x]$ denotes the largest integer that is not greater than x, $\tilde n=(m+n-i-k-p-i'-k'-p')$, $\tilde\beta=\alpha_0^2(\frac{A_1}{\alpha_0^2/2+A_1}+\frac{A_1^*}{\alpha_0^2/2+A_1^*})+\frac{1}{\sigma_\xi{}^2}$, and $D_{p,i,k}^{mn}(\xi,t)=\frac{m!n!a_1^ia_2^ka_3^p\epsilon_1{}^{(m-p-2i)}\delta_1{}^{(n-p-2k)}}{i!k!p!(m-p-2i)!(n-p-2k)!}$ with $\epsilon_1=\frac{\alpha_0(2A_1\xi-A_2)}{\alpha_0^2/2+A_1}$, $\delta_1=2(E-D\xi)+\frac{D(2A_1\xi-A_2)}{\alpha_0^2/2+A_1}$.

To see the physical effects of the IST clearly, in the following we investigate the special case of transition from the ground state to the first few excited states and ignoring the Brownian motion. By setting $\xi=0$ in Eq. (20), we have the transition probabilities from the ground state to higher excited states with solely the effect of the IST

$$\mathcal{P}_0(0\to m)=P_0(t)\frac{e^{(B_3+B_3^*)}H_m(\mu_0)H_m^*(\mu_0)}{2^m m!}\Big|\frac{v(t)}{u(t)}\Big|^m, \quad (21)$$

where $\mu_0=\frac{M\eta\omega q(0)}{\hbar\omega_0\alpha_0\sqrt{u(t)v(t)}}$, $u(t)=\sin(\omega t)\cosh(\frac{\eta t}{2})+i[\frac{\eta}{2\omega_0}\sinh(\frac{\eta t}{2})\sin(\omega t)-\frac{\omega}{\omega_0}\cosh(\frac{\eta t}{2})\cos(\omega t)]$, $v(t)=\sin(\omega t)\sinh(\frac{\eta t}{2})+i[\frac{\eta}{2\omega_0}\cosh(\frac{\eta t}{2})\sin(\omega t)-\frac{\omega}{\omega_0}\sinh(\frac{\eta t}{2})\cos(\omega t)]$, and $P_0(t)=P_0(0\to 0)=\frac{\omega}{\omega_0|u(t)|}$ is the probability for the system to remain in its ground state.[38,39] For comparison, here we also give the expressions for the transition probabilities ignoring both the Brownian motion and IST

$$P_0(0\to m)=P_0(t)\Big(\frac{m!}{2^m}\Big)\frac{|a_1|^m}{[(\frac{m}{2})!]^2}, \quad (22)$$

for even m and zero, otherwise. This is a special case of the more general rule: the transitions between eigenstates with different parities are forbidden due to the fact that the Hamiltonian of Eq. (9) does not possess the space-inversion symmetry.

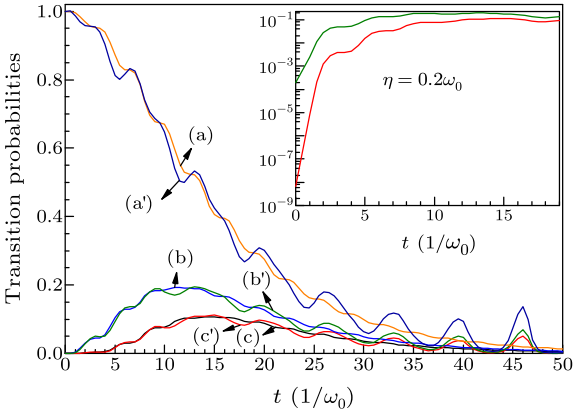

Fig. 1. Evolution of transition probabilities ignoring the Brownian motion when $\eta=0.2\omega_0$. Curve (a) is the probability for the system to remain in its ground state $P_0(t)$ ignoring the initial-slip term while (a′) is $\mathcal{P}_0(t)$ the same plot including the effect of the initial-slip term. Curves (b) and (b′) are the plots for $P_0(0\to 2)$ and $\mathcal{P}_0(0\to 2)$, curves (c) and (c′) are the plots for $P_0(0\to 4)$ and $\mathcal{P}_0(0\to 4)$. Note that the initial values of the curves (b′) and (c′) are finite constants: $\mathcal{P}_0(0\to 2)|_{t\to 0}=2\times 10^{-4}$, and $\mathcal{P}_0(0\to 4)|_{t\to 0}=\frac{2}{3}\times 10^{-8}$, both much less than unity; see the enlarged plot in the upper-right corner. The time t is in units of $\frac{1}{\omega_0}$, and $q(0)=1$ in units of $\frac{\hbar}{M\omega_0}$.

Having obtained the expressions for the transition probabilities, let us first take a look at the transitions from the ground to the first few even states ($m=0$, 2 and 4), which are allowed in the case when the IST is ignored and have been shown in Ref. [39]. Figure 1 shows the transition probabilities for $\mathcal{P}_0(t)$, $\mathcal{P}_0(0\to 2)$, $\mathcal{P}_0(0\to 4)$. To make comparison with the transition probabilities ignoring the IST, we also plot $P_0(t)$, $P_0(0\to 2)$ and $P_0(0\to 4)$ in the same graphs. Hence, in the absence of the Brownian motion, it is clear from the graphs that for those allowed transitions the IST will only add slight short-time fluctuations to the curves without the effect of IST, and the fluctuations become stronger as time increases.

From Eq. (21), we can see that the transition probabilities are not always zero for odd m. Therefore, strikingly different from the case ignoring the IST where only the transition to even states are allowed, it is evident that the transition from the ground to odd states are possible now. In other words, in the absence of Brownian motion, the IST can induce transitions between states of different parities. Note that as shown previously,[39] the Brownian motion can also cause such transitions when the IST is dropped but in a different manner. In Fig. 2, we plot the transition probabilities from the ground to the first ($m=1$) and second odd ($m=3$) states. It is evident that their behaviors are quite different, one always decays while

the other first increases then decays. Moreover, the scale of their largest values is in orders smaller than those transitions from the ground to even states, as shown in Fig. 1.

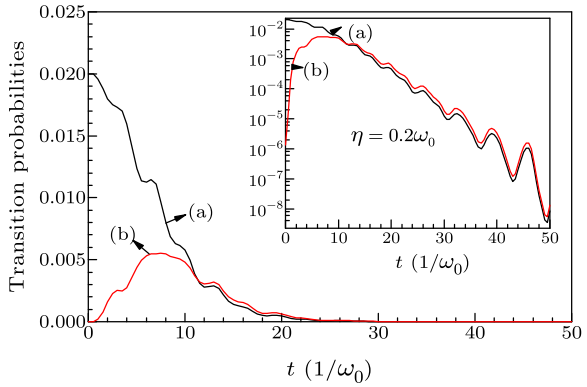

Fig. 2. Evolution of transition probabilities due to the initial-slip term while ignoring the Brownian motion when $\eta = 0.2\omega_0$. Curve (a) is the probability for the system to jump from the ground state to the first excited state $\mathcal{P}_0(0 \to 1)$. Curve (b) is the probability for the system to jump from the ground state to the third excited state $\mathcal{P}_0(0 \to 3)$. Note that its initial value $\mathcal{P}_0(0 \to 3)|_{t\to 0} = \frac{4}{3} \times 10^{-6} \ll 1$, thus it 'appears' to be zero in the scale we used in the plot, but actually not (see the enlarged plot in the upper-right corner). The time t is in units of $\frac{1}{\omega_0}$, and $q(0) = 1$ in units of $\frac{\hbar}{M\omega_0}$.

Another point worth mentioning is that the initial values of the transition probabilities are changed due to the presence of IST. In the limit of $t \to 0$, $u(t) \sim \frac{\omega}{\omega_0}$, thus $P_0(t) \to 1$. On the other hand, it can be readily shown that $B_3(t)|_{t\to 0} \to 0$. Therefore, together with Eq. (21) we have

$$\mathcal{P}_0(0 \to m)|_{t\to 0} = \frac{1}{2^m m!}\left(\frac{M\eta q(0)}{\hbar}\right)^{2m}. \quad (23)$$

This means that for non-zero $q(0)$, the IST will lift the initial transition probabilities from 0 to a finite value, as reflected in the enlarged plots in Figs. 1 and 2.

It should be emphasized that our calculation is restricted to the Ohmic bath and valid only when the coupling between the system and the bath is very weak, thus the effect of dissipation can be treated perturbatively. As noted in Ref. [41], the notion of transitions between discrete eigenstates becomes questionable if the coupling is not very weak. In that case, the discrete states of the harmonic oscillator are 'absorbed' into the continuum, and there are no longer any discrete states. It is also worthwhile mentioning a few points for the YS method itself. In the derivation of the YS method, (i) the frequency renormalization term is treated as a large constant which fails for the non-Markovian processes.[35] Thus the YS method is valid only for the Markovian processes. (ii) The cutoff frequency for the Ohmic bath has been taken to be infinity and this makes the final wave function appear to be independent of the cutoff frequency.

In summary, by employing the YS approach we have investigated the dissipation-induced transition probabilities between any two eigenstates of a simple harmonic oscillator. The general analytical expressions for the transition probabilities are obtained. It is shown that the IST plays a significant role in the transition processes. For instance, the IST can induce transitions between states of different parities when the Brownian motion is negligible. Moreover, the IST will lift the initial values of the transition probabilities. Therefore, instead of being simply dropped, the effects of the IST should be carefully examined.

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