Quantum-Classical Transition in Dissipative Double-Well Systems
—A Numerical Study by a New Monte Carlo Scheme—

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The thermodynamics of dissipative quantum systems with double-well potentials is studied by a path-integral Monte Carlo (PIMC) method without truncation to the two-state model. For efficient simulation at low temperatures, we develop a new local update scheme on the basis of the approximate decomposition of the Boltzmann weight to Gaussian distributions. The localization transition induced by ohmic dissipation is clarified numerically for arbitrary potential barriers.

KEYWORDS: Caldeira-Leggett model, quantum dissipation, path-integral Monte Carlo, localization transition

Quantum tunneling between distinct states subject to dissipation has been one of the central problems in both physics and chemistry for several decades.\textsuperscript{1,2} A number of studies on dissipative quantum systems have revealed that dissipation strongly affects the quantum nature of the system. In particular, the suppression/destruction of quantum superpositions has been studied extensively in the dissipative two-state model. The most striking feature of the two-state system is that localization transition occurs at a critical value of dissipation strength for ohmic damping.\textsuperscript{3–5} This phenomenon can be interpreted as a ‘quantum-classical transition’ driven by the coupling with the environment, which is unavoidable for macroscopic objects.

The dissipative two-state model is useful for the analysis of generic systems with a double-well-shaped potential in the large-barrier limit. For the small-barrier case, however, the truncation to the two-state model cannot be justified, and we must analyze the original generic system directly. Dissipation effects on generic systems are nontrivial, and have been considered only in a few studies. Aoki and Horikoshi have discussed localization transition in the double-well potential systems by a non-perturbative renormalization group approach with local approximation.\textsuperscript{6} They concluded that the critical value of dissipation strength is larger than that of the two-state model. Capriotti et al. have studied the thermodynamics of dissipative double-well systems by the path-integral Monte Carlo (PIMC) method.\textsuperscript{7} However, they have not discussed localization transition, because their algorithm based on the conventional update scheme significantly limits the accuracy of the simulation at low temperatures. Thus, neither the identification of localization transition nor the determination of critical dissipation strength have been achieved so far without approximations.

Recently, a significant improvement in the update scheme of the PIMC method has been presented by Werner and Troyer for periodic-potential systems.\textsuperscript{8,9} They introduced a novel update scheme by extending the cluster algorithm for classical Ising-spin systems to realize efficient change in the paths beyond the potential barrier. In addition, they adopted an efficient local update scheme by combining the fast random-number generation of the Gaussian distributions with stochastic acceptance. They demonstrated that their algorithm is much more efficient than conventional PIMC simulations,\textsuperscript{10–12} and determined the phase diagram successfully by the accurate calculation of response functions at low temperatures. This development of the Monte Carlo algorithm, in principle, enables us to study the thermodynamics of various types of dissipative systems in much wider parameter regions. The application of their method to double-well systems, however, is not straightforward.

In this paper, we propose a new scheme for efficient local update in the PIMC simulation, and demonstrate its efficiency for large system sizes. By combining this improved update with the cluster update by Werner and Troyer, we show for the first time the quantum-classical transition in generic double-well potential systems without truncation to the two-state model. We stress that our local update scheme has wide application to various classes of models and is not restricted to dissipative systems.

The dissipative system is described by the Caldeira-Leggett model:\textsuperscript{15,16}

\begin{equation}
H = \frac{p^2}{2m} + V(x) + \sum_\alpha \left\{ \frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} \left( y_\alpha - \frac{c_\alpha}{m_\alpha \omega_\alpha^2} x \right)^2 \right\}. \quad (1)
\end{equation}

The environment properties are uniquely determined by...
the spectral function
\[
J(\omega) = \frac{\pi}{2} \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha}\omega_{\alpha}} \delta(\omega - \omega_{\alpha}).
\]  
(2)

In this paper, we restrict our discussion to ohmic dissipation, for which the spectral function is given as \( J(\omega) = \gamma \omega \). The double-well potential is expressed by the quadratic-plus-quartic form
\[
V(x) = \frac{16V_0}{a^2} \left( x^2 - \frac{a^2}{4} \right)^2,
\]  
(3)
for a barrier height \( V_0 \) and a spatial distance \( a \) between two potential minima. In the following discussion, we rescale the length by \( a/2 \), the energy by \( V_0 \) and the frequency by \( \omega_0 = (32V_0/ma^2)^{1/2} \) for a small oscillation near the potential minima. Then, in the absence of dissipation, the system can be characterized by only one Trotter number.

We further define a dimensionless dissipation strength as \( \alpha = m\gamma a^2/(2\pi\hbar) \).

By integrating the variables of the harmonic oscillators, we can rewrite the partition function in terms of path integrals using the effective action as
\[
Z = \int Dx(\tau) \exp(-S[x(\tau)]),
\]  
(4)

\[
S[x(\tau)] = \frac{8}{g} \int_0^{\beta g} d\tau \left\{ \frac{1}{2} \left( \frac{dx}{d\tau} \right)^2 + \frac{1}{8}(x^2 - 1)^2 \right\}
\]
\[ - \int_0^{\beta g} d\tau \int_0^{\beta g} d\tau' k(\tau - \tau') x(\tau) x(\tau'),
\]  
(5)
where the memory kernel \( k(\tau) \) is given as
\[
k(\tau) = \frac{\alpha}{4 \sin^2((\pi/\beta g)\tau)}.
\]  
(6)

For the PIMC simulation, the path is discretized by the Trotter number \( N \), which is taken to be sufficiently large to satisfy \( \Delta \varepsilon \equiv \beta/N \ll 1 \). After the discretization, the action is obtained by the path片段 \( x_j = x((\beta g/N)j) \) as
\[
S[\{x_j\}] = -\sum_{i,j} K(i-j) x_i x_j + \Delta \varepsilon \sum_j (x_j^2 - 1)^2,
\]  
(7)
where the long-range kernel including the kinetic energy is given by
\[
K(i) = \frac{4N}{\beta g^2} (\delta_{i1} + \delta_{i,N-1}) + \frac{\alpha}{4 \sin^2((\pi/\beta g)N)}.
\]  
(8)
for \( i \neq 0 \). The value of \( K(0) \) is taken so that the zero-frequency Fourier component of the kernel becomes zero. In the conventional update scheme, one of the path fragments is changed as \( x_j^{\text{new}} = x_j^{\text{old}} + \varepsilon \) for a fixed \( j \). Then, this change is accepted with the probability \( \min(\exp(-S[\{x_j^{\text{new}}\})] - S[\{x_j^{\text{old}}\}],1) \).

The discretization \( \varepsilon \) is generated randomly by the uniform distribution with the range \([-\delta, \delta]\), where \( \delta \) is chosen appropriately to obtain the optimal acceptance rate. This algorithm, however, takes considerable time for one sweep of local updates on all the path fragments.

We now introduce a new update scheme. First, the Boltzmann weight of the potential term is approximately decomposed into \( M \) pieces of the Gaussian distribution as
\[
e^{-\Delta \varepsilon V(x)} \simeq \sum_{m=1}^{M} \mu_m e^{-\lambda(x-\sigma_m)^2},
\]  
(9)
where \( \lambda, \sigma_m \) and \( \mu_m \) are determined by fitting. For the double-well potentials, \( V(x) = (1 - x^2)^2 \), and this approximate decomposition can be carried out with a small value of \( M \). One example of fitting is shown in Fig. 1 for \( \Delta \varepsilon = 100/256 \simeq 0.4 \). Here, we used \( M = 4 \) Gaussian distributions, and the parameters were obtained as \( \lambda = 3.7683, -\sigma_1 = \sigma_2 = 0.9068, -\sigma_2 = \sigma_3 = 0.5858, \mu_1 = \mu_4 = 1.1169 \) and \( \mu_2 = \mu_3 = 0.3963 \). As seen in Fig. 1, the approximate fitting is almost in agreement with the original weight. In our calculation, we checked that the deviation from the exact weight is not distinguishably different for the obtained results up to \( N = 1024 \). By this decomposition, the partition function is written in the form
\[
Z = \sum_{\{m_j\}} \int \prod_j dx_j W(\{x_j\}, \{m_j\}).
\]  
(10)
Here, the new variables \( \{m_j\} \) play the role of auxiliary fields. Our update scheme consists of two steps. In the first step, the variables \( \{m_j\} \) are chosen for fixed \( \{x_j\} \) with the probability \( t(m_j|x_j) \). For this update, the weight is modified as \( W(\{x_j\}, \{m_j\}) = f(\{x_j\}) \times \prod_j w(x_j, m_j) \), where \( w(x_j, m_j) = \mu_m \exp(-\lambda(x_j - \sigma_m)^2) \) and \( f(\{x_j\}) \) is independent of \( \{m_j\} \). Then, the transition probability is given by the extended detailed valance condition as
\[
t(m_j|x_j) = \frac{w(x_j, m_j)}{\sum_{m_j} w(x_j, m_j)}.
\]  
(11)
Note that this update needs only the local information of each path fragment, thus, can be performed efficiently. In the second step, the path fragments \( \{x_j\} \) are updated for fixed \( \{m_j\} \). In this update, it is crucial that for fixed \( \{m_j\} \), the effective action defined by \( W(\{x_j\}, \{m_j\}) = \exp(-S) \) is written in a quadratic form.
of \{x_j\}. Using a Fourier transformation, the effective action can be written in the normal form

\[ S = \sum_n \left( c_n (\tilde{x}_n - \tilde{\sigma}_n)^2 - \sum_j \ln \mu_{m_j} \right) , \quad (12) \]

\[ c_n = \frac{16N^2}{\beta g^2} \sin^2 \frac{\pi n}{N} + \frac{\pi^2 \alpha}{2} |n| , \quad (13) \]

where \(\tilde{x}_n\) and \(\tilde{\sigma}_n\) are the Fourier components of \(x_j\) and \(\sigma_{m_j}\), respectively. The effective action can be modified further as

\[ S = \sum_n (c_n + \lambda N) \left( \tilde{x}_n - \frac{\lambda N \tilde{\sigma}_n}{c_n + \lambda N} \right)^2 + g(\{m_j\}) , \quad (14) \]

where \(g(\{m_j\})\) is independent of \(\{x_j\}\). Then, the new path is efficiently generated by the Gaussian distribution with mean \(\lambda N \tilde{\sigma}_n/(c_n + \lambda N)\) and standard deviation \((c_n + \lambda N)^{-1/2}/2\) for both real and imaginary parts of \(\tilde{x}_n\).\(^{18}\) Note that all the path fragments are updated immediately without rejection.

In the presence of large potential barriers, global change of the path across the barrier is strongly suppressed, even in the improved local update. To overcome this difficulty, we adopt the cluster update by Werner and Troyer.\(^8\) We first focus on the mirror symmetry \(V(x) = V(-x)\) for the potential energy, and flip the sign of the path without varying its amplitude, \(|x_j|\). Since the potential term in eq. (7) is unchanged by this update of the path, we can disregard this term in the following discussion. We define the Ising variables as \(s_j = s_j |x_j|\), and express the effective action by these variables as

\[ S[\{s_j\}] = - \sum_{i,j} J_{i,j} s_i s_j , \quad (15) \]

where \(J_{i,j} = K(\delta - j) |x_i| |x_j|\). This is simply the one-dimensional long-range Ising model. Then, the Wolff cluster algorithms can be applied directly.\(^{12}\) We note that the cluster update can deal with quantum tunneling processes efficiently through the creation (annihilation) of instantons and the change in their positions.

We show the effectiveness of our improved local update in Fig. 2. Here, the CPU time in an improved calculation is measured in a cluster computer consisting of eight Pentium 4 processors for the Monte Carlo sampling within the autocorrelation time in the correlation function \langle x(0)x(\beta/2) \rangle.\) The main figure in Fig. 2 shows the comparison between the conventional algorithm and the new algorithm for the local update at \(\alpha = 0\) (no dissipation) without the cluster update. As seen in this figure, our algorithm for the local update shows significant improvement in the simulation time. The improved CPU time is approximately proportional to \(N\) for large system sizes, for which the autocorrelation time is almost independent of \(N\). This system-size dependence indicates that the efficiency of our simulation is limited by the Fourier transformation, which requires time on the order of \(N \log N\). The inset in Fig. 2 shows the CPU time measured for \(\alpha \geq 0\) (nonzero dissipation) using both the new local update and the cluster update. This result shows that the efficiency of our algorithm is less affected by dissipation strength \(\alpha\).

Next, let us move onto the localization transition in double-well potential systems. We expect that this transition belongs to the Kosterlitz-Thouless type because of the same symmetry as the long-range Ising model with inverse square-law interactions.\(^{19}\) In accordance with ref. 19, the transition is determined by calculating the uniform susceptibility defined as

\[ \chi = N(\langle x_i x_j \rangle / N^2) / (\langle x^2_i / N \rangle) . \]

We use renormalization group analysis\(^{20}\) suggesting that

\[ \chi \sim \exp[A(\alpha - \alpha_c)^{-\nu} + B(\alpha - \alpha_c)^{-\nu} + \mathcal{O}((\alpha - \alpha_c)^{-\nu})] . \quad (16) \]

The critical value \(\alpha_c\) is then obtained by fitting. We show the data of the susceptibility at \(g = 2.0\) for large system sizes up to \(N = 2^{17} \approx 1.3 \times 10^7\) in the main panel of Fig. 3. To plot one point in this figure, we used 64 independent runs, each of which consisted of 500 Monte Carlo steps (MCS) for thermalization and next 600 MCS for measurement. In all the runs, we checked that the au-
tocolation time measured in the correlation function \(\langle x(0)x(\beta/2)\rangle\) is much less than 300 MCS. The inset shows the fitting for 1.42 \(\leq \alpha \leq 1.62\), where the data has almost converged on one curve with respect to the change in the system size. Stable fitting is obtained for each value of \(g\), and the critical dissipation strength \(\alpha_c\) is successfully determined within reasonable statistical errors.

Finally, the phase diagram is given in Fig. 4, where the closed squares show the critical values of dissipation strength for localization, \(\alpha_c\). We stress that it is the first time that transition points in the present system have been determined as a function of \(g\) without approximation.\(^{21}\) The error bar shown for the data at \(g = 1.5\) expresses the statistical error estimated from fitting using five independent Monte Carlo results. The error is reduced for larger values of \(g\), and becomes smaller than the symbol size at \(g = 4\). As \(g\) increases, \(\alpha_c\) is enhanced from the value \(\alpha_c = 1\), predicted in the two-state limit \(g \rightarrow 0\) (shown in the figure by the open square). Furthermore, the tendency of saturation is clearly observed for larger values of \(g\). The behavior of \(\alpha_c\) indicates that even for the infinitesimal potential barrier \((V_0 \ll \hbar \omega_0)\), a finite strength of dissipation is sufficient for the localization transition. This impressive result has already obtained for dissipative periodic-potential systems, where the critical value of dissipation strength is obtained as \(\alpha_c = 1\) in the small-barrier limit \(V_0/\hbar \omega_0 \rightarrow 0\).\(^{5,22}\) Note that the periodic-potential system is special because of the existence of a property called ‘duality’, which strongly suggests that the critical value \(\alpha_c\) is independent of the potential barrier.\(^{22}\) Actually, for the large-barrier limit, the critical value is also given as \(\alpha_c = 1\). Because double-well potential systems do not have such a property, the critical value can be derived from the limiting value.

The improved local update developed by us can be applied to other models, one of which is the nonlinear harmonic oscillator system such as the \(\phi^4\) chain. The present scheme is also useful for analyzing the nonlinear effects of phonons in dielectric substances. The extension of our algorithm to these systems will be studied elsewhere. The idea of Gaussian decomposition also suggests that a model with continuous variables can be mapped approximately into another model only with discrete variables after integrating out the continuous variables. This process will give a new insight into the original continuum model.

In summary, we considered the localization transition in dissipative double-well systems by a PIMC simulation improved by an approximate decomposition of the weight by several Gaussian distributions. We determined the transition point by fitting to the scaling expression for the Kosterlitz-Thouless transition. For potential barriers that are small compared with quantum fluctuations, the critical value of dissipation strength becomes larger than 1, and saturates at a finite value. We expect that the decomposition into Gaussian distributions is helpful for both creating algorithms and analyzing of other models with continuous variables.

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