Path integral Monte Carlo for dissipative many-body systems

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We address the possibility of performing numerical Monte Carlo simulations for the thermodynamics of quantum dissipative systems. Dissipation is considered within the Caldeira-Leggett formulation, which describes the system in the path-integral formalism through the inclusion of an influence action that is bilocal and quadratic in the system’s coordinates. At a first sight the usual direct approach of discretizing the path integral could seem feasible, but complications arise when one tries to introduce a physically meaningful dissipation kernel: in particular its imaginary-time dependence turns out to be severely singular and difficult to evaluate analytically, in spite of the simple expressions for its Matsubara components. We therefore propose to face the numerical problem using Fourier path-integral Monte Carlo, that can be formulated in two different ways: transforming the continuous paths and then truncating the high Fourier components (with possible improvements upon the truncation procedure), or performing the Fourier transformation upon the discretized paths. The latter choice leads to a simpler formulation and allows for a better control of the extrapolation to the limit of infinite Trotter number. The method is implemented for a single nonlinear particle with Ohmic dissipation and for a φ4 chain with Drude-like dissipation.

I. INTRODUCTION

In the last decades the interest in quantum dissipation has come mainly from the study of mesoscopic systems, which have been experimentally fabricated and theoretically analyzed. In such systems, the characteristic quantum effects involve a macroscopic number of particles. The sizeable dimension of the devices implies that the relevant dynamical variables can couple to a very large number of degrees of freedom of the surrounding environment (or dissipation bath): this coupling can be described macroscopically without caring for the details of the interaction, and can result in dramatic changes in the behavior of the system. For instance, the dissipative phase transition in Josephson-junction arrays (JJA).

While the classical thermodynamics is unaffected by dissipation, its quantum counterpart is substantially modified, and it constitutes therefore an ideal field to study the genuine interplay between quantum fluctuations and dissipation, which leads in general to interesting physics in the regimes of high quantum coupling and/or low temperature.

The issue of evaluating thermodynamic quantities in a quantum-dissipative system was recently faced by an extension of the effective-potential method that is very fruitful in the regime of intermediate quantum coupling. However, a more powerful tool is required when the aim is to study dramatic effects, as, for instance, the dissipative phase transition from superconducting to insulating behavior in JJA predicted by mean-field theory. Unfortunately, a suitable theoretical approach, allowing a faithful comparison with the experimental findings in the regime of high quantum coupling, is still lacking.

II. PATH-INTEGRAL FOR THE DISSIPATIVE SYSTEM

A. Formalism

In this paper, we discuss an efficient path-integral Monte Carlo (PIMC) approach can be implemented. In Section II the basic formalism and the connection with the phenomenological description dissipation are reviewed. The customary approach to Monte Carlo is set up in Section III, where some difficulties are pointed out; this leads us to consider Fourier PIMC basically extending the standard approach developed by many authors in the 80ies, involving the transformation to Matsubara components and their truncation by partial averaging, that by the way leads to a reformulation of the effective potential method. We propose a slightly different scheme for the numerical computation framework in Section IV which overcomes some ambiguities of the former. Eventually, in Section V the latter method is applied for two reference models: it appears that working with Fourier transformed variables, possibly using the knowledge of the exact quantum harmonic propagator, gives reliable results for many-body systems with reasonable numerical effort.
The Caldeira-Leggett (CL) model considers the system of interest as linearly interacting with a bath of harmonic oscillators, whose coordinates can be integrated out from the path integral, leaving the CL euclidean action:

$$S[q] = \int_0^{\beta \hbar} du \left[ \frac{m}{2} \dot{q}^2(u) + V(q(u)) \right] + S^{(nl)}[q]$$  \hspace{1cm} (2)$$

$$S^{(nl)}[q] = -\frac{m}{4\hbar} \int_0^{\beta \hbar} du \int_0^{\beta \hbar} du' k(u-u') \left[q(u)-q(u')\right]^2.$$  \hspace{1cm} (3)$$

The kernel \( k(u) \) depends on the temperature \( T = \beta^{-1} \) and is a symmetric and periodic function of the imaginary-time \( u \), \( k(u) = k(-u) = k(\beta \hbar - u) \); its functional form depends on the spectral density of the environmental bath and, moreover, it has a vanishing average, \( \int_0^{\beta \hbar} du k(u) = 0 \). Thanks to the last property, one can write the nonlocal dissipative action also as

$$S^{(nl)}[q] = \frac{m}{2\hbar} \int_0^{\beta \hbar} du \int_0^{\beta \hbar} du' k(u-u') q(u) q(u').$$  \hspace{1cm} (4)$$

The density matrix elements in the coordinate representation are expressed by Feynman’s path integral as

$$\rho(q'',q') = \int_{q'}^{q''} D[q] e^{-S[q]},$$  \hspace{1cm} (5)$$

where the path integration is defined as a sum over all paths \( q(u) \), with \( u \in [0,\beta \hbar] \), \( q(0) = q' \) and \( q(\beta \hbar) = q'' \), and the partition function reads

$$Z = \int D[q] e^{-S[q]}.$$  \hspace{1cm} (6)$$

The usual procedure for the phenomenological identification of \( k(u) \) consists in comparing its explicit expression (in terms of the dynamical variables of the oscillator bath) with the analogous expression of the (retarded) damping function \( \gamma(t) \) one gets in deriving the (classical or quantum) Langevin equation of motion from the same composite Hamiltonian:

$$m \ddot{q} + m \int dt' \gamma(t-t') \dot{q}(t') + V'(q) = f(t),$$  \hspace{1cm} (7)$$

where \( f(t) \) is the fluctuating force. The relation that is found between \( k(u) \) and \( \gamma(t) \) can be expressed in a simple way as a relation between their respective Matsubara transform,

$$k_n = \int_0^{\beta \hbar} du e^{-i\nu_n u} k(u), \hspace{1cm} \nu_n = \frac{2\pi n}{\beta \hbar},$$  \hspace{1cm} (8)$$

and Laplace transform,

$$\gamma(z) = \int_0^\infty dt e^{-zt} \gamma(t),$$  \hspace{1cm} (9)$$

and reads

$$k_n = |\nu_n| \gamma(z=|\nu_n|).$$  \hspace{1cm} (10)$$

Here it is apparent that \( k_0 = 0 \), i.e. the ‘local part’ is assumed to be fully included as a quadratic term in the potential. The following completeness/orthogonality relations have to be taken into account:

$$\sum_{n=-\infty}^{\infty} e^{i\nu_n u} = \beta \hbar \delta(u),$$  \hspace{1cm} (11)$$

where \( \delta(u) = \delta(u + \beta \hbar) \) is the periodic delta function, and its inverse

$$\int_0^{\beta \hbar} du e^{i\nu_n u} = \frac{\nu_n - 1}{i\nu_n} = \beta \hbar \delta_{n0}.$$  \hspace{1cm} (12)$$

B. Ohmic and Drude dissipation

In the above dynamical equation (7) the bath spectral density is assumed to be such to reproduce the most useful phenomenological models, namely:

i) Ohmic (or Markovian) dissipation. This is characterized by the absence of memory in the dissipative term, and corresponds to assuming a separation of time scales: the time scale with which the bath responds to changes in the system is much smaller than the system’s typical times. In this case dissipation can be described by one constant parameter, \( \gamma \):

$$\gamma(t) = \gamma \delta(t-0^+), \hspace{1cm} \gamma(z) = \gamma.$$  \hspace{1cm} (13)$$

ii) Drude-like dissipation. Here the bath responds on a time scale \( \omega_D^{-1} \) which is comparable to the system’s typical times:

$$\gamma(t) = \gamma \omega_D e^{-\omega_D t}, \hspace{1cm} \gamma(z) = \gamma \frac{\omega_D}{\omega_D + z}.$$  \hspace{1cm} (14)$$

Therefore, there are two parameters which describe dissipation, the intensity \( \gamma \) and the response frequency (or ‘spectral width’) \( \omega_D \); for \( \omega_D \to \infty \), i.e., fast bath response, the Ohmic form is recovered.

Note that \( \gamma(z) \) has the dimension of a frequency, while \( k_n \) is a squared frequency. Only the above two cases will be considered in what follows; although, of course, the actual physics of a problem could give more appropriate definitions of \( \gamma(t) \).

C. Imaginary-time kernel for Ohmic dissipation

From the above formulas it follows that the relation connecting the imaginary-time kernel \( k(u) \) with the (assumed known) Laplace transform \( \gamma(z) \) of the damping function \( \gamma(t) \) is

$$k(u) = \frac{1}{\beta \hbar} \sum_{n=-\infty}^{\infty} e^{i\nu_n u} |\nu_n| \gamma(z=|\nu_n|).$$  \hspace{1cm} (15)$$
The point is that the simple cases above give rather involute results for \( k(u) \). Let us calculate it in the Ohmic case \([13]\), invoking a criterion of mean convergence for the resummation:

\[
\frac{\beta h}{\gamma} \tilde{k}(u) = \sum_{n=-\infty}^{\infty} \nu_n | e^{i \nu_n u} - \frac{\beta h}{\pi} \left( \sin \frac{\pi u}{\beta h} \right)^{-2} . \tag{16}
\]

While it might be useful to note that

\[
- \frac{\pi}{\beta h} \left( \sin \frac{\pi u}{\beta h} \right)^{-2} = \partial_u \cot \frac{\pi u}{\beta h} = \frac{\beta h}{\pi} \partial_u^2 \ln \sin \frac{\pi u}{\beta h} ,
\]

so that one has alternative expressions,

\[
\tilde{k}(u) = \frac{\gamma}{\beta h} \partial_u \cot \frac{\pi u}{\beta h} = \frac{\gamma}{\beta h} \partial_u^2 \ln \sin \frac{\pi u}{\beta h} , \tag{17}
\]

one can see that the requirement \( k_0 = \int du \tilde{k}(u) = 0 \) is not satisfied and that to fulfil it one must subtract from the expression found – this is the reason why we used the tilde in the notation \( \tilde{k}(u) \) – the product of a (periodic) delta function \( \delta(u) \) by an infinite constant:

\[
k(u) = \tilde{k}(u) - \tilde{k}_0 \delta(u) \tag{19}
\]

where

\[
\tilde{k}_0 = \int_{\epsilon}^{\beta h} du \tilde{k}(u) = - \frac{2 \gamma}{\beta h} \cot \frac{\pi \epsilon}{\beta h} \mathop{\longrightarrow}_{\epsilon \to 0} - \infty ; \tag{20}
\]

one can indeed verify that the correct Matsubara transform \( | \nu_n | \gamma \) is obtained thanks to the cancelation of two divergences,

\[
k_n = \int_0^{\beta h} du \tilde{k}(u) (e^{-i \nu_n u} - 1) = \frac{\gamma}{\beta h} \int_0^{\beta h} du \partial_u \cot \frac{\pi u}{\beta h} (e^{-i \nu_n u} - 1) = \frac{\gamma}{\beta h} \left[ \cot \frac{\pi u}{\beta h} (e^{-i \nu_n u} - 1) \right]_{0}^{\beta h} - \epsilon + i \gamma \nu_n \int_0^{\beta h} du \cot \frac{\pi u}{\beta h} e^{-i \nu_n u}
\]

\[
= \frac{2 \gamma}{\beta h} \cot \frac{\pi \epsilon}{\beta h} (1 - \cos \frac{\pi \epsilon}{\beta h}) + i \gamma \nu_n \int_0^{\pi} \frac{dx}{\pi} \cot x e^{-2i \nu_n x} = O(\epsilon) + i \gamma \nu_n (-i \mathrm{sign}) = \gamma | \nu_n | . \tag{21}
\]

III. REAL-SPACE PIMC

The standard PIMC approach consists in approximating the partition function \([1]\) by discretizing the paths \( q(u) \) on a finite mesh. Namely, the imaginary-time interval \([0, \beta h]\) is divided into \( P \) slices of finite duration \( \epsilon = \beta h/P \), \( P \) being the so called Trotter number. Each whole path \( \{ q(u), u \in [0, \beta h] \} \) turns into the \( P \) discrete quantities \( \{ q_t = q(\epsilon t) \} \), with the periodicity condition \( q_0 = q_P \), and the action becomes:

\[
S_T = \frac{P}{\beta h^2} \tilde{V}(q_t - q_{t-1})^2 + \frac{\beta}{P} V(q_t) + S^{(nl)}_P \tag{22}
\]

\[
S^{(nl)}_P = \frac{2 \beta h}{4 P^2} \sum_{t, t' = 1}^{P} k_{t-t'} (q_t - q_{t'})^2 . \tag{23}
\]

The partition function is approximated by

\[
Z_T = \left( \frac{mP}{2\pi h^2} \mathop{\mathcal{P}}_{\beta} \right)^{P/2} \int P \int dq_t e^{-S_T} . \tag{24}
\]

In the standard PIMC procedure the thermodynamic averages \( \langle G, P \rangle \) obtained from this multiple integral are evaluated by a stochastic simulation, e.g., the Metropolis algorithm for configuration sampling; this is to be done for large enough values of \( P \), and the exact result \( G = G_{\infty} \) is estimated by extrapolating the calculated values \( G_P \). For the discrete kernel \( k_t \) that approximates the singular function \( k(u) \), it is reasonable to keep a piecewise approximation, namely, for \( \ell \neq 0 \)

\[
k_t = \frac{\gamma P}{(\beta h)^2} \left[ \cot \frac{\pi}{P}(\ell + \frac{\gamma}{\beta h}) - \cot \frac{\pi}{P}(\ell - \frac{\gamma}{\beta h}) \right] ; \tag{25}
\]

for large \( P \) one has

\[
k_t \simeq \frac{\gamma P}{(\beta h)^2} \left( \sin \frac{\pi}{P} \right)^{-2} \mathop{\mathcal{P}}_{\beta}^{2} \mathop{\mathcal{P}}_{\ell}^{2} ; \tag{26}
\]

and for \( \ell = 0 \)

\[
k_0 = \frac{1}{\beta h} \int_{-\beta h}^{\beta h} du \tilde{k}(u) = \frac{1}{\gamma} \left[ \int_{-\beta h/2}^{\beta h/2} du \tilde{k}(u) \right] = - \frac{1}{\beta h} \int_{-\beta h/2}^{0} du \tilde{k}(u) = \frac{2 \gamma P}{(\beta h)^2} \cot \frac{\pi}{2P} . \tag{27}
\]

The choice \([24]\) should be preferred to \([29]\) since it ensures the exact vanishing of the \( k_t \) for \( \ell \neq 0 \). However, it is apparent that \( k_0 \) does not contribute to the action \([23]\).

The interaction along the Trotter direction involves all pairs (which is very bad from the point of view of the code efficiency) although it is rapidly decreasing \( \sim \ell^{-2} \). This suggest the possibility of cutting the interaction beyond, say, \( R^{th} \) neighbors (keeping only \( | \ell - \ell'| < R \)); a rough calculation can be made assuming that the kinetic term dominates, i.e. that \( (x_{\ell} - x_{\ell-1})^2 \sim g^2/(\epsilon^2 P) \), which gives a ratio between the discarded and the included dissipative interaction energy \( \sim 1/\ln R \). In any case, it turns out that a simulation along these lines requires to deal with long-ranged summations whose short-range part is highly singular; moreover, if one would like to consider more physical dissipation kernels, e.g., the Drude one, the calculation of \( k(u) \) and of \( k_t \) becomes very involute in spite of the simple expression of \( k_n \).
IV. FOURIER PIMC WITH CONTINUOUS IMAGINARY TIME

In order to overcome the above mentioned difficulties, let us try now to face the problem from another point of view: since we know as ‘initial input’ the Matsubara components of the kernel, $k_n$, it is worth to explore the possibility of using the simulation technique based on the sampling of Fourier components of the path $q(u)$. We will follow the scheme of Refs. [8,9,10,11,12,13] with some modifications[4] that seem to improve upon their approach when the so called partial averaging is performed.

The Fourier transform of the closed path $q(u)$, $u \in [0, \beta \hbar]$, $q(0) = q(\beta \hbar)$, reads:

$$q(u) = \sum_{n=-\infty}^{\infty} q_n e^{-i \nu_n u} \equiv \bar{q} + \sum_{n=1}^{\infty} q_n(u)$$

$$q_n(u) = 2 \left( x_n \cos \nu_n u + y_n \sin \nu_n u \right), \tag{28}$$

where $q_n \equiv x_n + iy_n = q_n^{\pm}$ since $q(u)$ is real, so that $x_n = x_{-n}$ and $y_n = -y_{-n}$. Using the completeness and orthogonality relations, Eqs. (11) and (12), the inverse transform is found to be

$$q_n = \frac{1}{\beta \hbar} \int_0^{\beta \hbar} du \, q(u) e^{i \nu_n u}, \tag{29}$$

and obviously $q_0 \equiv \bar{q}$ is the average point of the path.

In terms of the transformed variables the action [4] takes the form

$$S[q] = \frac{\beta m}{2} \sum_{n=-\infty}^{\infty} (\nu_n^2 + k_n) |q_n|^2 + \int_0^{\beta \hbar} du \, V(q(u)), \tag{30}$$

which accounts in a simple way for the nonlocal dissipative part, at the price of leaving the integral involving the potential, whose argument is to be meant as expressed as in Eq. (28). The path integral [4] for the partition function transforms into

$$Z = C \prod_{n=1}^{\infty} \left[ \frac{\beta m \nu_n^2}{\pi} \right] \int d^2q_n \, e^{-\beta m (\nu_n^2 + k_n) |q_n|^2} \right] \times \exp \left\{ - \int_0^{\beta \hbar} du \, V(q(u)) \right\}, \tag{31}$$

where $|q_n|^2 = x_n^2 + y_n^2$ and $d^2q_n = dx_n dy_n$ and

$$C = \sqrt{\frac{m}{2 \pi \hbar^2 \beta}}. \tag{32}$$

The measure can be easily checked in the free-particle nondissipative limit. One can think this expression as the Gaussian average of the last exponential:

$$Z = C e^{-\beta \mu} \prod_{n=1}^{\infty} \left[ \frac{\beta m \nu_n^2}{\pi} \right] \int d^2q_n \, e^{-\beta \mu (\nu_n^2 + k_n) |q_n|^2} \right] \times \exp \left\{ - \int_0^{\beta \hbar} du \, V(q(u)) \right\}, \tag{33}$$

with

$$\mu = \frac{1}{\beta} \sum_{n=1}^{\infty} \ln \left( \frac{\nu_n^2 + k_n}{\nu_n^2} \right), \tag{34}$$

and the nonvanishing moments

$$\left\langle x_n^2 \right\rangle = \left\langle y_n^2 \right\rangle = \frac{1}{2 \beta m} \frac{1}{\nu_n^2 + k_n}, \tag{35}$$

i.e., the $n$-th component of $q(u)$ has the variance

$$\left\langle q_n^2(u) \right\rangle = 4 \left( \left\langle x_n^2 \right\rangle \cos^2 \nu_n u + \left\langle y_n^2 \right\rangle \sin^2 \nu_n u \right) \equiv \alpha_n \tag{36}$$

$$\alpha_n = \frac{2}{\beta m} \frac{1}{\nu_n^2 + k_n}. \tag{37}$$

A MC simulation based on Eq. (33) involves a Metropolis dynamics for the Fourier coefficients $\bar{q}$, $x_n$, and $y_n$, with a truncation of the series [23], say, at $n = P$; this should correspond to a standard simulation with Trotter number $P$.

On the other hand, the authors of of Refs. [8,9,10,11,12,13] always expand $q(u)$ after subtracting the initial point $q \equiv q(0)$, in a sin-only series, i.e.,

$$q(u) = q + \sum_{n=1}^{\infty} \alpha_n \sin \frac{\pi n u}{\beta \hbar}. \tag{38}$$

The difference of this choice resembles the one between the use of fixed boundary conditions (stationary waves, nonuniform amplitude) instead of periodic boundary conditions (plane waves, uniform amplitude).

A. Partial averaging

The partial averaging[4] improves upon the rude truncation of the Fourier series for $q(u)$, and basically relies upon the Jensen inequality[23]. Look again at Eqs. (31) and (33): these can be expressed as a superposition of uncorrelated Gaussian averages $\langle F(x_n, y_n) \rangle_n$ upon the variables $x_n$ and $y_n$, and for anyone of these averages we can choose to approximate

$$\langle e^F \rangle_n \approx e^{\langle F \rangle_n}. \tag{39}$$

Therefore, choosing to retain (and simulate) the Fourier components up to $n = P$, one can estimate what is left over in the exact average; separating the components that we want to keep (up to $n = P$) from those which are to be averaged out, i.e.,

$$q(u) = q_P(u) + \xi_P(u) \tag{40}$$

with

$$q_P(u) = \bar{q} + \sum_{n=1}^{P} q_n(u), \tag{41}$$

$$\xi_P(u) = \sum_{n=P+1}^{\infty} q_n(u), \tag{42}$$

one can immediately get

$$\left\langle \xi_P^2(u) \right\rangle = \sum_{n=P+1}^{\infty} \left\langle q_n(u) \right\rangle \equiv \alpha_P$$

$$\alpha_P = \sum_{n=P+1}^{\infty} \alpha_n = \frac{2}{\beta m} \sum_{n=P+1}^{\infty} \frac{1}{\nu_n^2 + k_n}, \tag{43}$$
and apply the Jensen inequality for this part getting the approximate (upper bound for the) partition function as a Gaussian average $\langle \cdots \rangle_\alpha$ over the finite set of the first $2P+1$ variables,

$$Z = C \, e^{-\beta\mu} \int d\bar{q} \exp \left\{ - \int_0^{\beta h} \frac{du}{h} V_{\alpha}(q_{\alpha}(u)) \right\},$$

(44)

with an effective potential $V_{\alpha}$ given as the Gaussian smearing $\langle \cdots \rangle_\alpha$ on the scale of $\alpha$, $\langle \cdots \rangle_\alpha = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + k_n + \omega^2} \beta \hbar^2$, \hspace{1cm} (45)

where $\langle \xi^2 \rangle_\alpha = \alpha$. What makes this result appealing compared to the previous approaches is the fact that $\alpha$ does not depend on $u$, as it occurs for the 'stationary wave' approach, so one can expect that even in the nondissipative case this could be an improvement for PIMC coding. Moreover, note that taking the roughest approximation, i.e. $P = 0$, one gets exactly the recipe for the effective potential introduced by Feynman:

$$Z = C \, e^{-\beta\mu} \int d\bar{q} \, e^{-\beta V_0(\bar{q})}$$

(46)

where $V_0(\bar{q}) = \langle V(\bar{q} + \xi_\alpha) \rangle_\alpha$ is broadened with

$$\alpha_0 = \frac{2}{\beta m} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + k_n + \omega^2} \beta \hbar^2$$

(47)

while $\mu \to 0$ for $k_n \to 0$.

\textbf{B. The variational effective potential}

In view of improving the technique, one can speculate whether it is possible to better account for the harmonic part, in the spirit of Refs. \cite{16,17,18}. Let us first review how the improved variational approximation arises in the present context. The aim is to incorporate a frequency term in the Gaussian averages \cite{53}, i.e., in the variances appearing in Eq. (52), and since there is an overall integration over $\bar{q}$, the frequency $\omega = \omega(\bar{q})$ can depend on it. Thus we rewrite Eq. (52) as follows

$$Z \gtrsim C \int d\bar{q} \, e^{-\beta V_{\text{eff}}(\bar{q})}$$

(52)

$$V_{\text{eff}}(\bar{q}) = \langle \delta V(q(u)) \rangle$$

$$= \langle V(\bar{q} + \xi) \rangle - \frac{m}{2} \omega^2(\bar{q}) \, \alpha_0(\bar{q}) + \mu(\bar{q})$$

(53)

\begin{align}
\alpha_0(\bar{q}) &= \frac{2}{\beta m} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + k_n + \omega^2(\bar{q})} \\
&\quad \to k_n \to 0 \frac{\hbar}{2m \omega(\bar{q})} \left( \coth \frac{f}{2} - \frac{1}{f} \right),
\end{align}

(54)

Note that the dependence of $V_{\text{eff}}$ on $u$ disappears upon averaging. We have now to maximize the r.h.s. of Eq. (52), i.e. to minimize the effective potential (53), in order to determine $\omega^2(\bar{q})$.

$$\frac{\partial \mu}{\partial \omega^2} = \frac{m}{2} \alpha_0,$$

(55)

a cancelation occurs and what is left is the known determination,

$$\frac{\partial V_{\text{eff}}}{\partial \omega^2} = \frac{1}{2} \left( \langle V''(\bar{q} + \xi) \rangle - m \omega^2(\bar{q}) \right) \frac{\partial \alpha_0}{\partial \omega^2} = 0.$$

(56)

This concludes the derivation of the effective potential. Note that there is no need to introduce the parameter $w(\bar{q})$ of Refs. \cite{16,17,18} and to optimize it.

\textbf{C. Improved partial averaging}

In order to retain the exact calculation of the first $P$ fluctuation variables, let us split $q(u)$ as in Eqs. (44-45) and introduce the frequency $\omega^2 = \omega^2(q_0, ..., q_r)$ in the Gaussian variances we want to approximate, i.e., those labeled by $n = P+1, ..., \infty$:

$$Z = \sum_{n=1}^{P} \prod_{n=P+1}^{\infty} \left[ \frac{\beta m \nu_n^2}{\pi} \int d^2 q_n \, e^{-\beta m (\nu_n^2 + k_n) |q_n|^2} \right] \times \prod_{n=P+1}^{\infty} \left[ \frac{\beta m \nu_n^2}{\pi} \int d^2 q_n \, e^{-\beta m (\nu_n^2 + k_n) |q_n|^2} \right] \times \exp \left\{ - \int_0^{\beta h} \frac{du}{h} \left[ V(q(u)) - \frac{m}{2} \omega^2(\xi(\bar{q})) \right] \right\},$$

(50)

where

$$\delta V(q(u)) = V(q(u)) - \frac{m}{2} \omega^2(q(u) - \bar{q})^2 + \mu.$$
\[ \equiv C \int d\bar{q} \left\{ \exp \left\{ - \int_0^{\beta n} \frac{du}{n} \delta V(q(u)) \right\} \right\}, \]  

(57)

where

\[ \delta V(q(u)) = V(q_{\mu}(u) + \xi_{\mu}(u)) - \frac{m}{2} \omega^2 \xi_{\mu}^2(u) + \mu_{\mu}, \]  

(58)

with

\[ \mu_{\mu} = \frac{1}{\beta} \left\{ \sum_{n=1}^{P} \ln \frac{\nu_n^2 + k_n}{\nu_n^2} + \sum_{n=p+1}^{\infty} \ln \frac{\nu_n^2 + k_n + \omega^2}{\nu_n^2} \right\}. \]  

(59)

In order to perform the partial averaging, we take now the Jensen approximation for the Gaussian components beyond the \( P \)-th one, so the relevant variance is

\[ \alpha_{\mu} = \langle \xi_{\mu}^2(u) \rangle = \frac{2}{\beta m} \sum_{n=p+1}^{\infty} \frac{1}{\nu_n^2 + k_n + \omega^2}, \]  

(60)

and the approximation reads

\[ Z \geq C \int d\bar{q} \left\{ \exp \left\{ - \int_0^{\beta n} \frac{du}{n} \right\} \right\}, \]  

(61)

with the effective potential

\[ V_{\mu}(q) = \langle V(q + \xi_{\mu}) \rangle_{\alpha_{\mu}} - \frac{m}{2} \omega^2 \alpha_{\mu} + \mu_{\mu}, \]  

(62)

that actually depends on \( \{q_0, ..., q_{\mu}\} \) since \( q = q_{\mu}(u) \) is given by Eq. (6). In order to optimize \( \omega \) we must minimize the integral of the effective potential,

\[ 0 = \frac{\partial}{\partial \omega^2} \int_0^{\beta n} \frac{du}{n} \left\{ \frac{1}{2} \left\langle V''(q_{\mu}(u) + \xi_{\mu}) \right\rangle_{\alpha_{\mu}} - m \omega^2 \frac{\partial \alpha_{\mu}}{\partial \omega^2} \right\} = 0, \]  

(63)

which, since \( \partial \mu_{\mu}/\partial \omega^2 = m \alpha_{\mu}/2 \), gives

\[ \int_0^{\beta n} \frac{du}{\beta n} \left\{ \frac{1}{2} \left\langle V''(q_{\mu}(u) + \xi_{\mu}) \right\rangle_{\alpha_{\mu}} - m \omega^2 \right\} \frac{\partial \alpha_{\mu}}{\partial \omega^2} = 0, \]  

(64)

and definitely

\[ m \omega^2 = \int_0^{\beta n} \frac{du}{\beta n} \left\langle V''(q_{\mu}(u) + \xi_{\mu}) \right\rangle_{\alpha_{\mu}}. \]  

(65)

The effective potential can therefore be written as

\[ V_{\mu}(q) = \langle V(q + \xi_{\mu}) \rangle_{\alpha_{\mu}} - \frac{\alpha_{\mu}}{2} \left\langle V''(q + \xi_{\mu}) \right\rangle_{\alpha_{\mu}} + \mu_{\mu}, \]  

(66)

or, using the differential operator \( \Delta_{\mu} = \frac{1}{2} \alpha_{\mu} \partial_{\mu}^2 \), as

\[ V_{\mu}(q) = (1 - \Delta_{\mu}) e^{\Delta_{\mu} V}(q) + \mu_{\mu}. \]  

(67)

Eqs. (64) and (68) are self-consistent for any choice of the arguments \( \{q_0, ..., q_p\} \).

### D. Low-coupling approximation (LCA)

In the above framework the frequency \( \omega^2(q_0, ..., q_{\mu}) \) depends on all simulated variables and the self-consistent Eqs. (60) and (61) give rise to a considerable complexity, even for one degree of freedom; indeed, one should practically solve those equations after each MC move except for very simple potentials as the quartic one just discussed. Some kind of LCA is then necessary; among several possibilities, the most reasonable choices for approximating \( \omega^2(q_0, ..., q_{\mu}) \) with some \( \omega_0^2 \) are:

1. leaving the only dependence on \( q_0 = \bar{q} \) by averaging over the fluctuation coordinates \( q_1, ..., q_{\mu} \), which leaves the need of tabulating the resulting \( \omega_0^2(\bar{q}) = \langle \omega^2(q_0, ..., q_{\mu}) \rangle_{\bar{q}} \); therefore, choosing to insert \( \omega \) in the first \( P \) Gaussian averages in order to better describe the resulting probability distribution, one has

\[ \omega_0^2(\bar{q}) = \langle V''(\bar{q} + \xi_0) \rangle = e^{\Delta} V''(\bar{q}), \]  

(68)

with \( \Delta = \frac{1}{2} \alpha \partial_{\mu}^2 \) and the full pure-quantum spread

\[ \alpha = \alpha_0 = \langle \xi_0^2 \rangle = \frac{2}{\beta m} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + k_n + \omega^2}. \]  

(69)

2. taking the above value in the minimum, \( \omega_0^2 = \omega_0^2(\bar{q} = \bar{q}_0) \) of course, it is also possible to take the improved LCA, i.e., the self-consistent HA (SCHA) of \( \omega_0^2(q) \), so that the above self-consistent equations are solved only once.

The first choice reduces the complexity of the self-consistent equations to the same one of the approach of Refs. (62), (63), and can then be used for problems with few degrees of freedom, while the latter appears to be necessary when facing many-body problems. In both cases the effective potential has to be expanded in the same way. After splitting

\[ \omega^2(q_0, ..., q_{\mu}) = \omega_0^2 + \delta \omega^2, \]  

(70)

where (for simplicity the integral is omitted)

\[ \delta \omega^2 = \frac{1}{m} e^{\Delta_{\mu} V''(q_{\mu}(u))} - \omega_0^2, \]  

(71)

we use \( \partial \mu_{\mu}/\partial \omega^2 = m \alpha_{\mu}/2 \) in expanding

\[ \mu_{\mu} \simeq \mu_{\mu} + \frac{m}{2} \alpha_{\mu} \left[ m^{-1} e^{\Delta_{\mu} V''(q_{\mu}(u))} - \omega_0^2 \right] \simeq \mu_{\mu} + \frac{m}{2} e^{\Delta_{\mu} \Delta_{\mu}} V'(q_{\mu}(u)) - \frac{m}{2} \alpha_{\mu} \omega_0^2, \]  

(72)

where terms of order \( \delta \omega^4 \) are neglected, and replacing this in the effective potential we get

\[ V_{\mu}(q) \simeq (1 - \Delta_{\mu} + \Delta_{\mu}) e^{\Delta_{\mu} V}(q) + \mu_{\mu} - \frac{m}{2} \alpha_{\mu} \omega_0^2 \simeq (1 - \delta \Delta_{\mu}) e^{\Delta_{\mu} + \delta \Delta_{\mu} V}(q) + \mu_{\mu} - \frac{m}{2} \alpha_{\mu} \omega_0^2, \]  

(73)

where for simplicity the integral is omitted. The correlation function becomes

\[ \langle V''(\bar{q} + \xi_0) \rangle = e^{\Delta} V''(\bar{q}), \]  

(74)
and, neglecting terms of order $\delta \Delta^2$, the LCA effective potential eventually reads

$$V_P(q) = e^{\Delta_0 P} V(q) + \mu_{\text{eff}} - \frac{m}{2} a_{\text{eff}} \omega_0^2 . \quad (73)$$

Eventually, the expression for the partition function suitable for numerical simulation reads

$$Z = C \int dq \exp \left\{ - \int_0^{\beta \hbar} \frac{du}{\hbar} V_P(q(u)) \right\} . \quad (74)$$

Other possibilities for a LCA are explored in Ref. [14], where the above described approach was also implemented for the Morse potential.

V. FOURIER PIMC WITH DISCRETE IMAGINARY TIME

In order to numerically evaluate the integral appearing in Eq. (74), we have seen in Section III that the standard PIMC method divides the imaginary-time interval $[0, \beta \hbar]$ into $P$ slices of width $\varepsilon = \beta \hbar / P$, and that the coordinate $q(u)$ turns into the discrete quantities $q_\ell = q(\ell \varepsilon)$. The partition function $Z$ and the other macroscopic thermodynamic quantities are obtained as the $P \rightarrow \infty$ extrapolation of Eq. (74) and of the estimators generated from it.

As mentioned in Section III, the application of this direct PIMC approach to a dissipative system is made difficult by the fact that the kernel $k(u-u')$ is explicitly known in terms of its Matsubara transform $k_n$, i.e. Eq. (10), rather than in the imaginary-time domain. In fact, it is given in terms of the Laplace transform of the damping function $\gamma(t)$ appearing in the phenomenological Langevin equation (1), and we have seen for Ohmic dissipation $\gamma(t) = \gamma$ that this makes $k(u-u')$ long-ranged, while for a more realistic Drude dissipation $k(u-u')$ becomes very hard to evaluate.

In the previous Section we realized that the Fourier path integral is very convenient as far as the treatment of the dissipative nonlocal action is concerned, because it enters the relevant expressions trough the (assumed known) Matsubara components $k_n$. However, the continuous imaginary-time approach used there has a general drawback (also present in the nondissipative case) arising from the appearance of the integral of the potential in the last exponent of Eq. (11).

The alternative we propose here is to start from the finite-$P$ expression (24) of the standard PIMC for the partition function and make there a lattice (discrete) Fourier transform, changing the integration variables from $q_\ell$ to $q_n$ by setting:

$$q_\ell = \tilde{q} + \sum_{n=1}^{P-1} q_n e^{i 2 \pi \ell n / P} , \quad (75)$$

so that:

$$Z_P = C^{1/P} \int d \tilde{q} \prod_{\ell=1}^{P-1} dq_n$$

$$\times \exp \left\{ - \frac{m}{2} \sum_{n=1}^{P-1} \left[ (\nu_{P,n} + k_n) |q_n|^2 \right] \right\} . \quad (76)$$

where $C$ is a temperature-independent normalization and $k_n$ is as given in Eq. (11). Comparing with the previous expression (24), two significant differences appear: firstly, the last term (integral of the potential along a path) is converted to a well-defined summation that doesn’t require further approximations; secondly, the kinetic-energy term contains the finite-$P$ Matsubara frequencies

$$\nu_{P,n} \equiv \frac{2 P}{\beta \hbar} \sin \frac{\pi n}{P} \quad (77)$$

rather than $\nu_n = 2 m n / \beta \hbar$, which are approached for $P \rightarrow \infty$. Thanks to these features the expression we got is exactly equivalent to the standard finite-$P$ expression (24), a property that gives us control onto the extrapolation of the results to $P \rightarrow \infty$.

Estimators for the relevant thermodynamic quantities can be obtained in the usual way: for example, from the thermodynamic relation $U = - \beta \partial \ln Z$, the following estimator for the internal energy is found:

$$U_P = V_P + \frac{P}{2 \beta} \sum_{n=1}^{P-1} \left[ \frac{2 m P^2}{\beta^2 \hbar^2} \sin^2 \frac{\pi n}{P} - m k_n \right] |q_n|^2 . \quad (78)$$

For a given potential $V(\tilde{q})$, it is convenient to devise a characteristic energy scale $\epsilon$ (e.g., the barrier height for a double well potential, the well depth for physical potentials that vanish at infinity, etc.) and length scale $\sigma$ (such that variations of $V$ comparable to $\epsilon$ occur on this length scale) and write

$$V(\tilde{q}) = \epsilon v(\tilde{q} / \sigma) . \quad (79)$$

In this way one better deals with the dimensionless coordinate $\tilde{x} = \tilde{q} / \sigma$. If $x_m$ is the absolute minimum of $v(x)$, the harmonic approximation (HA) of the system is characterized by the frequency $\omega_0$ given by

$$\omega_0^2 = \frac{\epsilon v''}{m \sigma^2} , \quad v'' \equiv v''(x_m) ; \quad (80)$$

the coupling parameter $g$ for the system can be defined as the ratio between the HA quantum energy-level splitting $\hbar \omega_0$ and the overall energy scale $\epsilon$,

$$g = \frac{\hbar \omega_0}{\epsilon} = \frac{\hbar^2 \omega_0^2}{m \epsilon \sigma^2} . \quad (81)$$

The case of weak (strong) quantum effects occurs when $g$ is small (large) compared to 1. It is then easy to make use of dimensionless variables only, i.e. to give energies in units of $\epsilon$, lengths in units of $\sigma$, frequencies in units of $\omega_0$, and so on; the reduced temperature is $t = 1/(\epsilon \beta)$, the reduced damping intensity is $\tilde{\gamma} = \gamma / \omega_0$. 
We can finally write a dimensionless expression for the partition function (82) for odd Trotter number $P = 2N + 1$:

$$Z_P = C \int \mathcal{D} \bar{x} \int \prod_{n=1}^{N} \mathcal{D} a_n db_n \times \exp \left\{ -\sum_{n=1}^{N} \left[ \frac{4v''_n t P^2}{g^2} \sin^2 \frac{\pi n}{P} + \frac{v''}{t} K_n \right] (a_n^2 + b_n^2) \right\} , \quad (82)$$

where $x_\ell = \bar{x} + 2 \sum_{n=1}^{N} [a_n \cos \frac{2\pi t n}{P} + b_n \sin \frac{2\pi t n}{P}]$, $K_n = k_n/\omega_0^2$ and we have used the symmetry properties of $k(u)$, so that $K_{P-n} = K_n$. The real Fourier variables $\bar{x}$, $a_n$ and $b_n$ are dimensionless; the integrals in Eq. (82) may be numerically evaluated by standard Monte Carlo sampling techniques, e.g., the Metropolis one.

VI. FOURIER PIMC WITH DISCRETE IMAGINARY TIME: APPLICATIONS

A. Single particle in the double-well potential

As a first application we consider a particle in a quartic double well potential $v(x) = (1-x^2)^2$ in presence of Ohmic dissipation, i.e., $k_n = 2\pi (t/g) \Gamma n$, where $\Gamma$ is the damping strength in units of $\omega_0$: the same model was already investigated in Ref. 3 by means of the effective-potential method outlined in Section IV B. In Fig. 1 we show the Fourier PIMC results for the average potential energy $\langle v(x) \rangle$ at the strong quantum coupling $g = 5$, for different values of the damping strength. The Monte Carlo data reported in the figure represent the extrapolation to $P \to \infty$ of the results obtained at $P = 17$, 33, 65, and 129. First of all, for the non-dissipative system ($\Gamma = 0$) we observe the perfect agreement between the exact results (obtained by numerical solution of the Schrödinger equation) and the PIMC data, proving the reliability of the PIMC code; for the dissipative model, the PIMC data provide a novel reference to check the validity of the previous effective-potential results. In particular, the latter turns out to be reliable at lower and lower temperature as the damping strength increases: indeed, this is expected since the coordinate fluctuations decrease with $\Gamma$, i.e., the coordinate-dependent quantities tend to the classical behavior as an effect of dissipation.

B. One-dimensional $\phi^4$ chain

Let us now consider a many-body dissipative system, namely, the quantum discrete $\phi^4$ chain, whose Hamiltonian may be written as

$$\mathcal{H} = \varepsilon_k \left[ \frac{Q^2 R}{3} \sum_{i=1}^{M} \hat{p}_i^2 + V(\hat{q}) \right] , \quad (83)$$

where $\varepsilon_k$ is the quantum coupling and $\mathcal{R}$ is the kink energy and length, respectively, in the classical continuum limit. In the above Hamiltonian the number of particles in the chain is $M$ and periodic boundary conditions are assumed. The canonical variables are such that $[\hat{q}_i, \hat{p}_j] = i \delta_{ij}$ and the harmonic excitations of this system have the dispersion relation $\Omega_k = Q \varepsilon_k \sqrt{1 + 4R^2 \sin^2 \frac{k}{2}}$.

We assume independent baths coupled to each degree of freedom of the chain, so that for this system Eq. (82) is easily generalized as

$$Z_P = C \int \mathcal{D} \bar{x} \int \prod_{n=1}^{N} \mathcal{D} db_n e^{-S_P} , \quad (85)$$

where the action reads

$$S_P = \sum_{i=1}^{M} \left\{ \sum_{n=1}^{N} \left[ \frac{6t P^2}{Q^2 R} \sin^2 \frac{\pi n}{P} + \frac{3}{2} R K_n \right] (a_n^2 + b_n^2) \right. \right. \left. \left. \left. + \frac{3R}{4t} \left( \hat{q}_i - \hat{q}_{i-1} \right)^2 \right. \right. \right. \left. \right. \right. \left. \left. + \frac{3R}{2t} \sum_{n=1}^{N} \left( a_{in} - a_{i-1,n} \right)^2 + \left( b_{in} - b_{i-1,n} \right)^2 \right) \right\} , \quad (86)$$

with the coordinates expressed in terms of their Fourier components as

$$q_{i\ell} = \bar{q}_i + 2 \sum_{n=1}^{N} \left( a_{in} \cos \frac{2\pi n \ell}{P} + b_{in} \sin \frac{2\pi n \ell}{P} \right) , \quad (87)$$

FIG. 1: Temperature dependence of the average potential energy $\langle v(x) \rangle$ for the single particle in a quartic double well, for $g = 5$ and different values of the damping strength $\Gamma$. Empty symbols are PIMC data, lines the predictions from the effective potential method and the filled circles are the exact results for $\Gamma = 0$. $V(\hat{q}) = \frac{3}{2R} \sum_{i=1}^{M} \left[ v(\hat{q}_i) + \frac{R^2}{2} (\hat{q}_i - \hat{q}_{i-1})^2 \right] , \quad (84)
FIG. 2: $\langle q_i^2 \rangle$ vs temperature for the $\phi^4$ chain, with $Q = 0.2$, $R = 5$, $\Omega_D = 100$ and different values of $\Gamma$. The empty symbols are PIMC data (extrapolated for $P \rightarrow \infty$) and the lines are the predictions from the effective potential method. \( \Gamma = 0 \): circles and solid line; \( \Gamma = 20 \): squares and short-dashed line; \( \Gamma = 100 \): triangles and long-dashed line. The inset reports the average $\langle v(q_i) \rangle$.

and the dimensionless temperature reads $t = (\beta \varepsilon_K)^{-1}$.

The average quantities for the dissipative $\phi^4$ chain presented in the figures have been obtained for periodic chains of length (~10^2 sites) large enough to be representative of the thermodynamic limit for each set of physical parameters and by extrapolating to $P \rightarrow \infty$ the results given by simulations at finite $P$. A Drude-like spectral density, as introduced in Section II B, was assumed for the environmental interaction, so that the dissipative kernel reads

$$K_n \equiv \frac{k_n}{\Omega^2} = \frac{\Gamma \Omega_D}{1 + Q \Omega_D/(2\pi t_n)} \ , \tag{88}$$

where the dissipation strength $\Gamma \equiv \gamma/\Omega$ and the cut-off frequency $\Omega_D \equiv \omega_D/\Omega$ are also measured in units of the characteristic frequency $\Omega = Q \varepsilon_K$.

The comparison of our PIMC results with those of the effective-potential method, shown in Figs. 2 and 3, clearly indicates that the predictions of the latter are very accurate; this accuracy is preserved for fairly large values of the quantum coupling, close to the predicted limits of applicability of the effective-potential approximation, as it appears in Fig. 4 which reports data for $Q = 1$.

Moreover, in order to get a reliable thermodynamic limit, finite-size effects have to be negligible, i.e., the number $M$ of sites must be large enough. In this condition, reaching high Trotter numbers becomes more and more computationally demanding and the extrapolation to $P \rightarrow \infty$ problematic. However, such difficulty can sometimes be overcome by means of a simple trick devised to improve the bare Monte Carlo outcomes. According to Eqs. (38) and (44) of Ref. 22 any finite-$P$ PIMC estimate $G(P)$ of a given thermodynamic quantity $G$ can be corrected by the known error affecting the same quantity for the corresponding SCHA system (of course, including the dissipative action). This error, that can be calculated in a simple way, is just the difference between the ‘exact’ ($P \rightarrow \infty$) SCHA value, $G_{HA}^{(h)}$ and the finite-$P$ SCHA estimate $G_{HA}^{(h)}(P)$. Note that any thermodynamic quantity of interest for a quadratic action in presence of dissipation at finite $P$ can be obtained starting from the density matrix given by Eq. (A14) of Ref. 4 with $w = 0$ and $C$ and $\Lambda$ given by Eqs. (36) and (37) of the same reference, with $\infty$ replaced by $N$ in the limits of the summations. We thus correct the bare PIMC data $G(P)$ to the improved values

$$G_{HA}(P) = G(P) + \left[ G_{HA}^{(h)} - G_{HA}^{(h)}(P) \right] \ . \tag{89}$$

This procedure is shown to be very effective also for dissipative systems, as shown in Fig. 5 where the improved estimates for the internal energy $U_{HA}(P)$ display a very
FIG. 5: Internal energy (per site) $U$ vs $1/P^2$ for the $\phi^4$ chain with $Q = 1$, $R = 3$, $\Omega_D = 10$, $\Gamma = 20$, at the temperature $t = 0.2$. The full triangles are the bare PIMC results $U(P)$, while the empty ones report the harmonically-corrected data $U_{HA}(P)$. The lines are linear fits.

We think that the above formulation of the Fourier path-integral Monte Carlo can make it affordable to investigate the thermodynamics of quantum many-body dissipative systems. The examples we reported testify to the power of the method and confirm that the effective-potential approach is valid in the expected parameter range (weak quantum coupling and/or strong dissipation). The further developments involve the implementation of the Fourier PIMC procedure beyond the limits of the effective-potential method. It is expected that it will permit to study the behavior of strongly quantum systems in presence of dissipation and thus open the possibility to approach problems like the dissipative transition in Josephson-junction arrays.

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