Simulating Quantum Dissipation in Many-Body Systems

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Abstract

An efficient Path Integral Monte Carlo procedure is proposed to simulate the behavior of quantum many-body dissipative systems described within the framework of the influence functional. Thermodynamic observables are obtained by Monte Carlo sampling of the partition function after discretization and Fourier transformation in imaginary time of the dynamical variables. The method is tested extensively for model systems, using realistic dissipative kernels. Results are also compared with the predictions of a recently proposed semiclassical approximation, thus testing the reliability of the latter approach for weak quantum coupling. Our numerical method opens the possibility to quantitatively describe real quantum dissipative systems as, e.g., Josephson junction arrays.
The description of open quantum systems has significant implications in the fundamental concepts of quantum mechanics. It involves issues as the breakdown of the Schrödinger picture and the connection between the ‘reversible’ and the ‘irreversible’ world [1]. These basic problems gave the first strong boost to the research in this field in the early 50’s and still are among the most fascinating aspects of the topic.

In the recent years a renewed interest in the study of quantum dissipation has come mainly from condensed-matter physics, as systems with an intermediate (mesoscopic) scale have been experimentally developed and theoretically analyzed. The fundamental issues in quantum and statistical mechanics are closely tied to technical applications, such as the single electron transistors [2], the Josephson quantum-bits [3], the SQUIDS [4], and many others. 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 (infinite) number of degrees of freedom of the surrounding environment (or dissipation bath). The interaction between the open system and its environment leads in general to dissipation, fluctuation, decoherence and irreversible processes. These result in dramatic changes in the behavior of the system, for instance the dissipative phase transition in Josephson junction arrays [5].

At variance with classical thermodynamics, which is unaffected by dissipation, quantum thermodynamics is 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. Unfortunately, a suitable theoretical approach, allowing a faithful comparison with the experimental findings in the regime of high quantum coupling, is still lacking. In this Letter, we present an original Path Integral Monte Carlo (PIMC) approach, which allows one to efficiently deal with the quantum thermodynamics of many-body open systems in a wide range of couplings and temperature; we will show how working with Fourier transformed variables, and taking advantage of our knowledge of the exact quantum propagator of harmonic systems, allows us to get reliable results for many body-systems with reasonable numerical efforts.

We address the problem of quantum dissipation within the Caldeira-Leggett (CL) framework [6], where dissipation is described as the result of a linear coupling of the physical system of interest with a bath of harmonic oscillators. By generalizing the CL formalism to many-body systems, the partition function of a quantum dissipative system is given by the
The path integral

\[ Z = \int \mathcal{D}[q] \ e^{-S[q]}, \tag{1} \]

with the Euclidean action

\[ S[q] = \int_0^{\beta h} \frac{du}{\hbar} \left[ \frac{1}{2} \dot{q}(u) \ A \ \dot{q}(u) + V(q(u)) \right] + S_{\text{nl}}[q]. \tag{2} \]

Here, \( q \equiv \{q_i\}_{i=1,...,M} \) denotes the vector whose components are the \( M \) coordinates of the investigated system and \( A \equiv \{A_{ij}\} \) is the mass matrix; the effects of dissipation are contained in the influence action,

\[ S_{\text{nl}}[q] = \frac{1}{2\hbar} \int_0^{\beta h} \int_0^{\beta h} \ q(u) \ K(u-u') \ q(u') \tag{3} \]

Within the many-body CL formalism the kernel \( K(u) \equiv \{K_{ij}(u)\} \) is an \( M \times M \) matrix, which is in general nonlocal in space, i.e., nondiagonal. Thus the dissipation bath can drive also the spatial correlations of the system as it is expected, for instance, in the case of shunted Josephson junction arrays. The kernel matrix \( K(u) \), depends on the temperature \( T = \left(k_B \beta\right)^{-1} \), is a symmetric and periodic function of the imaginary time \( u \), \( K(u) = K(-u) = K(\beta \hbar - u) \), and has a vanishing average over a period.

In order to numerically evaluate the integral appearing in Eq. (1), the standard PIMC method divides the imaginary-time interval \([0, \beta \hbar]\) into \( P \) slices of width \( \varepsilon = \beta h/P \), \( P \) being the so called \textit{Trotter number}. The coordinates \( q(u) \) turn into the discrete quantities \( q_\ell = q(\ell \varepsilon) \), \( q(u) \to P(\beta h)^{-1}(q_\ell - q_{\ell-1}) \), and the partition function \( Z \) is obtained as the \( P \to \infty \) extrapolation of

\[ Z_P = C \beta^{-M} \prod_{i=1}^{M} \int dq_{i0} \prod_{\ell=1}^{P-1} dq_{\ell} \ e^{-S_P[\{q_\ell\}]} \tag{4} \]

where \( S_P[\{q_\ell\}] \) is the discretized form of the action (2) and \( C \) is a temperature-independent normalization; the related macroscopic thermodynamic quantities are obtained through the accordingly generated estimators.

The application of the standard PIMC approach to dissipative systems is made difficult by the fact that the kernel \( K(u-u') \) is usually not explicitly known in the imaginary-time domain, but rather in the Matsubara frequency one. In fact, it is generally given in terms of the bath spectral density or in terms of the Laplace transform of the damping function appearing in the phenomenological Langevin equation [7]. This makes \( K(u-u') \) long-ranged,
cumbersome to evaluate and sometimes ill-defined as, e.g., in the case of the widely used Ohmic (or Markovian) dissipation. A possible way to avoid such problem could be the use of Fourier path-integral approaches, possibly supported by the partial-averaging scheme [8]: the latter method, however, still deals with the problem of evaluating path averages of the potential over continuous paths.

What we propose here is to start from the finite-\(P\) expression (4) of the standard PIMC for the partition function and make there a lattice (discrete) Fourier transform, changing the integration variables from \(q_{i\ell}\) to \(q_{ik}\) by setting:

\[
q_{\ell} = \bar{q} + \sum_{k=1}^{P-1} q_k e^{i 2\pi \ell k / P}
\]

so that:

\[
Z_P = C \beta^{-\frac{PM}{2}} \prod_{i=1}^{M} \int d\bar{q}_i \int_{\ell=1}^{P-1} dq_{i\ell} \exp \left\{ -\sum_{k=1}^{P-1} q_k \left[ \frac{2P^2}{\beta h^2} \sin^2 \frac{\pi k}{P} A + \frac{\beta}{2} K_k \right] q_k^* - \frac{\beta}{P} \sum_\ell V(q_{\ell}) \right\},
\]

where \(K_k \equiv \{ K_{ij,k} \}\) is the usual Matsubara transform \(K_k = \int_0^{\beta h} du \ K(u) \ e^{-i\nu_k u}\) of the dissipative kernel matrix at the Matsubara frequency \(\nu_k = 2\pi k / \beta h\).

We must however observe that the change of variables above is not enough to get a really efficient procedure to simulate many-body systems. In fact, in order to get a reliable thermodynamic limit finite-size effects have to be negligible; as a consequence the number \(M\) must be large enough, so that reaching high values of \(P\) may become computationally very demanding, making the extrapolation to \(P \to \infty\) problematic. However, such difficulty can be largely circumvented by making use of our knowledge of both the finite- and infinite-\(P\) exact partition function of pure bilinear actions [9]. According to Ref. [9] [Eqs. (38) and (44)] any Monte Carlo estimate \(G(P)\) of a given quantity \(G\) obtained at finite \(P\) can be corrected by adding the exact \((P \to \infty)\) value \(G_{HA}^{(h)}\) and subtracting the finite-\(P\) estimate \(G_{HA}^{(h)}(P)\) of the same quantity [10] for the (self-consistent) harmonic approximation of the dissipative action, getting:

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

As it will clearly appear in the following applications, the last step turns out to be essential and truly effective in the investigation of many-body systems.
As a preliminary test, we take a single particle of mass \( m \) in a non-linear potential \( V(q) = \epsilon v(q/\sigma) \), where \( \epsilon \) and \( \sigma \) define the energy and length scale, respectively. In order to better examine the combined effects of quantum fluctuations and dissipation, it is useful to introduce the reduced temperature \( t = (\beta \epsilon)^{-1} \) and the quantum coupling \( g = \hbar \omega_0 / \epsilon \), where \( \omega_0 = \sqrt{\epsilon c^2 / m \sigma^2} \) and \( c^2 = v''(x_m) \), \( x_m \) being the absolute minimum of \( v(x) \). For odd Trotter number, \( P = 2N + 1 \), we get:

\[
Z_P = C t^P \int d\bar{x} \prod_{k=1}^N da_k db_k \exp \left\{ -\frac{1}{tP} \sum_{\ell} v(x_\ell) + \sum_{k=1}^N \left[ \frac{4c^2 t P^2}{g^2} \sin^2 \frac{\pi k}{P} + \frac{c^2}{t} \kappa_k \right](a_k^2 + b_k^2) \right\},
\]

(8)

where \( x_\ell = \bar{x} + 2 \sum_{k=1}^N (a_k \cos \frac{2\pi k \ell}{P} + b_k \sin \frac{2\pi k \ell}{P}) \), \( \kappa_k = K_k / \omega_0^2 \) and we have used the symmetry properties of \( K(u) \), so that \( \kappa_{P-k} = \kappa_k \). The real Fourier variables \( \bar{x}, a_k \) and \( b_k \) are dimensionless, and the integrals in Eq. (8) may be numerically evaluated by standard Monte Carlo sampling techniques, e.g. the Metropolis one.

Fig. 1 shows the results obtained for the average potential energy when a quartic double-well potential \( v(x) = (1 - x^2)^2 \) and Ohmic dissipation, i.e., \( \kappa_k = 2\pi (t/g) \Gamma k \), are considered (\( \Gamma \) is the damping strength in units of \( \omega_0 \)); the same model was already investigated in Ref. [11] by means of the pure-quantum self-consistent harmonic approximation (PQSCHA), a semiclassical approach. Data in Fig. 1 refer to \( g = 5 \) and different values of damping. The reported Monte Carlo data represent the extrapolation to \( P \to \infty \) of the results obtained at \( P = 17, 33, 65, \) and 129; the reliability of the algorithm is proven by the perfect agreement between the exact results and the PIMC data in the non-dissipative system (\( \Gamma = 0 \)). For the dissipative model, the PIMC data provide therefore a reference, still lacking until now, to verify the validity of the PQSCHA [12].

Let us turn now to a true many-body dissipative system, and consider the quantum discrete \( \phi^4 \) chain, whose Hamiltonian may be written as [12]

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

(9)

\[
V(\vec{q}) = \frac{3}{2R} \sum_{i=1}^M \left[ v(q_i) + \frac{R^2}{2} (q_i - q_{i-1})^2 \right],
\]

(10)

where \( v(x) = (1 - x^2)^2 / 8 \), \( Q \) is the quantum coupling, and \( \varepsilon_k \) and \( R \) are the kink energy and length, respectively, in the classical continuum limit.
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 are PQSCHA predictions (Ref. \[11\]) and filled circles are the exact results for \( \Gamma = 0 \).

Assuming identical independent baths \[12\] for each degree of freedom, i.e. \( K_{ij}(u) = \delta_{ij}K(u) \), Eq. (6) gives

\[
Z_P = C t^P \prod_{i=1}^M \int d\tilde{q}_i \int \prod_{k=1}^N da_{ik} db_{ik} e^{-S_P},
\]

where we set \( q_{i\ell} = \tilde{q}_i + 2 \sum_{k=1}^N (a_{ik} \cos \frac{2\pi k \ell}{P} + b_{ik} \sin \frac{2\pi k \ell}{P}) \), again with \( P = 2N + 1 \); using the dimensionless temperature \( t = (\beta \varepsilon_k)^{-1} \), the discretized action reads

\[
S_P = \sum_{i=1}^M \left\{ \sum_{k=1}^N \left[ 6 t P^2 \sin^2 \frac{\pi k}{P} + \frac{3}{2 R t} K_k \right] (a_{ik}^2 + b_{ik}^2) + \frac{3R}{4t} [(\tilde{q}_{i+1} - \tilde{q}_i)^2 + 2 \sum_{k=1}^N (a_{ik} - a_{i-1k})^2 + (b_{ik} - b_{i-1k})^2] + \frac{3}{2 R t P} \sum_{\ell=1}^P v(q_{i\ell}) \right\}.
\]

The average quantities for the dissipative \( \phi^4 \) chain presented in Figs. 2–4 have been obtained for periodic chains of length (\( \sim 10^2 \) sites) large enough to be representative of the thermodynamic limit for each set of physical parameters and by extrapolating to \( P \to \infty \) the results given by simulations at finite \( P \). A Drude-like spectral density was assumed for the environmental interaction \[7, 12\], so that the dissipative kernel reads

\[
K_k = \Gamma \Omega_d \frac{(2\pi tk/Q)}{\Omega_d + (2\pi tk/Q)},
\]

(12)
FIG. 2: $\langle q_i^2 \rangle$ and $\langle v(q_i) \rangle$ (inset) vs temperature for the $\phi^4$ chain, with $Q = 0.2$, $R = 5$, $\Omega_D = 100$ and different values of $\Gamma$. Empty symbols are PIMC data ($P \to \infty$ extrapolations) and lines are PQSCHA predictions (Ref. [12]). $\Gamma = 0$: circles and solid line; $\Gamma = 20$: squares and short-dashed line; $\Gamma = 100$: triangles and long-dashed line.

FIG. 3: $\langle q_i^2 \rangle$ vs temperature for the $\phi^4$ chain, with $Q = 1$, $R = 3$, $\Omega_D = 10$ and different values of $\Gamma$. Full symbols are PIMC data at finite Trotter number ($P = 81$, for finite $\Gamma$, $P = 11$ for $\Gamma \to \infty$); empty symbols are $P \to \infty$ extrapolations. Lines are PQSCHA predictions.

where the dissipation strength $\Gamma$ and the cut-off frequency $\Omega_D$ are measured in units of $\Omega = Q\varepsilon_K$. Comparison of the PIMC results with those of the PQSCHA [12], shown in Fig. 2, clearly indicates that the predictions of the latter are impressively accurate. Remarkably, the accuracy is also preserved for fairly large values of quanticity, quite close to the predicted limits of applicability of the PQSCHA scheme, as it appears in Fig. 3.

The role played by the correction scheme of Eq. (7) is clearly shown in Fig. 4 (a), where
FIG. 4: Internal energy (per site) $U$ for the $\phi^4$ chain, with $Q = 1$, $R = 3$, $\Omega_d = 10$, and different values of $\Gamma$. (a): $P$-dependence of $U$ for $\Gamma = 20$, and $t = 0.2$. Full symbols: bare PIMC results $U(P)$; empty symbols: harmonically-corrected data $U_{HA}(P)$. Lines are quadratic fits. (b): temperature dependence of $U$. Full symbols: PIMC data for $P = 101$; empty symbols: harmonically-corrected $P \to \infty$ extrapolations. Lines are PQSCHA predictions.

$U_{HA}(P)$ displays a very weak dependence on $P$, thus allowing to get reliable estimates of the $P \to \infty$ extrapolation even by starting from results obtained for relatively small values of $P$. The relevance of the harmonic correction is more and more evident for increasing dissipation strength [Fig. 4 (b)]: indeed, in this regime the finite-$P$ bias essentially comes from the bilinear contribution of the influence functional and the latter can be easily healed by the above correction scheme, so that, for instance, the characteristic almost flat behavior of $U$ at low temperature [12] is obtained without using exceedingly high values of $P$.

In conclusion, we have introduced a formulation of the Path Integral Monte Carlo method which greatly simplifies the numerical investigation of the thermodynamics of quantum dissipative systems with bilinear influence action, making it possible to afford also many-body systems. The combined use of both the discrete Fourier transformed representation of the dynamical variables and the correction scheme of Eq. (7) is essential to efficiently circumvent the numerical difficulties arising from the non locality in time and space of the
action describing an open many-body system. The application to a double-well potential and to a $\phi^4$ chain have shown the power of the method and have given, as a byproduct, a direct confirmation of the validity of the semi-classical approach of Refs. [11, 12] in the expected parameter region, i.e., weak quantum coupling and/or strong dissipation. The numerical approach introduced here does not suffer of such limitations, and we expect it to be useful for getting meaningful insight on the behavior of strongly quantum systems in presence of dissipation, thus making it possible to address interesting problems of mesoscopic physics as, e.g., the dissipative transition in Josephson junction arrays [5].

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[1] W.H. Zurek, Phys. Today, 44, 36 (1991).

[2] M. H. Devoret and R. J. Schölkopf, Nature, 406, 1039 (2000).

[3] Y. Nakamura, Yu. A. Pashkin, and J. S. Tsai, Nature, 398, 786 (1999).

[4] J. R. Friedman, V. Patel, W. Chen, S. K. Tolpygo, and J. E. Lukens, Nature, 406, 43 (2000).

[5] Y. Takahide, R. Yagi, A. Kanda, Y. Ootuka, and S. I. Kobayashi, Phys. Rev. Lett. 85, 1974 (2000).

[6] A. O. Caldeira and A. J. Leggett, Phys. Rev Lett. 46, 211 (1981); Ann. of Phys. 149, 374 (1983).

[7] U. Weiss, Quantum Dissipative Systems (World Scientific, Singapore, 2nd edition, 1999).

[8] See, e.g., M. Eleftheriou, J. D. Doll, E. Curotto, and D. L. Freeman, J. Chem. Phys. 110, 6657 (1999); S. L. Mielke, J. Srinavasan, and D. G. Trulhar, J. Chem. Phys. 112, 8758 (2000); and references cited therein.

[9] A. Cuccoli, A. Macchi, G. Pedrolli, V. Tognetti and R. Vaia, Phys. Rev. B 51, 12369 (1995).

[10] For a quadratic action with CL dissipation, any thermodynamic quantity at finite $P$ can be exactly obtained starting from the density matrix given by Eqs. (A14), (36), and (37) of
Ref. [12], with $w = 0$ and $\infty$ replaced by $N$ (as defined in Eqs. (8) and (11)) in the summation limits.

[11] A. Cuccoli, A. Rossi, V. Tognetti, and R. Vaia, Phys. Rev. E 55, 4849 (1997).

[12] A. Cuccoli, A. Fubini, V. Tognetti and R. Vaia, Phys. Rev. E 60, 231 (1999).