On oscillator–bath system: exact propagator, reduced density matrix and Green’s function

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Abstract
The exact form of a quantum propagator of a quantum oscillator, interacting with a bosonic bath consisting of \(N\)-distinguished quantum oscillators with different frequencies, is obtained in the Heisenberg picture. A reduced density matrix for the oscillator is obtained. The kernel or Green’s function connecting the initial density matrix of the oscillator to the density matrix in an arbitrary time is obtained, and its connection to the Feynman–Vernon influence functional is discussed. A weak coupling regime and squared mean values for position, momentum, and energy of the oscillator are obtained in equilibrium.

Keywords: propagator, bosonic-bath, density-matrix, memory function, Green’s function

1. Introduction
The theory of open quantum systems has been extensively studied and developed after the seminal works reported in [1–4]. This theory has found applications in fields such as statistical mechanics, chemical physics [5–9], condensed matter [10–12], quantum optics [13–16], quantum information and atomic physics [17]. The dynamics of an open quantum system can be described in terms of generalized master equations [18, 19] and Langevin equations [20, 21]. Due to the complexity of correctly incorporating different physical parameters, various approximations such as weak-coupling regime, Markovian limit, high temperature or the initial factorizing condition are usually invoked. These approximations are not valid for open quantum systems in the low temperature regime or in the presence of initial correlations between the system and its environment or in the case of driven nonequilibrium quantum systems [22].

Ford, Kac and Mazur [20] proposed the system–bath model for investigating classical and quantum dissipative systems coupled linearly to a bosonic bath of harmonic oscillators. A formal approach to the system–bath model was introduced by Feynman and Vernon [2], who derived an influence functional for the system by tracing out the bath degrees of freedom in the context of path integral formalism [23–26]. This approach was later applied by Caldeira and Leggett [8] to derive the high temperature behaviour of the master equation for a quantum harmonic oscillator coupled to a bath of harmonic oscillators. Agarwal derived some exact results for a dissipative harmonic oscillator in [14], and Hu, Paz and Zhang solved the same problem exactly and discovered that the diffusion constants are time dependent [27]. In all of these approaches, the crucial assumption was that the initial state of the system–bath was considered to be a product state and Hakim and Ambegaokar showed that the evolution of the density matrix is highly dependent on the initial state [28]. In [29] and [30] the authors showed that the initial correlations make one-photon phase control of physico-chemical systems possible. Also in [31], it was shown that the initial correlations between a system and its environment are relevant in allowing for a coherent character of excitonic energy transfer in photosynthetic light-harvesting systems. An exact quantum master equation for a driven Brownian oscillator was constructed in [32] via a Wigner phase-space Gaussian wave packet approach. The phase space propagator was also derived in [33].

Usually dissipative quantum systems are investigated using path integrals or, in the Heisenberg picture, in the framework of the Langevin or master equations. Here we are interested in the time evolution of the quantum state of the oscillator–bath system. The initial state can be considered to be an arbitrary state; for example, it can be a product state, a maximally entangled state, a coherent state, etc. Therefore, we are interested in the exact quantum propagator for the
oscillator–bath system. Knowing the exact propagator, we can formally obtain all information about the combined system or a particular subsystem by integrating out the other subsystem degrees of freedom. Also, we can focus on the oscillator subsystem and find the amount of energy flowing from the oscillator to the bath or find the probability of decaying rates. The explicit expressions obtained here can be used for numerical investigation of engineered bath models containing a few or a large number of bath oscillators. The main feature of the present approach is its simplicity: only the properties of the propagator are used to obtain the exact form of the propagator. Also, the results are in terms of the coupling constants $f_j$, which can be adjusted by experimental data directly or through the susceptibility of the medium.

The paper is organized as follows. In section 2, the model is introduced and reviewed briefly. In section 3, using symmetry and the initial condition properties of the quantum propagator, the exact form of the quantum propagator for a quantum oscillator interacting with a bosonic bath consisting of $N$-distinguished quantum oscillators, with different frequencies, is obtained in the Heisenberg picture. In section 4, knowing the propagator of the total system, the reduced density matrix for the oscillator is obtained. The kernel or properties of the propagator are used to obtain the exact form of the propagator. Also, the results are in terms of the coupling constants $f_j$, which can be adjusted by experimental data directly or through the susceptibility of the medium.

The total Lagrangian of the oscillator–bath system can be written as [34]

$$ L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 + \sum_j \left( \frac{1}{2} \dot{X}_j^2 - \frac{1}{2} \omega_j^2 X_j^2 \right) + \sum_j f_j \dot{X}_j x, $$

where the second term is a collection of independent harmonic oscillators with different frequencies, and the last term represents the interaction between the main oscillator (system) and the bath oscillators through a linear coupling with coupling constants $f_j$. Since a total time derivative can be removed from the Lagrangian without changing the physics of the problem, we can consider the interaction term as $\sum_j f_j X_j \dot{x}$, which classically resembles the friction proportional to the velocity; of course, other equivalent forms can be obtained through unitary transformations. The Lagrangian (1) leads to the Hamiltonian (6), which resembles the coupling of a charge particle to a black body radiation and also a renormalized mass (7). The conjugate canonical momenta for the system and bath oscillators are defined by

$$ p = \frac{\partial L}{\partial \dot{x}} = m \dot{x}, $$

$$ P_j = \frac{\partial L}{\partial \dot{X}_j} = \dot{X}_j + f_j x, $$

respectively. The total system is now quantized by imposing equal-time commutation relations

$$ [x, p] = i \hbar, $$

$$ [X_j, P_k] = i \hbar \delta_{jk}. $$

The Hamiltonian can be rewritten as

$$ H = p \dot{x} + \sum_j P_j \dot{X}_j - L, $$

$$ = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 + \sum_j \left( \frac{P_j^2}{2} + \frac{1}{2} \omega_j^2 X_j^2 \right) + \sum_j f_j x, $$

$$ = \frac{p^2}{2m} + \frac{1}{2} m \Omega^2 x^2 + \sum_j \left( \frac{P_j^2}{2} + \frac{1}{2} \omega_j^2 X_j^2 \right) - \sum_j f_j x, $$

where $\Omega^2 = \omega^2 + \sum f_j^2$ is the shifted frequency, and it is implicitly assumed that the summation $\sum_j f_j^2$ exists and is finite. From Hamiltonian (6) and using Heisenberg equations, one can obtain the equations of motion for the system and bath oscillators as

$$ \ddot{x} + \omega^2 x = \frac{1}{m} \sum_j f_j \dot{X}_j, $$

and

$$ \ddot{X}_j + \omega_j^2 X_j = -f_j \dot{x}, $$

respectively. Equation (9) has the formal solution [35]

$$ X_j(t) = X_j^{(0)}(t) - f_j \int_0^t dt' G_j(t - t') \dot{x}(t'), $$

where
\[ X_j^N(t) = \cos(\omega_j t)X_j^N(0) + \frac{\sin(\omega_j t)}{\omega_j} P_j^N(0) \]  

is the homogeneous solution. The homogeneous solution \( X_j^N(t) \) depends on the initial position and momentum of the corresponding bath oscillator and, due to the unknown initial conditions of position and momentum of each bath-oscillator, can be interpreted as a noise field leading to the noise force \( mf_j^N(t) \) given in (14). The Green’s function of equation (9) is defined by

\[ G_j(t - t') = \frac{\sin(\omega_j (t - t'))}{\omega_j} \theta(t - t'), \]

which is a retarded Green’s function, and \( \theta(t - t') \) is the Heaviside step function. Inserting (10) into (8) leads to [35]

\[ \ddot{x} + \omega^2 x(t) + \int_0^t dt' \gamma(t - t') \dot{x}(t') = f^N(t), \]

where

\[ f^N(t) = \frac{1}{m} \sum_j f_j X_j^N(t) \]

\[ = \frac{1}{m} \sum_j \left[ \cos(\omega_j t) P_j^N(0) - \omega_j \sin(\omega_j t) X_j^N(0) \right] \]

is the scaled noise force. The memory function or susceptibility of the medium or bosonic bath is defined by [35]

\[ \gamma(t - t') = \frac{1}{m} \sum_j f_j^2 \cos(\omega_j (t - t')). \]

We can rewrite (15) in terms of the spectral density function \( g(\omega) \) as

\[ \gamma(\tau) = \int_0^\infty d\omega g(\omega) \cos(\omega \tau), \]

where

\[ g(\omega) = \frac{1}{m} \sum_j \frac{f_j^2}{\omega} \delta(\omega - \omega_j). \]

Equation (16) is the cosine Fourier transform and can be inverted, leading to [36]

\[ g(\omega) = \frac{2}{\pi} \int_0^\infty d\tau \gamma(\tau) \cos(\omega \tau), \]

which can be rewritten in terms of the real part of the Fourier transform of the memory function [35]

\[ \tilde{\gamma}(\omega) = \int_0^\infty d\tau \gamma(\tau)e^{i\omega \tau}, \]

as

\[ g(\omega) = \frac{2}{\pi} \Re\{\tilde{\gamma}(\omega)\}. \]

Note that if the bosonic bath is a collection of harmonic oscillators with continuum frequency (as is the case), then we use the substitution

\[ \sum_j f_j^2 h(\omega_j) \rightarrow \int_0^{\infty} d\omega f^2(\omega)h(\omega), \]

where \( h(\omega) \) is an arbitrary function of \( \omega_j \). In this case, from (20) we will find [35]

\[ f^2(\omega) = \frac{2m \rho \omega}{\pi} \Re\{\tilde{\gamma}(\omega)\}. \]

The transition from the discrete to the continuum case can be achieved easily throughout the paper; in this case, vectors, matrices, and their inverse should be considered as states and operators over the semi-infinite interval frequency \([0, \infty)\).

Taking the Laplace transform of (13), we find

\[ s^2 \tilde{x}(s) - sx(0) - \dot{x}(0) + \omega^2 \tilde{x}(s) + \tilde{\gamma}(s)(\tilde{x}(s) - x(0)) = \tilde{f}^N(s); \]

therefore,

\[ \tilde{x}(s) = \frac{s + \tilde{\gamma}(s)}{s^2 + \omega^2 + s\tilde{\gamma}(s)} x(0) + \frac{1}{s^2 + \omega^2 + s\tilde{\gamma}(s)} \dot{x}(0) \]

Let us define for simplicity

\[ \alpha(t) = L^{-1}\left[ \frac{s + \tilde{\gamma}(s)}{s^2 + \omega^2 + s\tilde{\gamma}(s)} \right], \]

\[ \beta(t) = L^{-1}\left[ \frac{1}{s^2 + \omega^2 + s\tilde{\gamma}(s)} \right], \]

\[ \delta_j(t) = L^{-1}\left[ \frac{s}{(s^2 + \omega_j^2)(s^2 + \omega^2 + s\tilde{\gamma}(s))} \right], \]

\[ \eta_j(t) = L^{-1}\left[ \frac{\omega_j}{(s^2 + \omega_j^2)(s^2 + \omega^2 + s\tilde{\gamma}(s))} \right]. \]

Note that \( \delta_j(t) = \eta_j(t)/\omega_j \). Now, taking the inverse Laplace transform of (24) and using (25)–(28), we find

\[ x(t) = \alpha(t)x(0) + \beta(t)\frac{P(0)}{m} + \frac{1}{m} \sum_j \left[ \delta_j(t) P_j^N(0) - \omega_j \eta_j(t)X_j^N(0) \right]. \]

We will make use of this equation in the next section to find the total quantum propagator.

### 3. Propagator

In this section we find the quantum propagator of the total system, using properties of the propagator in the framework of the Heisenberg approach. In the Heisenberg picture, the time
evolution of the oscillator position operator is given by
\[
x(t) = U^{\dagger}(t)x(0)U(t) \Rightarrow U(t)x(t) = x(0)U(t)\quad (30)
\]
the matrix elements of the last equality in the position space of the total system \(\langle x|\otimes|X_1, X_2, \ldots, \rangle \equiv \langle x|X\rangle\) is
\[
\langle x| U(t)x(t)|x'\rangle = \langle x| U(x(0)U(t)|x'\rangle. \quad (31)
\]
Now from (29) and the definition of propagator \(K(x, X|U(t)|x', X')\), we easily find
\[
\beta(t) \frac{\partial}{\partial x} + \sum_{j} f_j \delta_j(t) \frac{\partial}{\partial X_j} K(x, X; t, x', X') = \frac{-i}{\hbar} x - \alpha(t)x' + \frac{1}{m} \sum_{j} f_j \eta_j(t) \omega_j X_j \times K(x, X; t, x', X'), \quad (32)
\]
or, equivalently,
\[
\left[ \beta(t) \frac{\partial}{\partial x} + \sum_{j} f_j \delta_j(t) \frac{\partial}{\partial X_j} \right] \ln K(x, X; t, x', X') = \frac{-i}{\hbar} x - \alpha(t)x' + \frac{1}{m} \sum_{j} f_j \eta_j(t) \omega_j X_j. \quad (33)
\]
Equations (33) is the partial differential equation that the propagator should fulfill. Since the oscillator–bath system is described by two coupled differential equations (8), (9), we need another equation that comes from the time evolution of the bath oscillator positions \(X_j(t)\), which we now determine. By taking the Laplace transform of (10), we find
\[
\tilde{X}_j(s) = \tilde{X}_j^N(s) - \int_{s} \tilde{G}_j(s)(s\tilde{x}(s) - x(0)), \quad (34)
\]
and by taking the inverse Laplace transform, we find
\[
X_j(t) = \frac{\alpha^2 f_j}{\omega_j} \eta_j(t)x(0) - \frac{f_j}{m \omega_j} \dot{\eta}_j p(0) + \sum_k \left[ M_{jk} P^N_k(0) \right. \quad (36)
\]
where for notational simplicity we have defined the matrices
\[
M_{jk} = \cos \left( \omega_j t \right) \delta_{jk} + Q_{jk} \left( \omega_k^2 \right) \quad (37)
\]
and
\[
Q_{jk}(t) = Q_{kj}(t) = L^{-1} \left[ (f_j f_k s) / \left( m \left( x^2 + \omega_j^2 \right) \right) \left( s^2 + \omega_k^2 \right) \right] \quad (38)
\]
Now, similarly to (30), we have
\[
X_j(t) = U^{\dagger}(t)X_j(0)U(t) \Rightarrow U(t)X_j(t) = X_j(0)U(t)\quad (39)
\]
using
\[
\langle x, X| U(t)X_j(0)|x', X'\rangle = \langle x, X| X_j(0)U(t)|x', X'\rangle. \quad (40)
\]
Following the same steps that led to (33), we will find
\[
\left[ \frac{f_j}{\omega_j} \eta_j(t) \frac{\partial}{\partial x'} + \frac{m}{2} \sum_k \frac{1}{\omega_k^2} M_{jk} \frac{\partial}{\partial X_k} \right] \ln K(x, X; t, x', X') = \frac{i}{\hbar} X_j - \frac{\alpha^2 f_j}{\omega_j} \eta_j x' - \sum_k M_{jk} X_k. \quad (41)
\]
The form of the quantum propagator can now be determined from equations (33) and (41). The right-hand side of these partial differential equations suggests that we can assume the following general quadratic form for the logarithm of propagator
\[
\ln K(x, X; t, x', X') = A + B_0 x' + B \cdot X' + \frac{1}{2} C_0 x'^2 + \frac{1}{2} D_{ij} X_i X_j, \quad (42)
\]
where the coefficients \(A, B_0, B, C_0, C,\) and \(D_{ij}\) can depend on time and unprimed variables \(x, \{X_j\}\). Inserting (42) into equations (33), (41) and matching the coefficients on both sides of these equations, we will find
\[
B_0 = -\frac{i}{\hbar} x - \frac{i}{2 \hbar} \sum_{jl} \xi_j \mathcal{N}_{lj}^{-1} \lambda_l, \quad (43)
\]
\[
B_k = \frac{i}{\hbar} \sum_{l} \mathcal{N}_{lk}^{-1} \lambda_l, \quad (44)
\]
\[
C_0 = \frac{i}{\hbar} \sum_{l} \mathcal{N}_{li}^{-1} \mu_l, \quad (45)
\]
\[
C_k = -\frac{2i}{\hbar} \sum_{l} \mathcal{N}_{kl}^{-1} \mu_l, \quad (46)
\]
where for notational simplicity we have defined
\[ \xi_k(t) = \frac{\xi_k}{\omega_k}, \]
\[ \lambda_k = X_k - \frac{x}{\beta} \xi_k, \]
\[ \mu_j(t) = \omega^2 \xi_j(t) + \frac{\alpha}{\beta} \xi_j, \]
\[ N_{jk} = \frac{m}{\omega^2} M_{jk} = -\frac{m}{\omega_j} \sin \left( \omega_j t \right) \delta_{jk} + m \hat{Q}_{jk} - \frac{f_{jk} \hat{p}_{jk}}{\beta \omega_j \omega_k}, \]
\[ \mathcal{L}_{jk} = m \mathcal{M}_{jk} = \frac{f_{jk} \hat{p}_{jk}}{\beta \omega_j \omega_k}, \]
\[ = -\frac{m}{\omega_j} \sin \left( \omega_j t \right) \delta_{jk} + m \hat{Q}_{jk} - \frac{f_{jk} \hat{p}_{jk}}{\beta \omega_j \omega_k}. \]

By inserting coefficients (42)–(46) into (42) and making use of the symmetry property \( K(x, X; t; x', X') = K(x', X', t; x, X) \), we can write the propagator as
\[ K(x, X; t; x', X') = g(t) e^{i \hat{H} \left( t^{r+2} + t^{l+2} \right) a(t) - 2 t_{ij} + \frac{1}{4} \delta_{ij} - \frac{1}{4} \delta(t^{r+2}) - 2 t_{ij} + \frac{1}{4} \delta_{ij}}, \]
\[ = e^{i \hat{H} \left( t^{r+2} + t^{l+2} \right) a(t) - 2 t_{ij} + \frac{1}{4} \delta_{ij} - \frac{1}{4} \delta(t^{r+2}) - 2 t_{ij} + \frac{1}{4} \delta_{ij}}. \]

and \( g(t) \) is a time-dependent function that can be determined from the identity
\[ \int dx^* \prod_{k=1}^{N} dX_k^* K(x, X; t; x^*, X^*) \]
\[ \times K^*(x', X', t; x^*, X^*) \]
\[ = \delta(x - x') \prod_k \delta(X_k - X_k). \]

up to a phase factor \( e^{i \theta} \)
\[ g(t) = e^{i \theta} \frac{m}{\sqrt{2 \pi \hbar}} \left( \frac{m}{\sqrt{2 \pi \hbar}} \right)^{N} \frac{1}{\sqrt{\det \mathcal{N}}} \].

The phase factor can be obtained from the limiting case \( f_k = 0, \forall k \), or simply \( f = 0 \). In this case, the oscillator is not coupled to the bath oscillators, and the form of \( g(t) \) is known in this case. Inserting the limits
\[ \lim_{t \to 0} \beta(t) = \frac{\sin(\omega t)}{\omega}, \]
\[ \lim_{t \to 0} N_{jk}(t) = -\frac{m}{\omega_j} \frac{\sin(\omega_j t)}{\omega_j} \delta_{jk}. \]

into (59) leads to
\[ g(t) = e^{i \theta} \frac{m}{\sqrt{2 \pi \hbar}} \left( \frac{m}{\sqrt{2 \pi \hbar}} \right)^{N} \frac{1}{\sqrt{\det \mathcal{N}}} \]
\[ = \frac{m}{\sqrt{2 \pi \hbar}} \left( \frac{m}{\sqrt{2 \pi \hbar}} \right)^{N} \frac{1}{\sqrt{\det \mathcal{N}}} \]
\[ = \frac{m}{\sqrt{2 \pi \hbar}} \left( \frac{m}{\sqrt{2 \pi \hbar}} \right)^{N} \frac{1}{\sqrt{\det \mathcal{N}}} \]

Finally, the explicit form of the total propagator is
\[ K(x, X; t; x', X') \]
\[ = e^{i \hat{H} \left( t^{r+2} + t^{l+2} \right) a(t) - 2 t_{ij} + \frac{1}{4} \delta_{ij} - \frac{1}{4} \delta(t^{r+2}) - 2 t_{ij} + \frac{1}{4} \delta_{ij}}. \]

The propagator (65) is exact, but it depends on the matrices \( \mathcal{N}^{-1} \) and \( \mathcal{L} \), defined by (51) and (52), respectively. Therefore, for a finite but large number of bath oscillators, numerical calculations are unavoidable.

**Example 1.** Consider a charged harmonic oscillator with mass \( m \) and charge \( q \) oscillating along the \( x \)-axis inside an \( n \)-mode cavity. We assume that the walls of the cavity are far enough from the oscillator so ignore them from the confinement effects. In the electric dipole approximation [37], the vector potential in the place of the oscillating charge can be written as [37]
\[ A_i = \sum_{k=1}^{n} c_k (\hat{a}_k + \hat{a}_k^*), \]

where \( c_k \) are some constant dependent on the polarization directions inside the cavity, and \( \hat{a}_k \) (\( \hat{a}_k^* \)) are annihilation (creation) operators of \( k \)-mode photons. The total Hamiltonian of the charged oscillator and the electromagnetic field modes can be written as [37]
where each electromagnetic mode with frequency \( \omega_k \) is replaced with its corresponding harmonic oscillator Hamiltonian. From the relation between the position and momentum of the \( k \)-mode oscillator and the ladder operators

\[
\hat{a}_k = \frac{1}{\sqrt{2\hbar\omega_k}} (X_k + iP_k),
\]

\[
\hat{a}_k^\dagger = \frac{1}{\sqrt{2\hbar\omega_k}} (X_k - iP_k),
\]

we can rewrite (66) as

\[
A_k = \sum_{k=1}^n c_k \sqrt{2\omega_k} X_k.
\]

The Hamiltonian (67) can be obtained from the Lagrangian

\[
L = \frac{1}{2} \dot{X}_k^2 - \frac{1}{2} \frac{m}{\hbar^2} \dot{X}_k^2 - \sum_{k=1}^n \left( \omega^2_k - \omega^2_k \right) X_k^2 + \sum_{k=1}^n \frac{g_k}{\hbar} X_k \dot{X}_k,
\]

\[
L = \frac{1}{2} \dot{X}_k^2 - \frac{1}{2} \frac{m}{\hbar^2} \dot{X}_k^2 - \sum_{k=1}^n \left( \omega^2_k - \omega^2_k \right) X_k^2 + \sum_{k=1}^n \frac{g_k}{\hbar} X_k \dot{X}_k,
\]

where \( g_k = q c_k \sqrt{2\omega_k} \). The Lagrangian (71) is equivalent to the Lagrangian (1), since they differ by a total time derivative, and the only modification is replacing the coupling constants \( f_k \) with the new couplings \( -g_k \). The quantum propagator for this system is given by (65), where \( f_k \) should be replaced with \( -g_k \).

Let us go back to the Hamiltonian (67). Expanding the term inside the parenthesis, we find

\[
H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 + \sum_{k=1}^n \frac{1}{2} \left( P_k^2 + \omega^2_k X_k^2 \right) - \frac{1}{2} \sum_{k=1}^n \sum_{j=1}^n g_k g_j X_k X_j,
\]

\[
H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 + \sum_{k=1}^n \frac{1}{2} \left( P_k^2 + \omega^2_k X_k^2 \right) - \frac{1}{2} \sum_{k=1}^n \sum_{j=1}^n g_k g_j X_k X_j,
\]

where the last term, which is the diamagnetic term \( q^2 A^2 / 2m \), can be written in terms of the ladder operators as

\[
\frac{1}{2m} \sum_{j=1}^n g_j X_j X_j = \frac{1}{2m} \sum_{k=1}^n \sum_{j=1}^n \frac{g_k g_j}{\sqrt{2\omega_k \omega_j}} \times \left( \hat{a}_k \hat{a}_j + \hat{a}_j \hat{a}_k \right).
\]

The diamagnetic term is usually neglected in system–field interactions. In [38] it was shown that for a single-mode cavity and in the electric dipole approximation, keeping the diamagnetic term causes a frequency shift of the mode. Here we generalize this to an \( n \)-mode cavity via canonical transformations. For this purpose, consider the following canonical transformations

\[
p = U_{pq} P_q,
\]

\[
\dot{q} = P_q U_{pq}^\dagger.
\]

Therefore, we can remove the diamagnetic term \( (q^2 A^2 / 2m) \) and replace the frequency modes \( \omega_k \) with \( s_k^2 \). Now the unitary transformation [39]
\[ U = e^{i\int \frac{p^2}{2m} + \frac{1}{2} \omega_0^2 x^2 \, dt}, \] (83)

interchanges the position and momentum of the oscillator
\[ x \to U^\dagger x \quad U = -\frac{p}{m \omega_0}, \] (84)
\[ p \to U^\dagger p \quad U = \max, \] (85)

and leaves the oscillator modes unchanged. The Hamiltonian transforms to the equivalent Hamiltonian
\[ H' = U^\dagger H U = \frac{p^2}{2m} + \frac{1}{2} \omega_0^2 x^2 + \sum_{k=1}^{n} \left( P_k^2 + \omega_k^2 X_k^2 \right) + \sum_{k=1}^{n} d_k X_k x, \] (86)

where the new coupling constants are defined by \( d_k = -\sigma_k m \omega_0 \). The Hamiltonian (86) can be diagonalized via canonical transformation [3]
\[ p = \sum_{i=0}^{n} \sqrt{m} T_0 P_i^r, \]
\[ x = \sum_{i=0}^{n} \frac{1}{\sqrt{m}} T_0 X_i^r, \]
\[ P_k = \sum_{i=0}^{n} T_k P_i^r, \]
\[ X_k = \sum_{i=0}^{n} T_k X_i^r, \] (87)

where the unitary matrix \( T^\dagger T = 1 \) diagonalizes the symmetric matrix [3]
\[
W = \begin{pmatrix}
\omega_0^2 & \frac{d_1}{\sqrt{m}} & \frac{d_2}{\sqrt{m}} & \cdots & \frac{d_n}{\sqrt{m}} \\
\frac{d_1}{\sqrt{m}} & \omega_1^2 & 0 & \cdots & 0 \\
\frac{d_2}{\sqrt{m}} & 0 & \omega_2^2 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{d_n}{\sqrt{m}} & 0 & 0 & \cdots & \omega_n^2
\end{pmatrix},
\] (88)

therefore,
\[ T^\dagger W T = \begin{pmatrix}
\Omega_0^2 & 0 & 0 & \cdots & 0 \\
0 & \Omega_1^2 & 0 & \cdots & 0 \\
0 & 0 & \Omega_2^2 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & \Omega_n^2
\end{pmatrix}, \] (89)

where \( \Omega_k^2 \) are eigenvalues of the matrix \( W \) and corresponding eigenvectors are used to construct the transformation matrix \( T \). From the canonical transformations (87) and the normalization of the eigenvectors of the \( T \) matrix, one can easily show that the eigenvalues \( \Omega_k^2 \) satisfy equation [3]
\[ \omega^2 - \Omega_k^2 + \sum_{k=1}^{n} \frac{d_k^2}{m \left( \Omega_k^2 - \omega_k^2 \right)} = 0. \] (90)

The equivalent transformed Hamiltonian is now defined by
\[ H' = \frac{p^2}{2} + \frac{1}{2} \Omega_0^2 x^2 + \sum_{j} \left( \frac{p_j^2}{2} + \frac{1}{2} \omega_j^2 X_j^2 \right) - \sum_i P_i f_j x, \] (92)

under the unitary transformation
\[ U = e^{-i \int \sum_{j=1}^{n} \frac{\sum_{k=0}^{n} \frac{\omega_k}{\sqrt{m}} x_k^2 \, dt} \}, \] (93)

we have
\[ X_j \to U^\dagger X_j U = -\frac{P_j}{\omega_j}, \] (94)
\[ P_j \to U^\dagger P_j U = \omega_j X_j, \] (95)

and the Hamiltonian (92) transforms to
\[ H' = \frac{p^2}{2} + \frac{1}{2} \Omega_0^2 x^2 + \sum_{j} \left[ \frac{p_j^2}{2} + \frac{1}{2} \omega_j^2 X_j^2 \right] + \sum_i \epsilon_i X_i x, \] (96)

which is the Hamiltonian considered in [3] and \( \epsilon_j = -f_j \omega_j \). Also, one can show that the normal modes defined in [3] are the poles of the the Laplace transformed function \( \tilde{\rho}(s) \) defined in (26)
\[ \tilde{\rho}(s) = \frac{1}{s^2 + \omega^2 + s\tilde{\rho}(s)}. \] (97)

4. Density matrix

Having the propagator (65), we can find the total density matrix in any time. From the quantum Liouville’s equation we have
\[ \frac{\partial \rho}{\partial t} = -\frac{i}{\hbar} [H, \rho], \] (98)

and since the total Hamiltonian is time-independent, we can
solve (98) as

\[
\rho(t) = e^{-\frac{i}{\hbar} \mathcal{H} t} \rho(0) e^{\frac{i}{\hbar} \mathcal{H} t} = U(t) \rho(0) U^\dagger(t) .
\]

Therefore,

\[
\rho(x, X, x', X', t) = \langle x, X | \rho(t) | x', X' \rangle = \left( \langle x, X | U(t) \rho(0) U^\dagger(t) | x', X' \rangle \right) = \int dx_1 dx_2 dX_1 dX_2 K(x, X, t; x_1, X_1) \times \rho(x_1, X_1, x_2, X_2, 0) \times K^\dagger(x', X', t; x_2, X_2). \tag{100}
\]

For a given initial state, which is usually a product state \( \rho \otimes \rho_B \), where \( \rho \) is an arbitrary density matrix for the oscillator, and \( \rho_B \) can be chosen, for example, as a thermal state for the bath, we can find from (100) the total density matrix in an arbitrary time. If we are interested in the time evolution of the reduced density matrix, which is usually the case, then we can trace out the bath degrees of freedom and find

\[
\rho(x, x', t) = tr_B(\rho) = \int dX \rho(x, X, x', X, t),
\]

where the kernel or the reduced Green’s function \( G_{\text{red}} \) is defined by

\[
G_{\text{red}}(x, x'; x_1, x_2, t) = \int dX_1 dX_2 dX K(x, X, t; x_1, X_1) \times \rho_B(x_1, X_1, x_2, X_2, 0) \times K^\dagger(x', X', t; x_2, X_2). \tag{102}
\]

This kernel is in fact the same factor introduced by Feynman–Vernon in [2], known as an influence functional obtained from the path integral approach. If we define the operator \( K(x, x', t) \) on the Hilbert space of the environment oscillators for real parameters \( x, x', t \) as

\[
K(x, X, t; x', X') = \langle X' | K(x, x', t) | X \rangle,
\]

then we can rewrite (102) as

\[
G_{\text{red}}(x, x'; x_1, x_2, t) = \int dX_1 dX_2 dX \langle X' | K(x, x', t) \rangle \times \rho_B(x_1, X_1, x_2, X_2, 0) \times \langle X | K^\dagger(x_1, x_2, t) | X_1 \rangle \times tr \left[ \rho_B(0) K^\dagger(x', x_2, t) K(x, x_1, t) \right] = \left\{ K^\dagger(x', x_2, t) K(x, x_1, t) \right\}_{\text{eq}}. \tag{104}
\]

One can show that this recent equation can be rewritten as

\[
G_{\text{red}}(x, x', x_1, x_2, t) = \frac{m}{2\pi \hbar} \beta^N \left( \frac{m}{2\pi \hbar} \beta^N \right) e^{-\frac{m}{\hbar} \beta^N (x - x' - \frac{i}{\hbar} \mathcal{H} t)} \times e^{\frac{m}{\hbar} \beta^N (x_1 - x) + 2\beta (x_1 - x)} \times F_B(x' - x, x_2 - x_1, t), \tag{105}
\]

where \( F_B \) is defined by

\[
F_B(x' - x, x_2 - x_1, t) = \int dX \rho_B(X, X + q, 0) \times e^{\frac{m}{\hbar} X \left[ N^{-1} \mathcal{Q} - m N^{-1} q \right]}, \tag{106}
\]

and

\[
q = \frac{(x_2 - x_1)}{\beta} - (x' - x) \xi, \tag{107}
\]

\[
q' = (x_2 - x_1) \mu - \frac{(x' - x)}{\beta} \xi. \tag{108}
\]

**Example 2.** Let the initial state of the bath be a thermal state given by

\[
\rho_B(X, X', 0) = \prod_k \frac{(\omega_k)}{\pi \hbar} \coth \left( \frac{\omega_k \tau}{2} \right) \times e^{\frac{\pi}{\hbar} \sum_k (\omega_k x_k^2 - \omega_k \tau) - \frac{\pi}{\hbar} \sum_m (\omega_m x_m^2 - \omega_m \tau) - \frac{\pi}{\hbar} \sum_m (\omega_m x_m^2 - \omega_m \tau)} \tag{109}
\]

Then from the definition (106) we will find

\[
F_B(x' - x, x_2 - x_1, t) = \frac{2\pi}{\beta} e^{\pi \sum_k (\omega_k x_k^2 - \omega_k \tau)} \left[ q_k - \frac{\omega_k}{2\omega_k} \right]^2, \tag{110}
\]

where \( p_k \) is defined by

\[
p_k = \sum_j \left[ N^{-1} \mathcal{Q} \right]_{kj} q_j - m N^{-1} q_j. \tag{111}
\]

**5. Thermal equilibrium**

In thermal equilibrium, the density matrix of the total system is given by

\[
\rho(x, X, x', X'; T) = \frac{1}{Z(T)} \left\{ x, X | e^{-\frac{\beta}{\hbar} \mathcal{H}} | x', X' \right\} = \frac{1}{Z(T)} K(x, X, -i\tau; x', X') \tag{112}
\]

where \( \tau = it = \frac{\hbar}{k_B} \), and \( k_B \) is the Boltzmann constant, and the total partition function is given by

\[
Z(T) = \int dx \int d^{N}X \rho(x, X, x, X; T). \tag{113}
\]
The propagator function can be calculated using the formula [40]
\[ Z(T) = \frac{1}{\sqrt{2\pi \beta t}} \frac{m^\frac{3}{2}}{\sqrt{\det(E - mI)}} \left( 1 - \frac{1}{a - b + \frac{mc^2}{\beta}} \right), \] (115)
where
\[ \zeta(t) = \left( \frac{\epsilon}{\beta} + \beta \mu \right) \cdot \mathcal{N}^{-1}(\mathbf{L} - m\mathbf{1})^{-1} \cdot \left( \frac{\epsilon}{\beta} + \beta \mu \right). \] (116)

Note that throughout the section the time variable \( t \) should be replaced with \( -ir, \) \( (r = \frac{b}{\hbar s}) \) in the steady state or long time limit. Now the reduced density matrix of the oscillator can be obtained by tracing over bath variables \( \mathbf{X} \), leading to
\[ \rho(x, x', T) = \int \frac{d^nx}{(2\pi\hbar)^n} e^{\frac{i}{\hbar} S_{XX}} \left( \frac{1}{\sqrt{2\pi \beta t}} \frac{m^\frac{3}{2}}{\sqrt{\det(E - mI)}} \left( 1 - \frac{1}{a - b + \frac{mc^2}{\beta}} \right) \right), \] (117)

From equations (115), (117) we can define the effective partition function of the harmonic oscillator as \( \mathcal{Z}_e = 1 / \sqrt{2(a + b + \frac{mc^2}{\beta})} \), which in the absence of interaction reduces to 1/2 sinh \( (\alpha \beta) \), as expected. Therefore, the effective or large-time propagator of the oscillator can be written as
\[ K_{\mathbf{X}}(x, t; x', 0) = \sqrt{\frac{m}{2\pi \hbar \beta (t)}} \times e^{\frac{i}{\hbar} \left( (x^{2} + x'^{2})(\alpha(t)) - \frac{1}{2}(b - \frac{mc^2}{\beta})x' \right)}, \] (118)

By making use of (117), the mean squared position and momentum of the oscillator can be obtained in a general medium as
\[ \langle x^2 \rangle = \text{tr} \left( \rho x^2 \right) = \left. \frac{i\hbar \beta}{2m a - b + \frac{mc^2}{\beta}} \right|_{x = -ir}, \] (119)
\[ \langle p^2 \rangle = \text{tr} \left( \rho p^2 \right) = \left. \frac{m\hbar(a + b)}{2i\beta} \right|_{x = -ir}, \] (120)
and for energy, we find
\[ \langle H \rangle = \left. \frac{\hbar(a + b)}{4i\beta} + \frac{\hbar \omega^2 \beta}{4a - b + \frac{mc^2}{\beta}} \right|_{x = -ir}, \] (121)

6. Weak coupling regime

The propagator (65) is exact and more suitable for numerical calculations for a finite number of environment oscillators or engineered environments. Also, the density matrix (117) is exact, and numerical calculations can be applied. Here, by the weak coupling limit, we mean that the coupling constants \( f_j \) are small; that is, the dimensionless parameters satisfy \( f_j^2 / \hbar m \omega^2 \ll 1 \). In this limit, we can approximate the related functions up to the second order in coupling constants and ignore them from higher orders. As the expressions suggest, this limit is not suitable near the zero temperature and it should be applied in finite temperatures, far from the zero temperature. In the weak coupling regime we have
\[ \beta(t) \approx \frac{\sin (\omega t)}{\omega} - \sum_j \frac{f_j^2}{m} \times \left( \left[ \frac{\omega^2 + \omega_j^2}{\cos (\omega t) - (\omega(t)[\omega^2 - \omega_j^2])} \right] \right) \times \left[ \frac{\omega^2 - \omega_j^2}{2(\omega^2 - \omega_j^2)^2} \right], \] (122)

\[ \alpha(t) \approx \cos (\omega t) + \sum_j \frac{f_j^2}{m} \times \left[ \left[ \frac{\omega^2 + \omega_j^2}{[1 - \cos (\omega(t)][\cos (\omega(t)] - 1 \right] \right] \times \left[ 1 + \cos (\omega(t)]\eta_j^{(0)}(t) + \omega \sin (\omega(t))\eta_j^{(0)}(t) \right]^2, \] (123)

where
\[ \eta_j^{(0)}(t) = \frac{\omega \sin (\omega(t) - \omega_j \sin (\omega(t))}{\omega(\omega^2 + \omega_j^2)} \] (125)

is the zero order approximation of \( \eta_j(t) \) defined in (28). This is because according to the definitions (51), (52), (116), we only need the zero-order approximation of the \( \eta_j(t) \). Now from the definitions (56), we find
\[ a(t) \approx \alpha(t) - \sum_j \frac{f_j^2}{\hbar \omega \sin (\omega_j t)} \times \left[ \frac{\omega^2 \eta_j^{(0)}(t) + \omega \cot (\omega(t))\eta_j^{(0)}(t)}{\omega(\omega^2 + \omega_j^2)} \right], \] (126)

\[ b(t) \approx 1 + \sum_j \frac{f_j^2}{m} \frac{\omega \eta_j^{(0)}(t)}{\omega \sin (\omega_j t) \sin (\omega(t))}. \] (127)

In zero-order approximation, from (122) we find \( a(t) = \cos (\omega(t)), b(t) = 1, \) and \( \xi(t) = 0, \) and from relations (86), (87), (121) we recover the well-known expressions...
\[ \langle x^2 \rangle = \frac{\hbar}{2m} \coth \left( \frac{\hbar \omega}{2k_B T} \right), \quad (128) \]

\[ \langle p^2 \rangle = \frac{m \hbar \omega}{2} \coth \left( \frac{\hbar \omega}{2k_B T} \right), \quad (129) \]

\[ \langle H \rangle = \frac{\hbar \omega}{2} \coth \left( \frac{\hbar \omega}{2k_B T} \right), \quad (130) \]

For \( N = 2 \) and dimensionless parameters \( r_1 = f_1^2/\hbar \omega^2 = .01, \ r_2 = f_2^2/\hbar \omega^2 = .02, \ s_1 = \omega_1/\omega = .9, \) and \( s_2 = \omega_2/\omega = .8 \) the position, momentum and energy are plotted in units of \( l_0^2 = \hbar/2m\omega, \ m_p^2 = \hbar \omega/2 \) and \( E_0 = \hbar \omega/2 \) in figures 1, 2, and 3 respectively. The dimensionless variable is taken as \( u = \omega \tau = \hbar \omega/k_B T. \)

It should be noted here that these diagrams have been obtained in the weak coupling regime and not close to zero temperature. The diagrams show that for the values \( r_1 = f_1^2/\hbar \omega^2 = .01, \ r_2 = f_2^2/\hbar \omega^2 = .02, \ s_1 = \omega_1/\omega = .9, \) and \( s_2 = \omega_2/\omega = .8 \), all thermal mean values are increased, compared with the free central oscillator. For engineered environments consisting of a finite number of bath oscillators, more accurate results can be obtained numerically by calculating the inverse Laplace transforms (25)–(28) and inverse of matrices defined in (51), (52), which takes us far from the goals of the present work.

7. Conclusions

In the present, using the symmetry and initial condition properties of a quantum propagator, the exact form of the total propagator of a quantum oscillator interacting with a bosonic bath is obtained in the Heisenberg picture. Knowing the propagator of the total system, the reduced density matrix for the oscillator is obtained. The kernel or Green’s function connecting the initial density matrix of the oscillator to the density matrix in an arbitrary time is defined, and its connection to the Feynman–Vernon influence functional is discussed. The weak coupling regime and squared mean values for position, momentum, and energy of the oscillator are obtained in equilibrium.

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