Field-induced dynamics in the quantum Brownian oscillator: An exact treatment

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Abstract
We consider a quantum linear oscillator coupled to a bath in equilibrium at an arbitrary temperature and then exposed to an external field arbitrary in form and strength. We then derive the reduced density operator in closed form of the coupled oscillator in a non-equilibrium state at an arbitrary time.

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1. Introduction
One of the most successful approaches to non-equilibrium statistical mechanics is the linear response theory [1,2,3]. This allows us to predict the average response of a physical quantity of the system to external perturbations with weak strength. At the heart of linear response theory we have the fluctuation-dissipation theorem [4,5], which offers a clear-cut relationship between irreversible processes in a non-equilibrium state and thermal fluctuations in the (initial) equilibrium state. However, this approach is, in general, restricted to non-equilibrium states near equilibrium in validity.

As a prototype of quantum dissipative systems, the scheme of quantum Brownian motion has been studied deeply and widely over a long period [5]. At its heart we have a quantum harmonic oscillator linearly coupled to an independent-oscillator model of a heat bath [quantum Brownian oscillator] in equilibrium at a (low) temperature. Due to its mathematical simplicity, this system allows the linear response theory to yield an exact expression for an average response of the system operator $\hat{q}$ (position) [and also that of $\hat{p}$ (momentum)] to external forces $F$ arbitrary in form and strength as well as those for the equilibrium fluctuations $\langle \hat{q}^2 \rangle_\beta$ and $\langle \hat{p}^2 \rangle_\beta$, respectively [5,6]. Based on this well-known result, quantum Brownian oscillator has recently attracted considerable interest in investigating thermodynamic behaviors of small-scaled quantum systems coupled to quantum environments in the low-temperature regime [7,8,9,10,11,12,13,14] (“quantum thermodynamics” [15,16,17]). Here the finite coupling strength between system and environment yields some quantum subtleties and so cannot be neglected whereas ordinary quantum statistical mechanics is intrinsically based on a vanishingly small coupling between them.

On the other hand, response functions in a far-from-equilibrium state such as $\langle \hat{q}^n(t) \rangle$ and $\langle \hat{p}^n(t) \rangle$ with $n \geq 2$ in this system cannot be obtained directly from the linear response theory. To explicitly have such non-equilibrium quantities, we need to exactly treat the higher-order terms in the external field and accordingly go beyond the scheme of linear response theory [18,19]. The primary goal of this paper is to derive a reduced density operator in closed form of the coupled oscillator in a non-equilibrium state at an arbitrary time $t$, which can, obviously, provide all higher-order fluctuations of the non-equilibrium state. For numerical analysis we will also consider a variety of external fields (d.c. and a.c.) leading to explicit evaluation of the non-equilibrium fluctuations. In doing so, we will employ not only the $\hat{q}F(t)$ interaction Hamiltonian (“scalar-potential gauge”) but also the $\hat{p}A(t)$ interaction Hamiltonian (“vector-potential gauge”). The equivalence of the two interactions is based on the gauge transformation between their wavefunctions satisfying the corresponding (time-dependent) Schrödinger equations, respectively (for a detailed discussion of $\hat{q}F$ versus $\hat{p}A$ gauge problem, see Ref. [20]). And we will adopt the Drude model with a finite frequency cut-off for the spectral density of bath modes, which is a prototype for physically realistic damping [5].

The general layout of this paper is the following. In Sect. 2 we briefly review the general results of quantum Brownian oscillator needed for our later discussions. In Sect. 3 we explicitly derive an exact expression for the reduced...
density operator of the coupled oscillator in a non-equilibrium state. In Sect. 4 we perform numerical analysis for various non-equilibrium quantities induced from the reduced density operator. Finally we give the concluding remarks of this paper in Sect. 5.

2. General treatment of quantum Brownian oscillator

The quantum Brownian oscillator under consideration is described by the model Hamiltonian \( \hat{H} = \hat{H}_s + \hat{H}_{sb} \),

\[
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\]

where

\[
\hat{H}_s = \frac{\hat{p}^2}{2M} + \frac{M}{2} \omega_0^2 \hat{q}^2
\]

\[
\hat{H}_{sb} = \sum_{j=1}^{N} \left( \frac{\hat{p}_j^2}{2m_j} + \frac{m_j}{2} \omega_j^2 \left( \dot{\xi}_j - \frac{c_j}{m_j \omega_j^2} \hat{q} \right)^2 \right) .
\]

The Hamiltonian \( \hat{H}_{sb} \) can split into the bath and the coupling terms such as

\[
\hat{H}_b = \sum_{j=1}^{N} \left( \frac{\hat{p}_j^2}{2m_j} + \frac{m_j}{2} \omega_j^2 \xi_j^2 \right)
\]

\[
\hat{H}_{sb} = -\hat{q} \sum_{j=1}^{N} c_j \dot{\xi}_j + \hat{q}^2 \sum_{j=1}^{N} \frac{c_j^2}{2m_j \omega_j^2} ,
\]

respectively. The interaction Hamiltonian \( \hat{H}_{sb} \) contains a term of quadrature completion modifying the frequency of the system oscillator \( \hat{H}_s \). This quadrature term is needed not only for later exact calculations; in fact, the model Hamiltonian without the quadrature completion has a significant defect, as was discussed in [21]. The total system is assumed to be within the canonical thermal equilibrium state \( \hat{p}_b = e^{-\beta \hat{H}} / Z_\beta \) where \( \beta = 1/(k_B T) \), and \( Z_\beta \) is the partition function.

From the Heisenberg equations of motion for \( \hat{q} \) and \( \hat{p} \) we can derive the quantum Langevin equation [5, 6]

\[
M \ddot{q}(t) + M \int_0^t d\tau \gamma(t-\tau) \dot{q}(\tau) + M \omega_0^2 \hat{q}(t) = \dot{\xi}(t) ,
\]

where we used \( \hat{p}(t) = M \ddot{q}(t) \), and the damping kernel and the noise operator are, respectively, given as

\[
\gamma(t) = \frac{1}{M} \sum_{j=1}^{N} \frac{c_j^2}{m_j \omega_j} \cos(\omega_j t) ; \quad \dot{\xi}(t) = -M \gamma(t) \dot{q}(0) + \sum_{j=1}^{N} c_j \left( \ddot{\xi}_j(0) \cos(\omega_j t) + \frac{\hat{p}(0)}{m_j \omega_j} \sin(\omega_j t) \right) .
\]

Here the expectation value of the noise operator vanishes, \( \text{Tr} \{ \dot{\xi}(t) \hat{p}_b \} = 0 \) or, equivalently, \( \langle \dot{\xi}(t) \rangle_{\hat{p}_b} = 0 \) with respect to the initial bath state, prepared as a shifted canonical equilibrium distribution, \( \hat{p}_b = e^{-\beta \hat{H}_{\text{eq}}} / Z_\beta \), in which a normalization constant \( Z_\beta \) is the properly defined partition function [5]. And the noise correlation is given as [8]

\[
S_{\xi \xi}(t-t') := \frac{1}{2} \left( \langle \dot{\xi}(t) \dot{\xi}(t') \rangle_{\hat{p}_b} + \langle \dot{\xi}'(t) \dot{\xi}(t) \rangle_{\hat{p}_b} \right) = \frac{h}{2} \sum_{j=1}^{N} \frac{c_j^2}{m_j \omega_j} \cos(\omega_j (t-t')) \coth \left( \frac{\beta \omega_j}{2} \right) .
\]

With \( h \to 0 \), the correlation \( S_{\xi \xi}(t-t') \) reduces to its classical counterpart, \( M \gamma(t-t') / \beta \) [22]. We also introduce a response function [6]

\[
\chi_{qp}(t) = \frac{i}{\beta} \left( \langle \dot{q}(t), \dot{q}(0) \rangle \right)_{\hat{p}_b} \Theta(t) ,
\]

where \( \Theta(t) \) represents a step function. Then we can have other response functions as well such as \( \chi_{qp}(t) = -\chi_{qp}(t) = M \dot{\chi}_{qp}(t) \), and \( \chi_{pp}(t) = -M^2 \ddot{\chi}_{qq}(t) \).
For a later purpose it is instructive to discuss the time-reversal dynamics of \( \tilde{q}(t) \) in terms of \( \tilde{r}(t) := \tilde{q}(-t) \) and its momentum \( \tilde{\chi}(t) := -\dot{\tilde{r}}(t) \). We can then derive the corresponding quantum Langevin equation \( 8 \)

\[
M \ddot{\tilde{r}}(t) + M \int_0^t dt' \gamma(t - t') \dot{\tilde{r}}(t') + M \omega_0^2 \tilde{r}(t) = \tilde{\xi}_-(t) .
\]  

(10)

While this is the same in form as equation (6), the two equations differ in the noise in such a way that \( \tilde{\xi}_-(t) \) is identical to \( \hat{\xi}(t) \), however, with the replacement of \( \dot{\tilde{r}}(0) \rightarrow -\dot{\tilde{r}}(0) \) in (7). And from equation (9) and stationarity of the equilibrium correlation function between operators \( F \) and \( \tilde{G} \) such as \( \langle \tilde{F}(t) \tilde{G}(0) \rangle_\beta = \langle \tilde{F}(0) \tilde{G}(-t) \rangle_\beta \) 6, we can easily obtain \( \chi_{\tau r}(t) = -\chi_{\tau q}(t) \) [note that \( \tilde{r}(0) = \tilde{q}(0) \)]. Likewise, it also appears that \( \chi_{\tau r}(t) = \chi_{\tau q}(0) \).

Now we intend to derive explicit expressions for \( \tilde{q}(t) \) and \( \dot{\tilde{r}}(t) \), respectively. To do so, we first apply the Laplace transform to equations (6) and (10), respectively. Let the Laplace transform \( \tilde{\chi}(s) = \mathcal{L}[\chi(t)](s) \), and so we have \( \mathcal{L}[\tilde{q}(t)](s) = s\tilde{q}(s) - \tilde{q}(0) \) and \( \mathcal{L}[\dot{\tilde{r}}(t)](s) = s^2\tilde{\chi}(s) - s\tilde{q}(0) - \tilde{q}(0) \) 23. We can then obtain the Fourier-Laplace transform of \( \tilde{q}(t) \), which reads as

\[
\tilde{q}(s) = \int_{0-}^{0+} e^{is\tau} \tilde{q}(\tau) d\tau ,
\]

and the Fourier-Laplace transform of \( \dot{\tilde{r}}(t) \),

\[
\tilde{\chi}(s) = \mathcal{L}[\chi(t)](s) = \frac{c_j}{m_j \omega_j^2} - \omega_j^2 .
\]

(13)

We introduce the susceptibility, defined as the Fourier-Laplace transform of \( \chi_{\tau q}(t) \) in (9), such as 56

\[
\tilde{\chi}_{\tau q}(s) := \int_{-\infty}^{\infty} dt \chi_{\tau q}(t) e^{ist} = \frac{1}{i} \langle [\tilde{q}(s), \tilde{q}](t) \rangle ,
\]

(14)

which easily reduces to \(-1/[M(\omega_0^2 + i\omega \tilde{\gamma}(s) - \omega_0^2)]\) with the aid of (11). And it then appears that

\[
\tilde{\chi}_{\tau q}(s) = \frac{1}{i} \langle [\tilde{q}(s), \tilde{q}](t) \rangle = \frac{c_j}{m_j (\omega_j^2 - \omega^2)} \tilde{\chi}_{\tau q}(s) ,
\]

\[
\tilde{\chi}_{\tau r}(s) = \frac{1}{i} \langle [\tilde{r}(s), \tilde{r}](t) \rangle = -\tilde{\chi}_{\tau q}(s) .
\]

\[
\tilde{\chi}_{\tau q}(s) = i\omega M \tilde{\chi}_{\tau q}(s) ,
\]

\[
\tilde{\chi}_{\tau q}(s) = i\omega M \tilde{\chi}_{\tau q}(s) .
\]

\[
\tilde{\chi}_{\tau q}(s) = -\tilde{\chi}_{\tau q}(s) \tilde{q} + \tilde{\chi}_{\tau q}(s) \tilde{p} - \sum_j [\tilde{\chi}_{\tau q}(s) \tilde{\chi}_j - \tilde{\chi}_{\tau q}(s) \tilde{p}_j] \]

\[
\tilde{\chi}_{\tau r}(s) = -\tilde{\chi}_{\tau r}(s) \tilde{q} + \tilde{\chi}_{\tau r}(s) \tilde{p} - \sum_j [\tilde{\chi}_{\tau r}(s) \tilde{\chi}_j - \tilde{\chi}_{\tau r}(s) \tilde{p}_j] .
\]

(17a)

(17b)

\[
\hat{q}(t) = -\chi_{\tau q}(t) \tilde{q} + \chi_{\tau q}(t) \tilde{p} - \sum_j [\chi_{\tau q}(t) \tilde{\chi}_j - \chi_{\tau q}(t) \tilde{\chi}_j] ,
\]

\[
\hat{r}(t) = -\chi_{\tau r}(t) \tilde{q} + \chi_{\tau r}(t) \tilde{p} - \sum_j [\chi_{\tau r}(t) \tilde{\chi}_j - \chi_{\tau r}(t) \tilde{\chi}_j] .
\]

(18a)

(18b)
where
\[
\chi_{qq}(t) = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega \chi_{qq}(\omega) e^{-i\omega t}.
\] (19)

The two equations will be used in Sect. 3 for derivation of the reduced density operator of the coupled oscillator in closed form.

For a later purpose it is useful to introduce well-known expressions for the equilibrium fluctuations in terms of the susceptibility \(\chi_{qq}(\omega)\) such as [24]
\[
\langle \hat{q}^2 \rangle_{\beta} = \frac{\hbar}{\pi} \int_{0}^{\infty} d\omega \coth \left( \frac{\hbar \omega}{2} \right) \text{Im} \{\chi_{qq}(\omega + i0^+)\} \]
(20)
and
\[
\langle \hat{p}^2 \rangle_{\beta} = \frac{\hbar^2}{\pi} \int_{0}^{\infty} d\omega \omega^2 \coth \left( \frac{\hbar \omega}{2} \right) \text{Im} \{\chi_{qq}(\omega + i0^+)\},
\]
(21)
respectively, which can be derived from the fluctuation-dissipation theorem [4, 5].

3. Reduced density operator of the coupled oscillator in a non-equilibrium state

Now we study the influence of an external field on a linear oscillator coupled to a bath. To do so, we first consider the equation of motion for the density operator of the total system (i.e., oscillator plus bath), which reads [5, 6]
\[
\dot{\hat{\rho}}(t) = e^{-\mu L_0} \hat{\rho}(0) - i \int_{0}^{t} dt e^{-i(\omega - \gamma)\frac{\hbar}{2}} \hat{L}_1(t) \hat{\rho}(t) .
\] (22)

In the scalar-potential gauge for the field-coupling, the total Hamiltonian reads as \(\hat{H}(t) = \hat{H} - \hat{q} F(t)\), and the corresponding Liouville operator \(\hat{L} = \hat{L}_0 + \hat{L}_1^{(1)}\) satisfies
\[
\hat{L}_0 \hat{\rho}(t) = \frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] ; \hat{L}_1^{(1)}(\tau) \hat{\rho}(\tau) = -\frac{i}{\hbar} [\hat{q}, \hat{\rho}(\tau)] F(\tau) .
\] (23)

In the vector-potential gauge, on the other hand, the total Hamiltonian is given as
\[
\hat{H}(t) = \frac{\{\hat{p} + p_{s}(t)\}^{2}}{2M} + \frac{M \omega_{0}^{2}}{2} \hat{q}^{2} + \hat{H}_{s-b},
\]
(24)
which is identical \(\hat{H} + p_{s}(t) \hat{p}/M + p_{s}^{2}(t)/(2M)\), and accordingly
\[
\hat{L}_0 \hat{\rho}(t) = \frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] ; \hat{L}_1^{(v)}(\tau) \hat{\rho}(\tau) = \frac{i}{\hbar} [\hat{p}, \hat{\rho}(\tau)] \frac{\hat{L}_1^{(v)}}{\hat{L}_0} .
\] (25)

Here the vector potential \(p_{s}(t) = \int_{0}^{t} F(\tau) d\tau\) is an impulse induced by field \(F\). For an uncoupled oscillator the equivalence of the two interactions is based on the gauge transformation \(\psi_{s}(q, t) = e^{i\varphi(q, t)}\psi(q, t)\) [20], where the wavefunctions \(\psi_{s}(q, t)\) and \(\psi(q, t)\) satisfy the time-dependent Schrödinger equations in the scalar-potential and the corresponding vector-potential gauges, respectively.

We substitute (23) into (22), with \(\hat{\rho}(0) = \hat{\rho}_{\beta}\), and make iterations for \(\hat{\rho}(t)\) in the integral. Then we can arrive at the expression
\[
\hat{\rho}_{s}(t) = \hat{\rho}_{\beta} + \frac{i}{\hbar} \int_{0}^{t} d\tau F(\tau) e^{-i(\omega - \gamma)\frac{\hbar}{2}} \left[ \hat{q}, \hat{\rho}_{\beta} \right] e^{i(\omega - \gamma)\frac{\hbar}{2}} + \left( \frac{i}{\hbar} \right)^{2} \int_{0}^{t} d\tau F(\tau) \int_{0}^{t} d\tau' F(\tau') e^{-i(\omega - \gamma)\frac{\hbar}{2}} \times
\]
\[
\left[ \hat{q}, e^{-i(\omega - \gamma)\frac{\hbar}{2}} \left[ \hat{q}, \hat{\rho}_{\beta} \right] e^{i(\omega - \gamma)\frac{\hbar}{2}} + \left( \frac{i}{\hbar} \right)^{3} \int_{0}^{t} d\tau F(\tau) \int_{0}^{t} d\tau' F(\tau') \int_{0}^{t} d\tau'' F(\tau'') e^{-i(\omega - \gamma)\frac{\hbar}{2}} \times
\]
\[
\left[ \hat{q}, e^{-i(\omega - \gamma)\frac{\hbar}{2}} \left[ \hat{q}, \hat{\rho}_{\beta} \right] e^{i(\omega - \gamma)\frac{\hbar}{2}} + \left( \frac{i}{\hbar} \right)^{4} \int_{0}^{t} d\tau F(\tau) \int_{0}^{t} d\tau' F(\tau') \int_{0}^{t} d\tau'' F(\tau'') \int_{0}^{t} d\tau''' F(\tau''') e^{-i(\omega - \gamma)\frac{\hbar}{2}} \times
\]
\[
\left[ \hat{q}, e^{-i(\omega - \gamma)\frac{\hbar}{2}} \left[ \hat{q}, \hat{\rho}_{\beta} \right] e^{i(\omega - \gamma)\frac{\hbar}{2}} \right] e^{i(\omega - \gamma)\frac{\hbar}{2}} + \cdots .
\] (26)

With the aid of \([\hat{p}, \hat{H}] = 0\), this equation easily reduces to the expression in terms of \(\dot{\hat{\rho}}(t) = e^{-\mu \frac{\hbar}{2}} \hat{q} e^{\frac{\hbar}{2}}\) such as
\[
\hat{\rho}_{s}(t) \equiv \hat{\rho}_{\beta} + \frac{i}{\hbar} \int_{0}^{t} d\tau F(\tau) \left[ \dot{\hat{\rho}}(t - \tau), \hat{\rho}_{\beta} \right] + \left( \frac{i}{\hbar} \right)^{2} \int_{0}^{t} d\tau F(\tau) \int_{0}^{t} d\tau' F(\tau') \left[ \dot{\hat{\rho}}(t - \tau), \dot{\hat{\rho}}(t - \tau'), \hat{\rho}_{\beta} \right] + \left( \frac{i}{\hbar} \right)^{3} \int_{0}^{t} d\tau F(\tau) \int_{0}^{t} d\tau' F(\tau') \int_{0}^{t} d\tau'' F(\tau'') \left[ \dot{\hat{\rho}}(t - \tau), \dot{\hat{\rho}}(t - \tau'), \dot{\hat{\rho}}(t - \tau''), \hat{\rho}_{\beta} \right] + \cdots .
\] (27)
where
\[ \hat{\rho}(t) = -\chi_{sp}(t) \hat{q}, \hat{p}_b + \chi_{sr}(t) (\hat{\rho}_{\hat{b}, \hat{p}} + \sum_j \chi_{sj}(t) \hat{\rho}_j, \hat{p}_j) . \] (28)

obtained directly from equation (18b). For the vector-potential gauge, on the other hand, we plug (25) into (22), and after making some calculations similar to those for (26) we can finally obtain the expression in terms of \( \hat{s}(t) = -e^{-\hat{H}t} \hat{\rho} e^{\hat{H}t} \) such as
\[ \hat{\rho}_s(t) = \hat{\rho}_b + \frac{i}{\hbar} \int_0^t dt \int_0^{\tau} d\tau \int_0^{\tau'} d\tau' \left[ \hat{s}(t - \tau), \hat{\rho}_{\hat{b}_s, \hat{p}} \right] + \left( \frac{i}{\hbar} \right)^2 \int_0^t dt \int_0^{\tau} d\tau \int_0^{\tau'} d\tau' \int_0^{\tau''} d\tau'' \left[ \hat{s}(t - \tau), \left[ \hat{s}(t - \tau'), \hat{\rho}_{\hat{b}_s, \hat{p}} \right] \right] + \cdots . \] (29)

From (28) and \( \hat{s}(t) = M \hat{s}(t) \) we can easily have
\[ \left[ \hat{s}(t), \hat{\rho}_{\hat{b}_s, \hat{p}} \right] = -\chi_{sp}(t) \hat{q}, \hat{p}_b + \chi_{sr}(t) (\hat{\rho}_{\hat{b}_s, \hat{p}} + \sum_j \chi_{sj}(t) \hat{\rho}_j, \hat{p}_j) . \] (30)

Let us now consider the reduced density operators for the coupled oscillator, \( \hat{\rho}_s(t) : = \text{Tr}_b \hat{\rho}(t) \) from (27) and (29), respectively. Here, \( \text{Tr}_b \) denotes the partial trace for the bath alone. The initial state \( \hat{\rho}(0) \) of the coupled oscillator, being the reduced operator of the canonical equilibrium state \( \hat{\rho}_b \), is known as \( [5, 23] \)
\[ \langle q | \hat{\rho}(0) | q' \rangle = \frac{1}{\sqrt{2\pi \hbar^2 q'}} \exp \left( \frac{\langle q' \rangle^2 - (q - q')^2}{2\hbar^2} \right) . \] (31)

First, from (28) we obtain
\[ \langle q | \text{Tr}_b \left[ \hat{\rho}(t), \hat{p}_b \right] | q' \rangle = \hat{S}_{qq}(t) \langle q | \hat{\rho}(0) | q' \rangle , \] (32)
where \( \hat{S}_{qq}(t) : = -i\hbar \chi_{sr}(t) \left( \hat{\partial}_q + \hat{\partial}_{q'} \right) - \chi_{sp}(t) (q - q') \), and similarly from (30) we can also have
\[ \langle q | \text{Tr}_b \left[ \hat{s}(t), \hat{p}_b \right] | q' \rangle = \hat{V}_{qq}(t) \langle q | \hat{\rho}(0) | q' \rangle , \] (33)
where \( \hat{V}_{qq}(t) : = -i\hbar \chi_{sr}(t) \left( \hat{\partial}_q + \hat{\partial}_{q'} \right) - \chi_{sp}(t) (q - q') \). Here we used
\[ \int_{-\infty}^{\infty} \prod_k |dx_k| \langle \hat{j}_x, \hat{p}_b | x_k \rangle = 0 \] (34a)
\[ \int_{-\infty}^{\infty} \prod_k |dp_k| \langle \hat{p}_k, \hat{p}_b | p_k \rangle = 0 . \] (34b)

From (18b), (34a) and (34b) it also appears that
\[ \int_{-\infty}^{\infty} \prod_k |dx_k| \langle \hat{j}_x, \hat{p}_b | x_k \rangle = 0 \] (35)

unless both \( \hat{\partial} \in [\hat{q}, \hat{p}] \) and \( \hat{\partial}' \in [\hat{q}, \hat{p}] \). Therefore we can arrive at the expressions,
\[ \langle q | \text{Tr}_b \left[ \hat{\rho}_b | \hat{p}(t), \hat{p}_b \right] | q' \rangle = \hat{S}_{qq}(t) \hat{S}_{qq}(\tau) \langle q | \hat{\rho}(0) | q' \rangle \] (36)
\[ \langle q | \text{Tr}_b \left[ \hat{s}_s | \hat{p}(t), \hat{p}_b \right] | q' \rangle = \hat{V}_{qq}(t) \hat{V}_{qq}(\tau) \langle q | \hat{\rho}(0) | q' \rangle . \] (37)

Here we also used
\[ \langle q | \text{Tr}_b \left[ \hat{\partial}_q | \hat{p}_b \right] | q' \rangle = (q - q')^2 \langle q | \hat{\rho}(0) | q' \rangle , \] (38)
and \([\hat{q}, [\hat{p}, \hat{p}_y]] = [\hat{p}, [\hat{q}, \hat{p}_y]]\). Along the same line, after making lengthy calculations, we can also obtain

\[
\langle q|T_\alpha^{\hat{t}}(\hat{t}), [\hat{f}(\tau), [\hat{f}(\tau'), \hat{p}_y]]|q'\rangle = \hat{S}_{qq^\prime}(\tau) \hat{S}_{qq^\prime}(\tau') \langle q|\hat{R}(0)|q'\rangle \quad (39)
\]

\[
\langle q|T_\beta^{\hat{t}}(\hat{t}), [\hat{s}(\tau), [\hat{s}(\tau'), \hat{p}_y]]|q'\rangle = \hat{V}_{qq^\prime}(\tau) \hat{V}_{qq^\prime}(\tau') \langle q|\hat{R}(0)|q'\rangle . \quad (40)
\]

With the help of equations (27), (32), (36), and (39) we can finally find the matrix elements of the reduced density operator in the scalar-potential gauge such as

\[
\langle q|\hat{R}_s(t)|q'\rangle = T e^{\hat{J}_s(t)} \langle q|\hat{R}(0)|q'\rangle , \quad (41)
\]

where the operator \(\hat{J}_s(t) := \int_0^t d\tau F(\tau) \hat{S}_{qq^\prime}(t-\tau)\) represents a time-evolution action, and \(T\) is the time ordering operator. For the vector-potential gauge, along the same line, from (29), (33), (37), and (40) we can arrive at the matrix elements

\[
\langle q|\hat{R}_v(t)|q'\rangle = T e^{\hat{J}_v(t)} \langle q|\hat{R}(0)|q'\rangle , \quad (42)
\]

where the operator \(\hat{J}_v(t) := (1/M) \int_0^t d\tau p_z(\tau) \hat{V}_{qq^\prime}(t-\tau)\).

Now we simplify the above expressions for \(\langle q|\hat{R}_s(t)|q'\rangle\) and \(\langle q|\hat{R}_v(t)|q'\rangle\). The operator \(\hat{J}_s(t)\) immediately reduces to \(i\hbar \langle \hat{q}(t)_s (\hat{a}_q + \hat{a}_q') + \langle \hat{p}(t)_s (q - q')\rangle\) from the well-known exact expression

\[
\langle \hat{O}(t) \rangle_s - \langle \hat{O}(0) \rangle = \int_0^t d\tau F(\tau) \chi_{\hat{O}}(t-\tau) , \quad (43)
\]

where \(\hat{O} \in \{\hat{q}, \hat{p}\}\), obtained directly from the linear response theory (note here that \(\langle \hat{q}(t) \rangle_s = 0\) and \(\langle \hat{p}(t) \rangle_s = M \langle \hat{q}(t) \rangle_s\)). Due to the fact that \([q - q', \hat{a}_q + \hat{a}_q'] = 0\), equation (41) then becomes

\[
\langle q|\hat{R}_s(t)|q'\rangle = e^{\hat{J}_s(t)} \langle q|\hat{R}(0)|q'\rangle \quad (44)
\]

Let \(y := q + q'\) so that \(\hat{a}_q + \hat{a}_q' = 2\hat{a}_y\). Then we can easily obtain

\[
\langle \hat{a}_q + \hat{a}_q' \rangle^\alpha \langle q|\hat{R}(0)|q'\rangle = 2^\alpha \left(\frac{z}{\sqrt{y}}\right)^\alpha \frac{1}{\sqrt{2\pi y}} \exp\left(-\frac{y^2}{8\sigma^2}\right) \langle q - q' | \hat{R}(0) | q' \rangle , \quad (45)
\]

which can subsequently be expressed in terms of the Hermite polynomial as

\[
\frac{1}{\sqrt{2\pi y}} \left(\frac{z}{\sqrt{y}}\right)^\alpha e^{-\frac{(\hat{J}_s(t))^2}{2\sigma^2}} e^{-z^2} H_\alpha(z) \quad (46)
\]

with \(z = y/\sqrt{2\sigma^2}\). Here we used the identity \(H_\alpha(z) = (-1)^\alpha e^z (d/dz)^\alpha e^{-z^2}\). Then, with the aid of the identity \(e^z e^{-z^2} = \sum_{n=0}^\infty \left[H_\alpha(z)/n!\right] z^n\), equation (44) finally reduces to the exact expression

\[
\langle q|\hat{R}_s(t)|q'\rangle = \frac{1}{\sqrt{2\pi y}} \exp\left(-\frac{(\hat{J}_s(t))^2}{2\sigma^2}\right) \exp\left\{ -\frac{1}{\sqrt{2\sigma^2}} \left(q^2 + q'^2 - \langle \hat{q}(t)_s \rangle^2 \right) - \frac{(\hat{p}(t)_s)^2}{2\sigma^2} \left(q - q' + \frac{\hbar}{\sigma} \langle \hat{p}(t)_s \rangle \right)^2 \right\} . \quad (47)
\]

The normalization \(\text{Tr} \hat{R}_s(t) = 1\) can easily be shown with the aid of (26)

\[
\int_0^\infty dq e^{-\omega q^2 - 2\hbar q} = \sqrt{\pi} e^{\beta\hbar} . \quad (48)
\]

For the vector-potential gauge, along the same line, after making some calculations leading to (44) with \(\hat{J}_v(t)\) in place of \(\hat{J}_s(t)\), we can obtain

\[
\langle q|\hat{R}_v(t)|q'\rangle = e^{\hat{J}_v(t)} \langle q|\hat{R}(0)|q'\rangle \quad (49)
\]
where we identified \( \langle \hat{q}(t) \rangle_s \) and \( \langle \hat{p}(t) \rangle_s \), respectively, as \( \int_0^t d\tau \, p_c(\tau) \chi_{sp}(t-\tau) \) and \( \int_0^t d\tau \, p_c(\tau) \chi_{sp}(t-\tau) \) [note that \( \chi_{sp}(t) = -M\chi_{sp}(t) \) and \( \chi_{sp}(t) = -M\chi_{sp}(t) \)], verified directly from the linear response theory with \((25)\) in place of \((24)\). In fact, with the aid of integration by parts it can easily be shown that

\[
\langle \hat{q}(t) \rangle_s = \langle \hat{q}(t) \rangle_v + p_c(t).
\]  

Consequently we can immediately obtain

\[
\langle q|\hat{R}_s(t)\rangle q' = \langle q|\hat{R}_v(t)\rangle q' = e^{-\frac{1}{2}\tau(q-q')^2} \langle q|\hat{R}_v(t)\rangle q'.
\]  

Obviously, we have \( \text{Tr} \hat{R}_s(t) = 1 \) from \((47)\).

It is instructive now to consider \( \langle \hat{q}^2(t) \rangle \) and \( \langle \hat{p}^2(t) \rangle \) in both scalar-potential and the vector-potential gauges. Using \((47)\) we can easily obtain

\[
\langle \hat{q}^2(t) \rangle_s = \langle \hat{q}^2(t) \rangle_v + \hat{q}^2(t),
\]

\[
\langle \hat{p}^2(t) \rangle_s = \langle \hat{p}^2(t) \rangle_v + \hat{p}^2(t).
\]

Similarly, we can also have

\[
\langle \hat{q}^2(t) \rangle_v = \text{Tr} \left[ \hat{q}^2 \hat{R}_v(t) \right] = \langle \hat{q}^2(t) \rangle_s,
\]

\[
\langle \hat{p}^2(t) \rangle_v = \langle \hat{p}^2(t) \rangle_s + \hat{p}^2(t).
\]

As a result, the instantaneous internal energy in the scalar-potential gauge

\[
\langle \hat{H}_s(t) \rangle_s = \frac{\langle \hat{p}^2(t) \rangle_s}{2M} + \frac{M}{2} \omega_0^2 \langle \hat{q}^2(t) \rangle_s
\]

is not necessarily identical to its vector-potential gauge counterpart, namely,

\[
\langle \hat{H}_s(t) \rangle_s - \langle \hat{H}_s(t) \rangle_v = \frac{1}{2M} \left( \langle \hat{p}(t) \rangle_v^2 - \langle \hat{p}(t) \rangle_s^2 \right) \neq 0.
\]

At first glance, it looks like a paradox. However, we have a rather simple justification for this \((27)\): In the scalar-potential-gauge problem, the experiment is performed in such a way that we turn on an external field at \( t = 0 \) and then turn off at \( t = t_f \). Afterwards we measure the fluctuation \( \langle \hat{p}^2(t_f) \rangle_s \). In the vector-potential-gauge setting, on the other hand, we need to turn off the vector potential \( p_c(t_f) = \int_0^{t_f} F(\tau) \, d\tau \) rather than the external field. Consequently the fluctuation \( \langle \hat{p}^2(t_f) \rangle_v \) differs from its scalar-potential counterpart in such a way that

\[
\langle \hat{p}^2(t_f) \rangle_v = \langle \hat{p}^2(t_f) \rangle_s + \langle \hat{p}(t_f) \rangle_s - p_c(t_f),  
\]

which is actually accordance with the result in \((53b)\) with \((50)\). It is, however, in general physically unrealistic to carry out an experiment in which the vector potential is turned off.

Comments deserve here. First, it is interesting to note a time-independent behavior of the purity measure

\[
\text{Tr} \hat{R}_s^2(t) = \text{Tr} \hat{R}_v^2(t) = \frac{\hbar}{2\sqrt{\langle \hat{q}^2 \rangle_v \langle \hat{p}^2 \rangle_v}},
\]

obtained directly from \((47)\) and \((51)\) with \((48)\), respectively.

Secondly, as was shortly pointed out in Sect. 4, whereas the equilibrium quantities \( \langle \hat{q}^2 \rangle_v \) and \( \langle \hat{p}^2 \rangle_v \) in equations \((20)\) and \((21)\) can exactly be obtained from the scheme of linear response theory, this is not the case for their non-equilibrium counterparts \( \langle \hat{q}^2(t) \rangle \) and \( \langle \hat{p}^2(t) \rangle \); in fact, by using \((27)\) we can arrive at the expression

\[
\langle \hat{q}^2(t) \rangle_s = \langle \hat{q}^2(t) \rangle_v + \int_0^t d\tau \chi^{(1)}(t-\tau) F(\tau) + \int_0^t d\tau F(\tau) \int_0^\tau d\tau' F(\tau') \chi^{(2)}(t-\tau, t-\tau'),
\]
where \( \chi^{(1)}(t) = \chi_{qq}(t) = \langle \mathbf{q_2}^2(t), \mathbf{q_1} \rangle_\beta = 0 \), and the 2nd-order response function \( \chi^{(2)}(t, \tau) = \langle [\mathbf{q_2}, \hat{\mathbf{r}}(t)], \hat{\mathbf{r}}(\tau) \rangle_\beta \) can be obtained from the cyclic invariance of the trace, which subsequently reduces to \( 2 \chi_{qq}(t) \chi_{qq}(\tau) \) with the aid of (18b).

The relation \( \chi \) obtained from the cyclic invariance of the trace, which subsequently reduces to 2\( \chi_{qq}(t) \chi_{qq}(\tau) \) with the aid of (18b).

The relation
\[
\int_0^\Omega d\tau \int_0^\Omega d\tau' = \int_0^\Omega d\tau' \int_0^\Omega d\tau [28]\text{ then allows equation (58) to become}
\[
\langle \mathbf{q_2}^2(t) \rangle_s - \langle \mathbf{q_2}^2 \rangle_s = 2 \int_0^\Omega d\tau' \mathbf{F}(\tau') \chi_{qq}(t - \tau') \int_0^\Omega d\tau \mathbf{F}(\tau) \chi_{qq}(t - \tau),
\]
which is also identical to
\[
2 \int_0^\Omega d\tau' \mathbf{F}(\tau') \chi_{qq}(t - \tau') \int_0^\Omega d\tau \mathbf{F}(\tau) \chi_{qq}(t - \tau) \tag{59}
\]
directly resulting from (58) with exchange of the two variable \( \tau \) and \( \tau' \). From (43), (59) and (60) we can immediately recover the exact result in (52a). Similarly we can do the same job for \( \langle \mathbf{\hat{p}_2}^2(t) \rangle_s \) and then for their vector-potential gauge counterparts, respectively.

Subsequently, we can also obtain, with the aid of (44), the higher-order fluctuations such as
\[
\langle \mathbf{\hat{q}_2}^2(t) \rangle_s = \langle \mathbf{\hat{q}(t)} \rangle_s \left[ 3 \langle \mathbf{\hat{q}_2}^2 \rangle_s + \langle \mathbf{\hat{q}(t)} \rangle_s^2 \right] \tag{61a}
\]
and
\[
\langle \mathbf{\hat{p}_2}^2(t) \rangle_s = \langle \mathbf{\hat{p}(t)} \rangle_s \left[ 3 \langle \mathbf{\hat{p}_2}^2 \rangle_s + \langle \mathbf{\hat{p}(t)} \rangle_s^2 \right] \tag{61b}
\]
and
\[
\langle \mathbf{\hat{q}_2}^4(t) \rangle_s = 3 \langle \mathbf{\hat{q}_2}^2 \rangle_s^2 + 6 \langle \mathbf{\hat{q}_2}^2 \rangle_s \langle \mathbf{\hat{q}(t)} \rangle_s \tag{62a}
\]
and
\[
\langle \mathbf{\hat{p}_2}^4(t) \rangle_s = 3 \langle \mathbf{\hat{p}_2}^2 \rangle_s^2 + 6 \langle \mathbf{\hat{p}_2}^2 \rangle_s \langle \mathbf{\hat{p}(t)} \rangle_s \tag{62b}
\]

etc. Their vector-potential counterparts immediately appear with the replacement of \( \langle \mathbf{\hat{p}(t)} \rangle_s \rightarrow \langle \mathbf{\hat{p}(t)} \rangle_s \).

4. Numerical Analysis within the Drude damping model

We carry out the numerical analysis in the scheme of the well-known Drude model (with a cut-off frequency \( \omega_d \) and a damping parameter \( \gamma_d \)), which is a prototype for physically realistic damping. It is then known that
\[
\langle \mathbf{\hat{q}_2}^2(d) \rangle_s = \frac{1}{M} \sum_{l=1}^{3} \lambda_d^{(l)} \left\{ \frac{1}{\omega_d} + \frac{1}{\omega} \psi \left( \frac{\Omega \omega}{\omega_d^2} \right) \right\} \tag{63a}
\]
and
\[
\langle \mathbf{\hat{p}_2}^2(d) \rangle_s = -\frac{M}{\sqrt{\omega_d}} \sum_{l=1}^{3} \lambda_d^{(l)} \left\{ \frac{1}{\omega_d^2} + \frac{1}{\omega} \psi \left( \frac{\Omega \omega}{\omega_d^2} \right) \right\} \tag{63b}
\]
in terms of the digamma function \( \psi(y) = d \ln \Gamma(y)/dy \) [26], where \( \omega_1 = \Omega, \omega_2 = z_1, \omega_3 = z_2 \), and the coefficients
\[
\lambda_d^{(1)} = \frac{z_1 + z_2}{(\omega - z_1)(\omega - z_2)} \quad \lambda_d^{(2)} = \frac{\Omega^2 + z_2}{(\omega - z_1)(\omega - z_2)} \quad \lambda_d^{(3)} = \frac{\Omega^2 + z_1}{(\omega - z_1)(\omega - z_2)} \tag{64}
\]
Here we have employed, in place of \( (\omega_0, \omega_d, \gamma_d) \), the parameters \( (w_0, \Omega, \gamma) \) through the relations
\[
\omega_0 := w_0 \frac{\Omega}{\Omega + \gamma} ; \quad \omega_d := \Omega + \gamma ; \quad \gamma_0 := \gamma \frac{\Omega + \gamma + w_0^2}{(\Omega + \gamma)^2} \tag{65}
\]
and then \( z_1 = \gamma/2 + iw_1 \) and \( z_2 = \gamma/2 - iw_1 \) with \( w_1 = \sqrt{(w_0)^2 - (\gamma/2)^2} \). For the underdamped case \( (w_0 \geq \gamma/2) \) we have \( z_2 = \bar{z}_1 \) whereas \( z_1, z_2 > 0 \) for the overdamped case \( (w_0 < \gamma/2) \). The susceptibility in the Drude damping model is also well-known as
\[
\chi_{qq}^{(d)}(\omega) = -\frac{1}{M} \omega + i(\Omega + z_1 + z_2) \tag{66}
\]
With the aid of (19) we can easily obtain the response function
\[
\chi_{qq}^{(d)}(t) = -\frac{1}{M} \left( \frac{z_1 - z_2}{\Omega - z_1} e^{-\Omega t} + \frac{z_2 - \Omega z_1}{\Omega - z_1} e^{z_1 t} + \left( \Omega^2 - z_1^2 \right) e^{-z_1 t} \right). \tag{67}
\]
This is real-valued and holds true for both underdamped and overdamped cases.

We first apply a static external field $F_1(t) = A_1 \Theta(t)$ (d.c. field) and then an oscillatory field $F_2(t) = A_2 \sin \omega t$ (a.c. field). By substituting equation (67) to (41) we can easily obtain both $\langle \hat{q}(t) \rangle^{(d)}$ and $\langle \hat{p}(t) \rangle^{(d)}$ within the Drude damping model in closed form for the two different forms of external force, respectively. Similarly we can also have their vector-potential counterparts in closed form. Figures 1-4 demonstrate temporal behaviors of $\langle \hat{q}(t) \rangle^{(d)}$ with $n = 1, 2$ for different damping and control parameters. Further, it is instructive to study a temporal behavior of a distance between the initial equilibrium state $\hat{R}(0)$ and the non-equilibrium state $\hat{R}(t)$. To do so, we adopt a well-defined measure $D^2(t) = \text{Tr} \left( (\hat{R}(t) - \hat{R}(0))^2 \right)$, introduced in (29), which is, independent of the dimension of the Liouville space, between 0 and 2. With the aid of (68) we can then have

$$D^2(t) = \frac{h}{\sqrt{\langle \hat{q}^2 \rangle (\langle \hat{p}^2 \rangle)}} \left( 1 - \exp \left\{ -\frac{1}{2} \left( \frac{\langle \hat{q}(0)^2 \rangle}{\langle \hat{q}^2 \rangle} + \frac{\langle \hat{p}(0)^2 \rangle}{\langle \hat{p}^2 \rangle} \right) \right\} \right)$$

and $D^2(t) = D^2(t)|_{\langle \hat{p}(0) \rangle \rightarrow \langle \hat{p}(0) \rangle}$. In figure 5 this measure within the Drude damping model is demonstrated for different external fields and temperatures.

5. Concluding remarks

In summary, we have discussed the field-induced dynamics in the scheme of quantum Brownian oscillator at an arbitrary temperature. We have then derived the reduced density operator in closed form of the coupled oscillator in a non-equilibrium state at an arbitrary time. In doing so, we have applied both scalar-potential and vector-potential gauges for the interaction Hamiltonian. We believe that this exact expression for the reduced density operator will provide a useful starting point, e.g., for later useful discussions of quantum thermodynamics and quantum information theory within quantum Brownian oscillator.

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Figure 1. $y = \langle \hat{q}(t) \rangle^{(d)}_F$ versus time $t$ for a static field $F_1(t) = A_1 \Theta(t)$. The response $\langle \hat{q}(t) \rangle^{(d)}_F$ is temperature-independent, refer to equations (43) and (67). Here $w_0 = \Omega = M = 1$. (1) dash ($\gamma = 5$, overdamped): From bottom to top, (black, $A_1 = 1$), (violet, $A_1 = 1.5$), and (red, $A_1 = 2$); (2) solid ($\gamma = 0.1$, underdamped): From bottom to top, (blue, $A_1 = 1$), (maroon, $A_1 = 1.5$), and (green, $A_1 = 2$).

Figure 2. $y = \langle \hat{q}(t) \rangle^{(d)}_F$ versus time $t$ for an oscillatory field $F_2(t) = A_2 \sin \omega_0 t$. The response $\langle \hat{q}(t) \rangle^{(d)}_F$ is temperature-independent. Here $w_0 = \Omega = M = A_2 = 1$; (1) violet dot: $\gamma = 0.1$ (underdamped) and $\omega_f = 1 \approx \omega_0$, resonant [cf. (65)]; (2) blue dash: $\gamma = 0.1$ (underdamped) and $\omega_f = 1.5$; (3) black dash: $\gamma = 5$ (overdamped) and $\omega_f = 1$; (4) red solid: $\gamma = 5$ (overdamped) and $\omega_f = 1.5$.

Figure 3. $y = \langle \hat{q}^2(t) \rangle^{(d)}_F$ versus time $t$ for $F_1(t) = A_1 \Theta(t)$. For $\langle \hat{q}^2(t) \rangle^{(d)}_F$ refer to equations (52a) and (63a). Here $h = k_B = w_0 = \Omega = M = 1$. (1) black dot ($\gamma = 5$, overdamped, and $\omega_f = 1$): From bottom to top, dimensionless temperature $k_B T/\hbar w_0 = 0.01, 2, 5$; (2) blue dash ($\gamma = 0.1$, underdamped, and $A_1 = 1$): From bottom to top, $k_B T/\hbar w_0 = 0.01, 2, 5$; (3) red solid ($\gamma = 0.1$, underdamped, and $A_1 = 2$): From bottom to top, $k_B T/\hbar w_0 = 0.01, 2, 5$..

Figure 4. $y = \langle \hat{q}^2(t) \rangle^{(d)}_F$ versus time $t$ for $F_2(t) = A_2 \sin \omega_0 t$. Here $h = k_B = w_0 = \Omega = M = A_2 = 1$. (1) black dot ($\gamma = 5$, overdamped, and $\omega_f = 1$): From bottom to top, $k_B T/\hbar w_0 = 0.01, 2, 5$; (2) blue dot ($\gamma = 0.1$, underdamped, and $\omega_f = 1$, resonant): From bottom to top, $k_B T/\hbar w_0 = 0.01, 2, 5$; (3) red dash ($\gamma = 0.1$, underdamped, and $\omega_f = 1.5$): From bottom to top, $k_B T/\hbar w_0 = 0.01, 2, 5$.

Figure 5. $y = D^2_F(t)$ versus time $t$ within the Drude damping model. For $D^2_F(t)$ refer to (65). Here $h = k_B = w_0 = \Omega = M = A_1 = A_2 = 1$, and $\gamma = 0.1$, underdamped. (1) dash (for d.c. field): From top to bottom, dimensionless temperature $k_B T/\hbar w_0 = 0.01, 2, 5$; (2) solid (for a.c. field): the same as for dash, with $\omega_f = 1 \approx \omega_0$, resonant.
Figure 1:
Figure 2:
Figure 3:
Figure 5: