General non-Markovian dynamics of open quantum systems

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We present a general theory of non-Markovian dynamics for open quantum systems. We explore the non-Markovian dynamics by connecting the exact master equations with the non-equilibrium Green functions. Environmental back-actions are fully taken into account. The non-Markovian dynamics consists of non-exponential decays and dissipationless oscillations. Non-exponential decays are induced by the discontinuity in the imaginary part of the self-energy corrections. Dissipationless oscillations arise from band gaps or the finite band structure of spectral densities. The exact analytic solutions for various non-Markovian environments show that the non-Markovian dynamics can be largely understood from the environmental-modified spectra of the open systems.

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Understanding the dynamics of open quantum systems is one of the most challenging topics in physics, chemistry, and biology. The environment-induced quantum dissipation and decoherence dynamics are the main concerns in the study of open quantum systems. [12]. Decoherence control has also recently become a key task for practical implementations of nanoscale solid-state quantum information processing, where the decoherence is mainly dominated by non-Markovian dynamics due to the strong back-actions from the environment. A fundamental issue is how to accurately take into account non-Markovian memory effects, which have attracted considerable attention very recently both in theory [4 12] and in experiments [13 12].

The non-Markovian dynamics of an open quantum system can be described by the master equation of the reduced density matrix $\rho(t)$. This is obtained by tracing over the environmental degrees of freedom, $\rho(t) = \text{tr}[\rho_{\text{tot}}(t)]$, where $\rho_{\text{tot}}(t)$ is the density matrix of the total system. The standard approach to the non-Markovian dynamics uses the Nakajima-Zwanzig operator projective technique [10] where the master equation is formally written as

$$\frac{d\rho(t)}{dt} = \int_{t_0}^{t} d\tau K(t-\tau)\rho(\tau).$$

(1)

The non-Markovian memory effects are taken into account by the time non-local integral kernel $K(t-\tau)$. In practice, very few systems can be exactly solved from (1). Therefore, the generality of non-Markovian dynamics has not been fully understood.

In general, there are three typical timescales in an open system to characterize non-Markovian dynamics: (i) the timescale of the system $\sim 1/\varepsilon_s$, where $\varepsilon_s$ is a typical energy scale of that system; (ii) the timescale of the environment $\sim 1/d$, where $d$ is the bandwidth of the environmental spectral density; (iii) the mutual timescale arising from the coupling between the system and the environment $\sim 1/\Gamma$, where $\Gamma$ is the dominant coupling strength. It is usually believed that non-Markovian memory effects strongly rely on the relations among these different timescales. However, such relationships have not been quantitatively established yet.

Here, we show that the general behavior of non-Markovian dynamics is mainly determined by the band structure of the environment and the coupling between the system and the environment. We explore the non-Markovian dynamics from the analytical solution, solved by connecting the exact master equation with the non-equilibrium Green functions. Exact master equations have been derived only for limited system-environment couplings [6 17 18]. Establishing the connection between the master equation and the non-equilibrium Green functions provides a new way to explore the non-Markovian dynamics even if the exact master equation of the open system is unknown.

Exact master equation and non-equilibrium Green functions.—We begin with a fermionic (bosonic) many-body system consisting of $N$ single-particle energy levels $\varepsilon_i$ ($i = 1, 2, \cdots, N$), coupled, via particle-particle exchanges, to a fermionic (bosonic) environment, $H_{SB} = \sum_{aki}[V_{aki}b_\alpha^{\dagger}b_\beta + V_{aki}^{\ast}b_\alpha b_\beta^{\dagger}]$. The environment can contain many different reservoirs, each reservoir is specified by its spectral density $J_{\alpha ij}(\omega) = 2\pi \sum_k V_{aki}V_{akj}^{\ast}\delta(\omega - \varepsilon_k)$, where $V_{aki}$ is a coupling strength between the system and reservoir $\alpha$. The operators $a_\alpha^{\dagger}$ ($a_\alpha$) and $b_\alpha^{\dagger}$ ($b_\alpha$) are the particle creation (annihilation) operators of the discrete energy level $i$ of the system and the continuous level $k$ of reservoir $\alpha$, respectively. These creation-annihilation operators obey the standard anticommutation (commutation) relationship for fermions (bosons). Nonlinear particle-particle interactions in the system are not included. Using the coherent-state path-integral method [20] to the Feynman-Vernon influence functional [21], the exact master equation of such an open system can be de-
The inhomogenous non-local time integral in (4b) with the integral kernel \(g(\tau', \tau')\), depicts the fluctuation arisen from the environment. Because \(v(t_0, t) = 0\), we can analytically solve Eq. (4b):

\[
v(\tau, t) = \int_{t_0}^{\tau} d\tau_1 \int_{t_0}^{t} d\tau_2 u(\tau, \tau_1) g(\tau_1, \tau_2) u^\dagger(\tau_2, t).
\]  

This solution shows that Eq. (4b) is a generalized non-equilibrium fluctuation-dissipation theorem in the time domain (the reduction to the equilibrium fluctuation-dissipation theorem is given in [23]). The fluctuation-dissipation theorem is a consequence of the unitarity of the whole system. It guarantees the positivity of the reduced density matrix during the non-Markovian time evolution.

Based on the above intrinsic features of open quantum systems, we can now explore the general properties of non-Markovian dynamics. From Eqs. (3), we can express the Green function \(u(t, t_0)\) in terms of the dissipation coefficient \(\gamma(t)\) as

\[
u(t, t_0) = \mathcal{T} \exp \left\{ -\int_{t_0}^{t} d\tau [i\varepsilon(\tau) + \gamma(\tau)] \right\},
\]

where \(\mathcal{T}\) is the time-ordering operator. This solution indicates that \(u(t, t_0)\) fully determines the dissipation dynamics of the system. However, due to the time-dependence of the dissipation coefficients, the detailed dissipation dynamics can vary significantly for different environments.

Explicitly, equation (5) show that \(\mathbf{g}(\tau, \tau') = \mathbf{g}(\tau' - \tau')\) and \(\mathbf{g}(\tau, \tau') = \mathbf{g}(\tau' - \tau')\). Thus we can write \(u(t, t_0) = u(t - t_0)\). Using the modified Laplace transform \(U(z) = \int_{t_0}^{\infty} dt u(t)e^{z(t-t_0)}\), it is easy to obtain

\[
U(z) = \frac{i}{z \mathbf{I} - \varepsilon_s - \mathbf{\Sigma}(z)},
\]

where \(\mathbf{I}\) is the identity, \(\mathbf{\Sigma}(z)\) is the Laplace transform of the known exact master equation and the non-equilibrium Green functions for open quantum systems.

General non-Markovian dynamics.— Different from the Nakajima-Zwanzig master equation, the exact master equation (2) is local in time, characterized by the dissipation and the fluctuation coefficients, \(\gamma(t)\) and \(\tilde{\gamma}(t)\). Non-Markovian memory effects are manifested as follows:

(i) The coefficients \(\gamma(t)\) and \(\tilde{\gamma}(t)\) are microscopically and non-perturbatively determined by the non-equilibrium Green functions from the Dyson equations (4). The non-Markovian memory effect is fully coded into the homogenous non-local time integrals in (4) with the integral kernel \(g(\tau, \tau')\). In other words, the self-energy correction \(\mathbf{g}(\tau, \tau')\) serves as a memory kernel that count all the back-actions from the environment.

(ii) The coefficients \(\gamma(t)\) and \(\tilde{\gamma}(t)\) are constrained by the non-equilibrium fluctuation-dissipation theorem. The inhomogenous non-local time integral in (4b) with the integral kernel \(g(\tau, \tau')\), depicts the fluctuation arisen from the environment. Because \(v(t_0, t) = 0\), we can analytically solve Eq. (4b):

\[
v(\tau, t) = \int_{t_0}^{\tau} d\tau_1 \int_{t_0}^{t} d\tau_2 u(\tau, \tau_1) g(\tau_1, \tau_2) u^\dagger(\tau_2, t).
\]
The first term in (10) corresponds to localized modes \( U \) function
\[
\Sigma(z) = \sum_{\alpha} \int \frac{d\omega}{2\pi} \frac{J_\alpha(\omega)}{z - \omega} \Delta(\omega) + \frac{i}{2} \sum_{\alpha} J_\alpha(\omega),
\]
and \( \Delta(\omega) = \sum_{\alpha} \mathcal{P} \int \frac{d\omega'}{2\pi} \frac{1}{\omega - \omega'} \) is the principal value of the integral. It can be shown that the general solution of \( u(t, t_0) \) is given by
\[
u(t, t_0) = \sum_i \mathcal{Z}_i e^{-i\omega_i(t-t_0)} + \sum_k \int_{B_k} \frac{d\omega}{2\pi} \left[ U(\omega + i0^+) - U(\omega - i0^+) \right] e^{-i\omega(t-t_0)}. \tag{10}
\]

Thus, the whole picture of non-Markovian dynamics is fully characterized by the dissipation and fluctuation coefficients of (10). The non-exponential decay part of (10) makes the dissipation coefficient \( \gamma(t) \) oscillates between positive and negative values, representing the back-flow of information from the system to the environment. Non-exponential decays alone give \( \gamma(t) \) a non-zero asymptotic value. If there are localized modes, \( \gamma(t) \) will vanish in the steady-state limit, resulting in dissipationless oscillations. In the weak coupling region, \( \gamma(t) \) can still be time-dependent but keeps positive, the corresponding dynamics gives simple exponential-like decays, observed mainly in the Markovian limit. Furthermore, Eqs. (9) and (10) together show that except for the initial environmental temperature dependence, the time-dependence of the fluctuation coefficient \( \gamma(t) \) behaves similar to \( \gamma(t) \), due to the fluctuation-dissipation theorem. In conclusion, non-Markovian dynamics can be fully understood from the solution of the Green function \( u(t, t_0) \).

**Examples and discussion** — To be more specific, let us first examine the non-Markovian dynamics of a single-mode bosonic nanosystem, such as a nanophotonic or optomechanical resonator, coupled to a general non-Markovian environment with spectral density
\[
J(\omega) = 2\pi \eta \omega \left( \frac{\omega}{\omega_c} \right)^{s-1} \exp\left( -\frac{\omega}{\omega_c} \right), \tag{11}
\]
where \( \eta \) is the coupling constant between the system and the environment, and \( \omega_c \) is the frequency cutoff. When \( s = 1, < 1 \) and \( > 1 \), the corresponding environments are Ohmic, sub-Ohmic and super-Ohmic, respectively. Following the above general procedure, the analytical solution of the non-Markovian dissipation dynamics is given by (setting \( t_0 = 0 \) for simplicity):
\[
u(t) = Z e^{-\omega t} + \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)e^{-i\omega t}}{4[\omega - \varepsilon_s - \Delta(\omega)]^2 + J^2(\omega)}, \tag{12}
\]
where \( \Delta(\omega) = \frac{1}{2}[\Sigma(\omega + i0^+) + \Sigma(\omega - i0^+)] \) and the Laplace transform of the self-energy correction
\[
\Sigma(\omega) = \begin{cases}
\eta\omega_c \left[ \pi \sqrt{-\omega} e^{-\bar{\omega}} \text{erfc}(\sqrt{-\bar{\omega}}) - \sqrt{\pi} \right] & \text{s} = 1/2 \\
\eta\omega_c \left[ \bar{\omega} \exp(-\bar{\omega}) \text{Ei}(\bar{\omega}) - 1 \right] & \text{s} = 1 \\
\eta\omega_c \left[ \bar{\omega}^3 e^{-\bar{\omega}} \text{Ei}(\bar{\omega}) - \bar{\omega}^2 - \bar{\omega} - 2 \right] & \text{s} = 3
\end{cases} \tag{13}
\]
with \( \bar{\omega} = \omega/\omega_c \). Due to the vanishing spectral density for \( \omega < 0 \), a localized mode at \( \omega' = \varepsilon_s - \Sigma(\omega') < 0 \) occurs when \( \eta\omega_c \Gamma(s) > \varepsilon_s \), here \( \Gamma(s) \) is a gamma function. The localized mode leads to the dissipationless process. The corresponding residue is \( Z = [1 - \Sigma'(\omega')]^{-1} \). This analytical solution precisely reproduces the exact numerical solution in the previous work. Figure 2 shows that
for a small $\eta$, the dissipation dynamics is an exponential-like decay. The corresponding $\gamma(t)$ and $\bar{\gamma}(t)$ are time-dependent but positive (corresponding to Markovian dynamics). When $\eta \geq 0.3$, the non-exponential decay dominates, and $\gamma(t)$ and $\bar{\gamma}(t)$ oscillate in positive and negative values with nonzero asymptotical values. When $\eta \geq 0.6$, the localized state occurs, and $u(t)$ does not decay to zero. Correspondingly, $\gamma(t)$ and $\bar{\gamma}(t)$ asymptotically approach to zero.

The second example is a fermionic system, a single electron transistor in nanostructures which consists of a quantum dot coupled to a source and a drain. The source and drain are treated as two reservoirs of the electron transistor in nanostructures which consists of a quantum dot coupled to a source and a drain. The solutions of these examples can further be written with a sharp cutoff to simulate a finite band for the environment. Their spectral densities take a Lorentzian form with a sharp cutoff, and $\gamma(t)$ and $\bar{\gamma}(t)$ oscillate in positive and negative values with nonzero asymptotical values.

The two localized states are located outside of the band, i.e., $\omega_f^j = \varepsilon_s + \Sigma(\omega_f^j)$, with $\omega_f^j < \omega_c - \Omega$, and $\omega_f^j > \omega_c + \Omega$. The corresponding residue is given by $Z_j = [1 - \Sigma'(\omega_f^j)]^{-1}$. Again, the localized modes lead to a dissipationless process and the integral term shows a non-exponential decay. Taking $\Omega \to \infty$, the two localized modes are excluded, and the solution of $u(t)$ reproduces the exact non-Markovian dynamics of the usual Lorentzian spectral density (for detailed derivation, see [25]).

The third example is a two-level system involving single-photon processes (spontaneous emission). In general, a multi-level atomic open system does not obey the master equation [2]. However, the Schrödinger equation of a two-level atomic system with only spontaneous single-photon emission processes (at zero temperature) can be reduced to the Dyson equation of [10]. Explicitly, the spectral density of the photonic crystals takes $J(\omega) = \frac{2\varepsilon_s}{\sqrt{\omega - \omega_c}}\Theta(\omega - \omega_c)$.

From Eq. (10), we directly obtain the analytical solution of the spontaneous emission dynamics

$u(t) = \frac{2\omega_r}{3\omega_r + \Delta} e^{i(\omega_r - \omega_c)t} + \frac{C}{\pi} \int_{\omega_r}^{\infty} d\omega \frac{\sqrt{\omega - \omega_r} e^{-i\omega t}}{(\omega - \varepsilon_s)^2(\omega - \omega_c) + C^2}$

where $\omega_r$ is the real root given by $(\omega_r + \Delta)\sqrt{\omega_r} = C$, and $\Delta = \varepsilon_s - \omega_c$ is the detuning. This analytical solution recovers both the exact analytical and numerical solutions given in [34].

The above examples show that very different open systems coupled to very different environments obey the same solution, Eq. (10), of the non-Markovian dynamics. The solutions of these examples can further be written in general as $u(t - t_0) = \int_{-\infty}^{\infty} d\omega D(\omega) \exp\{-i\omega(t - t_0)\}$ with

$D(\omega) = 2\pi\sum_j Z_j \delta(\omega - \omega_j^s) + \frac{J(\omega)}{|\omega - \varepsilon_s - \Delta(\omega)|^2 + J^2(\omega)/4}$

Equation (13) shows that the environment modifies the system spectrum as a combination of localized modes (dissipationless process) plus a continuum spectrum part.
(non-exponential decays). Remarkably, the result obtained from these simple examples gives indeed the general structure of two-point correlation functions in arbitrary complicated systems, see Ref. [3]. This indicates that alternatively, non-Markovian dynamics can be fully characterized by the environmental-modified spectrum of the system. If the spectrum of the open system can be measured, the non-Markovian dynamics can be extracted from its Fourier transform. This largely simplifies the exploration of the general properties of non-Markovian dynamics for many-body systems, we derive a general analytical solution of non-Markovian dynamics for open quantum systems, i.e., Eq. (10) or (18). From the analytical solution, we show that the general non-Markovian dynamics consists of non-exponential decays and dissipationless oscillations.

**Conclusion.**—By connecting the exact master equation with the non-equilibrium Green functions in many-body systems, we derive a general analytical solution of non-Markovian dynamics for open quantum systems, i.e., Eq. (10) or (18). From the analytical solution, we show that the general non-Markovian dynamics consists of non-exponential decays and dissipationless oscillations.

The dissipationless processes arise from band gaps or finite band structures of the environmental spectral densities. The non-exponential decays are induced by the discontinuity in the imaginary part of the self-energy corrections from the environment. The exponential decays observed in Markovian limit is a special case in the weak coupling limit. Since the non-equilibrium Green functions are well-defined for arbitrary quantum systems, this theory may also provide a new approach to explore non-Markovian dynamics for more complicated open systems whose exact master equation may be unknown.

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[23] Explicitly, \( \mathbf{v}_{ij}(\tau, t) = \langle a_i^\dagger(t) a_j(\tau) \rangle - \langle a_i^\dagger(t) a_j(\tau) \rangle \langle a_i^\dagger(t) a_j(\tau) \rangle \), where \( \langle \cdot \rangle \) denotes the initial state expectation value. In the standard non-equilibrium Green function formalism, \( G_{ij}(\tau, t) \equiv \langle \psi^\dagger(t) | a_i(t) a_j(\tau) \rangle \) is the so-called lesser Green function. On the other hand, \( u_{ij}(t, \tau) = \langle [a_i(t), a_j^\dagger(\tau)] \rangle \) is often called the spectral Green function, see [23].
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