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Non-Markovian Fermionic Stochastic Schrödinger Equation for Open System Dynamics

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This paper presents an exact Grassmann stochastic Schrödinger equation for the dynamics of an open fermionic quantum system coupled to a reservoir consisting of a finite or infinite number of fermions. We use this stochastic Schrödinger equation as a generic open system tool to derive the exact master equation for an electronic system strongly coupled to fermionic reservoirs. The generality and applicability of this Grassmann stochastic approach are justified and exemplified by several quantum fermionic system problems concerning quantum coherence coupled to vacuum or finite-temperature fermionic reservoirs. Our studies show that the quantum coherence property of a quantum dot system can be profoundly modified by the environmental memory.

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I. INTRODUCTION

Quantum dynamics of quantum systems coupled to fermionic or bosonic environments has recently attracted wide-spread interest in quantum open systems, quantum dissipative systems, quantum transport, quantum computing, and nanoscience [1–4]. For example, the size reduction of quantum devices in microelectronics requires controllable systems consisting of only a few electrons, where quantum coherence and quantum interference become dominant. In addition, quantum dots coupled to electrons of a metal is an interesting setup in quantum information processing where the quantum coherence of qubits is of essential importance [5]. The non-Markovian open systems arise in many important situations such as the strongly coupled system-environment, structured environment, time-delayed external control etc. [6]. Intuitively speaking, while the Markov evolution is an irreversible process, in the case of non-Markovian dynamics, the system energy (or phase information) dissipated into the environment may come back to the system in a finite time [7]. For open systems immersed in a bosonic environment, apart from the master equation and path integral approaches [8–10], a versatile stochastic formalism for quantum open system dynamics was developed to provide a powerful tool in studying quantum systems in a non-Markovian regime [11–17]. Such a stochastic pure state approach has several advantages in numerical simulations, perturbation and the derivation of the corresponding master equations. For a Markov environment (bosons or fermions), both the quantum state diffusion equations [18, 19] and Lindblad master equations [20] can be used to describe quantum dynamics of the system of interest. Several important theoretical tools in dealing with nonequilibrium fermionic systems have been developed including nonequilibrium Green's function (NEGF) theory, fermionic path integral etc [1, 21–26]. However, for a generic non-Markovian fermionic environment where the system-environment coupling is not weak or the environment cannot be treated as a broadband reservoir [4, 21–29], establishing a stochastic theory analogous to the non-Markovian quantum state diffusion equation [13] is a long standing problem.

The purpose of this paper is to develop a general non-Markovian stochastic theory of electronic systems coupled to a fermionic environment. The theory developed here is versatile enough to deal with a wide spectrum of open system problems ranging from a "small" environment (one fermion or a few fermions) to a large environment consisting of an infinite number of fermions irrespective of the details of spectral distribution of the fermionic environment. As an illustration of the power of the stochastic approach developed here, we derive several exact master equations governing the reduced density operators of the electronic systems coupled to vacuum and finite-temperature reservoirs.

The paper is organized as follows. In Sec. II, we establish the fermionic stochastic Schrödinger equation (SSE) for a class of open system models consisting of an electronic system coupled to a fermionic reservoir. In particular, we show how to derive the time-local SSE. We introduce a new type of Novikov theorem emerged from the Grassmann noise. We demonstrate the derivation of the corresponding exact master equation from the SSE. In Sec. III, a many-fermion model is considered. We show explicitly that the exact fermionic SSE and the corresponding master equation can be established. In Sec. IV, we establish the finite temperature fermionic SSE through a Bogoliubov transformation, and we provide an explicit construction of the exact time-local master equation as well as the so-called $\hat{Q}$ operator for this model. Then, in Sec. V, the finite temperature model is generalized into a more realistic case consisting of double quantum dots coupled to two fermionic reservoirs (source

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and drain). Both the time-local fermionic SSE and the exact master equation are derived. The numerical simulations of the double quantum dots based on the exact master equation are provided. Finally, we conclude the paper in Sec.VI. Some details about the Grassmann noise, the fermionic SSE, the $\hat{Q}$ operator, a proof of the Novikov theorems and the Heisenberg operator approach are left to Appendix.

II. FERMIONIC STOCHASTIC SCHRÖDINGER EQUATION AND NON-MARKOVIAN MASTER EQUATION

A. Model

To begin with, we consider a simplified model involving an electronic system in contact with a single fermionic reservoir, where the system anti-commutes with the bath [30]. The generalization to a more physically interesting model with two reservoirs (*e.g.*, source and drain) can be established in a similar way. With necessary modifications, the formalism is versatile enough to deal with stochastic gate potentials and nonlinear couplings. The total Hamiltonian for the system plus environment may be written as [1],

$$\hat{H}_{\rm tot} = \hat{H}_{\rm S} + \hat{H}_{\rm R} + \hat{H}_{\rm I}, \tag{1}$$

where $\hat{H}_{\rm S}$ is the Hamiltonian of the electronic system in the absence of the environment, $\hat{H}_{\rm R}$ is the Hamiltonian for a fermionic reservoir; $\hat{H}_{\rm R} = \sum_{\mathbf{k}\alpha} \hbar\omega_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}\alpha}\hat{b}_{\mathbf{k}\alpha}$ where $\hat{b}^\dagger_{\mathbf{k}\alpha}, \hat{b}_{\mathbf{k}\alpha}$ are the fermionic creation and annihilation operators $\{\hat{b}_{\mathbf{k}\alpha}, \hat{b}^\dagger_{\mathbf{k}'\alpha'}\} = \delta_{\mathbf{k}\alpha,\mathbf{k}'\alpha'}$, and the interaction Hamiltonian $\hat{H}_{\rm I}$ is given by

$$\hat{H}_{\rm I} = \hbar \sum_{\mathbf{k}\alpha} (t_{\mathbf{k}\alpha} \hat{L}^\dagger \hat{b}_{\mathbf{k}\alpha} + t_{\mathbf{k}\alpha} \hat{b}^\dagger_{\mathbf{k}\alpha} \hat{L}), \tag{2}$$

where $\hat{L}$ is the system coupling operator and $t_{\mathbf{k}\alpha}$ are the coupling constants. Note that $\hat{H}_{\rm S}$ is an arbitrary Hamiltonian operator that may contain interaction terms for the system particles (*e.g.*, Coulomb interactions between two electrons). The coupling operator $\hat{L}$ may, in general, be represented by a set of fermionic operators which are coupled to all the participating external agents such as the source and drain reservoirs.

The purpose of this paper is to develop a systematic stochastic theory for the models described by Eq. (1) and (2), those are relevant to quantum open systems, non-equilibrium statistical mechanics, path-integral theory and quantum devices based on quantum dots and mesoscopic electronics [6, 8–10, 29]. In the framework of the stochastic Schrödinger equation (SSE) for a bosonic bath, the state of the open quantum system is described by a stochastic pure state, which is generated by a complex Gaussian stochastic process. For the fermionic environment considered in this paper, similar to the fermionic path integral, the fermionic stochastic theory will involve a Grassmann Gaussian stochastic process. Remarkably, we show that the reduced density matrix of the system of interest can be reconstructed from the pure states by taking the statistical mean over the Grassmann noise [30]. As such, in principle, the exact master equation governing the reduced density operator for the open system can be recovered from the SSE, as illustrated by several physically interesting models below.

B. Fermionic stochastic Schrödinger equation

In this subsection, we will establish the fermionic stochastic Schrödinger equation (SSE) for an open electronic system coupled to a fermionic reservoir. Consider the model described by the total Hamiltonian in Eq. (1), in the interaction picture with respect to the fermionic reservoir, it becomes (setting $\hbar = 1$),

$$\hat{H}^I_{\rm tot}(t) = \hat{H}_{\rm S} + (\sum_j t_j \hat{L}^\dagger \hat{b}_j e^{-{\rm i}\omega_j t} + {\rm h.c.}), \tag{3}$$

here the subscript $\mathbf{k}\alpha$ is suppressed as j. In order to trace out the environmental variables, we introduce the fermionic coherent states $|\boldsymbol{\xi}\rangle$ which is defined as

$$|\boldsymbol{\xi}\rangle \equiv \prod_k (1 - \xi_k \hat{b}^\dagger_k)|{\rm vac}\rangle_{\rm R}. \tag{4}$$

And this state satisfies $\hat{b}_j|\boldsymbol{\xi}\rangle = \xi_j|\boldsymbol{\xi}\rangle$. Here, ξ_j is a Grassmann variable, satisfying $\{\xi_i, \xi_j\} = \{\xi^*_i, \xi_j\} = 0$, and $\{\xi_i, \hat{b}_j\} = \{\xi_i, \hat{b}^\dagger_j\} = 0$ [31, 32]. As shown below, the derivations and results for fermionic SSE are more complex than the bosonic case. Using the fermionic coherent state, we define

$$|\psi_t(\boldsymbol{\xi}^*)\rangle \equiv \langle \boldsymbol{\xi}| {\rm e}^{{\rm i}\hat{H}_{\rm R}t} {\rm e}^{-{\rm i}\hat{H}_{\rm tot}t} |\psi_{\rm tot}(0)\rangle, \tag{5}$$

where $|\psi_{\rm tot}(0)\rangle$ is the total initial state of both system and bath, and we assume the bath is initially prepared in vacuum state, *i.e.* $|\psi_{\rm tot}(0)\rangle = |\psi_{\rm S}(0)\rangle \wedge |{\rm vac}\rangle_{\rm R}$ ("$\wedge$" stands for an antisymmetrized wave function). The thermal state case will be discussed later. Taking the time derivative on the both sides of Eq. (5), one obtains

$$\begin{aligned}
&\partial_t|\psi_t(\boldsymbol{\xi}^*)\rangle \\
=& -{\rm i}\langle \boldsymbol{\xi}|\hat{H}^I_{\rm tot}(t)|\psi^I_{\rm tot}(t)\rangle \\
=& -{\rm i}[\hat{H}_{\rm S} + \sum_k (t_k \hat{L}^\dagger \overrightarrow{\partial}_{\xi^*_k} {\rm e}^{-{\rm i}\omega_k t} + t_k \xi^*_k \hat{L} {\rm e}^{{\rm i}\omega_k t})]|\psi_t(\boldsymbol{\xi}^*)\rangle \\
=&(-{\rm i}\hat{H}_{\rm S} - \hat{L}^\dagger \int_0^t {\rm d}s \sum_k \frac{\partial \xi_t}{\partial \xi_k} \frac{\partial \xi^*_s}{\partial \xi^*_k} \overrightarrow{\delta}_{\xi^*_s} - \hat{L}\xi^*_t)|\psi_t(\boldsymbol{\xi}^*)\rangle \\
=&[-{\rm i}\hat{H}_{\rm S} - \hat{L}\xi^*_t - \hat{L}^\dagger \int_0^t {\rm d}s\, K(t,s) \overrightarrow{\delta}_{\xi^*_s}]|\psi_t(\boldsymbol{\xi}^*)\rangle,
\end{aligned} \tag{6}$$

where $\xi^*_t \equiv -{\rm i}\sum_k t_k {\rm e}^{{\rm i}\omega_k t}\xi^*_k$ is the Grassmann Gaussian noise, $\overrightarrow{\delta}_{\xi^*_s}$ is the left functional derivative with respect to ξ_s^*, and the explicit form of function $K(t,s)$ is

$$K(t,s) \equiv \sum_k \frac{\partial \xi_t}{\partial \xi_k}\frac{\partial \xi_s^*}{\partial \xi_k^*} = \sum_k |t_k|^2 \mathrm{e}^{-\mathrm{i}\omega_k(t-s)}. \qquad (7)$$

The Grassmann Gaussian process is defined by

$$\mathcal{M}[\xi_k] \equiv \int \prod_k \mathrm{d}\xi_k^* \cdot \mathrm{d}\xi_k \, \mathrm{e}^{-\xi_k^* \cdot \xi_k} \, \xi_k = 0,$$
$$\mathcal{M}[\xi_k \xi_k^*] \equiv \int \prod_k \mathrm{d}\xi_k^* \cdot \mathrm{d}\xi_k \, \mathrm{e}^{-\xi_k^* \cdot \xi_k} \, \xi_k \xi_k^* = 1, \qquad (8)$$

where "$\mathcal{M}$" stands for the statistical mean over the random Grassmann variables "ξ_k". It is easy to check that the mean and the correlation function are given by: $\mathcal{M}[\xi_t] = \mathcal{M}[\xi_t^*] = 0$ and $\mathcal{M}[\xi_t \xi_s^*] = K(t,s)$, respectively. Note that our fermionic SSE (6) is applicable to an arbitrary correlation function including both Markov and non-Markovian environments. Unlike the complex Gaussian noise used in bosonic case, the Grassmann Gaussian noise is a non-commutative noise at different times reflecting a fundamentally distinctive feature arising from the fermionic environment. Our fermionic stochastic Schrödinger equation is expected to have a close connection with the fermionic path integral as shown in the case of bosonic case [33, 34].

The fermionic SSE (6) can be written in a more compact form,

$$\partial_t |\psi_t(\boldsymbol{\xi}^*)\rangle = -\mathrm{i}\hat{H}_{\mathrm{eff}} |\psi_t(\boldsymbol{\xi}^*)\rangle, \qquad (9)$$

where the effective Hamiltonian is given by,

$$\hat{H}_{\mathrm{eff}} = \hat{H}_{\mathrm{S}} - \mathrm{i}\hat{L}\xi_t^* - \mathrm{i}\hat{L}^\dagger \int_0^t \mathrm{d}s \, K(t,s) \overrightarrow{\delta}_{\xi_s^*}, \qquad (10)$$

Eq. (6) or (9) may serve as a fundamental equation for open fermionic systems coupled to a fermionic environment. Our stochastic method will provide a new insight into the individual physical process described by the SSE. Although the stochastic method is fundamentally equivalent to density matrix or NEGF formalism, it can be advantageous over the density operator and NEGF in several interesting cases such as fast tracking of information for quantum coherence and entanglement [35]. Moreover, it is known that perturbative master equations typically lead to unphysical effect such as violation of positivity, however, the stochastic equation can yield a systematic perturbative method that can be implemented numerically [14]. As an illustration of the power of the stochastic approach developed here, we derive several exact master equations governing the reduced density operators of the electronic systems coupled to vacuum and finite-temperature reservoirs.

Crucial to the practical applications of Eq. (9) is to express the Grassmann functional derivative under the memory integral in Eq. (10) in terms of system operators [12–17]. In order to calculate the functional derivative in the stochastic Schrödinger equation, we introduce an operator called the fermionic $\hat{Q}$ operator (similar to the $\hat{O}$ operator in bosonic case) as

$$\hat{Q}(t,s,\boldsymbol{\xi}^*)|\psi_t(\boldsymbol{\xi}^*)\rangle \equiv \overrightarrow{\delta}_{\xi_s^*} |\psi_t(\boldsymbol{\xi}^*)\rangle. \qquad (11)$$

With this definition, the effective Hamiltonian in Eq. (10) can be written as,

$$\hat{H}_{\mathrm{eff}} = \hat{H}_{\mathrm{S}} - \mathrm{i}\hat{L}\xi_t^* - \mathrm{i}\hat{L}^\dagger \bar{Q}, \qquad (12)$$

where

$$\bar{Q}(t,\boldsymbol{\xi}^*) \equiv \int_0^t \mathrm{d}s \, K(t,s) \hat{Q}(t,s,\boldsymbol{\xi}^*). \qquad (13)$$

The fermionic stochastic Schrödinger equation (9) is derived directly from the microscopic Hamiltonian without any approximation. It should be emphasized that the system Hamiltonian $\hat{H}_{\mathrm{S}}$ and the coupling operator $\hat{L}$ are entirely general. The evolution of the electronic system is governed by the anti-commutative stochastic differential equation (9). Although the mathematical form of the equation (9) is similar to the non-Markovian quantum state diffusion equation in the bosonic case, the behavior of the fermionic SSE can be very different due to the fermionic features of the environment [30]. Moreover, the Grassmann stochastic process has brought about several new features in dealing with the fermionic SSE such as a new type of Novikov theorem (see Appendix D).

From the consistency condition for the fermionic SSE

$$\overrightarrow{\delta}_{\xi_s^*} \partial_t |\psi_t(\boldsymbol{\xi}^*)\rangle = \partial_t \overrightarrow{\delta}_{\xi_s^*} |\psi_t(\boldsymbol{\xi}^*)\rangle, \qquad (14)$$

the fermionic $\hat{Q}$ operator can be shown to satisfy the following equation (see Appendix B),

$$\partial_t \hat{Q} = -\mathrm{i}[\hat{H}_{\mathrm{eff}}, \hat{Q}] - \mathrm{i}\,\overrightarrow{\delta}_{\xi_s^*}(\hat{H}_{\mathrm{eff}} - \hat{H}_{\mathrm{S}}). \qquad (15)$$

Once the fermionic $\hat{Q}$ operator is determined, the SSE can be cast into a time-local stochastic equation with the Grassmann type noise.

C. Non-Markovian master equation

Note that the reduced density operator for the open fermionic system can be obtained by taking the statistical average over all the Grassmann quantum trajectories which are the solutions to the SSE (9),

$$\hat{\rho}_r = \int \prod_k \mathrm{d}\xi_k^* \cdot \mathrm{d}\xi_k \mathrm{e}^{-\xi_k^* \cdot \xi_k} \hat{P}, \qquad (16)$$
$$\hat{P} = |\psi_t(\boldsymbol{\xi}^*)\rangle\langle\psi_t(-\boldsymbol{\xi})|, \qquad (17)$$

and in the rest of the paper, we will use the shorthand notations $\mathcal{D}_g[\boldsymbol{\xi}] \equiv \prod_k \mathrm{d}\xi_k^* \cdot \mathrm{d}\xi_k \mathrm{e}^{-\xi_k^* \cdot \xi_k}$ and $|\psi_t\rangle \equiv |\psi_t(\boldsymbol{\xi}^*)\rangle$, $|\psi_t^-\rangle \equiv |\psi_t(-\boldsymbol{\xi}^*)\rangle$ to represent the Grassmann Gaussian measure and the quantum trajectories, respectively (for more details, see Appendix C). Then taking the time derivative on

$$\hat{\rho}_r = \int \mathcal{D}_g[\boldsymbol{\xi}]|\psi_t\rangle\langle\psi_t^-|, \tag{18}$$

and substituting the fermionic SSE (9) into it, we can get the equation of motion for the reduced density operator,

$$\partial_t\hat{\rho}_r = -\mathrm{i}[\hat{H}_\mathrm{S},\hat{\rho}_r] + \int \mathcal{D}_g[\boldsymbol{\xi}]\{(-\hat{L}^\dagger\bar{Q} - \hat{L}\xi_t^*)\hat{P} + \hat{P}(-\bar{Q}_-^\dagger\hat{L} + \xi_t\hat{L}^\dagger)\}, \tag{19}$$

where $\bar{Q}_-$ is a short hand notation of $\bar{Q}(-\boldsymbol{\xi})$.

In order to calculate the terms $\int\mathcal{D}_g[\boldsymbol{\xi}]\,\xi_t^*\hat{P}$, we need to prove an extension of Novikov theorem for Grassmann Gaussian noise (for the bosonic case, see Ref. [14]). In the fermionic case, we have two kinds of Novikov-type theorems corresponding to the left and right functional derivatives.
Left type:

$$\int \mathcal{D}_g[\boldsymbol{\xi}]\,\xi_t^*\hat{P} = -\int_0^t \mathrm{d}s\sum_k \frac{\partial\xi_t^*}{\partial\xi_k^*}\frac{\partial\xi_s}{\partial\xi_k}\int\mathcal{D}_g[\boldsymbol{\xi}]\,\hat{P}\overleftarrow{\delta}_{\xi_s}; \tag{20}$$

Right type:

$$\int \mathcal{D}_g[\boldsymbol{\xi}]\,\hat{P}\xi_t = -\int_0^t \mathrm{d}s\sum_k \frac{\partial\xi_t}{\partial\xi_k}\frac{\partial\xi_s^*}{\partial\xi_k^*}\int\mathcal{D}_g[\boldsymbol{\xi}]\,\overrightarrow{\delta}_{\xi_s^*}\hat{P}; \tag{21}$$

where $\overleftarrow{\delta}_{\xi_s^*}$ ($\overrightarrow{\delta}_{\xi_s^*}$) is the right (left) functional derivative with respect to ξ_s^*. Applying the Novikov theorem for the Grassmann noise to Eq. (19), the formal exact master equation can be simplified into a compact form

$$\partial_t\hat{\rho}_r = -\mathrm{i}[\hat{H}_\mathrm{S},\hat{\rho}_r] + \{\int\mathcal{D}_g[\boldsymbol{\xi}][\bar{Q}\hat{P},\hat{L}^\dagger] + \mathrm{h.c.}\}, \tag{22}$$

Similar to the derivation for the SSE, the above derivation for non-Markovian master equation is only valid for the vacuum reservoir, in which we assume the system and environment are initially in the state $|\psi_\mathrm{tot}(0)\rangle = |\psi(0)\rangle_\mathrm{S}\wedge|\mathrm{vac}\rangle_\mathrm{R}$. However, the finite temperature case can be easily incorporated in our approach, as shown in the examples below.

In a special case where the fermionic $\hat{Q}$ operator is independent of noise, the master equation Eq. (22) takes a very simple form,

$$\partial_t\hat{\rho}_r = -\mathrm{i}[\hat{H}_\mathrm{S},\hat{\rho}_r] + \{[\bar{Q}\hat{\rho}_r,\hat{L}^\dagger] + \mathrm{h.c.}\}. \tag{23}$$

If we take the Markovian correlation function $K(t,s) = \Gamma\delta(t,s)$, then $\bar{Q}$ reduces to $\bar{Q} = \Gamma\hat{L}/2$, and the master equation will reduce to the standard Lindblad Markov master equation,

$$\partial_t\hat{\rho}_r = -\mathrm{i}[\hat{H}_\mathrm{S},\hat{\rho}_r] + \{\Gamma/2[\hat{L}\hat{\rho}_r,\hat{L}^\dagger] + \mathrm{h.c.}\}. \tag{24}$$

III. MANY-FERMION SYSTEM COUPLED TO A VACUUM FERMIONIC RESERVOIR

The first example considers a many-fermion open system coupled to a fermionic bath initially in the vacuum state. The total Hamiltonian is

$$\hat{H}_\mathrm{tot} = \sum_{j=1}^N \Omega_j\hat{d}_j^\dagger\hat{d}_j + \sum_k \omega_k\hat{b}_k^\dagger\hat{b}_k + \sum_{j,k} t_{j,k}\hat{d}_j^\dagger\hat{b}_k + t_{j,k}\hat{b}_k^\dagger\hat{d}_j, \tag{25}$$

where $\hat{d}_j$ and $\hat{d}_j^\dagger$ ($j=1$ to N) are the annihilation and creation operators of the fermions in the system, and $\hat{b}_k$ and $\hat{b}_k^\dagger$ are the fermionic annihilation and creation operators for the bath. Here $\hat{H}_\mathrm{S} = \sum_j\Omega_j\hat{d}_j^\dagger\hat{d}_j$, and the coupling operator is $\hat{L} = \sum_j\hat{d}_j$. Then, the fermionic SSE is given by

$$\mathrm{i}\partial_t|\psi_t\rangle = (\sum_j\Omega_j\hat{d}_j^\dagger\hat{d}_j - \mathrm{i}\sum_j\hat{d}_j\xi_t^* - \mathrm{i}\sum_j\hat{d}_j^\dagger\bar{Q})|\psi_t\rangle, \tag{26}$$

where the $\hat{Q}$ operator is given by $\hat{Q} = \sum_j f_j(t,s)\hat{d}_j$. Substituting the $\hat{Q}$ operator into the Eq. (15), we obtain the differential equations for the time-dependent coefficients $f_j(t,s)$ as

$$\frac{\partial}{\partial t}f_j(t,s) = \mathrm{i}\Omega_j f_j(t,s) + \sum_{k=1}^N F_k(t)f_j(t,s) \tag{27}$$

with the final condition $f_j(t,s=t)=1$. $F_j(t)$ is defined as $F_j(t) = \int_0^t \mathrm{d}s\,K(t,s)f_j(t,s)$. Thus, the exact $\hat{Q}$ operator is fully determined. Then one immediately obtains the exact master equation,

$$\partial_t\hat{\rho}_r = -\mathrm{i}[\hat{H}_\mathrm{S},\hat{\rho}_r] + \{[(\sum_{j=1}^N F_j(t)\hat{d}_j)\hat{\rho}_r,\sum_{j=1}^N\hat{d}_j^\dagger] + \mathrm{h.c.}\}. \tag{28}$$

As a special case of interest, we consider both the system and the reservoir just containing one mode with equal frequencies (resonant condition). Then the exact master equation reduces to

$$\partial_t\hat{\rho}_r = -\mathrm{i}\Omega[\hat{d}^\dagger\hat{d},\hat{\rho}_r] + \{[g\tan(gt)\hat{d}\hat{\rho}_r,\hat{d}^\dagger] + \mathrm{h.c.}\}, \tag{29}$$

where g is the coupling constant. This case is an extreme case of the non-Markovian evolution with the non-Markovianity being infinity [7]. In general, the negative values of the coefficients dictate the features of the non-Markovian evolution of an open quantum system. A more complete studies on non-Markovian fermonic systems will be conducted in the future publications [36].

IV. SINGLE QUANTUM DOT (QD) COUPLED TO A FINITE-TEMPERATURE FERMIONIC BATH

To illustrate how to establish a fermionic SSE for the case of finite temperature reservoirs, for simplicity, we use the example of a single QD coupled to a finite-temperature fermionic bath. As stated before, a realistic generalization to two finite temperature reservoirs is straightforward. In the standard Hamiltonian in Eq. (1) and Eq. (2), we choose $\hat{H}_{\rm S}=\omega_0\hat{d}^\dagger\hat{d}$ and $\hat{L}=\hat{d}$, then the total Hamiltonian is now given by,

$$\hat{H}_{\rm tot}=\omega_0\hat{d}^\dagger\hat{d}+\sum_k t_k(\hat{d}^\dagger\hat{b}_k+\hat{b}_k^\dagger\hat{d})+\sum_k\omega_k\hat{b}_k^\dagger\hat{b}_k. \quad (30)$$

It is known that the finite temperature model can be transformed into the vacuum case by introducing a fictitious reservoir "c" (a "hole" system with negative energies), which is decoupled from the system and reservoir "b", so the quantum dynamics will not be affected [13, 17]. With the fictitious reservoir $\hat{H}_{\rm R}^{fic}=\sum_k(-\omega_k)\hat{c}_k^\dagger\hat{c}_k$, the total Hamiltonian may be written as,

$$\begin{aligned}\hat{H}'_{\rm tot}=\omega_0\hat{d}^\dagger\hat{d}&+\textstyle\sum_k t_k(\hat{d}^\dagger\hat{b}_k+\hat{b}_k^\dagger\hat{d})\\&+\textstyle\sum_k\omega_k(\hat{b}_k^\dagger\hat{b}_k-\hat{c}_k^\dagger\hat{c}_k).\end{aligned} \quad (31)$$

By properly choosing the parameters of bath "c", the combined bath "$b+c$" can be initially prepared in a pure state which is equivalent to the vacuum corresponding to bath "$b'+c'$". The relation between the original bath and the transformed baths are given by the following Bogoliubov transformations,

$$\begin{aligned}\hat{b}'_k&=\sqrt{1-\bar{n}_k}\,\hat{b}_k-\sqrt{\bar{n}_k}\,\hat{c}_k^\dagger, & \hat{b}'^\dagger_k&=\sqrt{1-\bar{n}_k}\,\hat{b}_k^\dagger-\sqrt{\bar{n}_k}\,\hat{c}_k,\\ \hat{c}'_k&=\sqrt{1-\bar{n}_k}\,\hat{c}_k+\sqrt{\bar{n}_k}\,\hat{b}_k^\dagger, & \hat{c}'^\dagger_k&=\sqrt{1-\bar{n}_k}\,\hat{c}_k^\dagger+\sqrt{\bar{n}_k}\,\hat{b}_k;\\ \hat{b}_k&=\sqrt{1-\bar{n}_k}\,\hat{b}'_k+\sqrt{\bar{n}_k}\,\hat{c}'^\dagger_k, & \hat{b}_k^\dagger&=\sqrt{1-\bar{n}_k}\,\hat{b}'^\dagger_k+\sqrt{\bar{n}_k}\,\hat{c}'_k,\\ \hat{c}_k&=\sqrt{1-\bar{n}_k}\,\hat{c}'_k-\sqrt{\bar{n}_k}\,\hat{b}'^\dagger_k, & \hat{c}_k^\dagger&=\sqrt{1-\bar{n}_k}\,\hat{c}'^\dagger_k-\sqrt{\bar{n}_k}\,\hat{b}'_k;\end{aligned} \quad (32)$$

where $\bar{n}_k=\frac{1}{1+{\rm e}^{\beta(\hbar\omega_k-\mu)}}$, and μ is the chemical potential. After tracing out the fictitious bath "c" on the effective vacuum, the real bath "b" is then prepared in the initial thermal state, *i.e.*,

$$\hat{\rho}_b(0)={\rm Tr}_c[\hat{\rho}_{bc}(0)]=\exp[-\frac{\hat{H}_b-\mu\hat{N}_b}{k_BT}]/Z \quad (33)$$

where $Z={\rm Tr}\exp[-\frac{\hat{H}_b-\mu\hat{N}_b}{k_BT}]$ is the partition function. In such a way, the finite temperature model can be transformed into an effective vacuum case whose SSE has already been established in the previous sections.

Now we define the new coupling strength,

$$g_k\equiv\sqrt{1-\bar{n}_k}t_k,\quad f_k\equiv\sqrt{\bar{n}_k}t_k,$$

then the total Hamiltonian takes the following form,

$$\begin{aligned}\hat{H}'_{\rm tot}=\omega_0\hat{d}^\dagger\hat{d}&+\sum_k(g_k\hat{d}^\dagger\hat{b}'_k+f_k\hat{d}^\dagger\hat{c}'^\dagger_k+g_k\hat{b}'^\dagger_k\hat{d}\\&+f_k\hat{c}'_k\hat{d})+\sum_k\omega_k(\hat{b}'^\dagger_k\hat{b}'_k-\hat{c}'^\dagger_k\hat{c}'_k).\end{aligned} \quad (34)$$

The coherent states for the two baths can be defined as $|\boldsymbol{\xi}\rangle\equiv\prod_{k,l}(1-\xi_{b',k}\hat{b}'^\dagger_k)(1-\xi_{c',l}\hat{c}'^\dagger_l)|{\rm vac}\rangle_{\rm R}$. Thus, two independent Grassmann noises are defined,

$$\begin{aligned}\xi^*_{b',t}&\equiv-{\rm i}\sum_k g_k{\rm e}^{{\rm i}\omega_k t}\xi^*_{b',k},\\ \xi^*_{c',t}&\equiv-{\rm i}\sum_k f_k{\rm e}^{-{\rm i}\omega_k t}\xi^*_{c',k}.\end{aligned} \quad (35)$$

Then, the corresponding $\hat{Q}$ ($\bar{Q}$) operators and correlation functions are defined as

$$\begin{aligned}\hat{Q}_{b'}(t,s,\boldsymbol{\xi}^*)|\psi_t\rangle&\equiv\overrightarrow{\delta}_{\xi^*_{b',s}}|\psi_t\rangle,\\ \hat{Q}_{c'}(t,s,\boldsymbol{\xi}^*)|\psi_t\rangle&\equiv\overrightarrow{\delta}_{\xi^*_{c',s}}|\psi_t\rangle,\\ \bar{Q}_{b'}&\equiv\int_0^t{\rm d}s\,K_{b'}(t,s)\hat{Q}_{b'}(t,s,\boldsymbol{\xi}^*),\\ \bar{Q}_{c'}&\equiv\int_0^t{\rm d}s\,K_{c'}(t,s)\hat{Q}_{c'}(t,s,\boldsymbol{\xi}^*),\\ K_{b'}(t,s)&\equiv\sum_k g_k^2\,{\rm e}^{-{\rm i}\omega_k(t-s)},\\ K_{c'}(t,s)&\equiv\sum_k f_k^2\,{\rm e}^{{\rm i}\omega_k(t-s)}.\end{aligned} \quad (36)$$

With the above definitions, the SSE governing $|\psi_t\rangle$ can be written as

$${\rm i}\partial_t|\psi_t\rangle=[\hat{H}_{\rm S}+{\rm i}\hat{d}^\dagger(\xi^*_{c',t}-\bar{Q}_{b'})+{\rm i}\hat{d}(\bar{Q}_{c'}-\xi^*_{b',t})]|\psi_t\rangle. \quad (37)$$

Following the procedure of deriving master equation from the general SSE for the vacuum fermionic bath, we obtain the formal exact master equation of the case of finite temperature,

$$\begin{aligned}\partial_t\hat{\rho}_r=-{\rm i}[\hat{H}_{\rm S},\hat{\rho}_r]&+\int\mathcal{D}_g[\boldsymbol{\xi}]([\bar{Q}_{b'}\hat{P},\hat{d}^\dagger]\\&+[\hat{d},\bar{Q}_{c'}\hat{P}]+{\rm h.c.}).\end{aligned} \quad (38)$$

For the finite temperature case, the $\hat{Q}$ operators are not noise-free, hence we need to use the Heisenberg approach (see Appendix E) to derive the corresponding convolutionless master equation (an example of using Heisenberg approach in the case of bosonic bath can be found in Ref. [16, 17]).

The convolutionless master equation takes the following form,

$$\partial_t\hat{\rho}_r=-{\rm i}[\hat{H}_{\rm S},\hat{\rho}_r]+\{F_1(t)[\hat{d}\hat{\rho}_r,\hat{d}^\dagger]+F_2(t)[\hat{\rho}_r\hat{d},\hat{d}^\dagger]+{\rm h.c.}\} \quad (39)$$

where the time-dependent coefficients $F_i(t)$ $(i=1,2)$ are

$$F_i(t)=\int_0^t{\rm d}s\,[K_{b'}(t,s)u_i^{b'}(t,s)-K^*_{c'}(t,s)u_i^{c'}(t,s)], \quad (40)$$

and u_i^μ $(i=1,2,\ \mu=b'$ or $c')$ satisfy the following equations

$$\partial_s u_i^{b'}(t,s) = -\mathrm{i}\omega_0 u_i^{b'}(t,s) + [\int_s^t \mathrm{d}s'\, K_{c'}(s',s) - \int_0^s \mathrm{d}s'\, K_{b'}(s,s')] u_i^{b'}(t,s') + \int_0^t \mathrm{d}s'\, K_{c'}(s',s) u_i^{c'}(t,s'),$$
$$\partial_s u_i^{c'}(t,s) = -\mathrm{i}\omega_0 u_i^{c'}(t,s) + [\int_s^t \mathrm{d}s'\, K_{b'}^*(s',s) - \int_0^s \mathrm{d}s'\, K_{c'}^*(s,s')] u_i^{c'}(t,s') + \int_0^t \mathrm{d}s'\, K_{b'}^*(s',s) u_i^{b'}(t,s'), \qquad (41)$$

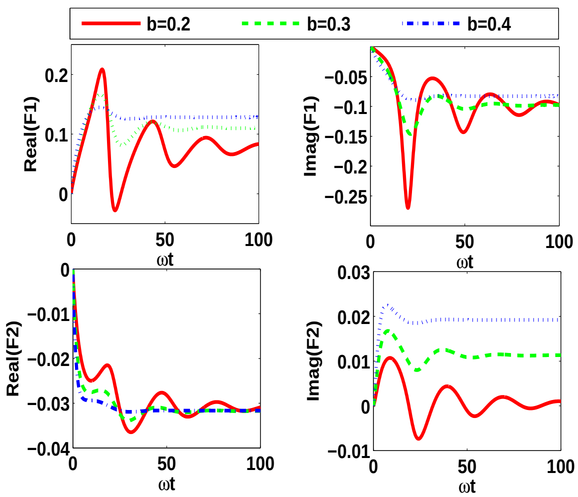

FIG. 1. Time evolution of the coefficients for the single quantum dot in a finite temperature bath with different bandwidths. The real (imaginary) part of the coefficients F_1 (F_2) are plotted separately. The parameters are $T = 100$mK, $\mu = 2\times10^{-5}$eV, $\omega_0 = 3\times10^{-5}$eV.

with the final conditions: $u_1^{b'}(t,s=t) = u_2^{c'}(t,s=t) = 1$, and $u_2^{b'}(t,s=t) = u_1^{c'}(t,s=t) = 0$.

Generally speaking, the time-dependent coefficients of the exact master equation may evolve in a complicated way (for example, taking negative values as a typical manifestation of non-Markovian behaviors, see [7]) and can be sensitively affected by the parameters of the environment. To show the temporal behavior of the exact master equation, we plot the Fig. 1 for the time-evolution of the coefficients $F_1(t)$ and $F_2(t)$; for simplicity, we choose a noise-free $\hat{Q}$ operator in our numerical simulations. The spectral density is chosen as the Lorentzian form

$$t_k^2(\omega_k)\Delta\omega = \frac{\Gamma b^2}{(1-\frac{\omega_k}{\omega_0})^2 + b^2}.$$

When the bandwidth b is wide, which corresponds to a white noise situation, the coefficients $F_1(t)$ and $F_2(t)$ must converge to constants rapidly, approaching the Markov limit [29]. On the contrary, if the bandwidth b is narrow, the distribution of the spectral density should represent a colored noise case, then we could expect that

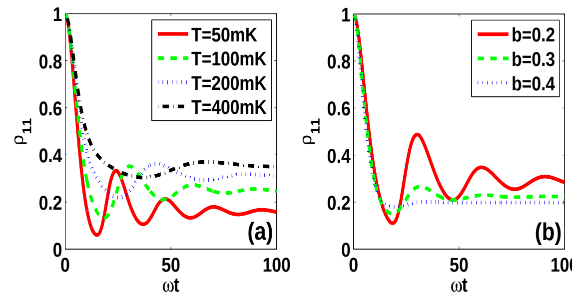

FIG. 2. Time evolution of ρ_{11} for the single quantum dot with different parameters of the bath. (a) is plotted with the different temperatures T, and (b) is plotted with the different bandwidths of the spectral density. The other parameters are $\mu = 2\times10^{-5}$eV, $\omega_0 = 3\times10^{-5}$eV.

the non-Markovian properties (*e.g.*, time-dependent coefficients) becomes dominant. As a direct result of using different $F_1(t)$ and $F_2(t)$, we could see that in Fig. 2 (b), the density matrix element ρ_{11} performs differently when it converges to the steady state. The wider the bandwidth b expands the faster the steady state could be approached, and significant fluctuations would come forth when b is small. Another parameter that will affect the non-Markovian properties is the temperature of the bath. As shown in Fig. 2 (a), the non-Markovian behaviors become more dominant in the low temperature regimes.

V. DOUBLE QDS COUPLED TO TWO FINITE-TEMPERATURE FERMIONIC BATHS

The model considered in this section is more involved, but physically more relevant. Here, we consider an electronic system coupled to two fermionic baths described by the following total Hamiltonian,

$$\begin{aligned}\hat{H}_{\rm tot} &= \omega_1 \hat{d}_1^\dagger \hat{d}_1 + \omega_2 \hat{d}_2^\dagger \hat{d}_2 + g\hat{d}_1^\dagger \hat{d}_2 + g^*\hat{d}_2^\dagger \hat{d}_1 \\ &+ \sum_k \omega_k (\hat{b}_{1,k}^\dagger \hat{b}_{1,k} + \hat{b}_{2,k}^\dagger \hat{b}_{2,k}) \\ &+ \{\sum_k t_{2,k}\hat{d}_2^\dagger \hat{b}_{2,k} + \sum_k t_{1,k}\hat{d}_1^\dagger \hat{b}_{1,k} + \text{h.c.}\}, \qquad (42)\end{aligned}$$

where $\hat{d}_i$ and $\hat{d}_i^\dagger$ ($i=1,2$) are the fermionic annihilation and creation operators of the two quantum dots in the

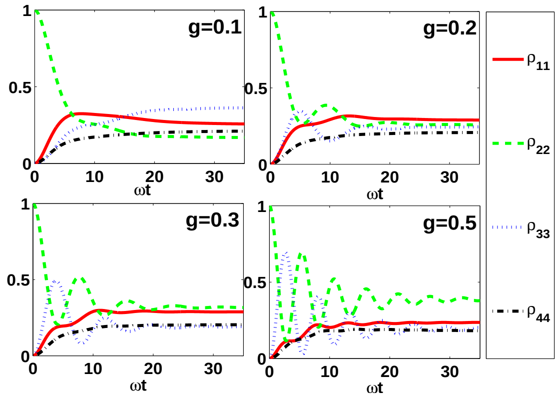

FIG. 3. Dynamic evolution for the double quantum dot from the initial state $d_1^\dagger|\text{vac}\rangle_{\text{S}}$ with different coupling strength g. The other parameters are $T = 100\text{mK}$, $\mu_1 = 2\times10^{-5}\text{eV}$, $\mu_2 = 4\times10^{-5}\text{eV}$, $\omega_1 = \omega = 2.5\times10^{-5}\text{eV}$, $\omega_2 = 3.5\times10^{-5}\text{eV}$.

system, and $\hat{b}_{i,k}$, $\hat{b}_{i,k}^\dagger$ are the annihilation and creation operators for the fermionic baths. This Hamiltonian describes a physical model that double quantum dots coupled to two fermionic baths with different chemical potentials, the "source" and the "drain". This model has been widely studied by using the fermionic path integral and the input-output approaches [28, 37].

Similar to the case of the single QD model discussed before, the exact SSE for the double QDs model can be established as,

$$\begin{aligned} \mathrm{i}\partial_t|\psi_t\rangle = (&\hat{H}_{\text{S}} - \mathrm{i}\hat{d}_1^\dagger\bar{Q}_{1,b'} - \mathrm{i}\hat{d}_1\xi^*_{1,b',t} + \mathrm{i}\hat{d}_1^\dagger\xi^*_{1,c',t} + \mathrm{i}\hat{d}_1\bar{Q}_{1,c'} \\ &- \mathrm{i}\hat{d}_2^\dagger\bar{Q}_{2,b'} - \mathrm{i}\hat{d}_2\xi^*_{2,b',t} + \mathrm{i}\hat{d}_2^\dagger\xi^*_{2,c',t} + \mathrm{i}\hat{d}_2\bar{Q}_{2,c'})|\psi_t\rangle, \end{aligned} \tag{43}$$

where $\bar{Q}_{\mu,\nu}|\psi_t\rangle \equiv \int_0^t \mathrm{d}s\, K_{\mu,\nu}(t,s)\overrightarrow{\delta}_{\xi^*_{\mu,\nu,s}}|\psi_t\rangle$ (the indices $\mu = 1,2$ represent the left and right baths, and $\nu = b', c'$ represent the fictitious baths b' and c' in the finite-temperature transformation). Therefore, the exact master equation for the double quantum dots system can be derived from the SSE,

$$\begin{aligned} \partial_t\hat{\rho}_r = -\mathrm{i}[\hat{H}_{\text{S}}, \hat{\rho}_r] + \{\sum_{j=1}^{2}[(F_1^j(t)\hat{d}_1 + F_2^j(t)\hat{d}_2)\hat{\rho}_r \\ + \hat{\rho}_r(F_3^j(t)\hat{d}_1 + F_4^j(t)\hat{d}_2), \hat{d}_j^\dagger] + \text{h.c.}\} \end{aligned} \tag{44}$$

where

$$F_i^j(t) \equiv \int_0^t \mathrm{d}s\,[K_{jb'}(t,s)u_i^{jb'}(t,s) - K^*_{jc'}(t,s)u_i^{jc'}(t,s)], \tag{45}$$

where $K_{j\mu}$ ($j = 1, 2$, $\mu = b'$ or c') are the correlation functions, and the equations for the coefficients u_i^μ ($i = 1, 2, 3, 4$, $\mu = 1b', 2b', 1c'$ or $2c'$) are

$$\begin{aligned} \partial_s u_j^{1b'}(t,s) &= -\mathrm{i}\omega_1 u_j^{1b'}(t,s) - \mathrm{i}g\, u_j^{2b'}(t,s) + [\int_s^t \mathrm{d}s'\, K_{1c'}(s',s) - \int_0^s \mathrm{d}s'\, K_{1b'}(s,s')]u_j^{1b'}(t,s') + \int_0^t \mathrm{d}s'\, K_{1c'}(s',s)u_j^{1c'}(t,s') \\ \partial_s u_j^{2b'}(t,s) &= -\mathrm{i}\omega_2 u_j^{2b'}(t,s) - \mathrm{i}g^* u_j^{1b'}(t,s) + [\int_s^t \mathrm{d}s'\, K_{2c'}(s',s) - \int_0^s \mathrm{d}s'\, K_{2b'}(s,s')]u_j^{2b'}(t,s') + \int_0^t \mathrm{d}s'\, K_{2c'}(s',s)u_j^{2c'}(t,s') \\ \partial_s u_j^{1c'}(t,s) &= -\mathrm{i}\omega_1 u_j^{1c'}(t,s) - \mathrm{i}g\, u_j^{2c'}(t,s) + [\int_s^t \mathrm{d}s'\, K^*_{1b'}(s',s) - \int_0^s \mathrm{d}s'\, K^*_{1c'}(s,s')]u_j^{1c'}(t,s') + \int_0^t \mathrm{d}s'\, K^*_{1b'}(s',s)u_j^{1b'}(t,s') \\ \partial_s u_j^{2c'}(t,s) &= -\mathrm{i}\omega_2 u_j^{2c'}(t,s) - \mathrm{i}g^* u_j^{1c'}(t,s) + [\int_s^t \mathrm{d}s'\, K^*_{2b'}(s',s) - \int_0^s \mathrm{d}s'\, K^*_{2c'}(s,s')]u_j^{2c'}(t,s') + \int_0^t \mathrm{d}s'\, K^*_{2b'}(s',s)u_j^{2b'}(t,s'), \end{aligned} \tag{46}$$

with the final conditions: $u_1^{1b'}(t,s=t) = u_2^{2b'}(t,s=t) = u_3^{1c'}(t,s=t) = u_4^{2c'}(t,s=t) = 1$, and the others are zero. We omit the mathematical details of solving this model, since the procedure is complicated however the main idea is still same to the single QD case.

Here, we only show some properties of this model by plotting the time evolution of the population; and the detailed study of this model will be discussed elsewhere [36]. In Fig. 3, we plot the dynamic evolution of the probabilities of all the four states with different coupling strength between the two QDs. In a long-time limit, the system trends to converge to a steady state. When t is small, the electron tunneling from one dot to the other can be significantly enhanced by the direct couplings between the two QDs.

VI. CONCLUSION

In this paper, we have developed an exact fermionic stochastic Schrödinger equation approach for solving the quantum open system coupled to a fermionic environment. The fundamental dynamic equation is derived directly from the microscopic quantum model without any approximations. By using the Grassmann noise, the stochastic Schrödinger equation approach is expanded from bosonic to fermionic environments. Three examples are presented to show the power of this approach. It is worth noting that the stochastic Schrödinger equation is versatile enough to deal with a generic fermionic environment incorporating cases from strong system-reservoir interaction to structured reservoirs. The exact stochastic approach can be applied to more realistic models when the approximation methods are used [36].

Note Added: After completion of this work, we became aware of an independent work by M. Chen and J. Q. You [38], who also derived a stochastic diffusive equation by using Grassmann coherent state approach.

ACKNOWLEDGEMENTS

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Appendix A: Fermionic coherent state and Grassmann noise

Fermionic coherent state: For any set $\boldsymbol{\xi} = \{\xi_j\}$ of independent Grassmann numbers, we define the fermionic coherent state $|\boldsymbol{\xi}\rangle$ as

$$|\boldsymbol{\xi}\rangle \equiv \prod_k (1 - \xi_k \hat{b}_k^\dagger)|\mathrm{vac}\rangle_{\mathrm{R}}. \tag{A1}$$

By our definition, it is easy to verify the results below,

$$\hat{b}_j|\boldsymbol{\xi}\rangle = \xi_j|\boldsymbol{\xi}\rangle = |\boldsymbol{\xi}\rangle\xi_j, \quad \hat{b}_j^\dagger|\boldsymbol{\xi}\rangle = -\overrightarrow{\partial}_{\xi_j}|\boldsymbol{\xi}\rangle = |\boldsymbol{\xi}\rangle\overleftarrow{\partial}_{\xi_j}. \tag{A2}$$

We can also check the validity of the completeness of the fermionic coherent states,

$$\hat{I} = \int \mathcal{D}_g[\boldsymbol{\xi}]|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}| = \prod_k \int \mathrm{d}\xi_k^* \,\mathrm{d}\xi_k \,\mathrm{e}^{-\xi_k^*\xi_k}|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}|, \tag{A3}$$

where $\mathcal{D}_g[\boldsymbol{\xi}]$ is the Grassmann Gaussian measure.

From the main text of this paper we know that the Grassmann Gaussian noises are generated as:

$$\xi_t \equiv \mathrm{i}\sum_k t_k \mathrm{e}^{-\mathrm{i}\omega_k t}\xi_k, \quad \xi_s^* \equiv -\mathrm{i}\sum_k t_k \mathrm{e}^{\mathrm{i}\omega_k s}\xi_k^*, \tag{A4}$$

through these definitions of the noises, we can calculate the correlation function as:

$$\mathcal{M}[\xi_t\xi_s^*] = \sum_k t_k^2 \mathrm{e}^{-\mathrm{i}\omega_k(t-s)}\mathcal{M}[\xi_k\xi_k^*]. \tag{A5}$$

It is easy to check that $\mathcal{M}[\xi_k\xi_k^*] = \int \mathcal{D}_g[\boldsymbol{\xi}]\xi_k\xi_k^* = 1$, so $\mathcal{M}[\xi_t\xi_s^*] = K(t,s) = \sum_k |t_k|^2 \mathrm{e}^{-\mathrm{i}\omega_k(t-s)}$.

Since time is a continuous index, so we can introduce the functional derivatives with respect to the Grassmann noise and the Taylor expansion of the Grassmann noise functional. Another useful feature is the chain rule; while deriving the SSE we only need to use a special case of the chain rule $\overrightarrow{\partial}_{\xi_k} = \int_0^t \mathrm{d}s \frac{\partial \xi_s}{\partial \xi_k}\overrightarrow{\delta}_{\xi_s}$ and $\overleftarrow{\partial}_{\xi_k} = \int_0^t \mathrm{d}s \frac{\partial \xi_s}{\partial \xi_k}\overleftarrow{\delta}_{\xi_s}$. The validity of this special chain rule is easy to check.

Appendix B: Derivation of the equation for fermionic $\hat{Q}$ operator

Applying the SSE Eq. (6) to both sides of the consistency condition,

$$\overrightarrow{\delta}_{\xi_s^*}\partial_t|\psi_t\rangle = \partial_t \overrightarrow{\delta}_{\xi_s^*}|\psi_t\rangle, \tag{B1}$$

we will obtain

$$\begin{aligned}\partial_t(\hat{Q})|\psi_t\rangle &= (\overrightarrow{\delta}_{\xi_s^*}\partial_t - \hat{Q}\partial_t)|\psi_t\rangle \\ &= (-\mathrm{i}\overrightarrow{\delta}_{\xi_s^*}\hat{H}_{\mathrm{eff}} + \mathrm{i}\hat{Q}\hat{H}_{\mathrm{eff}})|\psi_t\rangle \\ &= \{-\mathrm{i}[\hat{H}_{\mathrm{eff}}, \hat{Q}] - \mathrm{i}\overrightarrow{\delta}_{\xi_s^*}(\hat{H}_{\mathrm{eff}} - \hat{H}_{\mathrm{S}})\}|\psi_t\rangle. \end{aligned} \tag{B2}$$

So, the dynamics of $\hat{Q}$ operator is

$$\partial_t\hat{Q} = -\mathrm{i}[\hat{H}_{\mathrm{eff}}, \hat{Q}] - \mathrm{i}\overrightarrow{\delta}_{\xi_s^*}(\hat{H}_{\mathrm{eff}} - \hat{H}_{\mathrm{S}}). \tag{B3}$$

Appendix C: Recovering a reduced density operator from the Grassmann trajectories

First, note that the following two formulas for the Grassmann variables are necessary for our derivation.

1. For any two Grassmann functions $X(\boldsymbol{\xi})$ and $Y(\boldsymbol{\xi})$, one has

$$\begin{aligned}X(\boldsymbol{\xi})Y(\boldsymbol{\xi}) = \frac{1}{2}[&Y(\boldsymbol{\xi})X(\boldsymbol{\xi}) + Y(-\boldsymbol{\xi})X(\boldsymbol{\xi}) \\ &+ Y(\boldsymbol{\xi})X(-\boldsymbol{\xi}) - Y(-\boldsymbol{\xi})X(-\boldsymbol{\xi})].\end{aligned} \tag{C1}$$

2. The resolution of identity for the fermionic coherent states is given by,

$$\hat{I}_{\mathrm{tot}} = \sum_{\boldsymbol{n}} \int \mathcal{D}_g[\boldsymbol{\xi}]\,|\boldsymbol{n}\rangle_{\mathrm{S}}|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}|\langle\boldsymbol{n}|_{\mathrm{S}}. \tag{C2}$$

We start the derivation from a lemma [36] without its proof

$$\hat{\rho}_r \equiv \sum_{\boldsymbol{n},\boldsymbol{l},\boldsymbol{m}} |\boldsymbol{n}\rangle_{\mathrm{S}}\langle\boldsymbol{l}|_{\mathrm{R}}\langle\boldsymbol{n}|_{\mathrm{S}}\hat{\rho}_{\mathrm{tot}}|\boldsymbol{m}\rangle_{\mathrm{S}}|\boldsymbol{l}\rangle_{\mathrm{R}}\langle\boldsymbol{m}|_{\mathrm{S}}. \tag{C3}$$

Inserting Eq. (C2) into Eq. (C3), and using Eq. (C1) to exchange some terms, we can get the reduced density operator in the fermionic coherent state representation.

$$
\begin{aligned}
\hat{\rho}_r &= \int \mathcal{D}_g[\boldsymbol{\xi}] \sum_{\boldsymbol{n},\boldsymbol{l},\boldsymbol{m},\boldsymbol{n}'} |\boldsymbol{n}\rangle_{\rm S}\langle \boldsymbol{l}|_{\rm R}\langle \boldsymbol{n}|_{\rm S}|\boldsymbol{n}'\rangle_{\rm S}|\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}|\langle \boldsymbol{n}'|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{m}|_{\rm S} \\
&= \int \mathcal{D}_g[\boldsymbol{\xi}] \sum_{\boldsymbol{n},\boldsymbol{l},\boldsymbol{m},\boldsymbol{n}'} \frac{1}{2}(|\boldsymbol{n}\rangle_{\rm S}\langle\boldsymbol{\xi}|\langle \boldsymbol{n}'|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}\langle\boldsymbol{n}|_{\rm S}|\boldsymbol{n}'\rangle_{\rm S}|\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S} \\
&\quad + |\boldsymbol{n}\rangle_{\rm S}\langle-\boldsymbol{\xi}|\langle \boldsymbol{n}'|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}\langle\boldsymbol{n}|_{\rm S}|\boldsymbol{n}'\rangle_{\rm S}|\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S} + |\boldsymbol{n}\rangle_{\rm S}\langle\boldsymbol{\xi}|\langle \boldsymbol{n}'|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}\langle\boldsymbol{n}|_{\rm S}|\boldsymbol{n}'\rangle_{\rm S}|-\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S} \\
&\quad - |\boldsymbol{n}\rangle_{\rm S}\langle-\boldsymbol{\xi}|\langle \boldsymbol{n}'|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}\langle\boldsymbol{n}|_{\rm S}|\boldsymbol{n}'\rangle_{\rm S}|-\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S}).
\end{aligned}
$$

Using some trick of changing the integration variables, these four terms can be merged into only one term.

$$
\begin{aligned}
\hat{\rho}_r &= \int \mathcal{D}_g[\boldsymbol{\xi}] \sum_{\boldsymbol{n},\boldsymbol{l},\boldsymbol{m},\boldsymbol{n}'} |\boldsymbol{n}\rangle_{\rm S}\langle\boldsymbol{\xi}|\langle \boldsymbol{n}'|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}\langle\boldsymbol{n}|_{\rm S}|\boldsymbol{n}'\rangle_{\rm S}|-\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S} \\
&= \int \mathcal{D}_g[\boldsymbol{\xi}] \sum_{\boldsymbol{n},\boldsymbol{l},\boldsymbol{m}} |\boldsymbol{n}\rangle_{\rm S}\langle\boldsymbol{\xi}|\langle \boldsymbol{n}|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}|-\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S}.
\end{aligned}
$$

In the last row of the above formula, the term $\sum_{\boldsymbol{l}} |\boldsymbol{m}\rangle_{\rm S}|\boldsymbol{l}\rangle_{\rm R}\langle\boldsymbol{l}|_{\rm R}|-\boldsymbol{\xi}\rangle$ actully equals $|\boldsymbol{m}\rangle_{\rm S}|-\boldsymbol{\xi}\rangle$. (it is true, but we do not want to provide the details) That means the density operator could be written as

$$
\hat{\rho}_r = \int \mathcal{D}_g[\boldsymbol{\xi}] \sum_{\boldsymbol{n},\boldsymbol{m}} |\boldsymbol{n}\rangle_{\rm S}\langle\boldsymbol{\xi}|\langle \boldsymbol{n}|_{\rm S}\hat{\rho}_{\rm tot}|\boldsymbol{m}\rangle_{\rm S}|-\boldsymbol{\xi}\rangle\langle\boldsymbol{m}|_{\rm S}
$$

After using a short hand notation, the density operator shows us the familiar form [13, 14]

$$
\hat{\rho}_r = \int \mathcal{D}_g[\boldsymbol{\xi}]\, \langle\boldsymbol{\xi}|\hat{\rho}_{\rm tot}|-\boldsymbol{\xi}\rangle = \int \mathcal{D}_g[\boldsymbol{\xi}]\, |\psi_t\rangle\langle\psi_t^-|, \tag{C4}
$$

where $\hat{\rho}_{\rm tot} \equiv |\psi^I_{\rm tot}(t)\rangle\langle\psi^I_{\rm tot}(t)|$ is the density operator for a pure state of the total system, and $\langle\psi_t^-| \equiv \langle\psi_t(-\boldsymbol{\xi})|$ is a quantum trajectory corresponding to a noise $-\xi_t$.

Appendix D: Proof of the extended Novikov theorem

We first separate the Grassmann Gaussian measure into two parts: Grassmann measure part and Gaussian part, then give them new notations

$$
\mathcal{D}[\boldsymbol{\xi}] \equiv \prod_k {\rm d}\xi_k^* \cdot {\rm d}\xi_k, \quad G(\boldsymbol{\xi}) \equiv \prod_k {\rm e}^{-\xi_k^*\cdot\xi_k}.
$$

Then we can prove the left-Novikov theorem:

$$
\begin{aligned}
\int \mathcal{D}_g[\boldsymbol{\xi}]\, \xi_t^* \hat{P} &= \sum_k \frac{\partial \xi_t^*}{\partial \xi_k^*} \int \mathcal{D}[\boldsymbol{\xi}] G(\boldsymbol{\xi})\, \xi_k^* \hat{P} \\
&= \sum_k \frac{\partial \xi_t^*}{\partial \xi_k^*} \int \mathcal{D}[\boldsymbol{\xi}] \overrightarrow{\partial}_{\xi_k} G(\boldsymbol{\xi})\, \hat{P} \\
&= \sum_k \frac{\partial \xi_t^*}{\partial \xi_k^*} \int \mathcal{D}[\boldsymbol{\xi}] \{ \overrightarrow{\partial}_{\xi_k} [G(\boldsymbol{\xi})\hat{P}] \\
&\quad - \overrightarrow{\partial}_{\xi_k} \hat{P}\, G(\boldsymbol{\xi}) \} \\
&= - \sum_k \frac{\partial \xi_t^*}{\partial \xi_k^*} \int \mathcal{D}[\boldsymbol{\xi}] \overrightarrow{\partial}_{\xi_k} \hat{P}\, G(\boldsymbol{\xi}) \\
&= \sum_k \frac{\partial \xi_t^*}{\partial \xi_k^*} \int \mathcal{D}_g[\boldsymbol{\xi}]\, \hat{P}^{\sim} \overleftarrow{\partial}_{\xi_k} \\
&= \int_0^t {\rm d}s \sum_k \frac{\partial \xi_t^*}{\partial \xi_k^*} \frac{\partial \xi_s}{\partial \xi_k} \int \mathcal{D}_g[\boldsymbol{\xi}]\, \hat{P}^{\sim} \overleftarrow{\delta}_{\xi_s}
\end{aligned} \tag{D1}
$$

From the third row to fourth row we use some special features of Grassmann variables

$$
\int {\rm d}\xi_k = \overrightarrow{\partial}_{\xi_k}, \quad \overrightarrow{\partial}_{\xi_k} \overrightarrow{\partial}_{\xi_k} = 0.
$$

In the fifth row "$^{\sim}$" is one kind of fermionic parity operation, and under the even state assumption, we have the conclusion $\hat{P}^{\sim} = \hat{P}$. Right-Novikov theorem can be proved similarly.

Appendix E: Heisenberg approach and convolutionless master equation

In the interaction picture, the dynamics of an operator $\hat{a}$ is

$$
\partial_t \hat{a}(t) = {\rm i}{\rm e}^{{\rm i}\hat{H}_{\rm tot}t}{\rm e}^{-{\rm i}\hat{H}_{\rm R}t}[\hat{H}^I_{\rm tot}(t), \hat{a}]{\rm e}^{{\rm i}\hat{H}_{\rm R}t}{\rm e}^{-{\rm i}\hat{H}_{\rm tot}t}. \tag{E1}
$$

For the single QD model,

$$\hat{H}^{I}_{\rm tot} = \omega_0\hat{d}^\dagger\hat{d} + \sum_k (g_k e^{-i\omega_k t}\hat{d}^\dagger\hat{b}'_k + f_k e^{-i\omega_k t}\hat{d}^\dagger\hat{c}'^\dagger_k + g_k e^{i\omega_k t}\hat{b}'^\dagger_k\hat{d} + f_k e^{i\omega_k t}\hat{c}'_k\hat{d}). \tag{E2}$$

Thus, the evolution of the reservoir operators are

$$\hat{b}'_k(s) = \hat{b}'_k + \int_0^s ds'\,\frac{\partial\xi^*_{b',s'}}{\partial\xi^*_{b',k}}\hat{d}(s'),$$
$$\hat{c}'_k(s) = \hat{c}'_k - \int_0^s ds'\,\frac{\partial\xi^*_{c',s'}}{\partial\xi^*_{c',k}}\hat{d}^\dagger(s'),$$

$$\hat{b}'^\dagger_k(s) = \hat{b}'^\dagger_k(t) - \int_s^t ds'\,\frac{\partial\xi_{b',s'}}{\partial\xi_{b',k}}\hat{d}^\dagger(s'),$$
$$\hat{c}'^\dagger_k(s) = \hat{c}'^\dagger_k(t) + \int_s^t ds'\,\frac{\partial\xi_{c',s'}}{\partial\xi_{c',k}}\hat{d}(s'). \tag{E3}$$

Define $\hat{U}(t) \equiv e^{i\hat{H}_{\rm R}t}e^{-i\hat{H}_{\rm tot}t}$, then we can prove

$$\langle\boldsymbol{\xi}|\hat{U}(t)\hat{d}(s)|\psi_{\rm tot}(0)\rangle = \hat{Q}_{b'}(t,s,\boldsymbol{\xi}^*)|\psi_t\rangle,$$
$$\langle\boldsymbol{\xi}|\hat{U}(t)\hat{d}^\dagger(s)|\psi_{\rm tot}(0)\rangle = -\hat{Q}_{c'}(t,s,\boldsymbol{\xi}^*)|\psi_t\rangle. \tag{E4}$$

Using these relations, we could derive a set of closed differential equations with respect to the time s.

Define

$$\hat{R}_{b'}(t,s) \equiv \int \mathcal{D}_g[\boldsymbol{\xi}]\,\hat{Q}_{b'}(t,s,\boldsymbol{\xi}^*_{b'})\hat{P},$$
$$\hat{R}_{c'}(t,s) \equiv \int \mathcal{D}_g[\boldsymbol{\xi}]\,\hat{Q}_{c'}(t,s,\boldsymbol{\xi}^*_{c'})\hat{P}, \tag{E5}$$

then, the equations for $\hat{R}_{b'}$ and $\hat{R}_{c'}$ are given by

$$\partial_s\hat{R}_{b'}(t,s) = -i\omega_0\hat{R}_{b'}(t,s) - \int_0^s ds'\,K_{b'}(s,s')\hat{R}_{b'}(t,s') + \int_s^t ds'\,K_{c'}(s',s)\hat{R}_{b'}(t,s') - \int_0^t ds'\,K^*_{c'}(s,s')\hat{R}^\dagger_{c'}(t,s').$$
$$\partial_s\hat{R}_{c'}(t,s) = i\omega_0\hat{R}_{c'}(t,s) - \int_0^s ds'\,K_{c'}(s,s')\hat{R}_{c'}(t,s') + \int_s^t ds'\,K_{b'}(s',s)\hat{R}_{c'}(t,s') - \int_0^t ds'\,K^*_{b'}(s,s')\hat{R}^\dagger_{b'}(t,s'). \tag{E6}$$

The solutions of $\hat{R}_{b'}$ and $\hat{R}_{c'}$ may be written as

$$\hat{R}_{b'}(t,s) = u^{b'}_1(t,s)\hat{d}\hat{\rho}_r(t) + u^{b'}_2(t,s)\hat{\rho}_r(t)\hat{d},$$
$$-\hat{R}^\dagger_{c'}(t,s) = u^{c'}_1(t,s)\hat{d}\hat{\rho}_r(t) + u^{c'}_2(t,s)\hat{\rho}_r(t)\hat{d}. \tag{E7}$$

Substitution of Eq. (E7) into Eq. (E6), the equations for u^μ_i ($i = 1,2$, $\mu = b'$ or c') will be derived just as it is shown in Eq. (41). Then the exact master equation can be derived given by Eq. (39).

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