Stochastic Equation of Motion Approach to Fermionic Dissipative Dynamics. I. Formalism

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In this work, we establish formally exact stochastic equations of motion (SEOM) theory to describe the dissipative dynamics of fermionic open systems. The construction of the SEOM is based on a stochastic decoupling of the dissipative interaction between the system and fermionic environment, and the influence of environmental fluctuations on the reduced system dynamics is characterized by stochastic Grassmann fields. Meanwhile, numerical realization of the time-dependent Grassmann fields has remained a long-standing challenge. To solve this problem, we propose a minimal auxiliary space (MAS) mapping scheme, with which the stochastic Grassmann fields are represented by conventional c-number fields along with a set of pseudo-levels. This eventually leads to a numerically feasible MAS-SEOM method. The important properties of the MAS-SEOM are analyzed by making connection to the well-established time-dependent perturbation theory and the hierarchical equations of motion (HEOM) theory. The MAS-SEOM method provides a potentially promising approach for accurate and efficient simulation of fermionic open systems at ultra-low temperatures.

I. INTRODUCTION

The dissipative dynamics of a quantum system embedded in a macroscopic environment is a fundamental problem in modern physics and chemistry. To address this problem, a number of formally exact quantum dissipation theories (QDTs) have been established over the past two decades. One of the most popular QDTs is the hierarchical equations of motion (HEOM) theory proposed first by Tanimura and Kubo and extended later by many authors. Accurate and efficient numerical schemes have been developed for the HEOM which have led to a wide range of applications including quantum-state evolution, optical spectroscopy, energy and heat transfer, charge transfer and transport, exciton dynamics in realistic molecular aggregates, and quantum phase transition. Despite its great success, the applicability of HEOM is often limited by the considerable cost of computer memory, which tends to increase drastically with the lowering of temperature. This is because the construction of HEOM is based on unraveling the non-Markovian environmental memory. A large memory basis set is usually needed to achieve an accurate unraveling at low temperatures, which inevitably requires a large amount of computer memory to store all the auxiliary density operators.

Apart from the deterministic HEOM theory, there is another class of QDTs which adopts a stochastic framework. Since a stochastic process can be realized via mutually independent trajectories, the numerical implementation of a stochastic QDT is memory-friendly and highly parallelizable.

The stochastic QDTs have been well established for bosonic dissipative systems. For instance, the quantum state diffusion (QSD) theory using a wavefunction description pioneered by Diósi and Gisin and Percival has been extended to capture the non-Markovian effects by Strunz et al. and many others. Alternatively, using a density operator description, Kubo has developed a stochastic Liouville equation for quantum systems as early as in 1963. Later, Stockerger and Grabert and Shao have independently established the formally exact stochastic equations of motion (SEOM) theory. In contrast to the HEOM theory, the SEOM formalism does not involve the unraveling of environmental memory. Instead, stochastic fields are introduced to represent the environmental fluctuations and to decouple the dynamics of system and the environment.

For bosonic environments, the stochastic fields are conveniently realized by c-number random noises. Yan and Shao et al. have proved the formal equivalence between the HEOM and the SEOM theories for bosonic environments, as well as the equivalence between the HEOM and the non-Markovian QSD theories. They have also applied the SEOM to study the dynamics of a spin-boson model at zero temperature. Hsieh and Cao have proposed a unified SEOM formalism for various types of environments. Besides, hybrid stochastic and hierarchical equations of motion (sHEOM) formalisms have also been established.

In contrast to the bosonic counterparts, the stochastic QDTs for fermionic open systems have remained far from
mature. Historically, the pioneering works can be traced back to the early attempts of Barnett et al., Applebaum et al., and Rogers who have derived stochastic dynamical equations to describe fermionic Brownian motion. In recent years, the non-Markovian QSD theory has been extended to address fermionic environments by Yu et al. and others. Moreover, the SEOM for fermionic environments has been formally established. Since the creation and annihilation operators of fermions satisfy the anti-commutation relationship, the random fluctuations in a fermionic environment are to be represented by stochastic Grassmann-number (g-number) fields.

It should be pointed out that, all the previous efforts on the stochastic formulations of fermionic open systems ended up with deterministic dynamical equations. The inability to implement such stochastic formulations is due to intrinsic difficulties originating from the nature of Grassmann variables.

Any conventional variable, continuous or discrete, can be viewed as a function in some configuration space. Alternatively, as it is done in algebraic geometry, one can view functions as the basic object, with the underlying space being retrieved once the algebra of functions is given. The fermionic SEOM theory can be formulated in terms of functions which satisfy the Grassmann algebra, while completely avoiding the notion of points. However, the underlying space of points associated with the Grassmann variables does not exist. This makes the applications of Monte Carlo sampling of high-dimensional or path integrals to the integrals over Grassmann variables highly problematic. Consequently, the implementation of stochastic g-numbers is rather difficult in practice. For instance, a set of \( N \) matrices with the size of \( 2^N \times 2^N \) are needed to represent \( N \) g-numbers. Here, \( N \) could be the number of time steps considered in a dynamical process. Apparently, as \( N \) increases, the size of matrix will soon exceed the limit of current computers.

Recently, we have proposed a mapping strategy for the stochastic g-number fields, based on which a numerically feasible SEOM approach has been developed. This has enabled the stochastic simulation of fermionic dissipative dynamics. Although the main idea has been given in Ref. [107], a lot of details about the practical SEOM approach are yet to be elucidated. To this end, we give a comprehensive account of the fermionic SEOM theory and related numerical approach in a series of two full papers. In this paper (paper I), we shall focus on the analytic formalism of the SEOM theory. We will not only give detailed derivation of the SEOM theory, but also provide important insights into the mapping strategy that is essential for achieving a numerically feasible SEOM approach. In a succeeding paper (paper II), we will elaborate on the numerical aspects of the SEOM approach with numerical demonstrations.

The remainder of this paper is organized as follows. In Sec. III we utilize a stochastic decoupling scheme to derive a formally exact SEOM for open fermionic systems. In addition, the equivalence between the fermionic SEOM and HEOM formalisms is established by using the Ito calculus. In Sec. III we elaborate on the mapping scheme for the stochastic g-number fields, with which the formally exact yet numerically unfeasible SEOM is converted into a numerically feasible SEOM. In Sec. IV we assess the exactness or non-exactness of the SEOM with two different analytic approaches. Finally, we give concluding remarks in Sec. V.

II. A STOCHASTIC FRAMEWORK FOR OPEN FERMIONIC SYSTEMS

A. Fermionic dissipative systems

In this work, we consider a generic system coupled to fermionic environments (such as electron reservoirs). The total system (system plus environment) is described by the Hamiltonian

\[
H_T = H_S + H_B + H_{SB}.
\]

Here, \( H_S, H_B \) and \( H_{SB} \) are the Hamiltonian of the system, the Hamiltonian of the bath environment, and the system-bath interaction, respectively. In particular, for a single-level system in contact with a non-interacting fermion bath, we have \( H_B = \sum_j \epsilon_j \hat{d}_j^\dagger \hat{d}_j \) and \( H_{SB} = \hat{c}^\dagger \hat{F} + \hat{F}^\dagger \hat{c} \), where \( \hat{c}, \hat{c}^\dagger \) and \( \hat{d}, \hat{d}^\dagger \) are the annihilation (creation) operators acting on the system level and \( j \)-th single-particle state of the fermion bath. \( \hat{F} = \sum_j t_j \hat{d}_j \) is the system-bath coupling strength.

The dynamics of the total system is determined by the Schrödinger equation,

\[
i\dot{\rho}_T = [H_T, \rho_T],
\]

where \( \rho_T \) is the density matrix of the total system. In this paper, we use the atomic units \( (\hbar = 1) \) and \( k_B = 1 \). The straightforward computation of Eq. 2 is intractable, because the fermion bath includes an infinite degrees of freedom (DOF) in the \( H_B \).

For a quantum dissipative system, we are interested in its reduced dynamics as well as its static and dynamical properties. The dissipative dynamics is characterized by the system reduced density matrix \( \rho_S(t) = \text{tr}_B[\rho_T(t)] \). In the following, we establish a rigorous stochastic formalism for the evaluation of \( \rho_S(t) \). For simplicity, the environment consists of a single fermion bath. As will be shown later, the derivation is easily extended to systems coupled to multiple fermion baths.

B. Fermionic coherent states and Grassmann algebra

For a single-level system, \( \hat{c}^\dagger \) and \( \hat{c} \) are respectively associated with the fermionic creation and annihilation op-
The identity operator is reproduced by
\[ |\psi\rangle \equiv e^{-\bar{\psi}^\dagger |0\rangle} = (1 - \psi^\dagger |0\rangle) = |0\rangle - \psi |1\rangle \] (3)
\[ \langle \tilde{\psi}| \equiv (0) e^{\bar{\psi}^\dagger} = |0\rangle (1 + \bar{\psi} \tilde{\psi}) = |0\rangle - |1\rangle , \] (4)
where \(|0\rangle\) and \(|1\rangle\) are the Fock states with the particle occupation number being zero and one, respectively. \(\psi\) and \(\tilde{\psi}\) are g-numbers. They satisfy the anti-commutation relation of \(\bar{\psi}\tilde{\psi} = -\bar{\psi}\tilde{\psi}\), and hence \((\bar{\psi}\tilde{\psi})^2 = (\bar{\psi})^2 = 0\). It can be easily verified that \(|\psi\rangle\) and \(|\tilde{\psi}\rangle\) are the eigenstates of operators \(\hat{c}\) and \(\hat{c}^\dagger\), with the eigenvalues \(\psi\) and \(\tilde{\psi}\), respectively.
\[ \hat{c}|\psi\rangle = \psi|\psi\rangle \quad \text{and} \quad \langle \tilde{\psi}| \hat{c}^\dagger = \langle \tilde{\psi}| \tilde{\psi}\tilde{\psi}\. \] (5)
In addition, we also have
\[ \hat{c}^\dagger |\psi\rangle = -\frac{\partial}{\partial \psi}|\psi\rangle \quad \text{and} \quad \langle \tilde{\psi}| \hat{c} = \frac{\partial}{\partial \tilde{\psi}}\langle \tilde{\psi}|\. \] (6)
The inner product of two fermionic coherent states is
\[ \langle \tilde{\psi}| \psi\rangle = 1 + \bar{\psi}\psi = e^{\bar{\psi} \tilde{\psi}}. \] (7)
All the fermionic coherent states form an overcomplete set, and thus the identity operator in the system’s Hilbert space, \(\hat{I}\), is expressed as
\[ \hat{I} = |0\rangle \langle 0| + |1\rangle \langle 1| = \int d\bar{\psi} d\psi e^{-\bar{\psi} \tilde{\psi}} |\psi\rangle \langle \tilde{\psi}|. \] (8)

The above definitions and relations can be extended to a system with \(N_{\nu}\) DOF. In such a case, define
\[ |\psi\rangle \equiv |\{\psi_{\nu}\}\rangle = e^{-\sum_{\nu=1}^{N_{\nu}} \psi_{\nu} c_{\nu}^\dagger} |0\rangle - \sum_{\nu=1}^{N_{\nu}} \psi_{\nu} |1_{\nu}\rangle \] (9)
\[ \langle \tilde{\psi}| \equiv \langle \{\tilde{\psi}_{\nu}\}| = 0 e^{\sum_{\nu=1}^{N_{\nu}} \tilde{\psi}_{\nu} c_{\nu}} = 0 - \sum_{\nu=1}^{N_{\nu}} |1_{\nu}\rangle. \] (10)
Here, \(|0\rangle\equiv |0_{1}, \cdots, 0_{N_{\nu}}\rangle\) is the anti-symmetrized vacuum state of the system, and \(|0_{\nu}\rangle\) and \(|1_{\nu}\rangle\) are the Fock states associated with the \(\nu\)th level. The inner product is evaluated by
\[ \langle \tilde{\psi}| \psi\rangle = 1 + \sum_{\nu=1}^{N_{\nu}} \tilde{\psi}_{\nu} \psi_{\nu} = e^{\sum_{\nu=1}^{N_{\nu}} \tilde{\psi}_{\nu} \psi_{\nu}}. \] (11)
The identity operator is reproduced by
\[ \hat{I} = \prod_{\nu=1}^{N_{\nu}} d\bar{\psi}_{\nu} d\psi e^{-\sum_{\nu=1}^{N_{\nu}} \bar{\psi}_{\nu} \psi_{\nu}} |\psi_{\nu}\rangle \langle \bar{\psi}_{\nu}|. \] (12)

C. Stochastic decoupling of system and environment dynamics

For a fermionic open system, the stochastic decoupling of system and bath is done by following a procedure similar to that adopted for a bosonic open system.\(^{22,22}\) The evolution of the density matrix of the total system is formally described by
\[ \rho_{T}(t) = \hat{U}_{T}(t, 0) \rho_{T}(0) \hat{U}_{T}^\dagger(t, 0). \] (13)
where \(\hat{U}_{T}(t, 0)\) and \(\hat{U}_{T}^\dagger(t, 0)\) are the forward and backward quantum evolution operators of the total system, respectively. Denote \(\hat{U}_{S}(t, 0)\) and \(\hat{U}_{S}^\dagger(t, 0)\) as the corresponding quantum propagators in the fermionic coherent state representation, and discretize the time domain by an infinitesimal time interval \(\Delta t = t_{i+1} - t_{i} = t/N\) with \(t_{0} = 0\) and \(t_{N} = t\). The quantum propagator is expressed as follows.
\[ \hat{U}_{T}(t, 0) = \langle \tilde{\psi}_{N} \tilde{\theta}_{N} | \hat{U}_{T}(t, 0) | \psi_{\theta_{0}} \rangle \]
\[ = \lim_{N \to \infty} \int D\psi D\tilde{\theta} \prod_{i=0}^{N-1} <\tilde{\psi}_{i+1} \tilde{\theta}_{i+1} | \hat{U}_{T}(t_{i+1}, t_{i}) | \psi_{\theta_{i}} > \]
\[ = \lim_{N \to \infty} \int D\psi D\tilde{\theta} \prod_{i=0}^{N-1} \hat{U}_{T}(t_{i+1}, t_{i}). \] (14)
Here, the g-numbers \(\{\bar{\psi}_{i}, \psi_{i}, \tilde{\theta}_{i}, \theta_{i}\}\) are eigenvalues of the system and bath operators \(\{\lambda \bar{c}^\dagger, \lambda \bar{c}, \lambda^2 \bar{F}^\dagger, \lambda - \bar{F}\}\), and \(\lambda\) is a reference energy that could take any positive value (\(\lambda > 0\)).
\[ D\psi D\tilde{\theta} \equiv \prod_{i=1}^{N-1} \frac{1}{(\Delta t)^2} d\psi_{i} d\tilde{\psi}_{i} d\theta_{i} d\tilde{\theta}_{i} e^{\bar{\psi}_{i} \psi_{i + 1} \psi_{i} + \tilde{\theta}_{i + 1} \theta_{i + 1} \Delta t} \]
\[ \text{is the metric of the integral. The overcompleteness of fermionic coherent states gives rise to the equality} \]
\[ \hat{I} = \frac{1}{(\Delta t)^2} \int d\psi_{i} d\tilde{\psi}_{i} d\theta_{i} d\tilde{\theta}_{i} e^{-\tilde{\psi}_{i} \psi_{i+1} \psi_{i} \Delta t} e^{-\bar{\theta}_{i+1} \theta_{i+1} \Delta t} |\psi_{i} \tilde{\theta}_{i}\rangle \langle \psi_{i} \tilde{\theta}_{i}|. \] (15)
In the limit of \(N \to \infty\) (\(\Delta t \to 0\)), the propagator \(\hat{U}_{T}(t_{i+1}, t_{i})\) can be further split into three parts,
\[ \hat{U}_{T}(t_{i+1}, t_{i}) = \hat{U}_{S}(t_{i+1}, t_{i}) \hat{U}_{SB}(t_{i+1}, t_{i}) \hat{U}_{SB}(t_{i+1}, t_{i}). \] (16)
The last part associated with the system-bath coupling, \(\hat{U}_{SB}\), is recast into the fermionic coherent state representation as
\[ \hat{U}_{SB}(t_{i+1}, t_{i}) = \langle \bar{\psi}_{i+1} \bar{\theta}_{i+1} | \hat{U}_{SB}(t_{i+1}, t_{i}) | \psi_{\theta_{i}} > \]
\[ = \exp\{-i(\bar{\psi}_{i+1} \theta_{i} + \bar{\theta}_{i+1} \psi_{i}) \Delta t\} \]
\[ = \exp\{-i\bar{\psi}_{i+1} \theta_{i} \Delta t\} \exp\{-i\bar{\theta}_{i+1} \psi_{i} \Delta t\}. \] (17)
The products of g-numbers corresponding to the system and bath operators can be decoupled by using the property of Grassmann Gaussian integrals. We have the fol-
lowing equalities:

\[
e^{-i\hat{\psi}_i^+\hat{\theta}_i^+\Delta t} = \frac{1}{\Delta t} \int d\tilde{\eta}_1 \, d\eta_1 \, e^{-\bar{\eta}_1\eta_1 \Delta t} \times \exp \left[ -i e^{\pi/4} (\bar{\psi}_1 + \eta_1 \hat{\eta}_1) \Delta t \right],
\]

\[
e^{-i\hat{\theta}_i^+\hat{\psi}_i^+\Delta t} = \frac{1}{\Delta t} \int d\tilde{\eta}_2 \, d\eta_2 \, e^{-\bar{\eta}_2\eta_2 \Delta t} \times \exp \left[ -i e^{\pi/4} (\bar{\theta}_1 + \eta_2 \hat{\eta}_2) \Delta t \right],
\]

where \( \eta_1, \tilde{\eta}_1, \eta_2, \tilde{\eta}_2 \) are time-dependent auxiliary Grassmann fields (AGFs) for \( 0 \leq i < N \). Equation (18) can be regarded as a fermionic version of the Hubbard-Stratonovich transformation for \( \mathcal{U}_{\text{SN}} \). Inserting Eq. (18) into Eq. (17), we have

\[
\mathcal{U}_{\text{SN}}(t_{i+1}, t_i) = \frac{1}{(\Delta t)^2} \int d\tilde{\eta}_1 \, d\eta_1 \, d\tilde{\eta}_2 \, d\eta_2 \, e^{-\bar{\eta}_1\eta_1 \Delta t} \times e^{-\bar{\eta}_2\eta_2 \Delta t} \times e^{-i e^{\pi/4} (\bar{\psi}_1 + \eta_1 \hat{\eta}_1 + \bar{\psi}_2 + \eta_2 \hat{\eta}_2) \Delta t} \times e^{-i e^{\pi/4} (\bar{\theta}_1 + \eta_2 \hat{\eta}_2 + \bar{\eta}_1 \hat{\eta}_1) \Delta t}.
\]

In the continuous time limit, the forward propagator of Eq. (11) becomes a weighted average over the AGFs \( \{\eta, \tilde{\eta}\} = \{\eta_{j\tau}, \tilde{\eta}_{j\tau}\} \).

\[
\mathcal{U}_f(t, 0) = \int \mathcal{D} \eta \, \mathcal{D} \tilde{\eta} \, e^{-\int_0^t \eta \cdot S \, d\tau} \mathcal{U}_{\text{SN}}^f(t, 0) \mathcal{U}_{\text{SN}}^b(t, 0) \equiv \langle \mathcal{U}_{\text{SN}}^f(t, 0) \mathcal{U}_{\text{SN}}^b(t, 0) \rangle.
\]

Here, \( \langle \ldots \rangle \) denotes the stochastic average over the AGFs. With Eq. (20), the system and bath are formally decoupled from each other. Instead, they are coupled to the AGFs \( \{\eta_{j\tau}, \tilde{\eta}_{j\tau}\} \) \((j = 1, 2)\), where \( \mathcal{U}_{\text{SN}}^f(t, 0) \) and \( \mathcal{U}_{\text{SN}}^b(t, 0) \) are the stochastic system and bath propagators, respectively. The weight \( e^{-\int_0^t \eta \cdot S \cdot d\tau} = e^{-\int_0^t (\eta_1 \hat{\eta}_1 + \eta_2 \hat{\eta}_2) \, d\tau} \) is a Gaussian distribution. The AGFs anti-commute with each other, i.e., \( \eta_{j\tau} \tilde{\eta}_{j'\tau'} = -\delta_{jj'} \delta_{\tau\tau'} \), and their stochastic averages satisfy the relations \( \langle \eta_{j\tau} \rangle = \langle \tilde{\eta}_{j\tau} \rangle = 0 \) and \( \langle \eta_{j\tau} \tilde{\eta}_{j'\tau'} \rangle = \delta_{jj'} \delta(t-\tau) \). The backward propagator can be decoupled similarly by introducing the AGFs \( \{\eta_{j\tau}, \tilde{\eta}_{j\tau}\} \) with \( j = 3, 4 \).

Suppose the initially density matrix has a factorized form of \( \rho_b(0) = \rho_s(0) \rho_b(0) \), the dynamics of the total system is given by

\[
\rho_s(t) = \Gamma \rho_s(0) \rho_b(0).
\]

Here, \( \langle \ldots \rangle \) denotes the stochastic average over the AGFs \( \{\eta_{j\tau}, \tilde{\eta}_{j\tau}\} \). The time evolution of the decoupled stochastic system and bath density matrices is formally described by

\[
\begin{align*}
\rho_s(t) &= \hat{U}_f^b \rho_s(0) \hat{U}_b^f(0, t), \\
\rho_b(t) &= \hat{U}_b^f \rho_b(0) \hat{U}_f^b(0, t).
\end{align*}
\]

where \( \hat{U}_f^b \) and \( \hat{U}_b^f \) are the effective forward and backward evolution operators for the decoupled system/bath, respectively. Specifically, the forward evolution operators take the time-ordered form of

\[
\hat{U}_b^f(t, 0) = \exp_+ \left\{ -i \int_0^t \frac{d\tau}{\lambda^Z} \left[ H_s + e^{\pi/4} \lambda^Z \hat{F} \hat{F}^\dagger \hat{F} \hat{F}^\dagger \hat{F} \hat{F}^\dagger \right] \right\},
\]

\[
\hat{U}_f^b(t, 0) = \exp_+ \left\{ -i \int_0^t \frac{d\tau}{\lambda^Z} \left[ H_b + e^{\pi/4} \lambda^{-Z} \hat{F} \hat{F}^\dagger \hat{F} \hat{F}^\dagger \right] \right\}.
\]

\( \hat{U}_b^f(0, t) \) can be expressed similarly. These operators result in the following SEOM for the decoupled stochastic system and bath density matrices:

\[
\hat{\rho}_b = -i[H_b, \rho_b] + e^{\pi/4} \lambda^Z \left( \hat{c} \eta_1 + \bar{\eta}_2 \hat{c} \right) \rho_b + e^{\pi/4} \lambda^{-Z} \left( \bar{\eta}_1 \hat{F} + \hat{F}^\dagger \eta_2 \right) \rho_b,
\]

\[
\hat{\rho}_b = -i[H_b, \rho_b] + e^{\pi/4} \lambda^{-Z} \left( \bar{\eta}_1 \hat{F} + \hat{F}^\dagger \eta_2 \right) \rho_b + e^{\pi/4} \lambda^{-Z} \rho_b.
\]

The system reduced density matrix is obtained as

\[
\hat{\rho}_s = \langle \rho_s \, \hat{U}_b^f \rho_b(0) \hat{U}_f^b \rangle.
\]

Obviously, \( \text{tr}_b(\rho_b) \) is the weight of each quantum trajectory of \( \rho_s \). Therefore, although there is no explicit coupling between system and bath in Eqs. (23) and (24), the evolution of the fermion bath still affects the system dynamics through the stochastic average of Eq. (25). Define \( \hat{\rho}_s = \rho_s \, \hat{U}_b^f \rho_b(0) \), so that \( \hat{\rho}_s = \langle \hat{\rho}_s \rangle \), i.e., the quantum trajectories of \( \hat{\rho}_s \) are equally weighted.

To verify the exactness of the stochastic decoupling, we show the original Schrödinger equation of Eq. (25) can be precisely recovered by Eqs. (26) and (27). Consider the Itô’s formula:

\[
d\rho_b(t) = d\rho_s(t) + d\rho_b(t) + d\rho_b^* \, d\rho_b(t).
\]

where \( d\rho_b(t) \sim \mathcal{O}(dt) \), and thus cannot be neglected. Taking the average over all the AGFs on both sides of Eq. (25), we have

\[
d\rho_s(t) = -i[H_s + H_b, \rho_s] \, dt + i\langle \hat{c}^\dagger \eta_1 + \bar{\eta}_2 \hat{c} \rangle \langle \hat{F}^\dagger \eta_2 \rangle \, dt + i\langle \rho_b \rangle \langle \hat{c}^\dagger \eta_3 + \bar{\eta}_4 \hat{c} \rangle \langle \hat{F}^\dagger \eta_4 \rangle \, dt^2
\]

\[
= -i[H_s + H_b + H_{\text{SN}}, \rho_s] \, dt.
\]

Here, we have used the causality principle that \( \rho_s(t) \) and \( \rho_b(t) \) depend only on \( \{\eta_j, \tilde{\eta}_j\} \) at \( \tau < t \), as well as the equalities \( \rho_b(\bar{\eta}_1 \hat{F} + \hat{F}^\dagger \eta_2) = \langle \eta_1 \hat{F} + \hat{F}^\dagger \eta_2 \rangle \rho_b \) and \( \rho_b(\hat{c}^\dagger \eta_3 + \bar{\eta}_4 \hat{c}) = \langle \hat{c}^\dagger \eta_3 + \bar{\eta}_4 \hat{c} \rangle \rho_b \). These equalities hold true because \( \rho_b \) and the operators \( F \) and \( F^\dagger \) (c and
\( \hat{c}^\dagger \) belong to different physical spaces, and the product of an AGF and a creation/annihilation operator commutes with any function of AGFs.

In relation to the three contributions on the right-hand side of Eq. (28), \( \langle \rho_s \Delta \rangle \) and \( \langle \Delta \rho_s \rangle \) result in the dynamics due to the pure system and pure bath, \( [H_s + H_B, \rho_s] \); while \( \langle \Delta \rho_s \Delta \rangle \) gives rise to the dynamics due to the system-bath interaction, \( [H_{sb}, \rho_s] \).

D. Capturing the non-Markovian memory of fermionic environment

In practice, the bath is considered to have an infinite DOF, and thus we normally avoid solving Eq. (26) explicitly. In Eq. (27), \( \text{tr}_n(\rho_n) \) is the weight of the trajectory of \( \rho_n \), which includes the AGFs \{\( \eta_{\tau}, \tilde{\eta}_{\tau} \). It captures the non-Markovian memory of the fermion bath on the reduced system dynamics, and it can be evaluated by analyzing Eq. (26).

In the \( H_B \)-interaction picture, the formal solution of Eq. (26) is worked out as

\[
\rho_n(t) = \tilde{U}_B^0(t) \tilde{U}_B^f(t,0) \rho_n(0) \tilde{U}_B^b(0,t) \tilde{U}_B^0(t). \tag{30}
\]

Here, \( \tilde{U}_B(t) = \exp(-iH_Bt) \) is the evolution operator for the isolated bath, with \( \tilde{F}(t) = \tilde{U}_B^0(t) \tilde{F} \tilde{U}_B^0(t) \). Using the cyclic permutation invariance of trace operation, we have

\[
\text{tr}_n(\rho_n) = \text{tr}_n \left[ \tilde{U}_B^f(t,0) \rho_n(0) \tilde{U}_B^b(0,t) \right]. \tag{31}
\]

Initially, the isolated bath is assumed to be in a thermal equilibrium state, i.e., \( \rho_n(0) = \rho_{eq} = e^{-\beta(H_B-N_{n0})} / Z \), where \( N_{n0} \) is the particle number operator, \( \rho_{eq} \) is the equilibrium chemical potential, \( \beta = 1/T \) is the inverse temperature, and \( Z = \text{tr}_n[e^{-\beta(H_B-N_{n0})}] \) is the partition function of the bath, respectively.

For a non-interacting fermion bath which satisfies the Gaussian statistics, Eq. (26) can be formally solved by using the Magnus expansion107 and the Baker-Campbell-Hausdorff formula111. This leads to the following expression of \( \text{tr}_n(\rho_n) \):

\[
\text{tr}_n(\rho_n) = e^{\int_0^t d\tau \left[ (\tilde{\eta}_{\tau} - i\eta_{\tau}) g_\tau^- + (\eta_{\tau} - i\tilde{\eta}_{\tau}) g_\tau^+ \right]}. \tag{32}
\]

The non-Markovian memory effects are accounted for by the following memory-convoluted AGFs107:

\[
\begin{align*}
g^- &= \lambda^{-1} \int_0^t \left\{ [C^+(t-\tau)]*\eta_{\tau} - iC^-(t-\tau) \eta_{\tau} \right\} d\tau, \\
g^+ &= \lambda^{-1} \int_0^t \left\{ [C^-(t-\tau)]*\tilde{\eta}_{\tau} - iC^+(t-\tau) \tilde{\eta}_{\tau} \right\} d\tau,
\end{align*}
\]

where \( C^+(t-\tau) = \text{tr}_n \left[ \tilde{F}(t) \tilde{F}(\tau) \rho_{eq}^n \right] \) and \( C^-(t-\tau) = \text{tr}_n \left[ \tilde{F}(t) \tilde{F}(\tau) \rho_{eq}^n \right] \) are two-time correlation functions of the fermion bath. They are related to the bath spectral density, \( J(\omega) = \pi \sum_k |\epsilon_k|^2 \delta(\omega - \epsilon_k) \), via the fluctuation-dissipation theorem as follows,

\[
C^\sigma(t) = \int_{-\infty}^{+\infty} d\omega \epsilon e^{i\epsilon t} f^\sigma(\omega) J(\omega). \tag{34}
\]

Here, \( \sigma = \pm \) and

\[
f^\sigma(\omega) = \frac{1}{1 + e^{\beta(\omega - \mu)}}, \tag{35}
\]

is the Fermi function for electron (\( \sigma = + \)) or hole (\( \sigma = - \)) at temperature \( T = 1/\beta \), and \( \mu \) is the bath chemical potential.

To obtain quantum dynamical trajectories of the reduced system with equal weights, we refer to the SEOM for bosonic environments.\(^{82,83}\) The Girsanov transformation has been utilized to absorb the weight function \( \text{tr}_n(\rho_n) \) into the dynamical variable.\(^{82,112}\) The fermionic analogue is expressed as

\[
\langle e^{-\bar{\theta} n} f(\theta, \bar{\theta}) \rangle = \int d\bar{\theta} d\theta e^{-\bar{\theta}(\theta+n)} f(\theta, \bar{\theta}) = \langle f(\theta - \eta, \bar{\theta}) \rangle, \tag{36}
\]

where \( f(\theta, \bar{\theta}) \) is any analytic function of the g-numbers \( \theta \) and \( \bar{\theta} \), and \( \eta \) is another g-number. Applying Eq. (36) to the system reduced density matrix of Eq. (27), and making use of Eq. (32), we have

\[
\bar{\rho}_S(t) = \langle \rho_s(t) \text{tr}_n(\rho_n) \rangle = \int D\bar{\eta} D\eta e^{-\frac{1}{2} \bar{\eta}_+ \eta_- d\tau \bar{\rho}_S(\eta, \bar{\eta}) \text{tr}_n(\rho_n)} \tag{37}
\]

Here, the third equality involves the following transformation of variables:

\[
\begin{align*}
\eta_{1\tau} &= \eta_{\tau} - g_{\tau}^- \\
\eta_{2\tau} &= \eta_{\tau} + g_{\tau}^+ \\
\eta_{3\tau} &= \eta_{\tau} + ig_{\tau}^- \\
\eta_{4\tau} &= \eta_{\tau} - ig_{\tau}^+.
\end{align*}
\]

Consequently, the dissipative dynamics of the system is described by the following SEOM

\[
\dot{\bar{\rho}}_S = -i[H_s, \bar{\rho}_S] + e^{-i\tau/4} \lambda^\frac{1}{2} \left\{ \hat{c}^\dagger g_\tau^- - g_\tau^+ \hat{c}, \bar{\rho}_S \right\} + e^{-i\tau/4} \lambda^\frac{1}{2} \left\{ \hat{c}^\dagger \eta_{3\tau} + \eta_{2\tau} \hat{c}, \bar{\rho}_S \right\} + e^{i\tau/4} \lambda^\frac{1}{2} \left\{ \hat{c} \eta_{3\tau} + \eta_{4\tau} \hat{c}, \bar{\rho}_S \right\}. \tag{39}
\]

The derivation is formally analogous to that for a boson bath, e.g., Eq. (17) in Ref. [52]. The non-Markovian bath
memory is captured by the memory-convoluted AGFs \( \{ g^\pm_n \} \), and the instantaneous AGFs \( \{ \eta_{lt}, \tilde{\eta}_{lt} \} \) characterize the fluctuations exerted by the bath to the system.

As will be verified in the next subsection, Eq. (39) is formally exact, as long as Eq. (32) is valid, i.e., if the fermion bath satisfies the Gaussian statistics and the quantum trajectories of \( \tilde{\rho}_s \) are equally weighted. However, the direct numerical implementation of Eq. (39) still faces fundamental difficulties, because of the problem in the realization of AGFs. Such difficulties severely hinder the practical use of Eq. (39) or its analogues for open fermionic systems. Consequently, all the previous efforts on fermionic SEOM ended up with formal derivations or transformation to deterministic approaches.

E. Equivalence between the formally exact SEOM and HEOM formalisms

We now analytically derive the equivalence between the SEOM of Eq. (39) and the rigorous HEOM. Similar to the derivation for a boson bath, we take the average on both sides of Eq. (39) over all the AGFs \( \{ \eta_{lt}, \tilde{\eta}_{lt} \} \). The reduced system dynamics is determined by the following EOM:

\[
\dot{\tilde{\rho}}_s = -i[H_s, (\tilde{\rho}_s)] + e^{-i\pi/4} \lambda^2 \left( \hat{c}^\dagger \langle g^+ \tilde{\rho}_s \rangle + \langle \tilde{\rho}_s g^+ \rangle \hat{c}^\dagger \right.
- \hat{c} \langle g^+ \hat{\rho}_s \rangle - \langle \hat{\rho}_s g^+ \rangle \hat{c} \right),
\]

where \( \langle \tilde{\eta}_{lt} \hat{\rho}_s \rangle = \langle \eta_{lt} \hat{\rho}_s \rangle = 0 \) because of the causality relation. Such an EOM is not self-close, because \( \langle \hat{\rho}_s g^+ \rangle \) and \( \langle \hat{g}_t \hat{\rho}_s \rangle \) are not an explicit function of \( \langle \hat{\rho}_s \rangle \). To proceed, we unravel the braided noncorrelation function \( C^\sigma(t) \) by a number of exponential functions,

\[
C^\sigma(t) = \sum_{m=1}^{M} C^\sigma_m(t) = \sum_{m=1}^{M} A^\sigma_m e^{\gamma^\sigma_m t},
\]

with the symmetry \( \gamma^+_m = (\gamma^-_m)^* \) satisfied, and the memory-convoluted AGFs are decomposed accordingly as \( g^\sigma_m = \sum_{m=1}^{M} g^\sigma_m(t) \). Each of the components, \( g^\sigma_m(t) \), satisfies a self-close EOM

\[
g^-_m = \lambda^{-1} \left[ -i \tilde{A}^-_m \eta_{lt} + (A^+_m)^* \eta_{lt} \right] + \gamma^-_m g^-_m,
\]

\[
g^+_m = \lambda^{-1} \left[ -i \tilde{A}^+_m \tilde{\eta}_{lt} + (A^-_m)^* \tilde{\eta}_{lt} \right] + \gamma^+_m g^+_m.
\]

In the path-integral formulation of HEOM, an \((I + J)\)th-tier auxiliary density operator (ADO) is defined by \((I \text{ and } J \text{ are arbitrary non-negative integers})\):

\[
\rho_{m_1 \cdots m_{I} n_{I+1} \cdots n_{J}} = \int D\bar{\psi} D\psi D\bar{\psi}' D\psi' e^{iS_{\psi}} F_{\psi} e^{-iS_{\bar{\psi}}}
\times B^-_{m_1} \cdots B^-_{m_I} B^+_n \cdots B^+_n \hat{\rho}_s(0),
\]

Here, \( \{ \tilde{\psi}, \tilde{\psi}' \} = \{ \psi, \psi' \} \) and \( \{ \psi, \psi' \} = \{ \tilde{\psi}, \tilde{\psi}' \} \) are g-numbers associated with \( \hat{c}^\dagger \) and \( \hat{c} \), respectively; \( S_{\psi} \) and \( S_{\bar{\psi}} \) are the forward and backward action functionals associated with \( F_{\psi} \) and \( \overline{F}_{\psi} \). The Feynman-Vernon influence functionals \( B^- \) and \( B^+ \) are the generating functionals:

\[
B^-_m = -i \int_0^t dt \left[ A^-_m \tilde{\psi}_\tau - (A^+_m)^* \tilde{\psi}'_\tau \right] e^{i\gamma^-_m (t-\tau)},
\]

\[
B^+_n = -i \int_0^t dt \left[ A^+_n \tilde{\psi}_\tau - (A^-_n)^* \tilde{\psi}'_\tau \right] e^{i\gamma^+_n (t-\tau)}.
\]

In the stochastic framework, such an \((I + J)\)th-tier ADO is retrieved as follows:

\[
\rho_{m_1 \cdots m_{I} n_{I+1} \cdots n_{J}} = \left( e^{i\pi/4} \lambda^2 \right)^{I+J} \langle g^-_{m_1} \cdots g^-_{m_I} g^+_n g^-_{n_{I+1}} \cdots g^-_{n_J} \rangle = \langle G^-_{m} \hat{\rho}_s g^+_n \rangle.
\]

For brevity, we will use the notation \( \prod \) to represent the ordered products, \( G^-_{m} \equiv \left( e^{i\pi/4} \lambda^2 \right)^I \prod_{j=1}^{I} g^-_{m_j} \), and \( G^+_{n} \equiv \left( e^{i\pi/4} \lambda^2 \right)^J \prod_{j=1}^{J} g^+_n \). In the ordered products, the indices \( \{ m_i \} \) and \( \{ n_j \} \) are arranged in the ascending order of \( i \) and \( j \). Accordingly, Eq. (40) is rewritten as

\[
\rho^{(0)}_{m} = -i[H_s, \rho^{(0)}_{m}] + i \sum_{m=1}^{M} \left( \hat{c} \rho_{m}^\dagger - \rho_{m} \hat{c}^\dagger \right)
+ \hat{c} \rho_{m}^\dagger - \rho_{m} \hat{c}^\dagger, \]

where \( \rho^{(0)}_{m} = \langle \tilde{\rho}_s \rangle \) is the reduced density matrix of the system, and \( \rho^{-}_{m} = e^{i\pi/4} \lambda^2 \langle g^-_{m} \hat{\rho}_s \rangle \) and \( \rho^{+}_{m} = e^{i\pi/4} \lambda^2 \langle \hat{\rho}_s g^+_n \rangle \) are the first-tier ADOs, respectively. Besides, an important equality is utilized in the derivation,

\[
\langle f(t) g^-_{m} \rangle = \langle g^-_{m} f(t) \rangle,
\]

which holds for any analytic function \( f(t) \) of the AGFs \( \{ \eta_{lt}, \tilde{\eta}_{lt} \} (j = 1, \cdots, 4) \).

To derive the EOM for the first-tier ADOs, we use the Ito’s formula to explore the differential of \( \hat{\rho}_s g^-_{m} \), which yields

\[
\frac{d}{dt} \hat{\rho}_s g^-_{m} = \langle d\hat{\rho}_s g^-_{m} \rangle + \langle d\hat{\rho}_s dg^-_{m} \rangle + \langle d\hat{\rho}_s dg^+_n \rangle + \langle d\hat{\rho}_s dg^+_{n} \rangle.
\]

Here, the first term on the right gives rise to ADOs at the second tier, while the last term retrieves the zeroth-tier ADO. Without loss of generality, the differential of \( \rho_{m_1 \cdots m_{I} n_{I+1} \cdots n_{J}} \) can be expressed as a sum of three parts,

\[
d\rho_{m_1 \cdots m_{I} n_{I+1} \cdots n_{J}} = \frac{d}{dt} \langle G^-_{m} \hat{\rho}_s G^+_n \rangle
= \langle dG^-_{m} \hat{\rho}_s G^+_n \rangle + \langle dG^-_{m} \hat{\rho}_s dG^+_n \rangle + \langle dG^-_{m} \hat{\rho}_s dG^+_n \rangle
= \Xi_1 + \Xi_2 + \Xi_3.
\]

Here, \( \Xi_1, \Xi_2 \) and \( \Xi_3 \) collect the contributions of ADOs
at the \((I + J + 1)\)th, \((I + J)\)th and \((I + J - 1)\)th tiers, respectively; whereas \((dg_m^- \rho \, dg_n^+) \sim O(dt^2)\) makes zero contribution. Presuming that the AGFs commute with the system creation and annihilation operators \(\hat{c}^\dagger\) and \(\hat{c}\) in the SEOM of Eq. (39), we have

\[
\Xi_1 = (g_m^- d \rho \, g_n^+) = -\sum_{i=1}^{M} [\hat{c}^\dagger \, \rho_{m_{-i}m_{-i+1}n_{-i+1}}] \, dt - \left( \sum_{i=1}^{M} [\hat{c}^\dagger \, \rho_{m_{-i}m_{-i+1}n_{-i+1}}] \right) \, dt
\]

Define the ordered products \(g_{m,-} \equiv (e^{i\pi/4\lambda^2})^{\sum_{i=1}^{N} g_{m,i}}\) and \(g_{m,-}^{-\infty} \equiv (e^{i\pi/4\lambda^2})^{\sum_{i=1}^{N} g_{m,i}}\), with which we have \(g_{m} = g_{m,-} \, g_{m,-}^{-\infty}\). Similarly, \(g_{n}^{-\infty} \) and \(g_{n}^{\infty}\) are introduced, and \(g_{m}^{-\infty} \, g_{n}^{-\infty}\) and \(g_{m}^{\infty} \, g_{n}^{\infty}\). Consequently, \(\Xi_2\) and \(\Xi_3\) are simplified as

\[
\Xi_2 = (dg_m^- \hat{\rho} \, g_n^+) + (g_m^- \hat{\rho} \, dg_n^+) = \left( \sum_{i=1}^{l} \langle g_{m_{-i}}^- \, d g_{m_{-i}} \, g_{m_{-i+1}}^- \, \rho \, g_{n_{-i+1}}^+ \rangle \right) + \left( \sum_{j=1}^{J} \langle g_{m_{-j}}^- \, \hat{\rho} \, g_{n_{-j}}^+ \, d g_{n_{-j}} \, g_{n_{-j+1}}^- \rangle \right) = \left( \sum_{i=1}^{l} \gamma_{m_{-i}} + \sum_{j=1}^{J} \gamma_{n_{-j}} \right) \rho_{m_{-i}m_{-i+1}n_{-i+1}} \, dt,
\]

and

\[
\Xi_3 = (dg_m^- \hat{\rho} \, g_n^+) + (g_m^- \hat{\rho} \, dg_n^+) = -\sum_{i=1}^{l} \left[ A_{m_{-i}}^- \hat{c} \langle g_{m_{-i}}^- \, \eta_{2t} \, g_{m_{-i+1}}^- \, \eta_{2t} \, \rho \, g_{n_{-i+1}}^+ \rangle \right] + \left( A_{m_{-i}}^+ \right)^* \langle g_{m_{-i}}^- \, \eta_{2t} \, g_{m_{-i+1}}^- \, \rho \, \eta_{2t} \, g_{n_{-i+1}}^+ \rangle \, \hat{c} \left( dt \right)^2
\]

Important equality,

\[
\langle g_{m_{-i}}^- \, \eta_{2t} \, g_{m_{-i+1}}^- \, \eta_{2t} \, \rho \, g_{n_{-i+1}}^+ \rangle \left( dt \right)^2 = \left( -1 \right)^{l-i} \langle \eta_{2t} \, \eta_{2t} \, g_{m_{-i}}^- \, \rho \, g_{m_{-i+1}}^- \, \eta_{2t} \, \rho \, g_{n_{-i+1}}^+ \rangle \left( dt \right)^2
\]

Equation (49) is finally recast into a compact form of

\[
\rho_{m_{-i}m_{-i+1}n_{-i+1}} = \left( -i \mathcal{L}_s + \sum_{i=1}^{l} \gamma_{m_{-i}} + \sum_{j=1}^{J} \gamma_{n_{-j}} \right) \rho_{m_{-i}m_{-i+1}n_{-i+1}} + \sum_{i=1}^{l} C_{m_{-i}}^- \, \rho_{m_{-i}m_{-i+1}n_{-i+1}} + \sum_{j=1}^{J} C_{n_{-j}}^+ \, \rho_{m_{-i}m_{-i+1}n_{-i+1}} + \sum_{i=1}^{M} A_{m_{-i}}^\sigma \, \rho_{m_{-i}m_{-i+1}n_{-i+1}}
\]

III. A NUMERICALLY FEASIBLE FERMIONIC SEOM METHOD

A. A minimal auxiliary space mapping scheme for the AGFs

In contrast with the bosonic case, the applications of the fermionic SEOM has been prohibited because of the numerical difficulty in realization of g-numbers. Different from the c-numbers, the g-numbers cannot be represented by scalars. Instead, it would require the use of N mutually anti-commutative matrices of the size \(2^N \times 2^N\) to represent a set of N g-numbers. The computer memory required to store these matrices will soon become too large with the increase of N.

To enable the direct stochastic simulation of fermionic dissipative dynamics by using the SEOM of Eq. (39) or its analogues, a mapping approach has been established in our previous work\textsuperscript{107}. In this subsection, we elaborate on this approach by providing more details and deeper insights.

Intuitively, one would attempt to “simplify” the time-dependent AGFs \(\{\eta_{j\tau}, \bar{\eta}_{j\tau}\}\) by separating the time dependence from the Grassmann character via the following mapping:

\[
\eta_{j\tau} \mapsto v_{j\tau} \xi_j, \quad \bar{\eta}_{j\tau} \mapsto v_{j\tau} \bar{\xi}_j \quad (j = 1, \ldots, 4),
\]
where \( \{ \xi_j, \tilde{\xi}_j \} \) are time-independent g-numbers, and \( \{ v_{j\tau} \} \) are Gaussian c-number noises with \( \mathcal{M}(v_{j\tau}) = 0 \) and \( \mathcal{M}(v_{j\tau} v_{j'\tau'}) = \delta_{jj'} \delta(t-\tau) \). Here, \( \mathcal{M}(\cdots) \) denotes the average over c-number noises. The mapping of Eq. (55) preserves the Grassmann character \( \eta_j \bar{\eta}_{j'} = -\bar{\eta}_{j'} \eta_j \), and the statistical properties \( \langle \eta_j \rangle = \langle \bar{\eta}_j \rangle = 0 \) and \( \langle \eta_j \bar{\eta}_j \rangle = \delta \delta(t-\tau) \). Meanwhile, such a mapping drastically reduces the memory cost for storing the AGFs, as the 8 time-independent g-numbers \( \{ \xi_j, \tilde{\xi}_j \} \) can be represented by 8 matrices of the size \( 2^j \times 2^j \). The system reduced density matrix can be obtained by

\[
\langle \tilde{\rho}_s \rangle = \int d\tilde{\xi} \ d\xi \ e^{-\xi \xi} \mathcal{M}(\tilde{\rho}_s),
\]

where \( \{ \xi, \tilde{\xi} \} \equiv \{ \xi_j, \tilde{\xi}_j \} \) \( (j = 1, \ldots, 4) \).

Unfortunately, the mapping of Eq. (55) cannot rigorously recover the result of Eq. (29). This is because some important properties of the original AGFs, such as

\[
\langle \eta_j \bar{\eta}_j \eta_{j'} \bar{\eta}_{j'} \rangle = \langle \eta_j \bar{\eta}_j \rangle \langle \eta_{j'} \bar{\eta}_{j'} \rangle - \langle \eta_j \bar{\eta}_{j'} \rangle \langle \eta_{j'} \bar{\eta}_j \rangle = [\delta(0) - \delta_{jj'}] \delta^2(t-\tau),
\]

are not preserved. The major drawback of Eq. (55) can be understood by considering the prototypical equation

\[
\hat{y} = y \left[ D(t) \eta_b + \int_0^t C(\tau) \bar{\eta}_r d\tau \right],
\]

where \( \eta_b \) and \( \bar{\eta}_r \) are time-dependent AGFs, and \( C(t) \) and \( D(t) \) are c-number functions. In Ref. 107 it has been shown that the mapping of Eq. (55) fails to reproduce the exact solution of Eq. (55).

To fix the above problem, we introduce a reduction procedure as a complement to Eq. (55). Such a procedure can be formally described by a linear operator \( \hat{r} \), which reduces any matching g-number pair (such as \( \xi_j, \tilde{\xi}_j \)) to 1 at each time step, i.e.,

\[
\hat{r}(1) = 1, \quad \hat{r}(\xi_j) = \xi_j, \quad \hat{r}(\tilde{\xi}_j) = \tilde{\xi}_j, \quad \hat{r}(\xi_j \tilde{\xi}_j) = 1.
\]

With the reduction procedure, any even-order moment of AGFs, including the one on the left-hand side of Eq. (55), is correctly reproduced. By applying Eq. (59) at each time step, the solution of Eq. (58) is exactly recovered; see the Supplemental Material of Ref. 107.

With the mapping of Eq. (55), \( \tilde{\rho}_s \) in the SEOM of Eq. (59) becomes an analytic function of \( \{ \xi_j, \tilde{\xi}_j \} \). The reduction procedure can be described by introducing the operators \( \{ \xi_j, \tilde{\xi}_j \} \), which can act on \( \tilde{\rho}_s \) from left or right:

\[
\hat{\xi}_j \tilde{\rho}_s = \hat{r}(\xi_j) \tilde{\rho}_s, \quad \tilde{\rho}_s \hat{\xi}_j = \hat{r}(\tilde{\xi}_j) \tilde{\rho}_s,
\]

\[
\hat{\tilde{\xi}}_j \tilde{\rho}_s = \hat{r}(\tilde{\xi}_j) \tilde{\rho}_s, \quad \tilde{\rho}_s \hat{\tilde{\xi}}_j = \hat{r}(\xi_j) \tilde{\rho}_s.
\]

More specifically, the left action results in

\[
\hat{\xi}_j 1 = \xi_j, \quad \hat{\xi}_j \xi_j = 0, \quad \hat{\xi}_j \tilde{\xi}_j = 1,
\]

\[
\hat{\tilde{\xi}}_j 1 = \tilde{\xi}_j, \quad \hat{\tilde{\xi}}_j \xi_j = 0, \quad \hat{\tilde{\xi}}_j \tilde{\xi}_j = -1.
\]  (61)

Similarly, for the right side action, we have

\[
\hat{\xi}_j 1 = \xi_j, \quad \xi_j \xi_j = 0, \quad \xi_j \tilde{\xi}_j = -1,
\]

\[
\hat{\tilde{\xi}}_j 1 = \tilde{\xi}_j, \quad \xi_j \tilde{\xi}_j = 0, \quad \tilde{\xi}_j \tilde{\xi}_j = 1.
\]  (62)

With Eq. (55) and the reduction operation, the time-dependent AGFs \( \{ \eta_j, \bar{\eta}_j \} \) are mapped to c-number noises \( \{ v_{j\tau} \} \) and a set of three elements \( \{ \xi_j, 1, \tilde{\xi}_j \} \).

Such a set is isomorphic to a minimal auxiliary space (MAS), \( S_j = \{ -1, 0, 1 \} \), via the following one-to-one correspondence:

\[
1 \rightarrow |0_j⟩, \quad \xi_j \rightarrow |−1_j⟩, \quad \tilde{\xi}_j \rightarrow |1_j⟩.
\]  (63)

Here, \(|0_j⟩, |−1_j⟩ \) and \(|1_j⟩ \) represent the three pseudo-Fock-states, i.e., the pseudo-vacuum, pseudo-hole and pseudo-particle states, of the \( j \)-th pseudo-level, respectively.

Accordingly, the operators \( \{ \xi_j, \tilde{\xi}_j \} \) correspond to the pseudo-operators \( \{ X_j^−, X_j^+ \} : \)

\[
\hat{\xi}_j \rightarrow X_j^−, \quad \hat{\tilde{\xi}}_j \rightarrow X_j^+.
\]  (64)

The AGFs \( \{ \eta_j, \bar{\eta}_j \} \) are finally represented by

\[
\eta_{j\tau} \rightarrow v_{j\tau} X_j^−, \quad \bar{\eta}_{j\tau} \rightarrow v_{j\tau} X_j^+ \quad (j = 1, \ldots, 4).
\]  (65)

Equation (65) is termed as the MAS mapping.

It is important to emphasize that, unlike normal operators which are associated with physical observables, the pseudo-operators are mathematical tools to assist tracking the time order of AGFs. For this purpose, the pseudo-operators are allowed to act on both the left and right sides of a pseudo-Fock-state (denoted by a ket), and the left and right actions may lead to different results. This is distinctly different from a normal operator. Specifically, the left actions of the pseudo-operators on the pseudo-Fock-states yield

\[
X_j^− |1_j⟩ = |0_j⟩, \quad X_j^− |0_j⟩ = |−1_j⟩, \quad X_j^− |−1_j⟩ = 0,
\]

\[
X_j^+ |1_j⟩ = 0, \quad X_j^+ |0_j⟩ = |1_j⟩, \quad X_j^+ |−1_j⟩ = −|0_j⟩.
\]  (66)

The actions from the right lead to

\[
|1_j⟩ X_j^− = −|0_j⟩, \quad |0_j⟩ X_j^− = |−1_j⟩, \quad |−1_j⟩ X_j^− = 0,
\]

\[
|1_j⟩ X_j^+ = 0, \quad |0_j⟩ X_j^+ = |1_j⟩, \quad |−1_j⟩ X_j^+ = |0_j⟩.
\]  (67)

Therefore, \( X_j^− \) and \( X_j^+ \) can be deemed as ladder-down and ladder-up pseudo-operators. Analogously to a spin system, we can also introduce the pseudo-spin-operator \( X_j^z \) as

\[
X_j^z |m_j⟩ = |m_j⟩ X_j^z = m_j |m_j⟩, \quad \text{for } m_j = 0, ±1.
\]  (68)
The pseudo-operators satisfy the following relations when acted from the left:

\[
\{ X^+_j, X^-_j \} = \delta_{jj'} X^+_j, \quad [ X^+_j, X^+_j ] = \pm \delta_{jj'} X^\pm_j ;
\]

while for the right action, we have

\[
\{ X^+_j, X^-_j \} = -\delta_{jj'} X^-_j, \quad [ X^-_j, X^-_j ] = \mp \delta_{jj'} X^\pm_j .
\]

Here, \[ \cdot, \cdot \] and \[ \cdot, \cdot \] represent the commutator and anti-commutator, respectively.

The MAS mapping preserves the exact solution of Eq. (65). However, such a mapping is intrinsically approximate because of the finite size of \( S_j \). For instance, some products of AGFs (such as \( \eta_{j\tau}, \bar{\eta}_{j\tau} \)) would become zero during the evolution, which inevitably leads to loss of memory. Consider another prototypical equation including a convolution integral,

\[
\dot{y} = y \left[ D(t) \eta_t + \int_0^t C(t - \tau) \bar{\eta}_\tau d\tau \right],
\]

where \( C(t) \) and \( D(t) \) are \( c \)-number functions. The MAS mapping of Eq. (65) does not recover the exact solution of \( \dot{y} \). Instead, it yields a reasonable approximation; see Ref. 107 for details.

### B. MAS-SEOM method for open fermionic systems

With the MAS mapping of Eq. (65), the stochastic reduced density matrix of the system \( \tilde{\rho}_s \) is now defined in the product space \( V = V_s \otimes S \), where \( V_s \) is the subspace of system, and \( S = S_1 \otimes S_2 \otimes S_3 \otimes S_4 \). In the product space \( V \), \( \tilde{\rho}_s(t) \) can be represented as

\[
\tilde{\rho}_s = \sum_{l_1 \in S_1} \sum_{l_2 \in S_2} \sum_{l_3 \in S_3} \sum_{l_4 \in S_4} \tilde{\rho}_{1l_1,2l_2,3l_3,4l_4},
\]

with \( \tilde{\rho}_{1l_1,2l_2,3l_3,4l_4} \) being a component corresponding to the pseudo-Fock-state \( |l_1, l_2, l_3, l_4 \rangle \) of the auxiliary space \( S \). In particular, we choose the initial condition to be \( \tilde{\rho}_s(0) = \rho_s(0) \otimes |0 \rangle \), where \( |0 \rangle = |0_1 \rangle \otimes |0_2 \rangle \otimes |0_3 \rangle \otimes |0_4 \rangle \) is the pseudo-vacuum state of \( S \).

The SEOM of Eq. (69) is cast into the following form:

\[
\dot{\tilde{\rho}}_s = -i[H_s, \tilde{\rho}_s] + e^{-i\pi/4} \lambda^* (\tilde{c} \tilde{c} Y_{1t} + Y_{2t} \tilde{c}) \tilde{\rho}_s + e^{i\pi/4} \lambda \tilde{\rho}_s (\tilde{c} \tilde{c} Y_{3t} + Y_{4t} \tilde{c}),
\]

where the pseudo-operators \( \{ Y_{j\tau} \} \) \( (j = 1, \cdots, 4) \) are defined by

\[
Y_{1t} \equiv v_{1t} X^+_1 + \tilde{g}_1, \quad Y_{2t} \equiv v_{2t} X^+_2 - \tilde{g}_2, \quad Y_{3t} \equiv v_{3t} X^+_3 - i\tilde{g}_3, \quad Y_{4t} \equiv v_{4t} X^+_4 + i\tilde{g}_4 .
\]

Through the MAS mapping, the memory-convoluted AGFs in Eq. (59), \( \{ g^\pm \} \), are replaced by \( \{ \tilde{g}^\pm \} \) as follows,

\[
\tilde{g}^- = \lambda^{-1} (\varphi_{4t} X^-_2 - i\varphi_{2t} X^-_2), \quad \tilde{g}^+ = \lambda^{-1} (\varphi_{3t} X^+_3 - i\varphi_{1t} X^+_1),
\]

where \( \{ \varphi \} \) \( (j = 1, \cdots, 4) \) are memory-convoluted \( c \)-number noises:

\[
\varphi_{1,2}(t) = \int_0^t d\tau C^\pm (t - \tau) v_{1,2}(\tau),
\]

\[
\varphi_{3,4}(t) = \int_0^t d\tau [C^\mp (t - \tau)]^* v_{3,4}(\tau).
\]

Based on Eqs. (66) and (67), \( \{ X^\pm \} \) acting on the left or right of \( \tilde{\rho}_s \) satisfy the following relation:

\[
X^\pm \tilde{\rho}_{1l_1,2l_2,3l_3,4l_4} = (-1)^{l_1 + l_2 + l_3 + l_4} \tilde{\rho}_{1l_1,2l_2,3l_3,4l_4} X^\pm .
\]

Equation (73) is termed as the MAS-SEOM, with which the reduced density matrix of system is obtained by projecting \( \tilde{\rho}_s(t) \) to the pseudo-vacuum state of the MAS, and then taking the stochastic average over all the Gaussian white noises \( \{ v_{j\tau} \} \) at \( 0 < \tau < t \):

\[
\tilde{\rho}_s = \mathcal{M} \{ \tilde{\rho}_s \} = \mathcal{M} (\tilde{\rho}_{s[0,0,0,0]}),
\]

where \( \mathcal{P} \equiv \{ 0 \} \) denotes the projection to the pseudo-vacuum state.

Compared with the space of the AGFs \( \{ \eta_{j\tau}, \bar{\eta}_{j\tau} \} \) \( (j = 1, \cdots, 4) \), the auxiliary space \( S \) is spanned by \( 3^4 \) pseudo-Fock-states, and hence the MAS mapping of Eq. (65) greatly reduces the computational cost. Consequently, the MAS-SEOM can be employed directly to do stochastic calculations. For a more general situation in which a multi-level system is coupled to more than one fermion baths, the MAS mapping is also applicable. The corresponding details of the MAS-SEOM will be elucidated in Sec. IV.C.

As the result of MAS mapping, the time-dependent AGFs in Eq. (59) are represented by time-dependent \( c \)-number fields with time-independent pseudo-levels. The stochastic transfers of particles between the system and the baths is replaced by the exchange of particle or hole from the system to the pseudo-levels. In the language of quantum chemistry, we can describe the AGFs \( \{ \eta_{j\tau}, \bar{\eta}_{j\tau} \} \) by the full configuration-interaction (CI) approach for the pseudo-levels in the auxiliary space. Nevertheless, the calculation of full CI is normally unfeasible in practice, so we truncate the auxiliary space by considering finite excitation configurations. In principle, the MAS is just an approximation at the single CI level, and the auxiliary space \( S_j \) is much smaller than the full space of AGFs. For instance, Eq. (73) only requires 4 matrices with the size of \( 3^4 \times 3^4 \) to represent all pseudo-operators, which can be directly applied to the simulation of fermionic dissipative dynamics. Although the MAS mapping (single CI) is an approximation for interacting systems, it leads to highly accurate results; see Ref. 107. In the next section, we will
assess the exactness or non-exactness of MAS-SEOM by different analytic approaches.

IV. APPROXIMATION PROPERTIES AND SOME IMPORTANT FEATURES OF MAS-SEOM

A. Approximate nature of MAS mapping

Although the MAS mapping of Eq. (39) preserves many important properties of the AGFs, such as \( \langle \eta_j \rangle = \langle \eta_j \rangle = 0 \) and \( \langle \eta_j \rangle \langle \eta_k \rangle = - \delta_{jk} \delta(t - \tau') \), the finite size of MAS inevitably causes the loss of memory. For instance, some products of AGFs, such as \( \eta_j \eta_k \eta_j \eta_k \), vanish during the evolution ofMAS-SEOM. In this section, we will scrutinize the difference between the formally exact SEOM of Eq. (39) and the MAS-SEOM of Eq. (73). In particular, we will focus on how the approximate nature of the MAS mapping affects the accuracy of the resulting SEOM. Two analytic approaches will be employed: the time-dependent perturbation theory approach and the HEOM approach.

B. Time-dependent perturbation theory

In this subsection, we assess the exactness or non-exactness of the MAS-SEOM by comparing the perturbation expansion of MAS-SEOM with the counterpart of the original Schrödinger equation of Eq. (2). Without loss of generality, we still choose a single-level system coupled to a fermion bath. The total Hamiltonian is \( H = H_0 + H_{sb} \) with \( H_0 = H_s + H_b \). In the Heisenberg interaction picture, the EOM of total density matrix is

\[
\hat{J}_t^\rho = -i [H_{\text{sb}}, \hat{J}_t^\rho] = -i \mathcal{L}_{\text{sb}}^1 \hat{J}_t^\rho.
\]

Here, \( \hat{J}_t^\rho = e^{iH_{0t}} \hat{\rho}_t e^{-iH_{0t}} \) and \( \mathcal{L}_{\text{sb}}^1 = e^{iH_{0t}} \tilde{L}_{\text{sb}} e^{-iH_{0t}} \) are the density matrix and the Liouville operator in the Heisenberg interaction picture, respectively. \( H_0 = \epsilon \hat{c} \hat{c}^\dagger \) is the Hamiltonian of the single-level system, and the system-bath coupling Hamiltonian \( H_{sb} = \kappa \hat{c} (\hat{c}^\dagger \hat{F} + \hat{F}^\dagger \hat{c}) \) with \( \kappa \) being the perturbation strength (\( \kappa > 0 \)) is taken as the perturbation.

We start with Eq. (73) and construct the deterministic time-dependent perturbation expansion in ascending order of the parameter \( \kappa \), i.e., \( \hat{\rho}_\gamma(t) = \text{tr}_B (\hat{\rho}_\gamma (t)) = \sum_{n=0}^{\infty} \hat{\rho}^{(2n)}(t) \). The nth-order response of system reduced density matrix to the perturbation is expressed as

\[
\hat{\rho}^{(2n)} = (-1)^n \int_0^t dt_1 \cdots \int_0^{t_{2n-1}} dt_{2n} \times \text{tr}_B [\mathcal{L}_{\text{sb}}^1 (t_1) \cdots \mathcal{L}_{\text{sb}}^1 (t_{2n}) \hat{\rho}_\gamma (0)],
\]

where the Liouville operators are arranged in the time-ordered form \( t > t_1 > \cdots > t_{2n-1} > t_{2n} \). The factorized initial condition \( \hat{\rho}_\gamma (0) = \rho_0 \hat{\rho}_b^{eq} \) is adopted, with \( \rho_0 = \hat{c} \hat{c}^\dagger = 1 - \hat{c}^\dagger \hat{c} \). In the following, we explicitly evaluate the low-order \((n = 1, 2)\) responses of \( \hat{\rho}_\gamma \) based on Eq. (59).

The first-order response of \( \hat{\rho}_\gamma \) is

\[
\hat{\rho}^{(2)}(t) = \kappa \int_0^t dt_1 \int_0^{t_1} dt_2 \text{tr}_B \{ [\hat{c} \hat{c}^\dagger (t_2) \rho_0 \hat{c} (t_1) \hat{F}^\dagger (t_2) \hat{F}(t_1) \}
\]

By using the definitions of two-time bath correlation functions, Eq. (51) results in

\[
\hat{\rho}^{(2)}(t) = \kappa \int_0^t dt_1 \int_0^{t_1} dt_2 \{ C^+(t_1 - t_2) \hat{c}^\dagger (t_2) \rho_0 \hat{c} (t_1) - \hat{c} (t_1) \hat{c}^\dagger (t_2) \rho_0 + C^+(t_2 - t_1) \}
\]

Here, \( \hat{c} (\tau) \equiv e^{-iH_0 \tau} \hat{c} e^{-iH_0 \tau} = e^{iH_s \tau} \hat{c} e^{-iH_s \tau} \), and \( C^+(\tau) \) are the bath correlation functions given by Eq. (34).

The second-order response of \( \hat{\rho}_\gamma \) to perturbation is expressed as

\[
\hat{\rho}^{(4)}(t) = \int_0^t dt_1 \cdots \int_0^{t_3} dt_4 \text{tr}_B [\mathcal{L}_{\text{sb}}^1 (t_1) \cdots \mathcal{L}_{\text{sb}}^1 (t_4) \hat{\rho}_\gamma (0)]
\]

where \( \gamma = (\gamma_1, \cdots, \gamma_4) \) with \( \gamma_j = L, R \). \( \hat{\rho}^{(4)} \) consists of 16 terms, and \( L (R) \) means that \( H_{sb}^1 \) acts on \( \hat{\rho}_\gamma \) (left (right)). Each term can be expressed as

\[
\hat{\rho}^{(4)}(t) = \kappa \cdots \int_0^t dt_1 \cdots \int_0^{t_3} dt_4 \hat{R}_{\gamma} (t_1, \cdots, t_4)
\]

where \( \{ \hat{R}_{\gamma} (t_1, \cdots, t_4) \} \) involve the four-time bath correlation functions. For example, \( \hat{R}_{\text{LLL}}^4 (t_1, \cdots, t_4) \) is expressed as

\[
\hat{R}_{\text{LLL}}^4 (t_1, \cdots, t_4) = \kappa^2 \hat{c} (t_1) \hat{c}^\dagger (t_2) \hat{c}^\dagger (t_3) \hat{c} (t_4) \rho_0
\]

Here, the second equality makes use of the Gaussian statistical property that a high-order bath correlation function can be fully expressed by the two-time correlation functions \( C^\pm (\tau) \). The other 15 members of \( \{ \hat{R}_{\gamma} (t_1, \cdots, t_4) \} \) can be expressed in a similar fashion.

In the following, we start with the MAS-SEOM, and build a perturbation expansion in the stochastic frame-
work. The results will be compared directly with the above formulas based on Eq. (79). In the interaction picture of $H_\alpha$, the MAS-SEOM of Eq. (80) can be expressed as the following:

$$\dot{\hat{\rho}}_s^1 = e^{-i\tau/4} \lambda^\frac{1}{2} \left[ \hat{c}^\dagger(t) Y_{1t} + Y_{2t} \hat{c}(t) \right] \hat{\rho}_{s0}^1$$

$$+ e^{i\tau/4} \lambda^\frac{1}{2} \hat{\rho}_{s0}^1 \left[ \hat{c}^\dagger(t) Y_{3t} + Y_{4t} \hat{c}(t) \right]$$

$$- i \hat{L}^1 \hat{\rho}_{s0}^1,$$

(86)

where $\hat{L}^1 \equiv e^{i H_s t} \hat{L} e^{-i H_s t}$ is the stochastic Liouville operator in the interaction picture, and the pseudo-operators $\{Y_{\gamma t}\}$ are defined by

$$Y_{1t} \equiv \kappa^\frac{1}{2} \left( \hat{v}_{1t} X_1^+ + \hat{g}_1^t \right),$$

$$Y_{2t} \equiv \kappa^\frac{1}{2} \left( \hat{v}_{2t} X_2^+ - \hat{g}_1^t \right),$$

$$Y_{3t} \equiv \kappa^\frac{1}{2} \left( \hat{v}_{3t} X_3^+ - i \hat{g}_1^t \right),$$

$$Y_{4t} \equiv \kappa^\frac{1}{2} \left( \hat{v}_{4t} X_4^+ + i \hat{g}_1^t \right).$$

We now take the stochastic Liouvillean as the perturbation, and construct the perturbation expansion in ascending order of the parameter $\kappa$. $\hat{\rho}_{s0}^n = \sum_{n=0}^\infty \hat{\rho}_s^{(2n)}$. Similar to Eq. (80), the $n$th-order response of system reduced density matrix is expressed as

$$\hat{\rho}_s^{(2n)} = (-1)^n \int_0^t dt_1 \cdot \int_0^{t_2-n} dt_2 \hat{L}^1(t_1) \cdot \hat{L}^1(t_2) \hat{\rho}_s(0),$$

(87)

where the Liouville operators are also arranged in the time-order form $(t > t_1 > \cdots > t_{2n-1} > t_{2n})$, and the initial condition is $\hat{\rho}_s(0) = \rho_0 \otimes |0\rangle$.

The first-order response of $\langle \hat{\rho}_s \rangle$ is

$$\langle \hat{\rho}_s^{(2)} \rangle = - \int_0^t dt_1 \int_0^{t_1} dt_2 \langle \hat{L}^1(t_1) \hat{L}^1(t_2) \hat{\rho}_s(0) \rangle$$

$$= \int_0^t dt_1 \int_0^{t_1} dt_2 \left[ - i \lambda \hat{c}(t_1) \hat{c}^\dagger(t_2) \rho_0 \mathcal{M}(Y_{2t_1} Y_{1t_2} | 0) \right]$$

$$+ \lambda \hat{c}(t_2) \rho_0 \hat{c}(t_1) \mathcal{M}(Y_{1t_2} Y_{2t_1} | 0)$$

$$+ i \lambda \rho_0 \hat{c}(t_2) \hat{c}^\dagger(t_1) \mathcal{M}(0 Y_{1t_2} Y_{2t_1})$$

$$+ \lambda \hat{c}^\dagger(t_1) \rho_0 \hat{c}(t_2) \mathcal{M}(Y_{1t_1} Y_{2t_2} Y_{4t_1} | 0)$$

$$= \kappa \int_0^t dt_1 \int_0^{t_1} dt_2 \left[ \hat{c}(t_1) \hat{c}^\dagger(t_2) \rho_0 \mathcal{M}(\varphi_{1t_1}, v_{1t_2} | 0) \right]$$

$$\times \mathcal{P}(X_1^+ X_1^- | 0)$$

$$+ \hat{c}(t_2) \rho_0 \hat{c}(t_1) \mathcal{M}(\varphi_{1t_2}, v_{1t_1} | 0) \mathcal{P}(0 X_1^+ X_1^-)$$

$$+ i \rho_0 \hat{c}(t_2) \hat{c}^\dagger(t_1) \mathcal{M}(0, 0) \mathcal{P}(X_1^+ X_1^-)$$

$$+ \hat{c}^\dagger(t_1) \rho_0 \hat{c}(t_2) \mathcal{M}(\varphi_{4t_1}, v_{4t_2} | 0) \mathcal{P}(0 X_1^+ X_1^-),$$

(88)

The second-order response of $\langle \hat{\rho}_s \rangle$ is

$$\langle \hat{\rho}_s^{(4)} \rangle = \int_0^t dt_1 \cdots \int_0^{t_4} dt_4 \hat{L}^1(t_1) \cdots \hat{L}^1(t_4) \hat{\rho}_s(0)$$

$$= \sum_\gamma \langle \hat{\rho}_s^{(4)} \rangle,$$

(89)

where $\gamma = (\gamma_1, \cdots, \gamma_4)$ with $\gamma_j = L, R$. Similar to Eq. (80), $\hat{\rho}_s^{(4)}$ consists of 16 terms, and L (R) means that the pseudo-operators $\{Y_{\gamma t}\}$ act on $\hat{\rho}_s$ from left (right). The statistical average of the second-order response is

$$\langle \hat{\rho}_s^{(4)} \rangle = \sum_\gamma \langle \hat{\rho}_s^{(4)} \rangle,$$

(90)

For example, for $\gamma = (LLLL)$, we have

$$\langle \hat{R}_{LLLL}^{(4)} \rangle = - \lambda^2 \hat{c}(t_1) \hat{c}^\dagger(t_2) \hat{c}(t_3) \hat{c}^\dagger(t_4) \rho_0$$

$$\times \mathcal{M}(Y_{2t_1} Y_{1t_2} Y_{2t_3} Y_{1t_4} | 0)$$

$$= \kappa^2 \hat{c}(t_1) \hat{c}^\dagger(t_2) \hat{c}(t_3) \hat{c}^\dagger(t_4) \rho_0 \mathcal{M}(\varphi_{1t_1}, v_{1t_2})$$

$$\times \mathcal{M}(\varphi_{1t_2}, v_{1t_1}) \mathcal{P}(X_1^+ X_1^- X_1^+ X_1^- | 0)$$

$$- \mathcal{M}(\varphi_{1t_2}, v_{1t_1}) \mathcal{M}(\varphi_{2t_3}, v_{2t_4})$$

$$\times \mathcal{P}(X_1^+ X_1^- X_2^+ X_2^- | 0) \mathcal{P}(X_1^+ X_1^- X_2^+ X_2^- | 0).$$

(91)

It can be verified that the final expression of $\langle \hat{R}_{LLLL}^{(4)} \rangle$ in Eq. (81) is identical to $\langle \hat{R}_{LLLL}^{(4)} \rangle$ of Eq. (80). Likewise, it is found that $\langle \hat{R}_\gamma^{(4)} \rangle = \hat{R}_\gamma^{(4)}$ holds for other $\gamma$, and thus $\langle \hat{\rho}_s^{(4)} \rangle = \hat{\rho}_s^{(4)}$. Therefore, the MAS-SEOM exactly reproduces the first- and second-order response of $\hat{\rho}_s$.

The discrepancy of the MAS-SEOM from the exact Liouville equation emerges from the third-order response. From Eq. (80), the third-order response of $\hat{\rho}_s$ is a summation of $2^6 = 64$ contributions,

$$\hat{\rho}_s^{(6)} = \sum_\gamma \int_0^t dt_1 \cdots \int_0^{t_6} dt_6 \hat{R}_\gamma^{(6)}(t_1, \cdots, t_6)$$

$$= \sum_\gamma \langle \hat{\rho}_s^{(6)} \rangle,$$

(92)

where $\gamma = (\gamma_1, \cdots, \gamma_6)$ with $\gamma_j = L, R$. For example, $\hat{R}_{LLLLLLL}^{(6)}$ is expressed as

$$\hat{R}_{LLLLLLL}^{(6)} = \kappa^3 \hat{c}(t_1) \hat{c}^\dagger(t_2) \hat{c}(t_3) \hat{c}^\dagger(t_4) \hat{c}(t_5) \hat{c}^\dagger(t_6) \rho_0$$

$$\times \text{tr}_B \left[ \hat{F}^\dagger(t_1) \hat{F}(t_2) \hat{F}^\dagger(t_3) \hat{F}(t_4) \hat{F}^\dagger(t_5) \hat{F}(t_6) \rho_B^0 \right]$$

$$= \kappa^3 \hat{c}(t_1) \hat{c}^\dagger(t_2) \hat{c}(t_3) \hat{c}^\dagger(t_4) \hat{c}(t_5) \hat{c}^\dagger(t_6) \rho_0$$

$$\times \hat{\tilde{R}}^{(6)}_{LLLLLLL},$$

(93)

where $\hat{\tilde{R}}^{(6)}_{LLLLLLL}$ is a sixth-order bath correlation function. Because of the Gaussian statistics, the trace over the bath DOF for the evaluation of $\hat{\tilde{R}}^{(6)}_{LLLLLLL}$ can be contracted.
by the Wick’s theorem into $3! = 6$ terms. Here, we only select one of them and use it as the reference for the perturbation analysis based on the MAS-SEOM. The selected term is
\[
\hat{r}^{(6)}_{LLLLLL}(t') = C^+(t_1 - t_6)C^-(t_2 - t_5)C^+(t_3 - t_4),
\]
where the vector $t' = \{t_1, t_6\}, \{t_2, t_5\}, \{t_3, t_4\}$ indicates the pairs of time instants corresponding to the contracted operator pairs.

Based on the MAS-SEOM, the third-order response of $\hat{\rho}_g$ is
\[
\hat{\rho}^{(6)}_g = -\sum_{\gamma} \int_0^t dt_1 \cdots \int_0^{t_3} dt_4 \hat{R}^{(6)}_\gamma(t_1, \ldots, t_6),
\]
where $\gamma = (\gamma_1, \ldots, \gamma_6)$ with $\gamma_3 = L, R$. In particular, the statistical average of $\hat{R}^{(6)}_{LLLLLL}(t_1, \ldots, t_6)$ is
\[
\langle \hat{R}^{(6)}_{LLLLLL} \rangle = -i\lambda^3 \hat{c}(t_1) \hat{c}^+(t_2) \hat{c}(t_3) \hat{c}^+(t_4) \hat{c}(t_5) \hat{c}^+(t_6) \rho_0 \times \mathcal{M}[\{Y_1, Y_{12}, Y_{14}, Y_{15}, Y_{16}\}|0]\rangle = \kappa^2 \hat{c}(t_1) \hat{c}^+(t_2) \hat{c}(t_3) \hat{c}^+(t_4) \hat{c}(t_5) \hat{c}^+(t_6) \rho_0 \times \langle \hat{r}^{(6)}_{LLLLLL} \rangle.
\]
In relation to Eq. (94), we explicitly write the component
\[
\langle \hat{r}^{(6)}_{LLLLLL} \rangle = C^+(t_1 - t_6)C^-(t_2 - t_5)C^+(t_3 - t_4) \times \mathcal{P}[X_1^+ X_2^+ X_1^- X_2^- X_1^- |0]\rangle
\]
(97)
Here, $X_1^-$ acts on the pseudo-vacuum state $|0\rangle$ twice consecutively, and thus yields the zero value of $\hat{r}^{(6)}_{LLLLLL}(t')$. Consequently, $\langle \hat{r}^{(6)}_{LLLLLL} \rangle \neq \hat{r}^{(6)}_{LLLLLL}(t')$. Similar discrepancies are also found for other components of $\{\hat{r}^{(6)}_g\}$—altogether 36 out of 384 components are different. Therefore, the third-order response of system reduced density matrix obtained from the MAS-SEOM, $\langle \hat{\rho}^{(6)}_g \rangle$, does not fully recover $\hat{\rho}^{(6)}_g$ of the original Liouville equation. It is thus clear that the finite size of auxiliary space $S_j$ indeed leads to loss of memory for the reduced system dynamics.

In this subsection, we have demonstrated on the time-dependent perturbation theory, we have demonstrated that the MAS-SEOM reproduces the exact reduced system dynamics up to the second-order response. The discrepancy of higher-order response is clearly ascribed to the finite size of the MAS. However, from the perturbation theory it is hard to tell how significantly the discrepancy will affect the accuracy of the numerical results of MAS-SEOM. In the following subsection, we will address this issue by making connection to the HEOM formalism.

C. Equivalence between the MAS-SEOM and a simplified HEOM method

For the convenience of analysis, we consider again a single-level system coupled to a fermion bath. Moreover, the number of pseudo-operators $\{X^\sigma_j\}$ involved in the MAS-SEOM of Eq. (73) are halved by assuming $X_1^\pm = X_3^\pm$ and $X_2^\pm = X_4^\pm$. Accordingly, the memory-convoluted fields $\tilde{g}_m^\pm$ are simplified as
\[
\tilde{g}_m^- = \lambda^{-1}(\varphi_{m\tau} - i\varphi_{m\tau}) X_{m\tau}^-,
\]
\[
\tilde{g}_m^+ = \lambda^{-1}(\varphi_{m\tau} - i\varphi_{m\tau}) X_{m\tau}^+,
\]
where $\{\varphi_{m\tau}\}$ are given in Eq. (76), and the resulting MAS-SEOM still has the form of Eq. (79).

We now examine the HEOM associated with the MAS-SEOM. By unraveling the bath correlation functions via Eq. (111), we have $\tilde{g}_m^\pm = \sum_{m=1}^M g_m^\pm(t)$, with
\[
\tilde{g}_m^- = \sum_{m=1}^M \lambda^{-1} \int_0^t dt \left[ -i A_m v_2 + (A_m) v_4 \right] e^{\gamma_m(t-\tau)} X_2^-,
\]
\[
\tilde{g}_m^+ = \sum_{m=1}^M \lambda^{-1} \int_0^t dt \left[-i A_m^* v_1 + (A_m^*) v_3 \right] e^{\gamma_m(t-\tau)} X_1^+,
\]
(99)
An $(J + J)$th-tier ADO of the HEOM is defined by
\[
\rho^{\langle\cdots\cdots\cdots\rangle}_{m_1\cdots m_J} = (e^{i\tau/4})^{J+J} \langle \tilde{g}_{m_1}^- \cdots \tilde{g}_{m_J}^- \tilde{g}_{m_1}^+ \cdots \tilde{g}_{m_J}^+ \rangle,
\]
where $\langle \cdots \rangle \equiv \mathcal{M}(\cdots)$, and the subscript of the ADO is determined by the sequence of $\{g_m^\pm\}$ and $\{g_\pm\}$ at the left and right of $\hat{\rho}_g$.

It is immediately recognized that the ADO is zero by definition if the right-hand side of Eq. (100) involves two or more identical pseudo-operators $X^\sigma_j$. This is because of the finite size of the MAS $S_j$, so that a pseudo-level can accommodate at most one particle or hole, and thus $\mathcal{P}[\{X^\sigma_j\}^p \tilde{\rho}_g] = \mathcal{P}[\tilde{\rho}_g X_1^\sigma]^p |0\rangle = 0$ for $p > 1$. For instance, $\tilde{\rho}_{m_1 m_2}^- = \langle \tilde{g}_{m_2}^- \tilde{g}_{m_1}^\tau \rangle = 0$, because $\mathcal{P}[X_2^- X_1^- \tilde{\rho}_g] = 0$. Likewise, the ADOs $\{\rho_{m_1 m_2}^\pm, \rho_{m_1 m_2} \rho_{m_1 m_2}^\pm, \rho_{m_1 m_2}^\pm \rho_{m_1 m_2} \}$ are all zero. By referring to the full HEOM of Eq. (75), these ADOs have a common feature: they involve two or more generating functionals $\{\mathcal{B}^\sigma_n\}$ that have the same $\sigma$ (different only in the index $m$). Such ADOs are termed as the interference ADOs.\(^22\)

Evidently, the HEOM corresponding to the MAS-SEOM of Eq. (73) is a finite hierarchy which terminates automatically at the second tier. The only nonzero ADOs in the hierarchy are $\{\rho_0, \rho_{m_1}, \rho_{m_2}, \rho_{m_1 m_2}\}$. Presuming that $X^\sigma_j$ commutes with $\hat{c}$ and $\hat{c}^+$ and using the equality $\langle X^\sigma_j \rho_o \rangle = -\langle \rho_o X^\sigma_j \rangle$, it can be proved that the EOM of any nonzero ADO has the same form of Eq. (74). Such a finite hierarchy with all the interference ADOs excluded is termed as the simplified HEOM (sim-HEOM). Its detailed derivation as well as the main features are provided in Ref.\(^22\).
To better understand the correspondence between the MAS mapping and the zero interference ADOs, we further consider a more general case in which a system of $N_\nu$ levels is coupled to $N_\alpha$ fermion baths. The corresponding MAS-SEOM is

\[
\dot{\tilde{\rho}}_\nu = -i[H_\nu, \tilde{\rho}_\nu] + \lambda_\nu^2 \sum_{\nu=1}^{N_\nu} \sum_{\alpha=1}^{N_\alpha} \left[ e^{i\sigma_\nu} (\tilde{c}_\nu^{\dagger} Y_{1\nu\alpha} + Y_{2\nu\alpha} \tilde{c}_\nu) \tilde{\rho}_\nu + e^{i\sigma_\nu} \tilde{\rho}_\nu (\tilde{c}_\nu^{\dagger} Y_{3\nu\alpha} + Y_{4\nu\alpha} \tilde{c}_\nu) \right].
\]

(101)

Here, $\nu$ and $\alpha$ label the system levels and the fermion baths, respectively. The pseudo-operators $\{Y_{j\nu\alpha}\} (j = 1, \cdots, 4)$ are defined by

\[
Y_{1\nu\alpha} \equiv v_{1\nu\alpha} X_{1\nu} - \tilde{g}_{1\nu\alpha}, \quad Y_{2\nu\alpha} \equiv v_{2\nu\alpha} X_{2\nu}^\dagger - \tilde{g}_{2\nu\alpha},
\]

\[
Y_{3\nu\alpha} \equiv v_{3\nu\alpha} X_{1\nu}^\dagger - i \tilde{g}_{3\nu\alpha}, \quad Y_{4\nu\alpha} \equiv v_{4\nu\alpha} X_{2\nu} + i \tilde{g}_{4\nu\alpha}.
\]

(102)

If there is no cross-correlation between any two system levels via the bath, we have $\tilde{g}_{j\nu\alpha} = \sum_m \tilde{g}_{j\nu\alpha}(t)$ by unraveling the bath memory, with

\[
\tilde{g}_{j\nu\alpha}(t) = \lambda_j^{-1} \int_0^t d\tau \left[ -i A_{j\nu\alpha} v_{j\nu\alpha\nu\alpha} + (A_{j\nu\alpha}^{\dagger})^* v_{j\nu\alpha\nu\alpha} \right] \times e^{\gamma_j \nu\alpha\nu\alpha(\tau - \tau')} X_{j\nu}(\tau - \tau').
\]

(103)

The Gaussian white noises satisfy $\mathcal{M}(v_{j\nu\alpha} v_{j'\nu'\alpha'\alpha'}) = \delta_{jj'}\delta_{\nu\nu'}\delta_{\alpha\alpha'}\delta(\tau - \tau')$.

In the following, we use $p$ and $q$ to denote the multi-component index $(\nu\alpha\nu\alpha)$. Based on the MAS-SEOM of Eq. (101), an $(I + J)$th-tier ADO is constructed by

\[
\hat{\rho}_{p_1 \cdots p_I q_1 \cdots q_J}^{(I + J)} \equiv \langle \psi_{\nu_1} \cdots \psi_{\nu_I} \tilde{\rho}_\nu \psi_{\nu_1} \cdots \psi_{\nu_I} \psi_{\nu_1} \cdots \psi_{\nu_I} \rangle.
\]

(104)

In the framework of HEOM the same ADO is defined as

\[
\hat{\rho}_{p_1 \cdots p_I q_1 \cdots q_J}^{(I + J)} \equiv \int D\bar{\psi}_1 D\psi_1 D\bar{\psi}_2 D\psi_2 e^{i S_h} F_{p_I} e^{-i S_h} \times B^{-\dagger}_{p_I \cdots p_I} B_{p_I \cdots p_I} \cdots B^{-\dagger}_{q_I \cdots q_I} B_{q_I \cdots q_I} \tilde{\rho}_\nu(0),
\]

(105)

with the generating functionals given by

\[
B_{\nu\alpha\nu\alpha} = -i \int_0^t d\tau \left[ A_{\nu\alpha\nu\alpha} \psi_{\nu\alpha} - (A_{\nu\alpha\nu\alpha}^{\dagger})^* \psi_{\nu\alpha} \right] e^{\gamma_{\nu\alpha\nu\alpha}(\tau - \tau')},
\]

\[
B_{\nu\alpha\nu\alpha}^+ = -i \int_0^t d\tau \left[ A_{\nu\alpha\nu\alpha} \psi_{\nu\alpha} - (A_{\nu\alpha\nu\alpha}^{\dagger})^* \psi_{\nu\alpha} \right] e^{\gamma_{\nu\alpha\nu\alpha}(\tau - \tau')}.
\]

(106)

If the ADO defined by Eq. (105) includes two or more generating functionals $(B^{\sigma}_{\nu\alpha\nu\alpha})$ that have the same $\sigma$ and $\nu$ (different only in $\alpha$ or $m$), it belongs to the interference ADOs. Based on the MAS-SEOM of Eq. (101), such an interference ADO must have a zero value because $\mathcal{P}[X_{\nu\nu}^\sigma] \rho\nu_{\nu\nu\nu} = \mathcal{P}[\tilde{\rho}_\nu X_{\nu\nu}^\sigma] = 0$ for $p > 1$. Therefore, the MAS-SEOM of Eq. (101) is formally equivalent to the sim-HEOM in which all the interference ADOs are excluded.

Alternatively, if $X_{\nu\nu}^\sigma$ is replaced by $X_{\nu\nu}^\sigma$ in Eqs. (102) and (103), the resulting MAS-SEOM is formally equivalent to the so-called sim-HEOM-\(\alpha\) formalism in which an interference ADO involves two or more generating functionals $(B^{\sigma}_{\nu\alpha\nu\alpha})$ that have the same $\sigma$, $\alpha$ and $\nu$ (different only in the index $m$). Apparently, the sim-HEOM-\(\alpha\) formalism is less approximate than the sim-HEOM, because in the former a smaller number of interference ADOs are excluded from the hierarchy.

From the above analysis, it is clear that the MAS mapping itself is intrinsically approximate, as it may cause loss of memory (or interference information) if the particle transfer event occurs consecutively through a same dissipation mode. Because the MAS-SEOM and the sim-HEOM (or the sim-HEOM-\(\alpha\)) are formally equivalent, they share the following common features:

(i) They yield the exact reduced dynamics, if the bath correlation functions $C^{\pm}_{\nu\nu}(t)$ have the form of a single exponential function. This is obvious because the index $m$ would become redundant, and hence there is no interference ADO in the original full HEOM.

(ii) They yield the exact single-particle properties for any non-interacting system. This is because for non-interacting systems the HEOM truncated at the second tier already yield the exact reduced single-particle density matrix and the interference ADOs have no influence on the latter, i.e., $\text{tr}_\gamma[\tilde{\rho}_{\nu\nu}(\tau)] = \text{tr}_\gamma[\tilde{\rho}_{\nu\nu}(0)] = 0$. Therefore, the interference ADOs can be safely omitted from the full hierarchy without affecting the exactness of the resulting single-particle properties.

(iii) For general interacting systems, they are in principle approximable, and the interference ADOs are supposedly important for the quantitative description of strong correlation effects such as the Kondo phenomena. Indeed, the discrepancies between the results of sim-HEOM and those of the full HEOM have been demonstrated in Ref. 22. Nevertheless, as shown in Ref. 107 and in our paper II in many cases the MAS-SEOM can still provide reasonably or even remarkably accurate predictions for the dissipative dynamics of an interacting system.

V. CONCLUDING REMARKS

To summarize, in this paper we first derive a rigorous SEOM for describing the dissipative dynamics of fermionic open systems. The SEOM of Eq. (38) is formally exact and is equivalent to the rigorous fermionic HEOM formalism. However, such an SEOM is numerically infeasible because of the difficulty in modeling g-numbers.

We then propose a MAS mapping scheme with which the time-dependent g-numbers are mapped to time-
With the HEOM method, the stationary state (thermal equilibrium state or non-equilibrium steady state) can be obtained either by propagating the HEOM to the asymptotic long-time limit, or by solving the hierarchically coupled linear equations resulted from the stationary condition. However, neither of these two approaches is currently available for the MAS-SEOM method. A related issue is that so far only the decoupled initial state has been considered for the MAS-SEOM. It remains unclear how to formulate the MAS-SEOM with a correlated initial state, which is important for many practical purposes. The imaginary-time SEOM is a potentially promising approach, but related works for fermionic environments have not been reported. Much effort is needed in this direction.

While the numerical aspects of MAS-SEOM are to be discussed in Ref. 108, we would like to point out here that, unlike the HEOM method, the MAS-SEOM does not require explicit unraveling of the bath correlation functions, and hence the cost of computer memory is trivial compared to the HEOM method. Therefore, the MAS-SEOM is particularly favorable for exploring the dissipative dynamics at ultra-low temperatures, which is still challenging for the present HEOM method. Furthermore, parallel computing techniques have been applied to the HEOM method, but related works for fermionic environments have not been reported. Massive parallelization is expected to be very easy for the MAS-SEOM, since the quantum trajectories are mutually independent and equally weighted.

Finally, because the MAS mapping is intrinsically approximate, for some interacting open systems, such as the strongly correlated quantum impurity systems, the numerical accuracy of the present MAS-SEOM might not be satisfactory. Even for these systems, the MAS-SEOM provides a valuable foundation for the future development of more sophisticated stochastic QDTs.

TABLE I. An overview of various aspects of the present fermionic HEOM method and the MAS-SEOM method. “Y” means the method possesses the specific feature or is feasible for the specific situation, while “N” means the method does not possess the feature or is unfeasible for the situation. See the main text in Sec. V for details.

| Aspect                                  | HEOM | MAS-SEOM |
|-----------------------------------------|------|----------|
| exactness (non-interacting system)      | Y    | Y        |
| exactness (interacting system)          | Y    | N        |
| short-time dynamics                     | Y    | Y        |
| long-time dynamics                      | Y    | N        |
| stationary state                        | Y    | N        |
| correlated initial state                | Y    | N        |
| ultra-low temperature                   | N    | Y        |
| massive parallel computation            | Y    | Y        |

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