Exact dynamics and thermalization of open quantum systems coupled to reservoirs through particle exchanges

Fei-Lei Xiong and Wei-Min Zhang[*]
Department of Physics and Center for Quantum Information Science, National Cheng Kung University, Tainan 70101, Taiwan

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In this paper, we study the exact dynamics of general open systems interacting with their environments through particle exchanges. The paper includes two main results. First, by taking advantage of the propagating function in the coherent state representation, we obtain the exact solution of the reduced density matrix, which is expressed in terms of the nonequilibrium Green functions. Second, in the dynamical perspective, we provide a rigorous thermalization process of open quantum systems.

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I. INTRODUCTION

In the real world, physical systems are inevitably coupled to environments, which makes the theory of open quantum systems vastly useful in very diverse research fields, including physics, chemistry, biology, and engineering. The systematic study of open quantum systems has aroused researcher interest since the 1960s [1–7], and has become more and more important for the developing fields of quantum information processing [7–9], quantum transport theory [10,11], and rapidly improving time-resolved measurement technologies [12,13]. One of the most crucial problems in dealing with open quantum systems is how to determine explicitly the evolution of open quantum system states, through which all the information about the system dynamics can be obtained. However, due to the contamination of a huge environment, the system dynamics is nonunitary and always involves complicated fluctuations and dissipation. As a consequence, to date most open quantum systems can only be dealt with perturbative methods, such as the Born-Markov approximation or cutting off in the Nakajima-Zwanzig operator projective technique [3–5]. Only for a few classes of open quantum systems, e.g., the harmonic oscillator in quantum Brownian motion [14,15] and the open systems interacting with particle-exchange coupling [16–20], can an exact master equation be obtained, let alone the exact state evolution.

In a series of papers [16–20], we have obtained the general exact master equation for open quantum systems whose interactions with reservoirs only involve particle exchanges. This large class of open quantum systems is an extension of the famous Fano-Anderson model [21,22] which characterizes many physical phenomena in different systems, such as Fano resonance in atomic physics and nanoelectronic systems [23], Anderson localization in condensed matter physics [21], photon-atom bound states in photonic crystals [24–26], quantum transport in various junctions [10], impurity defects in solids [27], etc. With the recent progress on the exact master equation for such a large class of noninteracting open quantum systems [16–19], various perspectives of open systems can be studied, e.g., memory effects [28–31], entanglement dynamics [32–34], non-Markovian decoherence [17,35,36], exact transient quantum transport [11,37,38], etc.

In this paper, one main result we obtained is the solution of the exact master equation, i.e., the exact form of the reduced density matrix of an open system at an arbitrary later time. Note that the time dependence of the reduced density matrix includes complete information about the system dynamics, and it offers more perspectives in studying the memory effects [28,29,39,40], entanglement dynamics, and dynamical phase transition [33,41]. Using the result of the reduced density matrix, in this paper we also study general thermalization, which is another important and hot topic for both experimentalists [42,43] and theorists [44–55] in recent years. In equilibrium statistic mechanics, the thermal distribution is based on the assumption of equal probability of all permissible microstates [56]. However, the foundation of thermalization has always been a tough problem and a long-term goal of physicists [53]. In the past decade, by taking the eigenstate thermalization hypothesis, researchers have studied the thermalization of closed quantum systems and have achieved some interesting results in understanding the underlying physics [44–46,48–54]. In contrast, in this paper, we discuss the thermalization of open systems from the dynamical perspective. With the exact evolution of open quantum systems, such an aim is achieved.

The rest of the paper is organized as follows. In Sec. II, we introduce the system we concern ourselves with and briefly review the previous results related to our present work. In Sec. III, we derive the exact solution of the reduced density matrix. In Sec. IV, we explain the physical consequences of the solution and discuss the general thermalization of open systems. A brief summary is given in Sec. V.

II. OVERVIEW OF THE EXACT MASTER EQUATION

The systems we are interested in are characterized by the bosonic (fermionic) Hamiltonian $H_S = \sum_{i,j=1}^{d} \epsilon_{ij} a_i^\dagger a_j$, and interact with a bosonic (fermionic) environment described by

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[*] wzhang@mail.ncku.edu.tw

$H_{\rm E}=\sum_k \epsilon_k b_k^\dagger b_k$, via the interaction $H_{\rm int}=\sum_{j,k}(V_{jk}a_j^\dagger b_k+$ H.c.). Here $a_j^\dagger$ and a_j are the creation and annihilation operators of the discrete single-particle energy level j in the system; $b_k^\dagger$ and b_k are the creation and annihilation operators of the continuous single-particle mode k in the environment; ϵ_{ii} and ϵ_k give the corresponding single-particle energy spectra of the system and the environment; ϵ_{ij} $(i\neq j)$ characterize the transitions between different single-particle levels; and V_{jk} is the interaction strength between the jth single-particle energy level in the system and mode k in the environment. If the creation and annihilation operators satisfy the commutation (anticommutation) relations, the corresponding systems is bosonic (fermionic).

We assume that initially the system and the environment are decoupled [57], i.e., $\rho_{\rm tot}(0)=\rho(0)\otimes\rho_{\rm E}(0)$, where $\rho(0)$ is an arbitrary physical state of the system and $\rho_{\rm E}(0)=\otimes_k e^{-\beta(\epsilon_k-\mu)b_k^\dagger b_k}/\mathcal{Z}$ is the thermal state of the environment with inverse temperature β and chemical potential μ. Here, $\mathcal{Z}=\prod_k[1\mp e^{-\beta(\epsilon_k-\mu)}]^{\mp1}$ denotes the grand partition function of the environment, with the upper and lower signs corresponding to the bosonic and fermionic cases respectively, and hereafter we keep to this convention. The dynamics of the open system is completely determined by the reduced density matrix which is obtained by tracing over all the environmental degrees of freedom from the total density matrix,

$$\rho(t)={\rm Tr}_{\rm E}[\mathcal{U}(t,0)\rho_{\rm tot}(0)\mathcal{U}^\dagger(t,0)], \tag{1}$$

where $\mathcal{U}(t,0)=\exp\{\frac{1}{i\hbar}(H_{\rm S}+H_{\rm E}+H_{\rm int})t\}$ is the time evolution operator of the total system.

In the coherent state representation, the reduced density matrix at generic time $t>0$ is connected to the initial state through the propagating function $\mathcal{J}(\boldsymbol{\eta}^\dagger,\boldsymbol{\eta}',t|\boldsymbol{\zeta}'^\dagger,\boldsymbol{\zeta},0)$ [17,19], i.e.,

$$\langle\boldsymbol{\eta}|\rho(t)|\boldsymbol{\eta}'\rangle=\int d\mu(\boldsymbol{\zeta},\boldsymbol{\zeta}')\langle\boldsymbol{\zeta}|\rho(0)|\boldsymbol{\zeta}'\rangle\mathcal{J}(\boldsymbol{\eta}^\dagger,\boldsymbol{\eta}',t|\boldsymbol{\zeta}'^\dagger,\boldsymbol{\zeta},0), \tag{2}$$

where $\boldsymbol{\zeta}^\dagger=(\zeta_1^*\ \cdots\ \zeta_d^*)$ and $\boldsymbol{\zeta}=(\zeta_1\ \cdots\ \zeta_d)^{\rm T}$, with the components being complex (Grassmannian) for bosons (fermions); $|\boldsymbol{\zeta}\rangle=e^{\boldsymbol{a}^\dagger\boldsymbol{\zeta}}|0\rangle$ and $\langle\boldsymbol{\zeta}|=\langle0|e^{\boldsymbol{\zeta}^\dagger\boldsymbol{a}}$ are the unnormalized coherent states, in which $\boldsymbol{a}^\dagger=(a_1^\dagger\ \cdots\ a_d^\dagger)$, $\boldsymbol{a}=(a_1\ \cdots\ a_d)^{\rm T}$, and $|0\rangle$ and $\langle0|$ are the vacuum states [58]; $d\mu(\boldsymbol{\zeta},\boldsymbol{\zeta}')=d\mu(\boldsymbol{\zeta})d\mu(\boldsymbol{\zeta}')$ is the integral measure, with $d\mu(\boldsymbol{\zeta})=\prod_{j=1}^d(d^2\zeta_j/\pi)e^{-\zeta_j^*\zeta_j}$ for bosons and $d\mu(\boldsymbol{\zeta})=\prod_{j=1}^d d\zeta_j^*d\zeta_je^{-\zeta_j^*\zeta_j}$ for fermions.

With the coherent state path-integral approach, the propagating function can be derived, reading [17,19]

$$\begin{aligned}\mathcal{J}(\boldsymbol{\eta}^\dagger,\boldsymbol{\eta}',t|\boldsymbol{\zeta}'^\dagger,\boldsymbol{\zeta},0)=[\det\boldsymbol{w}(t)]^{\pm1}\exp\{&\boldsymbol{\eta}^\dagger\boldsymbol{J}_1(t)\boldsymbol{\zeta}\pm\boldsymbol{\eta}^\dagger\boldsymbol{J}_2(t)\boldsymbol{\eta}'\\ &\pm\boldsymbol{\zeta}'^\dagger\boldsymbol{J}_3(t)\boldsymbol{\zeta}+\boldsymbol{\zeta}'^\dagger\boldsymbol{J}_1^\dagger(t)\boldsymbol{\eta}'\},\end{aligned} \tag{3}$$

where $\boldsymbol{w}(t)=[\mathbf{I}\pm\boldsymbol{v}(t)]^{-1}$, $\boldsymbol{J}_1(t)=\boldsymbol{w}(t)\boldsymbol{u}(t)$, $\boldsymbol{J}_2(t)=\mathbf{I}-\boldsymbol{w}(t)$, $\boldsymbol{J}_3(t)=\mathbf{I}-\boldsymbol{u}^\dagger(t)\boldsymbol{w}(t)\boldsymbol{u}(t)$, with $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ standing for the nonequilibrium Green functions. In the following, for simplicity of notation, we abbreviate the time dependence when encountering complicated formulas involving these quantities. More specifically, $\boldsymbol{u}(t)$ is the spectral Green function with elements defined as $u_{ij}(t)=\langle[a_i(t),a_j^\dagger(0)]_\mp\rangle$, and $\boldsymbol{v}(t)$ is the fluctuating correlation function originated from the environment [18,19], i.e.,

$$\boldsymbol{v}(t)=\int_0^t dt_1\int_0^t dt_2\,\boldsymbol{u}(t-t_1)\widetilde{\boldsymbol{g}}(t_1-t_2)\boldsymbol{u}^\dagger(t-t_2), \tag{4}$$

which has the same form as the Keldysh correlation Green function. Here, $\widetilde{\boldsymbol{g}}(t_1-t_2)=\int\frac{d\epsilon}{2\pi}f(\epsilon)\boldsymbol{J}(\epsilon)e^{-i\epsilon(t_1-t_2)}$ denotes a system-bath correction, with $f(\epsilon)=\frac{1}{e^{\beta(\epsilon-\mu)}\mp1}$ standing for the initial particle distribution of the environment and $J_{ij}(\epsilon)=2\pi\sum_k V_{ik}V_{jk}^*\delta(\epsilon-\epsilon_k)$ being the matrix element of the spectral density matrix $\boldsymbol{J}(\epsilon)$.

Taking advantage of Eqs. (2) and (3), the master equation has been derived [16–19], reading

$$\begin{aligned}\frac{d\rho(t)}{dt}=\frac{1}{i}[\widetilde{H}_{\rm S}(t),\rho(t)]+\sum_{ij}\{&\gamma_{ij}(t)[2a_j\rho(t)a_i^\dagger\\ &-a_i^\dagger a_j\rho(t)-\rho(t)a_i^\dagger a_j]+\widetilde{\gamma}_{ij}(t)[a_i^\dagger\rho(t)a_j\\ &\pm a_j\rho(t)a_i^\dagger\mp a_i^\dagger a_j\rho(t)-\rho(t)a_ja_i^\dagger]\}.\end{aligned} \tag{5}$$

In this master equation, $\widetilde{H}_{\rm S}(t)=\sum_{ij}\widetilde{\epsilon}_{ij}(t)a_i^\dagger a_j$ is the renormalized system Hamiltonian; $\gamma_{ij}(t)$ and $\widetilde{\gamma}_{ij}(t)$ characterize the dissipation and fluctuations induced by the system's coupling with the environment, respectively. The coefficients $\widetilde{\epsilon}_{ij}(t)$, $\gamma_{ij}(t)$, and $\widetilde{\gamma}_{ij}(t)$ are elements of Hermitian matrices and are determined entirely by the nonequilibrium Green functions $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$:

$$i\widetilde{\epsilon}_{ij}(t)+\gamma_{ij}(t)=-[\dot{\boldsymbol{u}}(t)\boldsymbol{u}^{-1}(t)]_{ij}, \tag{6a}$$

$$\widetilde{\gamma}_{ij}(t)=\dot{\boldsymbol{v}}_{ij}(t)-[\dot{\boldsymbol{u}}(t)\boldsymbol{u}^{-1}(t)\boldsymbol{v}(t)+{\rm H.c.}]_{ij}. \tag{6b}$$

The above formulation shows that the dynamics of open quantum systems are fully determined by $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ through the above master equation.

Furthermore, the general solution of the spectral Green function $\boldsymbol{u}(t)$ can be expressed as [16]

$$\boldsymbol{u}(t)=\sum_l\boldsymbol{Z}_le^{-i\epsilon_lt}+\int\frac{d\epsilon}{2\pi}\boldsymbol{D}(\epsilon)e^{-i\epsilon t}. \tag{7}$$

The quantities ϵ_l, $\boldsymbol{Z}_l$, and $\boldsymbol{D}(\epsilon)$ are all connected with the Green function in the energy domain,

$$\boldsymbol{U}(z)=\frac{1}{z\mathbf{I}-\boldsymbol{\epsilon}_{\rm S}-\boldsymbol{\Sigma}(z)}, \tag{8}$$

which is the modified Laplace transform of $\boldsymbol{u}(t)$ with respect to time; $\boldsymbol{\epsilon}_{\rm S}$ is the matrix formed by the parameters ϵ_{ij} in the system Hamiltonian and $\boldsymbol{\Sigma}(z)=\int\frac{d\epsilon}{2\pi}\frac{\boldsymbol{J}(\epsilon)}{z-\epsilon}$ is the self-energy correction of the system. Explicitly, ϵ_l is the pole of $\boldsymbol{U}(z)$ in the real axis and the energy of the lth localized state (or localized mode [16]); $\boldsymbol{Z}_l$ is the corresponding amplitude, reading $\boldsymbol{Z}_l=\frac{1}{2\pi i}\oint_{C_l}dz\boldsymbol{U}(z)$ with C_l standing for the positively oriented curve in the neighborhood of $z=\epsilon_l$; and $\boldsymbol{D}(\epsilon)$ is the continuous part of the Green function spectrum.

Physically, the first term (the discrete spectrum) of Eq. (7) describes the dissipationless dynamics of the system due to the localized states generated from the coupling between the system and environment. The second term (the continuous spectrum) describes the dissipation (spontaneous decay) of the system. The decay rates are given by Eq. (6a) in the master equation. In the weak-coupling regime, $\boldsymbol{D}(\epsilon)$ represents the spectrum broadening due to the coupling to the reservoir.

However, in the strong coupling regime, the energy renormalization marginalizes the system spectrum $\boldsymbol{\epsilon}_{\rm S}$ so that $\boldsymbol{D}(\epsilon)$ is dominated by the spectral density. This also results in the occurrence of the localized states, i.e., the first term in Eq. (7), when the pole condition $\det[\epsilon_l - \boldsymbol{\epsilon}_{\rm S} - \boldsymbol{\Sigma}(\epsilon_l)] = 0$ is satisfied. Once we have the general solution of $\boldsymbol{u}(t)$, the correlation Green function $\boldsymbol{v}(t)$ can be determined from Eq. (4), which is a manifestation of the fluctuation-dissipation theorem in the time domain [16]. This completes our exact master equation formulation. In fact, the spectral Green function $\boldsymbol{u}(t)$, the correlation Green function $\boldsymbol{v}(t)$, and their physical interpretation can also be seen from an alternative derivation in terms of the quantum Langevin equation given orginally in Refs. [20,59] and also in Appendix A.

III. THE EXACT SYSTEM STATE EVOLUTION

With the initial system state $\rho(0)$ and the solution of the Green functions $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$, the reduced density matrix $\rho(t)$ at an arbitrary instant can be determined in principle from the exact master equation (5). However, because the coefficients are all time dependent, it is not easy to solve the master equation directly. In fact, Eqs. (2) and (3) are already the exact solution of the reduced density matrix in the coherent state representation. In this section, we will attempt to find the general operator form of this solution. First, in Sec. III A, we shall introduce some conventions and derive the matrix elements of $\rho(0)$ in the coherent state representation. In Sec. III B, we obtain the matrix elements of $\rho(t)$ at arbitrary later time. In Sec. III C, the exact form of $\rho(t)$ will be given.

A. Representation of the initial system state

To obtain the density matrix elements at arbitrary time, one needs to carry out the integrals of Eq. (2) with the explicit expression of $\langle\boldsymbol{\zeta}|\rho(0)|\boldsymbol{\zeta}'\rangle$. Define the Fock state

$$|I\rangle = \frac{\boldsymbol{a}_I^\dagger}{\sqrt{i_1!\cdots i_d!}}|0\rangle, \quad \langle I| = \langle 0|\frac{\boldsymbol{a}_I}{\sqrt{i_1!\cdots i_d!}}, \tag{9}$$

where

$$\boldsymbol{a}_I^\dagger = (a_1^\dagger)^{i_1}\cdots(a_d^\dagger)^{i_d}, \tag{10a}$$

$$\boldsymbol{a}_I = (\boldsymbol{a}_I^\dagger)^\dagger = (a_d)^{i_d}\cdots(a_1)^{i_1}. \tag{10b}$$

In the formulas, $I = (i_1, i_2, \cdots, i_d)$ is a class of d-dim sequences corresponding to the particle occupation in the system, with i_n denoting the occupation number in the nth level. For fermions $i_n = 0, 1$ and for bosons $i_n = 0, 1, 2, \ldots$. The initial system density matrix can be generally expressed as

$$\rho(0) = \sum_{IJ}\rho_{IJ}(0)\frac{\boldsymbol{a}_I^\dagger|0\rangle\langle 0|\boldsymbol{a}_J}{\sqrt{i_1!\cdots i_d!j_1!\cdots j_d!}}, \tag{11}$$

where the summation is over all the possible physical pairs of I and J. For massive particles, the reduced density matrix elements with different massive particle number vanish; that is, there is no overlap between Fock states with different massive particle numbers. This is because massive particles cannot be generated or destroyed in the nonrelativistic regime even though they can be transferred. Thus, we further have the constraint $i_1 + \cdots + i_d = j_1 + \cdots + j_d$. With the initial state in Eq. (11) and the definition of coherent states, it is easy to find

$$\langle\boldsymbol{\zeta}|\rho(0)|\boldsymbol{\zeta}'\rangle = \sum_{IJ}\rho_{IJ}(0)\frac{\boldsymbol{\zeta}_I^\dagger\boldsymbol{\zeta}_J'}{\sqrt{i_1!\cdots i_d!j_1!\cdots j_d!}}, \tag{12}$$

where $\boldsymbol{\zeta}_I^\dagger$ and $\boldsymbol{\zeta}_J'$ follow conventions similar to those in Eq. (9), i.e., $\boldsymbol{\zeta}_I^\dagger = (\zeta_1^*)^{i_1}\cdots(\zeta_d^*)^{i_d}$ and $\boldsymbol{\zeta}_J' = (\zeta_d')^{j_d}\cdots(\zeta_1')^{j_1}$.

B. Evolution of the density matrix elements in the coherent state representation

Following Eqs. (3) and (12), Eq. (2) can be reexpressed as

$$\langle\boldsymbol{\eta}|\rho(t)|\boldsymbol{\eta}'\rangle = (\det\boldsymbol{w})^{\pm 1}e^{\pm\boldsymbol{\eta}^\dagger\boldsymbol{J}_2\boldsymbol{\eta}'}\sum_{IJ}\frac{\rho_{IJ}(0)}{\sqrt{i_1!\cdots i_d!j_1!\cdots j_d!}} \times\int d\mu(\boldsymbol{\zeta},\boldsymbol{\zeta}')\boldsymbol{\zeta}_I^\dagger\boldsymbol{\zeta}_J' e^{\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\zeta}+\boldsymbol{\zeta}'^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'+\boldsymbol{\zeta}'^\dagger\boldsymbol{J}_3\boldsymbol{\zeta}}. \tag{13}$$

In order to obtain the explicit form of $\langle\boldsymbol{\eta}|\rho(t)|\boldsymbol{\eta}'\rangle$, one needs to simplify the integral. The result is given in the following (see Appendix B for the details).

1. *Bosonic case*

In the bosonic case, the result is

$$\sum_{I'J'}P_+|(\boldsymbol{J}_3)_{J',I'}|_+(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1)_{\overline{I'}}(\boldsymbol{J}_1^\dagger\boldsymbol{\eta}')_{\overline{J'}}, \tag{14}$$

where we have used the following conventions:

(i) $I' = (i_1', i_2', \cdots, i_d')$ and $\overline{I'} = (\overline{i_1'}, \overline{i_2'}, \cdots, \overline{i_d'})$ are d-dim sequences of non-negative integers, with $i_k' + \overline{i_k'} = i_k$ for $1 \leqslant k \leqslant d$. The summation $\sum_{I'J'}$ is over all the possible pairs of I' and J' satisfying the constraint $i_1' + \cdots + i_d' = j_1' + \cdots + j_d'$.

(ii) $P_+ = C_{i_1'}^{i_1}\cdots C_{i_d'}^{i_d}C_{j_1'}^{j_1}\cdots C_{j_d'}^{j_d}$, with $C_k^n = \frac{n!}{k!(n-k)!}$ standing for the binomial coefficient.

(iii) $|(\boldsymbol{J}_3)_{J',I'}|_+ = \mathrm{perm}[(\boldsymbol{J}_3)_{J',I'}]$ stands for the *permanent* of the matrix $(\boldsymbol{J}_3)_{J',I'}$ [see Eq. (B5)].

(iv) $(\boldsymbol{J}_3)_{J',I'}$ is the matrix obtained by first taking j_m' copies of the mth row of $\boldsymbol{J}_3$ in Eq. (3) for each n and then taking i_n' copies of the nth column of the matrix obtained by the first step [see Eqs. (B6) and (B7)].

(v) $\boldsymbol{\eta}^\dagger\boldsymbol{J}_1$ and $\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'$ are vectors in d-dimensional spaces, and $(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1)_{\overline{I'}}$ and $(\boldsymbol{J}_1^\dagger\boldsymbol{\eta}')_{\overline{J'}}$ follow a convention similar to that in Eq. (12).

2. *Fermionic case*

In the fermionic scenario, the integral can be simplified to

$$\sum_{I'J'}P_-|(\boldsymbol{J}_3)_{J',I'}|_-(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1)_{\overline{I'}}(\boldsymbol{J}_1^\dagger\boldsymbol{\eta}')_{\overline{J'}}. \tag{15}$$

Here, we have used the following conventions:

(i) I', $\overline{I'}$, J', $\overline{J'}$, and the summation follow the same conventions as in the bosonic case, except that all the elements in the sequences are either 0 or 1.

(ii) $P_- = s(I, I')s(J, J')$, with $s(I, I')$ is the sign being defined through $\boldsymbol{\zeta}_I^\dagger = s(I, I')\boldsymbol{\zeta}_{I'}^\dagger\boldsymbol{\zeta}_{\overline{I'}}^\dagger$.

(iii) $|(\boldsymbol{J}_3)_{J',I'}|_- = \det[(\boldsymbol{J}_3)_{J',I'}]$ stands for the *determinant* of the matrix $(\boldsymbol{J}_3)_{J',I'}$.

(iv) $(\boldsymbol{J}_3)_{J',I'}$ follows the same convention as in the bosonic case. However, as all the elements in I' and J' are either 0 or 1, $(\boldsymbol{J}_3)_{J',I'}$ is in fact a submatrix of $\boldsymbol{J}_3$.

(v) $(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}}$ and $(\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}$ follow the same convention as in the bosonic case.

3. Common expression

Equations (14) and (15) can be summarized as

$$\sum_{I'J'} P_\pm |(\boldsymbol{J}_3)_{J',I'}|_\pm (\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}. \tag{16}$$

Thus, in the coherent state representation, the elements of $\rho(t)$ can be given by

$$\begin{aligned}\langle \boldsymbol{\eta}|\rho(t)|\boldsymbol{\eta}'\rangle = (\det \boldsymbol{w})^{\pm 1} \sum_{IJ} \frac{\rho_{IJ}(0)}{\sqrt{i_1! \cdots i_d! j_1! \cdots j_d!}} \\ \times \sum_{I'J'} P_\pm |(\boldsymbol{J}_3)_{J',I'}|_\pm (\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} e^{\pm \boldsymbol{\eta}^\dagger \boldsymbol{J}_2 \boldsymbol{\eta}'} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}.\end{aligned} \tag{17}$$

C. Exact form of the density matrix

The reduced density matrix $\rho(t)$ satisfying Eq. (17) can be explicitly written as

$$\rho(t) = \sum_{IJ} \rho_{IJ}(0) \sum_{I'J'} P_\pm \frac{|(\boldsymbol{J}_3)_{J',I'}|_\pm (\boldsymbol{a}^\dagger \boldsymbol{J}_1)_{\overline{I'}} \rho^{\text{th}}(t) (\boldsymbol{J}_1^\dagger \boldsymbol{a})_{\overline{J'}}}{\sqrt{i_1! \cdots i_d! j_1! \cdots j_d!}}, \tag{18}$$

where

$$\rho^{\text{th}}(t) = (\det \boldsymbol{w})^{\pm 1} \exp\{\boldsymbol{a}^\dagger \ln[\pm \boldsymbol{J}_2] \boldsymbol{a}\} \tag{19}$$

is a thermal-like state [47]; $\boldsymbol{a}^\dagger \boldsymbol{J}_1$ and $\boldsymbol{J}_1^\dagger \boldsymbol{a}$ stand for vector operators, and $(\boldsymbol{a}^\dagger \boldsymbol{J}_1)_{\overline{I'}}$ and $(\boldsymbol{J}_1^\dagger \boldsymbol{a})_{\overline{J'}}$ follow the same conventions as those in Eq. (9).

Equation (18) is directly obtained from Eq. (17) with the identity

$$\begin{aligned}\langle \boldsymbol{\eta}|(\boldsymbol{a}^\dagger \boldsymbol{J}_1)_{\overline{I'}} e^{\boldsymbol{a}^\dagger \ln[\pm \boldsymbol{J}_2] \boldsymbol{a}} (\boldsymbol{J}_1^\dagger \boldsymbol{a})_{\overline{J'}} |\boldsymbol{\eta}'\rangle \\ = (\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} e^{\pm \boldsymbol{\eta}^\dagger \boldsymbol{J}_2 \boldsymbol{\eta}'} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}},\end{aligned} \tag{20}$$

which can be easily derived with the properties of coherent states that

$$\langle \boldsymbol{\eta}|(\boldsymbol{a}^\dagger \boldsymbol{J}_1)_{\overline{I'}} = \langle \boldsymbol{\eta}|(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}}, \tag{21a}$$

$$(\boldsymbol{J}_1^\dagger \boldsymbol{a})_{\overline{J'}} |\boldsymbol{\eta}'\rangle = (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}} |\boldsymbol{\eta}'\rangle, \tag{21b}$$

and

$$\langle \boldsymbol{\eta}| e^{\boldsymbol{a}^\dagger \ln[\pm \boldsymbol{J}_2] \boldsymbol{a}} |\boldsymbol{\eta}'\rangle = e^{\pm \boldsymbol{\eta}^\dagger \boldsymbol{J}_2 \boldsymbol{\eta}'}. \tag{22}$$

IV. PHYSICAL INTERPRETATION OF THE SOLUTION AND THE THERMALIZATION

In this section, we shall discuss the underlying physics of the solution. The physical interpretation of the solution will be given in Sec. IV A, and the thermalization problem will be discussed in Sec. IV B.

A. Physical interpretation of the solution

To explain the physical consequences contained in Eq. (18), we consider two limiting cases first. One is that there is no particle in the environment initially, and the other is that there is no particle in the system initially. Finally, we shall consider the joint effect and the general solution.

1. No particle in the environment initially

In this case, the environment is initially in a vacuum state, so that $f(\epsilon) = 0$ and $\boldsymbol{v}(t) = 0$, namely there are no thermal fluctuations. Consequently, in Eqs. (18) and (19), $\boldsymbol{J}_1 \to \boldsymbol{u}$, $\boldsymbol{J}_2 \to \boldsymbol{0}, \boldsymbol{J}_3 \to \mathbf{I} - \boldsymbol{u}^\dagger \boldsymbol{u}$, and $\rho^{\text{th}}(t) \to |0\rangle\langle 0|$. As a result, $\rho(t)$ is simply reduced to

$$\begin{aligned}\rho(t) = \sum_{IJ} \rho_{IJ}(0) \\ \times \sum_{I'J'} P_\pm \frac{|(\mathbf{I} - \boldsymbol{u}^\dagger \boldsymbol{u})_{J',I'}|_\pm (\boldsymbol{a}^\dagger \boldsymbol{u})_{\overline{I'}} |0\rangle\langle 0| (\boldsymbol{u}^\dagger \boldsymbol{a})_{\overline{J'}}}{\sqrt{i_1! \cdots i_d! j_1! \cdots j_d!}}.\end{aligned} \tag{23}$$

Compared with the form of the initial state of Eq. (11), one can see that, under the time evolution, the factor

$$\boldsymbol{a}_I^\dagger |0\rangle\langle 0| \boldsymbol{a}_J \to \sum_{I'J'} P_\pm |(\mathbf{I} - \boldsymbol{u}^\dagger \boldsymbol{u})_{J',I'}|_\pm (\boldsymbol{a}^\dagger \boldsymbol{u})_{\overline{I'}} |0\rangle\langle 0| (\boldsymbol{u}^\dagger \boldsymbol{a})_{\overline{J'}}.$$

Note that $\boldsymbol{u}$ describes the dissipation (decay) dynamics of the system [16], i.e., initially $\boldsymbol{u}(t = 0) = \mathbf{I}$ and then it decays in time, as given by Eq. (7). The quantity $\mathbf{I} - \boldsymbol{u}^\dagger \boldsymbol{u}$ characterizes the probability of particles dissipating into the environment. As a result, the solution in Eq. (23) describes a pure *dissipation* process.

2. No particle in the system initially

In this case, the system initial state is in the vacuum state, $\rho(0) = |0\rangle\langle 0|$, so that no particle can be dissipated into the environment. This corresponds to the case where all the coefficients $\rho_{IJ}(0)$ are 0 except the one for which $I = J = \{0, \ldots, 0\}$. Following Eq. (18), one can easily find that

$$\rho(t) = \rho^{\text{th}}(t) = \frac{1}{[\det(\mathbf{I} \pm \boldsymbol{v})]^{\pm 1}} \exp\left\{\boldsymbol{a}^\dagger \ln\left(\frac{\boldsymbol{v}}{\mathbf{I} \pm \boldsymbol{v}}\right) \boldsymbol{a}\right\}. \tag{24}$$

Note that $\boldsymbol{v}(t)$ isthe time correlation function of the thermal fluctuating (noise) force induced from the environment, which can be derived explicitly from the quantum Langevin equation for the system operator by eliminating all the environmental degrees of freedom (see Refs. [20,59] or Appendix A). It is these thermal fluctuating processes that make the system thermalize with the environment, as we will discuss later. Therefore, the solution (24) is a consequence of thermal fluctuation processes induced by the environment.

3. Joint effect between fluctuation and dissipation

Now we consider the general result of Eq. (18). In Sec. IV A 1, we show that particles initially in the system will dissipate into the environment described by $\boldsymbol{u}$. From Sec. IV A 2, we learn that the thermal-like state $\rho^{\text{th}}(t)$, as a function of $\boldsymbol{v}$ only, is realized by the particle transitions induced by the thermal fluctuations from the environment.

In reality, these two processes must simultaneously occur due to the fluctuation-dissipation relation [16]. When initially particles exist in both the system and the environment, dissipation and fluctuations take place together, which results in the modification of $\mathbf{I}-\boldsymbol{u}^{\dagger}\boldsymbol{u} \to \mathbf{I}-\boldsymbol{u}^{\dagger}\frac{1}{\mathbf{I}\pm\boldsymbol{v}}\boldsymbol{u}=\boldsymbol{J}_3$ and $\boldsymbol{u} \to \frac{1}{\mathbf{I}\pm\boldsymbol{v}}\boldsymbol{u}=\boldsymbol{J}_1$, where $\frac{1}{\mathbf{I}\pm\boldsymbol{v}}$ is a factor due to thermal fluctuations as we discussed in the last subsection, IV A 2. Thus, mixing Eqs. (23) and (24) together with the above modification leads to the general solution of the reduced density matrix, i.e., Eq. (18). This is the result of various possible dissipation and fluctuation processes under the constraint of the fluctuation-dissipation relation, i.e., Eq. (4), during the time evolution of open quantum systems.

B. The thermalization

In this subsection, we shall study the asymptotic behavior of the state as the time approaches infinity. The absence or presence of localized states determines whether the system can be finally thermalized [38,46,47], so we consider these two cases separately from the general solution of the reduced density matrix.

In the case that there are no localized states (see Appendix A), $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ would finally evolve to

$$\lim_{t\to\infty}\boldsymbol{u}(t)=0, \tag{25a}$$

$$\lim_{t\to\infty}\boldsymbol{v}(t)=\int\frac{d\epsilon}{2\pi}f(\epsilon)\boldsymbol{D}(\epsilon):=\bar{\boldsymbol{n}}. \tag{25b}$$

In this case, the final state of the system would be (see Appendix C for the details)

$$\begin{aligned}\lim_{t\to\infty}\rho(t)&=\rho^{\mathrm{th}}(t\to\infty)\\&=\frac{1}{[\det(\mathbf{I}\pm\bar{\boldsymbol{n}})]^{\pm1}}\exp\left\{\boldsymbol{a}^{\dagger}\ln\left(\frac{\bar{\boldsymbol{n}}}{\mathbf{I}\pm\bar{\boldsymbol{n}}}\right)\boldsymbol{a}\right\}.\end{aligned} \tag{26}$$

Equation (26) shows that the final particle distribution in the system is completely characterized by the matrix $\bar{\boldsymbol{n}}$ [60], i.e.,

$$\mathrm{Tr}[\rho(\infty)a_j^{\dagger}a_i]=\bar{\boldsymbol{n}}_{ij}. \tag{27}$$

With the expression of $\bar{\boldsymbol{n}}$ in Eq. (25b) and the properties of the spectral function $\boldsymbol{D}(\epsilon)$ [that it is positive-semidefinite and $\int\frac{d\epsilon}{2\pi}\boldsymbol{D}(\epsilon)=\mathbf{I}$], the final particle distribution of the system can be seen as a weighted sum of the Bose-Einstein or Fermi-Dirac distribution over the spectral function $\boldsymbol{D}(\epsilon)$. That is, without the existence of localized states, the system would finally reach the thermal-like state of Eq. (26), instead of the Gibbs thermal state of the original system (characterized by $\boldsymbol{\epsilon}_{\mathrm{S}}$) contacting very weakly with the reservoir at given temperature and chemical potential, as we will discuss next.

When the coupling strength between the system and the environment is *very weak*, then the spectral density $\boldsymbol{J}(\epsilon)$ and the Lamb shift $\boldsymbol{\Delta}(\epsilon)$ both tend to vanish, i.e.,

$$\boldsymbol{J}(\epsilon)\to\mathbf{0},\quad \boldsymbol{\Delta}(\epsilon)\to\mathbf{0}. \tag{28}$$

Following

$$\boldsymbol{D}(\epsilon)=\frac{1}{\epsilon-\boldsymbol{\epsilon}_{\mathrm{S}}-\boldsymbol{\Delta}(\epsilon)+\frac{i\boldsymbol{J}(\epsilon)}{2}}\boldsymbol{J}(\epsilon)\frac{1}{\epsilon-\boldsymbol{\epsilon}_{\mathrm{S}}-\boldsymbol{\Delta}(\epsilon)-\frac{i\boldsymbol{J}(\epsilon)}{2}} \tag{29}$$

and the careful analysis in Appendix D, one can find that, under condition (28),

$$\boldsymbol{D}(\epsilon)\to 2\pi\delta(\epsilon\mathbf{I}-\boldsymbol{\epsilon}_{\mathrm{S}}). \tag{30}$$

That is, when the system-environment coupling becomes very weak, the spectrum broadening and Lamb shift of the system energy levels can be negligible, making the spectrum of the system converge to that of the isolated system. As a consequence of Eqs. (30) and (25b), $\bar{\boldsymbol{n}}$ approaches the Bose-Einstein or Fermi-Dirac distribution, i.e.,

$$\bar{\boldsymbol{n}}\to f(\boldsymbol{\epsilon}_{\mathrm{S}})=\frac{1}{e^{\beta(\boldsymbol{\epsilon}_{\mathrm{S}}-\mu)}\mp 1}. \tag{31}$$

Thus, Eq. (26) converges to

$$\rho(t\to\infty)=\frac{1}{\mathrm{Tr}[e^{-\beta\boldsymbol{a}^{\dagger}(\boldsymbol{\epsilon}_{\mathrm{S}}-\mu)\boldsymbol{a}}]}\exp\{-\beta\boldsymbol{a}^{\dagger}(\boldsymbol{\epsilon}_{\mathrm{S}}-\mu)\boldsymbol{a}\}, \tag{32}$$

which is exactly the Gibbs thermal state of the system with $H_{\mathrm{S}}=\boldsymbol{a}^{\dagger}\boldsymbol{\epsilon}_{\mathrm{S}}\boldsymbol{a}$ in the grand canonical ensemble at inverse temperature β and chemical potential μ of the environment. This provides a rigorous proof that, in the weak-coupling limit, the exact evolution of a noninteracting open quantum system would reproduce in the steady state limit the Gibbs thermal state in equilibrium statistical mechanics.

On the other hand, if there are localized states, their contribution to the oscillations in $\boldsymbol{u}(t)$ [see Eq. (7)] would survive as t approaches infinity, i.e.,

$$\boldsymbol{u}(t\to\infty)=\sum_l \boldsymbol{Z}_l e^{-i\epsilon_l t}. \tag{33}$$

Following the expression of the reduced density matrix in Eq. (18), the final state must be expressed in terms of the coefficients $\rho_{IJ}(0)$, i.e., the system keeps the memory of its initial state. Therefore, the system cannot be thermalized [38,46,47].

V. SUMMARY

In this paper, we investigated a general solution of open quantum systems interacting with the environment through particle exchanges. The exact evolution of the reduced density matrix is given in terms of the nonequilibrium Green functions. We explained the physical consequences of the solution. With the exact density matrix, we studied the thermalization process. We obtained the result of equilibrium statistical mechanics from the dynamical perspective and went beyond it. That is, when there are no localized states and the system-environment coupling is very weak, the final state would be as expected from the standard statistical mechanics; for no localized states but relatively strong coupling regime, the steady state would be thermal-like, which departs from the Gibbs thermal states; when there are localized states, the system keeps the memory on the initial state and therefore cannot be thermalized.

With the explicit expression of the reduced density matrix, one can obtain complete information about the system dynamics, which is quite important for the rapidly developing quantum thermodynamics and quantum information, because their central physical quantity, entropy, is directly related to the microstates of the system. It is also noteworthy that the model studied in our work involves non-Markovian nature. With the explicit form of the density matrix evolution, one can study the memory effects from more perspectives, e.g., quantum coherence, entanglement, and dynamical phase transition. Although we only considered the single-reservoir case, the results can be directly extended to the multireservoir case by just extending the corresponding expressions of the nonequilibrium Green functions $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ to multiple reservoirs (multiple leads in nanodevices or quantum devices, for example). Further works remain to be published in the future.

Finally, we should point out that the thermalization derived in this paper is for decoupled initial states between the system and the reservoir. We have shown that when the system and the environment are initially correlated with each other, the spectral Green function $\boldsymbol{u}(t)$ for dissipation is independent of the initial states, but the correlation Green function $\boldsymbol{v}(t)$ will contain the information of the initial system-reservoir correlations [61,62]. However, different types of initial correlations may result in different forms of master equations [61,63]. These may make the steady state different from the thermalized state we obtained in this work. In the weak-coupling regime, the initial system-environment correlation is negligible and our solution of thermalization is generic. On the other hand, in the strong coupling regime, it is not difficult to prepare experimentally the system in a state initially decoupled from the environment state. Then the thermalization solution given in this work can be experimentally explored also for the strong coupling regime, which is currently a very challenging topic in the study of quantum thermodynamics. The more general thermalization involving the system-environment initial correlations and interesting systems remains to be investigated further.

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APPENDIX A: CORRELATION GREEN FUNCTION $\boldsymbol{v}(t)$ AND ITS ASYMPTOTIC FORM

The Green function $\boldsymbol{v}(t)$ can be found to be the time correlation function of the thermal fluctuating (noise) force induced by the environment [20,59]. To see this physical picture clearly, one can derive the equation of motion for the creation and annihilation operators for both the system and the environment in the Heisenberg picture. Then one should formally solve the equation of motion for the environmental operators, and substitute the solution into the equation of motion for the system operator. Finally, one will arrive at the following exact quantum Langevin equation [59]:

$$\frac{d}{dt}a_i(t) + i\sum_j \epsilon_{ij}a_j(t) + \sum_j \int_0^t d\tau\, g_{ij}(t-\tau)a_j(\tau) = -i\sum_k V_{ik}b_k(0)e^{-i\epsilon_k t}, \tag{A1}$$

where $g_{ij}(t-\tau) = \int \frac{d\epsilon}{2\pi}J_{ij}(\epsilon)e^{-i\epsilon(t-\tau)}$. The quantum Langevin equation shows that the third term in the left-hand side of the above equation is the dissipation (damping) term and the term in right-hand side of the equation is the environment-induced noise force. Because of the linearity of the above equation, the general solution of Eq. (A1) can be written as

$$a_i(t) = \sum_j u_{ij}(t)a_j(0) + F_i(t). \tag{A2}$$

In the first term of Eq. (A2), $u_{ij}(t)$ is the spectral Green function obeying the Dyson equation,

$$\frac{d}{dt}u_{ij}(t) + i\sum_{j'} \epsilon_{ij'}u_{j'j}(t) + \sum_{j'}\int_0^t d\tau g_{ij'}(t-\tau)u_{j'j}(\tau) = 0, \tag{A3}$$

that describes the dissipation of the system. The second term in Eq. (A2),

$$F_i(t) = -i\sum_{j,k}\int_0^t d\tau u_{ij}(t-\tau)V_{jk}e^{-i\epsilon_k\tau}b_k(0), \tag{A4}$$

carries all the noise associated with the initial thermal state of the environment. The Green function $v_{ii'}(t)$ is the time correlation function of this noise force [59]:

$$v_{ii'}(\tau,t) = \langle F^{\dagger}_{i'}(t)F_i(\tau)\rangle = \sum_k f(\epsilon_k)\sum_{j'}\int_0^t dt_2 u^*_{i'j'}(t-t_2)V^*_{j'k}e^{i\epsilon_k t_2}\sum_j\int_0^\tau dt_1 u_{ij}(\tau-t_1)V_{jk}e^{-i\epsilon_k t_1} \tag{A5}$$

$$= \sum_{j,j'}\int_0^\tau dt_1\int_0^t dt_2\, u_{ij}(\tau-t_1)\,\widetilde{g}_{jj'}(t_1-t_2)\,u^*_{i'j'}(t-t_2), \tag{A6}$$

which is just Keldysh's correlation Green function, where $f(\epsilon_k) = \langle b^{\dagger}_k(0)b_k(0)\rangle$ is the particle distribution in the initial thermal state of the environment. When $\tau = t$, the above equation is reduced to Eq. (4).

In the following, we aim to find the expression of $\boldsymbol{v}(t)$ when t approaches infinity. To obtain the result, we first need to identify the asymptotic expression of the integrals in Eq. (A5). The integral in the third summation can be transformed to

$$\int_0^t d\tau\, u_{ij}(t-\tau)V_{jk}e^{-i\epsilon_k\tau} = i\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi}U_{ij}(\epsilon+i0^+)V_{jk}e^{-i\epsilon t}\int_0^t d\tau\, e^{i(\epsilon-\epsilon_k)\tau}. \tag{A7}$$

If there are no localized states in the total system, with the identity $\int_0^\infty d\tau\, e^{i(\epsilon-\epsilon_k)\tau} = \frac{i}{\epsilon-\epsilon_k+i0^+}$, Eq. (A5) is simply reduced to

$$\lim_{t\to\infty} v_{ii'}(t) \equiv \lim_{t\to\infty} v_{ii'}(t,t) = \sum_k f(\epsilon_k)\sum_{j,j'} V_{jk}V^\dagger_{kj'}U_{ij}(\epsilon_k+i0^+)U^\dagger_{j'i'}(\epsilon_k+i0^+). \tag{A8}$$

Take advantage of the definition of the spectral density, and take the continuous limit of k, the above equation can be transformed to

$$\lim_{t\to\infty} v_{ii'}(t) = \int\frac{d\epsilon}{2\pi}f(\epsilon)\sum_{j,j'}U_{ij}(\epsilon+i0^+)J_{jj'}(\epsilon)U^\dagger_{j'i'}(\epsilon+i0^+). \tag{A9}$$

In terms of the matrix representation, it can be expressed as

$$\lim_{t\to\infty}\boldsymbol{v}(t) = \int\frac{d\epsilon}{2\pi}f(\epsilon)\boldsymbol{U}(\epsilon+i0^+)\boldsymbol{J}(\epsilon)\boldsymbol{U}^\dagger(\epsilon+i0^+). \tag{A10}$$

Following Eq. (29), it can be further simplified to

$$\lim_{t\to\infty}\boldsymbol{v}(t) = \int\frac{d\epsilon}{2\pi}f(\epsilon)\boldsymbol{D}(\epsilon), \tag{A11}$$

which reproduces the general equilibrium fluctuation-dissipation theorem [14].

APPENDIX B: SIMPLIFICATION OF THE INTEGRAL IN EQ. (13)

1. Bosonic case

From Eq. (13), for bosons,

$$\begin{aligned}
&\int d\mu(\boldsymbol{\zeta},\boldsymbol{\zeta}')\zeta'^{\dagger}_I\zeta'_J e^{\boldsymbol{\zeta}'^\dagger\boldsymbol{J}_3\boldsymbol{\zeta}+\boldsymbol{\zeta}'^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'+\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\zeta}}\\
&\quad=\int\prod_{n=1}^{d}\frac{d^2\zeta_n d^2\zeta'_n}{\pi^2}\zeta'^{\dagger}_I\zeta'_J\exp\left\{-(\boldsymbol{\zeta}^\dagger\quad\boldsymbol{\zeta}'^\dagger)\begin{pmatrix}1&0\\-\boldsymbol{J}_3&1\end{pmatrix}\begin{pmatrix}\boldsymbol{\zeta}\\\boldsymbol{\zeta}'\end{pmatrix}+(\boldsymbol{\zeta}^\dagger\quad\boldsymbol{\zeta}'^\dagger)\begin{pmatrix}\boldsymbol{0}\\\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'\end{pmatrix}+(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\quad\boldsymbol{0})\begin{pmatrix}\boldsymbol{\zeta}\\\boldsymbol{\zeta}'\end{pmatrix}\right\}\\
&\quad=\partial_{\boldsymbol{\alpha}_J^*\boldsymbol{\alpha}_I}\int\prod_{n=1}^{d}\frac{d^2\zeta_n d^2\zeta'_n}{\pi^2}\exp\left\{-(\boldsymbol{\zeta}^\dagger\quad\boldsymbol{\zeta}'^\dagger)\begin{pmatrix}1&0\\-\boldsymbol{J}_3&1\end{pmatrix}\begin{pmatrix}\boldsymbol{\zeta}\\\boldsymbol{\zeta}'\end{pmatrix}+(\boldsymbol{\zeta}^\dagger\quad\boldsymbol{\zeta}'^\dagger)\begin{pmatrix}\boldsymbol{\alpha}\\\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'\end{pmatrix}+(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\quad\boldsymbol{\alpha}^\dagger)\begin{pmatrix}\boldsymbol{\zeta}\\\boldsymbol{\zeta}'\end{pmatrix}\right\}\Bigg|_{\boldsymbol{\alpha},\boldsymbol{\alpha}^\dagger=0}\\
&\quad=\partial_{\boldsymbol{\alpha}_J^*\boldsymbol{\alpha}_I}e^{\boldsymbol{\alpha}^\dagger\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\alpha}+\boldsymbol{\alpha}^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'}|_{\boldsymbol{\alpha},\boldsymbol{\alpha}^\dagger=0},
\end{aligned} \tag{B1}$$

where we have used the convention $\partial_{\boldsymbol{\alpha}_J^*\boldsymbol{\alpha}_I} := (\partial_{\alpha_d^*})^{j_d}\cdots(\partial_{\alpha_1^*})^{j_1}(\partial_{\alpha_1})^{i_1}\cdots(\partial_{\alpha_d})^{i_d}$ and the formula of the Gaussian integral [64].

$\partial_{\boldsymbol{\alpha}_J^\dagger\boldsymbol{\alpha}_I}e^{\boldsymbol{\alpha}^\dagger\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\alpha}^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'+\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\alpha}}|_{\boldsymbol{\alpha}=\boldsymbol{\alpha}^*=0}$ is only related to the coefficient of $\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}$ in the polynomial expansion of $e^{\boldsymbol{\alpha}^\dagger\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\alpha}^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'+\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\alpha}}$. Note

$$e^{\boldsymbol{\alpha}^\dagger\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\alpha}^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}'+\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\alpha}} = \sum_{k_1,k_2,k_3=0}^{\infty}\frac{(\boldsymbol{\alpha}^\dagger\boldsymbol{J}_3\boldsymbol{\alpha})^{k_1}}{k_1!}\frac{(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\alpha})^{k_2}}{k_2!}\frac{(\boldsymbol{\alpha}^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}')^{k_3}}{k_3!}. \tag{B2}$$

The terms with factor $\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}$ can be obtained through the following:

(i) $\frac{(\boldsymbol{\alpha}^\dagger\boldsymbol{J}_3\boldsymbol{\alpha})^{i'_1+\cdots+i'_d}}{(i'_1+\cdots+i'_d)!}$ contributes to $\alpha_d^{i'_d}\cdots\alpha_1^{i'_1}\alpha_1^{*j'_1}\cdots\alpha_d^{*j'_d}$,

(ii) $\frac{(\boldsymbol{\eta}^\dagger\boldsymbol{J}_1\boldsymbol{\alpha})^{\overline{i'_1}+\cdots+\overline{i'_d}}}{(\overline{i'_1}+\cdots+\overline{i'_d})!}$ contributes to $\alpha_d^{\overline{i'_d}}\cdots\alpha_1^{\overline{i'_1}}$,

(iii) $\frac{(\boldsymbol{\alpha}^\dagger\boldsymbol{J}_1^\dagger\boldsymbol{\eta}')^{\overline{j'_1}+\cdots+\overline{j'_d}}}{(\overline{j'_1}+\cdots+\overline{j'_d})!}$ contributes to $\alpha_1^{*\overline{j'_1}}\cdots\alpha_d^{*\overline{j'_d}}$,

where $i'_1,\ldots,i'_d, j'_1,\ldots,j'_d, \overline{i'_1},\ldots,\overline{i'_d}, \overline{j'_1},\ldots,\overline{j'_d}$ satisfy the constraints

$$i'_1,\ldots,i'_d, j'_1,\ldots,j'_d, \overline{i'_1},\ldots,\overline{i'_d}, \overline{j'_1},\ldots,\overline{j'_d} \in \{0,1,2,\ldots\}; \tag{B3a}$$

$$\overline{i'_1} = i_1 - i'_1, \quad \ldots, \quad \overline{i'_d} = i_d - i'_d; \tag{B3b}$$

$$\overline{j'_1} = j_1 - j'_1, \quad \ldots, \quad \overline{j'_d} = j_d - j'_d; \tag{B3c}$$

$$i'_1 + \cdots + i'_d = j'_1 + \cdots + j'_d. \tag{B3d}$$

Note,

(i) the coefficient of $\alpha_d^{i'_d} \cdots \alpha_1^{i'_1} \alpha_1^{*j'_1} \cdots \alpha_d^{*j'_d}$ in $\frac{(\boldsymbol{\alpha}^\dagger \boldsymbol{J}_3 \boldsymbol{\alpha})^{i'_1+\cdots+i'_d}}{(i'_1+\cdots+i'_d)!}$ is $\frac{\mathrm{perm}[(\boldsymbol{J}_3)_{J',I'}]}{i'_1!\cdots i'_d! j'_1! \cdots j'_d!}$ (see the following for the explanation of these symbols);

(ii) the coefficient of $\alpha_d^{\overline{i'_d}} \cdots \alpha_1^{\overline{i'_1}}$ in $\frac{(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1 \boldsymbol{\alpha})^{\overline{i'_1}+\cdots+\overline{i'_d}}}{(\overline{i'_1}+\cdots+\overline{i'_d})!}$ is $\frac{[(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_1]^{\overline{i'_1}} \cdots [(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_d]^{\overline{i'_d}}}{\overline{i'_1}! \cdots \overline{i'_d}!} = \frac{(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}}}{\overline{i'_1}! \cdots \overline{i'_d}!}$;

(iii) the coefficient of $\alpha_1^{*\overline{j'_1}} \cdots \alpha_d^{*\overline{j'_d}}$ in $\frac{(\boldsymbol{\alpha}^\dagger \boldsymbol{J}_1^\dagger \boldsymbol{\eta}')^{\overline{j'_1}+\cdots+\overline{j'_d}}}{(\overline{j'_1}+\cdots+\overline{j'_d})!}$ is $\frac{[(\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_d]^{\overline{j'_d}} \cdots [(\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_1]^{\overline{j'_1}}}{\overline{j'_1}! \cdots \overline{j'_d}!} = \frac{(\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}}{\overline{j'_1}! \cdots \overline{j'_d}!}$,

therefore, the coefficient of $\alpha_d^{i_d} \cdots \alpha_1^{i_1} \alpha_1^{*j_1} \cdots \alpha_d^{*j_d}$ in $\frac{(\boldsymbol{\alpha}^\dagger \boldsymbol{J}_3 \boldsymbol{\alpha})^{i'_1+\cdots+i'_d}}{(i'_1+\cdots+i'_d)!} \frac{(\boldsymbol{\alpha}^\dagger \boldsymbol{J}_1^\dagger \boldsymbol{\eta}')^{\overline{j'_1}+\cdots+\overline{j'_d}}}{(\overline{j'_1}+\cdots+\overline{j'_d})!} \frac{(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1 \boldsymbol{\alpha})^{\overline{i'_1}+\cdots+\overline{i'_d}}}{(\overline{i'_1}+\cdots+\overline{i'_d})!}$ is

$$\frac{\mathrm{perm}[(\boldsymbol{J}_3)_{J',I'}]}{i'_1! \cdots i'_d! j'_1! \cdots j'_d!} \frac{(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}}}{\overline{i'_1}! \cdots \overline{i'_d}!} \frac{(\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}}{\overline{j'_1}! \cdots \overline{j'_d}!}. \tag{B4}$$

The symbol perm[(·)] stands for the *permanant* of the square matrix (·). For an $n \times n$ matrix A, the permanant is defined as

$$\mathrm{perm}(A) = \sum_{\sigma \in S_n} \prod_{i=1}^{n} A_{i,\sigma(i)}, \tag{B5}$$

where S_n is the symmetric group of the set $\{1, 2, \ldots, n\}$, and $A_{i,\sigma(i)}$ is the matrix element of A in the ith row and $\sigma(i)$th column. The symbol $(\boldsymbol{J}_3)_{J',I'}$ stands for the block matrix

$$(\boldsymbol{J}_3)_{J',I'} = \begin{pmatrix} X_{j'_1 \times i'_1} & \cdots & X_{j'_1 \times i'_d} \\ \vdots & \ddots & \vdots \\ X_{j'_d \times i'_1} & \cdots & X_{j'_d \times i'_d} \end{pmatrix} \tag{B6}$$

with the block $X_{j'_m \times i'_n}$ standing for the $j'_m \times i'_n$ matrix whose elements are all $(\boldsymbol{J}_3)_{mn}$, i.e.,

$$X_{j'_m \times i'_n} = \begin{pmatrix} (\boldsymbol{J}_3)_{mn} & \cdots & (\boldsymbol{J}_3)_{mn} \\ \vdots & \ddots & \vdots \\ (\boldsymbol{J}_3)_{mn} & \cdots & (\boldsymbol{J}_3)_{mn} \end{pmatrix}. \tag{B7}$$

Here, $(\boldsymbol{J}_3)_{mn}$ stands for the matrix element of the matrix $\boldsymbol{J}_3$ in the mth row and nth column.

The total coefficient of $\alpha_d^{i_d} \cdots \alpha_1^{i_1} \alpha_1^{*j_1} \cdots \alpha_d^{*j_d}$ in Eq. (B2) is the summation of all the terms in Eq. (B4) with $i'_{(\cdot)}$'s and $j'_{(\cdot)}$'s satisfying Eq. (B3), i.e.,

$$\sum_{i'_1, \cdots, i'_d, j'_1, \cdots, j'_d} \frac{\mathrm{perm}[(\boldsymbol{J}_3)_{J',I'}]}{i'_1! \cdots i'_d! j'_1! \cdots j'_d!} \frac{(\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}}}{\overline{i'_1}! \cdots \overline{i'_d}!} \frac{(\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}}{\overline{j'_1}! \cdots \overline{j'_d}!}. \tag{B8}$$

Also note that

$$\partial_{\boldsymbol{\alpha}_J^\dagger \boldsymbol{\alpha}_I} \left(\alpha_d^{i_d} \cdots \alpha_1^{i_1} \alpha_1^{*j_1} \cdots \alpha_d^{*j_d} \right) = i_1! \cdots i_d! j_1! \cdots j_d!, \tag{B9}$$

therefore

$$\partial_{\boldsymbol{\alpha}_J^\dagger \boldsymbol{\alpha}_I} e^{\boldsymbol{\alpha}^\dagger \boldsymbol{J}_3 \boldsymbol{\alpha} + \boldsymbol{\alpha}^\dagger \boldsymbol{J}_1^\dagger \boldsymbol{\eta}' + \boldsymbol{\eta}^\dagger \boldsymbol{J}_1 \boldsymbol{\alpha}} \big|_{\boldsymbol{\alpha} = \boldsymbol{\alpha}^\dagger = 0} = \sum_{i'_1, \ldots, i'_d, j'_1, \ldots, j'_d} C_{i'_1}^{i_1} \cdots C_{i'_d}^{i_d} C_{j'_1}^{j_1} \cdots C_{j'_d}^{j_d} \mathrm{perm}[(\boldsymbol{J}_3)_{J',I'}] (\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}, \tag{B10}$$

where $C_k^n = \frac{n!}{k!(n-k)!}$ stands for the binomial coefficient. Denote

$$\sum_{I'J'} (\cdot) = \sum_{i'_1, \ldots, i'_d, j'_1, \ldots, j'_d} (\cdot), \quad P_+ = C_{i'_1}^{i_1} \cdots C_{i'_d}^{i_d} C_{j'_1}^{j_1} \cdots C_{j'_d}^{j_d}, \quad |(\boldsymbol{J}_3)_{J',I'}|_+ = \mathrm{perm}[(\boldsymbol{J}_3)_{J',I'}], \tag{B11}$$

in which the constraints over I' and J' are the same as those in Eq. (B3); then the result can be reexpressed as

$$\int d\mu(\boldsymbol{\zeta}, \boldsymbol{\zeta}') \boldsymbol{\zeta}_I'^\dagger \boldsymbol{\zeta}_J e^{\boldsymbol{\zeta}'^\dagger \boldsymbol{J}_3 \boldsymbol{\zeta} + \boldsymbol{\zeta}'^\dagger \boldsymbol{J}_1^\dagger \boldsymbol{\eta}' + \boldsymbol{\eta}^\dagger \boldsymbol{J}_1 \boldsymbol{\zeta}} = \sum_{I'J'} P_+ |(\boldsymbol{J}_3)_{J',I'}|_+ (\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}. \tag{B12}$$

2. Fermionic case

From Eq. (13), for fermions, we have

$$
\begin{aligned}
&\int d\mu(\boldsymbol{\zeta},\boldsymbol{\zeta}')\boldsymbol{\zeta}_I'^{\dagger}\boldsymbol{\zeta}_J' e^{-\boldsymbol{\zeta}'^{\dagger}\boldsymbol{J}_3\boldsymbol{\zeta}+\boldsymbol{\zeta}'^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'+\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\zeta}}\\
&=\int\prod_{n=1}^{d}(d\zeta_n^*d\zeta_nd\zeta_n'^*d\zeta_n')\boldsymbol{\zeta}_I'^{\dagger}\boldsymbol{\zeta}_J'\exp\left\{-(\boldsymbol{\zeta}^{\dagger}\quad\boldsymbol{\zeta}'^{\dagger})\begin{pmatrix}1&0\\ \boldsymbol{J}_3&1\end{pmatrix}\begin{pmatrix}\boldsymbol{\zeta}\\ \boldsymbol{\zeta}'\end{pmatrix}+(\boldsymbol{\zeta}^{\dagger}\quad\boldsymbol{\zeta}'^{\dagger})\begin{pmatrix}\boldsymbol{0}\\ \boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'\end{pmatrix}+(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\quad\boldsymbol{0})\begin{pmatrix}\boldsymbol{\zeta}\\ \boldsymbol{\zeta}'\end{pmatrix}\right\}\\
&=\partial_{\boldsymbol{\alpha}_J^*\boldsymbol{\alpha}_I}\int\prod_{n=1}^{d}(d\zeta_n^*d\zeta_nd\zeta_n'^*d\zeta_n')\exp\left\{-(\boldsymbol{\zeta}^{\dagger}\quad\boldsymbol{\zeta}'^{\dagger})\begin{pmatrix}1&0\\ \boldsymbol{J}_3&1\end{pmatrix}\begin{pmatrix}\boldsymbol{\zeta}\\ \boldsymbol{\zeta}'\end{pmatrix}+(\boldsymbol{\zeta}^{\dagger}\quad\boldsymbol{\zeta}'^{\dagger})\begin{pmatrix}\boldsymbol{\alpha}\\ \boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'\end{pmatrix}+(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\quad\boldsymbol{\alpha}^{\dagger})\begin{pmatrix}\boldsymbol{\zeta}\\ \boldsymbol{\zeta}'\end{pmatrix}\right\}\Bigg|_{\boldsymbol{\alpha},\boldsymbol{\alpha}^{\dagger}=0}\\
&=\partial_{\boldsymbol{\alpha}_J^*\boldsymbol{\alpha}_I}e^{-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha}+\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'}|_{\boldsymbol{\alpha},\boldsymbol{\alpha}^{\dagger}=0},
\end{aligned}
\tag{B13}
$$

where we have used the convention $\partial_{\boldsymbol{\alpha}_J^*\boldsymbol{\alpha}_I}:=(\partial_{\alpha_d^*})^{j_d}\cdots(\partial_{\alpha_1^*})^{j_1}(\partial_{\alpha_1})^{i_1}\cdots(\partial_{\alpha_d})^{i_d}$ and the formula of Grassmannian Gaussian integral [64].

$\partial_{\boldsymbol{\alpha}_J^{\dagger}\boldsymbol{\alpha}_I}e^{-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'+\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha}}|_{\boldsymbol{\alpha}=\boldsymbol{\alpha}^*=0}$ is only related to the coefficient of $\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}$ in the polynomial expansion of $e^{-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'+\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha}}$. Note

$$
e^{-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha}+\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}'+\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha}}=\sum_{k_1,k_2,k_3=0}^{\infty}\frac{(-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha})^{k_1}}{k_1!}\frac{(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha})^{k_2}}{k_2!}\frac{(\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')^{k_3}}{k_3!};
\tag{B14}
$$

the terms with factor $\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}$ can be obtained through the following:

(i) $\frac{(-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha})^{i_1'+\cdots+i_d'}}{(i_1'+\cdots+i_d')!}$ contributes to $\alpha_d^{i_d'}\cdots\alpha_1^{i_1'}\alpha_1^{*j_1'}\cdots\alpha_d^{*j_d'}$,

(ii) $\frac{(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha})^{\overline{i_1'}+\cdots+\overline{i_d'}}}{(\overline{i_1'}+\cdots+\overline{i_d'})!}$ contributes to $\alpha_d^{\overline{i_d'}}\cdots\alpha_1^{\overline{i_1'}}$,

(iii) $\frac{(\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')^{\overline{j_1'}+\cdots+\overline{j_d'}}}{(\overline{j_1'}+\cdots+\overline{j_d'})!}$ contributes to $\alpha_1^{*\overline{j_1'}}\cdots\alpha_d^{*\overline{j_d'}}$,

where $i_1',\ldots,i_d',j_1',\ldots,j_d',\overline{i_1'},\ldots,\overline{i_d'},\overline{j_1'},\ldots,\overline{j_d'}$ satisfy the constraint

$$
i_1',\ldots,i_d',\quad j_1',\ldots,j_d',\overline{i_1'},\ldots,\overline{i_d'},\overline{j_1'},\ldots,\overline{j_d'}\in\{0,1\};
\tag{B15a}
$$

$$
\overline{i_1'}=i_1-i_1',\quad\ldots,\quad\overline{i_d'}=i_d-i_d';
\tag{B15b}
$$

$$
\overline{j_1'}=j_1-j_1',\quad\ldots,\quad\overline{j_d'}=j_d-j_d';
\tag{B15c}
$$

$$
i_1'+\cdots+i_d'=j_1'+\cdots+j_d'.
\tag{B15d}
$$

Note that

(i) the coefficient of $\alpha_d^{i_d'}\cdots\alpha_1^{i_1'}\alpha_1^{*j_1'}\cdots\alpha_d^{*j_d'}$ in $\frac{(-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha})^{i_1'+\cdots+i_d'}}{(i_1'+\cdots+i_d')!}$ is $\det[(\boldsymbol{J}_3)_{J',I'}]$, where $\det[(\cdot)]$ stands for the *determinant* of the matrix $(\cdot)$ and $(\boldsymbol{J}_3)_{J',I'}$ is the block matrix similar to that in Eq. (B6) except that the $j_{(\cdot)}'$'s and $i_{(\cdot)}'$'s are either 0 or 1;

(ii) the coefficient of $\alpha_d^{\overline{i_d'}}\cdots\alpha_1^{\overline{i_1'}}$ in $\frac{(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha})^{\overline{i_1'}+\cdots+\overline{i_d'}}}{(\overline{i_1'}+\cdots+\overline{i_d'})!}$ is $(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1)_{\overline{I'}}$;

(iii) the coefficient of $\alpha_1^{*\overline{j_1'}}\cdots\alpha_d^{*\overline{j_d'}}$ in $\frac{(\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')^{\overline{j_1'}+\cdots+\overline{j_d'}}}{(\overline{j_1'}+\cdots+\overline{j_d'})!}$ is $(\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')_{\overline{J'}}$;

and

$$
\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}=s(I,I')s(J,J')\alpha_d^{i_d'}\cdots\alpha_1^{i_1'}\alpha_1^{*j_1'}\cdots\alpha_d^{*j_d'}\alpha_d^{\overline{i_d'}}\cdots\alpha_1^{\overline{i_1'}}\alpha_1^{*\overline{j_1'}}\cdots\alpha_d^{*\overline{j_d'}},
\tag{B16}
$$

where $s(I,I')$ is defined through the relation $\boldsymbol{\zeta}_I^{\dagger}=s(I,I')\boldsymbol{\zeta}_{I'}^{\dagger}\boldsymbol{\zeta}_{\overline{I'}}^{\dagger}$.

Therefore, the coefficient of $\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}$ in $\frac{(-\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_3\boldsymbol{\alpha})^{i_1'+\cdots+i_d'}}{(i_1'+\cdots+i_d')!}\frac{(\boldsymbol{\alpha}^{\dagger}\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')^{\overline{j_1'}+\cdots+\overline{j_d'}}}{(\overline{j_1'}+\cdots+\overline{j_d'})!}\frac{(\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1\boldsymbol{\alpha})^{\overline{i_1'}+\cdots+\overline{i_d'}}}{(\overline{i_1'}+\cdots+\overline{i_d'})!}$ is $s(I,I')s(J,J')\det[(\boldsymbol{J}_3)_{J',I'}](\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1)_{\overline{I'}}(\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')_{\overline{J'}}$. The total coefficient of $\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d}$ in Eq. (B14) is the summation of all the possible terms with $i_{(\cdot)}'$'s and $j_{(\cdot)}'$'s satisfying Eq. (B15), which is denoted as

$$
\sum_{i_1',\cdots,i_d',j_1',\cdots,j_d'}s(I,I')s(J,J')\det[(\boldsymbol{J}_3)_{J',I'}](\boldsymbol{\eta}^{\dagger}\boldsymbol{J}_1)_{\overline{I'}}(\boldsymbol{J}_1^{\dagger}\boldsymbol{\eta}')_{\overline{J'}}.
\tag{B17}
$$

Also note that for Grassmannian variables

$$
\partial_{\boldsymbol{\alpha}_J^{\dagger}\boldsymbol{\alpha}_I}(\alpha_d^{i_d}\cdots\alpha_1^{i_1}\alpha_1^{*j_1}\cdots\alpha_d^{*j_d})=1,
\tag{B18}
$$

therefore

$$\partial_{\boldsymbol{\alpha}_J^\dagger \boldsymbol{\alpha}_I} e^{-\boldsymbol{\alpha}^\dagger \boldsymbol{J}_3 \boldsymbol{\alpha} + \boldsymbol{\alpha}^\dagger \boldsymbol{J}_1^\dagger \boldsymbol{\eta}' + \boldsymbol{\eta}^\dagger \boldsymbol{J}_1 \boldsymbol{\alpha}} \big|_{\boldsymbol{\alpha}=\boldsymbol{\alpha}^\dagger=0} = \sum_{i_1',\cdots,i_d',j_1',\cdots,j_d'} s(I,I')s(J,J') \det[(\boldsymbol{J}_3)_{J',I'}](\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}. \tag{B19}$$

Denote

$$\sum_{I'J'}(\cdot) = \sum_{i_1',\ldots,i_d',j_1',\ldots,j_d'} (\cdot), \quad P_- = s(I,I')s(J,J'), \quad |(\boldsymbol{J}_3)_{J',I'}|_- = \det[(\boldsymbol{J}_3)_{J',I'}], \tag{B20}$$

in which the constraints over I' and J' are the same as those in Eq. (B15), then the final result can be formulated as

$$\int d\mu(\boldsymbol{\zeta},\boldsymbol{\zeta}') \zeta_I'^\dagger \zeta_J' e^{-\boldsymbol{\zeta}'^\dagger \boldsymbol{J}_3 \boldsymbol{\zeta} + \boldsymbol{\zeta}'^\dagger \boldsymbol{J}_1^\dagger \boldsymbol{\eta}' + \boldsymbol{\eta}^\dagger \boldsymbol{J}_1 \boldsymbol{\zeta}} = \sum_{I'J'} P_- |(\boldsymbol{J}_3)_{J',I'}|_- (\boldsymbol{\eta}^\dagger \boldsymbol{J}_1)_{\overline{I'}} (\boldsymbol{J}_1^\dagger \boldsymbol{\eta}')_{\overline{J'}}. \tag{B21}$$

APPENDIX C: EQUILIBRIUM STATE OF THE SYSTEM

If the total system possesses no localized states, the open system would finally reach an equilibrium state. Following the expression of the reduced density matrix in Eq. (18) and the asymptotic expression of $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ in Eq. (25), when t approaches infinity, only the terms with $\overline{I'} = \overline{J'} = \{0,\ldots,0\}$ would survive, i.e.,

$$\rho(\infty) = \sum_{IJ} \rho_{IJ}(0) \frac{|(\boldsymbol{J}_3)_{J,I}|_\pm \rho^{\text{th}}(\infty)}{\sqrt{i_1!\cdots i_d! j_1!\cdots j_d!}}. \tag{C1}$$

Because $\boldsymbol{J}_3$ reduces to the identity matrix $\mathbf{I}$ as $\boldsymbol{u}$ vanishes, the matrix $(\boldsymbol{J}_3)_{J,I}$ would approach a block-diagonal matrix in the form

$$(\boldsymbol{J}_3)_{J,I} = \begin{pmatrix} ((\boldsymbol{J}_3)_{J,I})_1 & & & \\ & ((\boldsymbol{J}_3)_{J,I})_2 & & \\ & & \ddots & \\ & & & ((\boldsymbol{J}_3)_{J,I})_d \end{pmatrix} \tag{C2}$$

where

$$((\boldsymbol{J}_3)_{J,I})_n = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix}_{j_n \times i_n}. \tag{C3}$$

The *permanent* and *determinant* of $(\boldsymbol{J}_3)_{J,I}$ then share a common expression, reading

$$|(\boldsymbol{J}_3)_{J,I}|_\pm = \begin{cases} 0 & (I \neq J), \\ i_1!\cdots i_d! & (I = J). \end{cases} \tag{C4}$$

Following Eq. (C1), $\rho(\infty)$ can be simplified to

$$\rho(\infty) = \sum_{I=J} \rho_{IJ}(0) \rho^{\text{th}}(\infty). \tag{C5}$$

With the normalization condition that $\sum_{I=J} \rho_{IJ}(0) = 1$, it can be finally written as

$$\rho(\infty) = \rho^{\text{th}}(\infty) = \frac{e^{\boldsymbol{a}^\dagger \ln(\frac{\boldsymbol{v}(\infty)}{\mathbf{I} \pm \boldsymbol{v}(\infty)}) \boldsymbol{a}}}{[\det(\mathbf{I} \pm \boldsymbol{v}(\infty))]^{\pm 1}} = \frac{e^{\boldsymbol{a}^\dagger \ln(\frac{\overline{\boldsymbol{n}}}{\mathbf{I} \pm \overline{\boldsymbol{n}}}) \boldsymbol{a}}}{[\det(\mathbf{I} \pm \overline{\boldsymbol{n}})]^{\pm 1}}. \tag{C6}$$

APPENDIX D: ASYMPTOTIC FORM OF $D(\epsilon)$ AS THE COUPLING STRENGTH VANISHES

When $\boldsymbol{J}(\epsilon) \to \mathbf{0}$ and $\boldsymbol{\Delta}(\epsilon) \to \mathbf{0}$, the spectrum

$$\boldsymbol{D}(\epsilon) = \frac{1}{\epsilon - \boldsymbol{\epsilon}_{\text{S}} - \boldsymbol{\Delta}(\epsilon) + i\frac{\boldsymbol{J}(\epsilon)}{2}} \boldsymbol{J}(\epsilon) \frac{1}{\epsilon - \boldsymbol{\epsilon}_{\text{S}} - \boldsymbol{\Delta}(\epsilon) - i\frac{\boldsymbol{J}(\epsilon)}{2}} \tag{D1}$$

is vanishing for the values of ϵ such that the matrices $\epsilon - \boldsymbol{\epsilon}_{\text{S}} - \boldsymbol{\Delta}(\epsilon) \pm i\frac{\boldsymbol{J}(\epsilon)}{2}$ are invertible. Because $\boldsymbol{J}(\epsilon) \to \mathbf{0}$ and $\boldsymbol{\Delta}(\epsilon) \to \mathbf{0}$, the condition can be simplified as $\epsilon - \boldsymbol{\epsilon}_{\text{S}}$ being invertible. Therefore, $\boldsymbol{D}(\epsilon)$ is nonvanishing only for ϵ equaling an eigenvalue ϵ_λ of $\boldsymbol{\epsilon}_{\text{S}}$. So in order to grasp the asymptotic behavior of $\boldsymbol{D}(\epsilon)$, one only needs to analyze the behavior of $\boldsymbol{D}(\epsilon)$ around $\epsilon = \epsilon_\lambda$.

Consider the behavior of $\frac{1}{\epsilon-\boldsymbol{\epsilon}_{\rm S}-\boldsymbol{\Delta}(\epsilon)\pm i\frac{\boldsymbol{J}(\epsilon)}{2}}$ for $\epsilon \approx \epsilon_\lambda$ in the weak-coupling limit. Denote the eigenspace of $\boldsymbol{\epsilon}_{\rm S}$ corresponding to the eigenvalue ϵ_λ as $\mathbb{H}_\lambda$; then the matrix $\epsilon - \boldsymbol{\epsilon}_{\rm S} - \boldsymbol{\Delta}(\epsilon) \pm i\frac{\boldsymbol{J}(\epsilon)}{2}$ can be written in blocks, reading

$$\epsilon - \boldsymbol{\epsilon}_{\rm S} - \boldsymbol{\Delta}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}(\epsilon) = \begin{pmatrix} (\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda - \boldsymbol{\Delta}_{\lambda\lambda}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}_{\lambda\lambda}(\epsilon) & \left[-\boldsymbol{\Delta}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}(\epsilon)\right]_{\lambda\lambda^\perp} \\ \left[-\boldsymbol{\Delta}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}(\epsilon)\right]_{\lambda^\perp\lambda} & \left[\epsilon - \boldsymbol{\epsilon}_{\rm S} - \boldsymbol{\Delta}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}(\epsilon)\right]_{\lambda^\perp\lambda^\perp} \end{pmatrix}, \tag{D2}$$

where the subscripts λ and $\lambda^\perp$ correspond to the space $\mathbb{H}_\lambda$ and its orthogonal complement, respectively. Because $\boldsymbol{J}(\epsilon) \approx \mathbf{0}$ and $\boldsymbol{\Delta}(\epsilon) \approx \mathbf{0}$, the inverse of $\epsilon - \boldsymbol{\epsilon}_{\rm S} - \boldsymbol{\Delta}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}(\epsilon)$ is approximately

$$\frac{1}{\epsilon - \boldsymbol{\epsilon}_{\rm S} - \boldsymbol{\Delta}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}(\epsilon)} \approx \begin{pmatrix} \frac{1}{(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda - \boldsymbol{\Delta}_{\lambda\lambda}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}_{\lambda\lambda}(\epsilon)} & \mathbf{0} \\ \mathbf{0} & \frac{1}{\epsilon - (\boldsymbol{\epsilon}_{\rm S})_{\lambda^\perp\lambda^\perp}} \end{pmatrix}, \tag{D3}$$

where $\mathbf{I}_\lambda$ is the identity in $\mathbb{H}_\lambda$. [In this equation, we have kept the term $(\epsilon - \epsilon_\lambda)\mathbf{I}_\lambda$ because we shall consider the behavior of the functions for $\epsilon \approx \epsilon_\lambda$.] Following Eqs. (D1) and (D3), and taking advantage of the property $\boldsymbol{J}(\epsilon) \approx \mathbf{0}$, the expression of $\boldsymbol{D}(\epsilon)$ around $\epsilon \approx \epsilon_\lambda$ can be approximately written as

$$\boldsymbol{D}(\epsilon) \approx \frac{1}{(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda - \boldsymbol{\Delta}_{\lambda\lambda}(\epsilon) + \frac{i}{2}\boldsymbol{J}_{\lambda\lambda}(\epsilon)}\boldsymbol{J}_{\lambda\lambda}(\epsilon)\frac{1}{(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda - \boldsymbol{\Delta}_{\lambda\lambda}(\epsilon) - \frac{i}{2}\boldsymbol{J}_{\lambda\lambda}(\epsilon)}. \tag{D4}$$

To obtain the limiting behavior, we first take the weak-coupling limit, and then let ϵ approach ϵ_λ. When the coupling is very weak, the real part of $(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda - \boldsymbol{\Delta}_{\lambda\lambda}(\epsilon) \pm \frac{i}{2}\boldsymbol{J}_{\lambda\lambda}(\epsilon)$ is dominated by $(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda$. Consequently, Eq. (D4) can be further simplified to

$$\boldsymbol{D}(\epsilon) \approx \frac{\boldsymbol{J}_{\lambda\lambda}(\epsilon)}{(\epsilon-\epsilon_\lambda)^2\mathbf{I}_\lambda + [\boldsymbol{J}_{\lambda\lambda}(\epsilon)]^2/4}. \tag{D5}$$

After expressing the right-hand side of the equation in the eigenbasis of $\boldsymbol{J}_{\lambda\lambda}(\epsilon)$, one can easily find that the diagonal elements all approach $2\pi\delta(\epsilon-\epsilon_\lambda)$ as $\boldsymbol{J}(\epsilon)$ vanishes. That is, for ϵ near ϵ_λ,

$$\boldsymbol{D}(\epsilon) \to 2\pi\delta(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda. \tag{D6}$$

For every λ, such a conclusion is always true. Therefore, for all ϵ,

$$\boldsymbol{D}(\epsilon) \to 2\pi\sum_\lambda \delta(\epsilon-\epsilon_\lambda)\mathbf{I}_\lambda = 2\pi\delta(\epsilon\mathbf{I} - \boldsymbol{\epsilon}_{\rm S}). \tag{D7}$$

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