

Nonequilibrium density-matrix description of steady-state quantum transportAbhishek Dhar,¹ Keiji Saito,² and Peter Hänggi^{3,4,5}¹*Raman Research Institute, Bangalore 560080, India*²*Graduate School of Science, University of Tokyo, 113-0033 Japan*³*Institute of Physics, University of Augsburg, Universitätsstrasse 1, D-86135 Augsburg, Germany*⁴*Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, Singapore 117546*⁵*Max Planck Institute for the Physics of Complex systems, Nöthnitzer Strasse 38, D-01187 Dresden, Germany*

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With this work we investigate the stationary *nonequilibrium* density matrix of current carrying nonequilibrium steady states of in-between quantum systems that are connected to reservoirs. We describe the analytical procedure to obtain the explicit result for the reduced density matrix of quantum transport when the system, the connecting reservoirs, and the system-reservoir interactions are described by quadratic Hamiltonians. Our procedure is detailed for both electronic transport described by the tight-binding Hamiltonian and for phonon transport described by harmonic Hamiltonians. For the special case of weak system-reservoir couplings, a more detailed description of the steady-state density matrix is obtained. Several paradigm transport setups for interelectrode electron transport and low-dimensional phonon heat flux are elucidated.

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I. INTRODUCTION

The theory of equilibrium statistical mechanics, as pioneered by Boltzmann and Gibbs, provides the prescription for the appropriate density-matrix (or density-operator) description of a system that is kept under various external constraints. Thus, for systems kept in isolation the microcanonical distribution yields the appropriate density matrix, while for systems in weak contact with a thermal and particle reservoir the grand-canonical density matrix describes the statistical state of the system. For classical systems, equilibrium statistical physics is governed by the phase space distribution of the system. A knowledge of the density matrix or the phase space distribution then enables one to find various equilibrium and also close to equilibrium properties of a system, as exemplified, for example, via linear response theory.

For systems taken far away from equilibrium there exists no general procedure in obtaining its density matrix. Particularly, this holds true for systems that have reached steady states. For classical Hamiltonian systems described by a Markovian stochastic dynamics, the steady state is determined by the stationary solution of the corresponding master equation; e.g., it is given by the stationary probability density of the Fokker-Planck generator for continuous Markovian processes [1]. Apart from specific situations, however, for example, (i) in the presence of symmetries such as (strict) detailed balance, or (ii) a single variable state space dynamics [1], the task of finding the closed form solution of such master equations presents a profound challenge which typically can be obtained only by the usage of extensive numerical simulations or algorithms.

In this context we remind the reader that even for the case of a system being in contact with a *single* bath the corresponding canonical equilibrium is typically not of the common Boltzmann-Gibbs structure, as encoded with the exponential of the (negative) bare system Hamiltonian and inverse temperature. The latter structure holds rigorously true for weak coupling. In the presence of strong coupling, however, the corresponding thermal (generalized canonical) density operator

then typically involves a temperature-dependent “Hamiltonian of mean force” [2] which includes entropic contributions that explicitly depend on the system-bath coupling strength.

Regrettably, no such general concept as the canonical Boltzmann-Gibbs density-matrix structure in terms of the bare (or even modified Hamiltonian of mean force) is available when the open system is subjected to steady state transport. Put differently, there are no generic results known for stationary nonequilibrium statistics. This latter situation, in fact, is not only substantially more complex but currently also less researched. It is thus of the utmost importance to gain further insight into this objective of obtaining the underlying nonequilibrium density matrices that govern quantum and/or classical transport. For example, the explicit form of a corresponding nonequilibrium density matrix not only determines the linear response due to an additional external perturbation of such a nonequilibrium steady state (NESS), but also its higher-order response functions.

A particular, exactly solvable case is that of heat conduction occurring in a one-dimensional ordered harmonic chain when connected to two baths at different temperatures. If the two baths are modeled therein as being *stochastic* with corresponding stochastic forces acting on the system of interest, the exact nonequilibrium steady-state phase space distribution for this problem was evaluated by Rieder, Lebowitz, and Lieb [3]. An extension to the case of higher dimensions was later obtained by Nakazawa [4]. Heat conduction in quantum harmonic oscillator chains has been studied by several authors [5–8], but thus far no explicit results are known for the precise form of the quantum mechanical *steady state* density matrix. Some formal results for the NESS density matrix of general quantum mechanical systems have been obtained in the works of Zubarev [9] and McLennan [10] and have more recently been discussed in specific models [11–13].

The problem of obtaining the NESS in explicit form presents a formidable challenge already for classical open systems (see above discussion). This objective, therefore, is typically even more intricate for a quantum NESS. Indeed, in the presence of general nonlinear interactions this task

is simply inaccessible without invoking also extensive and cumbersome numerical means and methods. To obtain general analytic insight over whole-parameter ranges thus necessitates confining the objective to stylized situations only, which allow for explicit closed form calculations.

With this work, we consider generic setups for steady-state quantum transport described by a bilinear Hamiltonian. The aim is to find a systematic procedure for obtaining explicit results for the NESS density matrix for this class of systems. We demonstrate that it is possible to obtain the complete NESS density matrix explicitly. We also show that when the coupling strength between the system and reservoirs is extremely weak, the NESS density matrix is given by an effective Gibbs state where each mode is formally only in equilibrium with a mode-dependent effective temperature that depends, however, in a complex manner on both bath temperatures.

We consider two generic setups for stationary nonequilibrium quantum transport, a first one involving fermions and the other one bosons as carriers. The first setup consists of electron and heat transport in a fermion setup of noninteracting particles that are connected to fermionic baths at different temperatures and chemical potentials. The second scenario consists of heat conduction occurring in harmonic crystals connected to oscillator baths kept at different temperatures. For both of these problems it is known from prior studies—using various approaches such as the nonequilibrium Green function formalism [14,15], the quantum Langevin equations approach [16–18], and the C^* algebra approach [19]—that it is possible to express all two-point correlations in the NESS in terms of appropriate Green functions. Because these systems are noninteracting it is evident that the two-point correlations contain necessary information on all higher-point correlations and hence should completely specify the NESS. With this study we give the procedure for finding the explicit NESS density matrices from a knowledge of the two-point correlations in these systems.

For the case of a weak coupling among system and the baths we are able to obtain explicit results. We further present explicit examples in simple one-dimensional models that illustrate our general procedure and also demonstrate the accuracy of the weak-coupling approximation.

The outline of the paper is as follows. In Sec. II we present the general procedure for construction of the NESS for the electron and phonon transport problems. The special case of weak coupling between system and bath is discussed in Sec. III. In Sec. IV we discuss some illustrative examples of models where both system and reservoirs are taken to be one-dimensional chains. Finally, we end with a discussion in Sec. V.

II. CONSTRUCTION OF STEADY-STATE DENSITY MATRIX

In this section, we outline the general procedure to obtain the steady-state density matrix in quantum transport described by a bilinear Hamiltonian. We focus on electric conduction as an example of fermionic transport, and phononic heat conduction as bosonic transport. Because the resulting NESS density matrix becomes Gaussian, the pertinent procedure first is in finding the explicit form of the two-point correlation

functions of physical quantities and next relating these to the Gaussian distribution.

A. Steady-state density matrix for noninteracting electron transport

We consider the typical setup of transport in the Landauer approach wherein a system is connected to two reservoirs initially kept at different temperatures and chemical potentials. At long times the system reaches a nonequilibrium steady state with a mean rate of flow of charge and energy current. One starts out by writing the full Hamiltonian of the system plus reservoirs, and here we consider a tight-binding approach of noninteracting electrons. We use the following notation: for sites on the system (S) we shall use the integer indices l, m, n, \dots ; for sites on the left reservoir (L) we employ the Greek indices α, ν ; and finally, for sites on the right reservoir (R) we use the primed Greek indices α', ν' . We consider quantum transport with the following overall Hamiltonian reading:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{LS} + \mathcal{H}_{RS}, \quad (2.1)$$

where

$$\begin{aligned} \mathcal{H}_S &= \sum_{lm} \mathbf{H}_{lm} c_l^\dagger c_m, & \mathcal{H}_L &= \sum_{\alpha\nu} \mathbf{H}_{\alpha\nu}^L c_\alpha^\dagger c_\nu, \\ \mathcal{H}_R &= \sum_{\alpha'\nu'} \mathbf{H}_{\alpha'\nu'}^R c_{\alpha'}^\dagger c_{\nu'}, & \mathcal{H}_{LS} &= \sum_{l\alpha} \mathbf{H}_{l\alpha}^{LS} [c_l^\dagger c_\alpha + c_\alpha^\dagger c_l], \\ \mathcal{H}_{RS} &= \sum_{l\alpha'} \mathbf{H}_{l\alpha'}^{RS} [c_l^\dagger c_{\alpha'} + c_{\alpha'}^\dagger c_l], \end{aligned}$$

where c^\dagger, c denote creation and annihilation operators satisfying the usual fermionic anticommutation rules and we assume that the matrices $\mathbf{H}, \mathbf{H}^L, \mathbf{H}^R$ are symmetric and real-valued while $\mathbf{H}^{LS}, \mathbf{H}^{RS}$ are real-valued. In the above setup we assume that the system possesses a finite number of lattice sites N while the left and right reservoirs have N_L and N_R sites, which will eventually be made infinite. The parts $\mathcal{H}_S, \mathcal{H}_L$, and \mathcal{H}_R denote the Hamiltonians of the isolated system, left, and right reservoirs, respectively, while \mathcal{H}_L and \mathcal{H}_R describe the coupling of the left and right reservoirs to the system, which have been taken to be real. To obtain a NESS for the system we consider an initial state at time $t = t_0$ given by the following product density matrix:

$$\rho(t_0) = \rho_S^0 \otimes \rho_L^0 \otimes \rho_R^0, \quad (2.2)$$

where $\rho_L^0 \sim e^{-(\mathcal{H}_L - \mu_L \mathcal{N}_L)/T_L}$ ($\rho_R^0 \sim e^{-(\mathcal{H}_R - \mu_R \mathcal{N}_R)/T_R}$) is the equilibrium grand-canonical density matrix of the left (right) reservoir, corresponding to temperature T_L (T_R) and chemical potential μ_L (μ_R) with $\mathcal{N}_L, \mathcal{N}_R$ the total number operators, while ρ_S^0 denotes an arbitrary initial density matrix for the system. We then time-evolve the whole system with the full Hamiltonian given in Eq. (2.1) so that at time t the full density matrix is given by

$$\rho(t) = e^{-i\mathcal{H}(t-t_0)/\hbar} \rho(t_0) e^{+i\mathcal{H}(t-t_0)/\hbar}. \quad (2.3)$$

Our principal objective is the long time limit of the steady-state reduced density matrix for the system under consideration, i.e.,

$$\rho_S = \lim_{t_0 \rightarrow -\infty} \lim_{\text{baths} \rightarrow \infty} \text{Tr}_{L,R} \rho(t), \quad (2.4)$$

where the trace, $\text{Tr}_{L,R}$, is over all the degrees of freedom of the two baths. In doing so we implicitly assume that the quantum transport setup is so that (i) it possesses a long time limit in the limit of infinite many bath degrees of freedom and (ii) that the interactions within the quantum system and the interaction with the bath degrees of freedom are such that the emerging asymptotic nonequilibrium steady-state density matrix indeed is time-independent.

Let us introduce the two-point correlation function

$$\langle c_m^\dagger c_l \rangle = \text{Tr}_S[c_m^\dagger c_l \rho_S] = \text{Tr}[c_m^\dagger c_l \rho], \quad (2.5)$$

where the first trace, Tr_S , is over system degrees of freedom and the second trace is over all degrees of freedom. Because of the quadratic form of the total Hamiltonian, the two-point correlations in the NESS can be exactly calculated using various methods [16,20,21].

The correlations can be expressed in terms of the following Green function:

$$\mathbf{G}^\pm(\omega) = \frac{1}{\hbar\omega - \mathbf{H} - \Sigma_L^\pm(\omega) - \Sigma_R^\pm(\omega)}, \quad (2.6)$$

where Σ_L^\pm and Σ_R^\pm are self-energy terms that model the effect of the infinite reservoirs on the isolated system Hamiltonian. The self-energies can be written in terms of the isolated reservoir Green functions $\mathbf{g}_L^\pm(\omega) = [\hbar\omega \pm i\epsilon - \mathbf{H}^L]^{-1}$, $\mathbf{g}_R^\pm(\omega) = [\hbar\omega \pm i\epsilon - \mathbf{H}^R]^{-1}$ and the coupling matrices \mathbf{H}^{LS} and \mathbf{H}^{RS} , reading

$$\begin{aligned} \Sigma_L^\pm(\omega) &= \mathbf{H}^{LS} \mathbf{g}_L^\pm(\omega) \mathbf{H}^{LS\dagger}, \\ \Sigma_R^\pm(\omega) &= \mathbf{H}^{RS} \mathbf{g}_R^\pm(\omega) \mathbf{H}^{RS\dagger}. \end{aligned} \quad (2.7)$$

Let us next define $\Gamma_L(\omega) = [\Sigma_L^- - \Sigma_L^+]/(2i)$, $\Gamma_R(\omega) = [\Sigma_R^- - \Sigma_R^+]/(2i)$. With these definitions one finds the following expressions for the steady-state correlation matrix:

$$\begin{aligned} \mathbf{C}_{ml} &= \langle c_m^\dagger c_l \rangle \\ &= \int_{-\infty}^{\infty} d\omega \frac{\hbar}{\pi} [(\mathbf{G}^+ \Gamma_L \mathbf{G}^-)_{lm} f(\omega, \mu_L, T_L) \\ &\quad + (\mathbf{G}^+ \Gamma_R \mathbf{G}^-)_{lm} f(\omega, \mu_R, T_R)], \end{aligned} \quad (2.8)$$

where $f(\omega, \mu, T) = 1/[e^{\beta(\hbar\omega - \mu)} + 1]$ denotes the Fermi function.

We demonstrate next how the NESS density matrix ρ_S can be fully expressed in terms of these correlations. Note that the matrix \mathbf{C} is Hermitian, since at any time $\text{Tr}[c_m^\dagger c_l \rho(t)] = \text{Tr}[c_m^\dagger c_l \rho(t)]^*$, where (*) indicates complex conjugation. This result can also be directly verified from the form in Eq. (2.8). Consequently the matrix \mathbf{C} can be diagonalized with a unitary matrix \mathbf{U} to read

$$\mathbf{U}^\dagger \mathbf{C} \mathbf{U} = \mathbf{D} = \text{diag}(d_1, d_2, \dots, d_{N-1}, d_N), \quad (2.9)$$

where the matrix \mathbf{D} is the diagonal matrix. Using the unitary transformation, we define new fermionic operators as

$$c'_s = \sum_l \mathbf{U}_{l,s} c_l, \quad s = 1, \dots, N. \quad (2.10)$$

Obviously, these new fermionic operators preserve the anti-commutation relations, $\{c'_s, c'^{\dagger}_{s'}\} = \delta_{s,s'}$. The steady-state density matrix is a diagonal matrix in terms of these new

fermion operators. Note that the two-point correlation of new fermionic operators reads $\langle c'_s c'^{\dagger}_{s'} \rangle = \delta_{s,s'} d_s$. From this we find the corresponding effective Fermi-Dirac distribution for each fermion s . Consequently, the steady-state matrix ρ_S is formally given by

$$\rho_S = \prod_{s=1}^N \frac{\exp[-a_s c'_s c'^{\dagger}_{s'}]}{[1 + \exp(-a_s)]} \quad (2.11)$$

$$= \frac{\exp[-\sum_{l,m} c_l^\dagger \mathbf{A}_{l,m} c_m]}{\prod_{s=1}^N [1 + \exp(-a_s)]}, \quad (2.12)$$

$$\mathbf{A} = \mathbf{U}^* \text{diag}(a_1, a_2, \dots, a_{N-1}, a_N) \mathbf{U}^T, \quad (2.13)$$

$$a_s = \ln(d_s^{-1} - 1). \quad (2.14)$$

To obtain Eq. (2.14) we used the relation $\langle c'_s c'^{\dagger}_{s'} \rangle = d_s = 1/[\exp(a_s) + 1]$. This completes our derivation of the expression for the steady-state density matrix for noninteracting electron transport.

B. Steady-state density matrix for noninteracting phonon transport

We next consider heat conduction in general harmonic networks. Examples of such a system are dielectric crystals for which the harmonic crystal provides a very good description. We again consider the usual Landauer-like framework of a system connected to two reservoirs kept at different temperatures [7,8]. The reservoirs are themselves modeled as collections of harmonic oscillators. Let us assume that the system has N Cartesian positional degrees of freedom $\{x_l\}$, $l = 1, 2, \dots, N$ with corresponding momenta $\{p_l\}$. These satisfy the usual commutation relations $[x_l, p_m] = i\hbar\delta_{l,m}$ and $[x_l, x_m] = [p_l, p_m] = 0$. Similarly, the left reservoir degrees of freedom are denoted by $\{x_\alpha^L, p_\alpha^L\}$, $\alpha = 1, \dots, N_L$ and the right reservoirs by $\{x_{\alpha'}^R, p_{\alpha'}^R\}$, $\alpha' = 1, \dots, N_R$. We will use the vector notation $\mathbf{X}^T = (x_1, x_2, \dots, x_N)$, $\mathbf{P}^T = (p_1, p_2, \dots, p_N)$, and similarly $\mathbf{X}^L, \mathbf{X}^R, \mathbf{P}^L, \mathbf{P}^R$. The general Hamiltonian for the system coupled to harmonic reservoirs is then given by

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{LS} + \mathcal{H}_{RS}, \quad (2.15)$$

where

$$\begin{aligned} \mathcal{H}_S &= \frac{1}{2} \mathbf{P}^T \mathbf{M}^{-1} \mathbf{P} + \frac{1}{2} \mathbf{X}^T \mathbf{K} \mathbf{X}, \\ \mathcal{H}_L &= \frac{1}{2} [\mathbf{P}^L]^T [\mathbf{M}^L]^{-1} \mathbf{P}^L + \frac{1}{2} [\mathbf{X}^L]^T \mathbf{K}^L \mathbf{X}^L, \\ \mathcal{H}_R &= \frac{1}{2} [\mathbf{P}^R]^T [\mathbf{M}^R]^{-1} \mathbf{P}^R + \frac{1}{2} [\mathbf{X}^R]^T \mathbf{K}^R \mathbf{X}^R, \\ \mathcal{H}_{LS} &= \mathbf{X}^T \mathbf{K}^{LS} \mathbf{X}^L, \quad \mathcal{H}_{RS} = \mathbf{X}^T \mathbf{K}^{RS} \mathbf{X}^R, \end{aligned}$$

where $\mathbf{M}, \mathbf{M}^L, \mathbf{M}^R$ and $\mathbf{K}, \mathbf{K}^L, \mathbf{K}^R$ denote, respectively, the mass matrix and the force-constant matrix of the system, left reservoir, and right reservoir, while \mathbf{K}^{LS} and \mathbf{K}^{RS} denote the linear coupling coefficients between the two reservoirs and the system.

Again we consider the time evolution of the coupled system plus reservoirs starting from an initial product density matrix of the form Eq. (2.2) with $\rho_L^0 \sim \exp(-\mathcal{H}_L/k_B T_L)$ and $\rho_R^0 \sim \exp(-\mathcal{H}_R/k_B T_R)$ and the system being in an arbitrary initial state. At long times the system reaches a NESS described by the reduced density matrix $\rho_S = \text{Tr}_{L,R} \rho(t \rightarrow \infty)$. In order to construct ρ_S , we start with defining the appropriate correlation

matrix as in the previous section for electron transport. In doing so, we consider the $2N \times 2N$ covariance matrix defined with the column vector $\varphi = (x_1, \dots, x_N, p_1, \dots, p_N)^T$,

$$\mathbf{C} = \langle \varphi \varphi^T \rangle = \text{Tr}_S[\varphi \varphi^T \rho_S]. \quad (2.16)$$

For this covariance matrix, we write the symmetric and antisymmetric parts as

$$\mathbf{C}_S = \frac{1}{2}(\mathbf{C} + \mathbf{C}^T), \quad (2.17)$$

$$\mathbf{C}_A = \frac{1}{2}(\mathbf{C} - \mathbf{C}^T) = \frac{i\hbar}{2} \mathbf{J}, \quad (2.18)$$

$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}, \quad (2.19)$$

where $\mathbf{1}$ and $\mathbf{0}$ are, respectively, $N \times N$ identity and zero matrices. The matrix expression of antisymmetric part \mathbf{C}_A is automatically determined by commutation relations between coordinate and momentum variables.

The symmetric part of covariance matrix \mathbf{C}_S is given by

$$\mathbf{C}_S = \begin{pmatrix} \langle XX^T \rangle & \frac{1}{2} \langle XP^T + [PX^T]^T \rangle \\ \frac{1}{2} \langle XP^T + [PX^T]^T \rangle & \langle PP^T \rangle \end{pmatrix}. \quad (2.20)$$

As for the electron case these correlations are known in terms of the following phonon Green function:

$$\mathbf{G}^\pm = \frac{1}{-\mathbf{M}\omega^2 + \mathbf{K} - \Sigma_L^\pm - \Sigma_R^\pm}, \quad (2.21)$$

where the self-energies can be expressed in terms of the isolated reservoir Green functions $\mathbf{g}_L^\pm(\omega) = [-\mathbf{M}^L(\omega \pm i\epsilon)^2 + \mathbf{K}^L]^{-1}$, $\mathbf{g}_R^\pm(\omega) = [-\mathbf{M}^R(\omega \pm i\epsilon)^2 + \mathbf{K}^R]^{-1}$, and the coupling elements $\mathbf{K}^{LS}, \mathbf{K}^{RS}$. These self-energies thus read

$$\Sigma_L^\pm(\omega) = \mathbf{K}^{LS} \mathbf{g}_L^\pm(\omega) [\mathbf{K}^{LS}]^T, \quad \Sigma_R^\pm(\omega) = \mathbf{K}^{RS} \mathbf{g}_R^\pm(\omega) [\mathbf{K}^{RS}]^T. \quad (2.22)$$

Defining $\Gamma_L(\omega) = \text{Im}[\Sigma_L^+]$, $\Gamma_R(\omega) = \text{Im}[\Sigma_R^+]$, we find [17,22,23]

$$\begin{aligned} \langle XX^T \rangle &= \int_{-\infty}^{\infty} d\omega \frac{\hbar}{2\pi} \sum_{a=L,R} \mathbf{G}^+ \Gamma_a \mathbf{G}^- g(\omega, T_a), \\ \langle PP^T \rangle &= \int_{-\infty}^{\infty} d\omega \frac{\hbar\omega^2}{2\pi} \sum_{a=L,R} \mathbf{M} \mathbf{G}^+ \Gamma_a \mathbf{G}^- \mathbf{M} g(\omega, T_a), \\ \frac{1}{2} \langle XP^T + [PX^T]^T \rangle &= \int_{-\infty}^{\infty} d\omega \frac{i\hbar\omega}{\pi} \sum_{a=L,R} \mathbf{G}^+ \Gamma_a \mathbf{G}^- \mathbf{M} g(\omega, T_a), \end{aligned} \quad (2.23)$$

where $g(\omega, T) = \coth(\hbar\omega/2k_B T)$.

We next show how the steady-state density matrix can be expressed in terms of the correlation matrix. For this it is necessary to consider symplectic transformations [24]. We first introduce the symplectic matrix \mathbf{S} , satisfying

$$\mathbf{S} \mathbf{J} \mathbf{S}^T = \mathbf{J}, \quad (2.24)$$

$$\mathbf{S} \mathbf{C}_S \mathbf{S}^T = \mathbf{D} = \text{diag}(d_1, \dots, d_N, d_1, \dots, d_N). \quad (2.25)$$

The procedure to find \mathbf{S} is detailed in the Appendix.

By using the symplectic transformation with the matrix \mathbf{S} , the new operators $\varphi' = (x'_1, \dots, x'_N, p'_1, \dots, p'_N)^T$ are defined as

$$\varphi'_s = \sum_{l=1}^N \mathbf{S}_{s,l} \varphi_l, \quad s = 1, \dots, N. \quad (2.26)$$

The most important property of the symplectic transformation, following from Eq. (2.24), is that it preserves the commutation relations, and we have $[x_s, p_{s'}] = i\hbar \delta_{s,s'}$ and $[x_s, x_{s'}] = [p_s, p_{s'}] = 0$. The steady-state density matrix can then be written in terms of these new operators, and we end up with the general main result:

$$\rho_S = \prod_{s=1}^N \frac{\exp[-a_s(x_s'^2 + p_s'^2)]}{Z_s} \quad (2.27)$$

$$= \frac{\exp[-\varphi'^T \mathbf{A} \varphi']}{\prod_{s=1}^N Z_s}, \quad (2.28)$$

$$\mathbf{A} = \mathbf{S}^T \text{diag}(a_1, \dots, a_N, a_1, \dots, a_N) \mathbf{S}, \quad (2.29)$$

$$Z_s = [2 \sinh(\hbar a_s)]^{-1}, \quad (2.30)$$

$$a_s = \hbar^{-1} \coth^{-1}(2d_s/\hbar). \quad (2.31)$$

In computing the normalization factor Z_s , we have used the second quantization representation $x'_s = \sqrt{\frac{\hbar}{2}}(b_s^\dagger + b_s)$, $p'_s = i\sqrt{\frac{\hbar}{2}}(b_s^\dagger - b_s)$, where b_s and b_s^\dagger satisfy $[b_s, b_{s'}^\dagger] = \delta_{s,s'}$. Then we obtain the expression $a_s(x_s'^2 + p_s'^2) = 2\hbar a_s(b_s^\dagger b_s + 1/2)$. The relation between d_s and a_s is then found by looking at the averages $\langle x_s'^2 \rangle$ and $\langle p_s'^2 \rangle$:

$$\langle x_s'^2 \rangle = \langle p_s'^2 \rangle = \frac{\hbar}{2} \coth(\hbar a_s) = d_s. \quad (2.32)$$

Finally, we also consider here the classical limit $\hbar \rightarrow 0$. In this limit, we have the simple relation $d_s = 1/(2a_s)$. Then, the matrix \mathbf{A} is given by

$$\mathbf{A} = \frac{1}{2} \mathbf{S}^T \mathbf{D}^{-1} \mathbf{S} \quad (\hbar \rightarrow 0). \quad (2.33)$$

Hence, from the relation $\mathbf{D}^{-1} = (\mathbf{S} \mathbf{C}_S \mathbf{S}^T)^{-1} = (\mathbf{S}^T)^{-1} \mathbf{C}_S^{-1} \mathbf{S}^{-1}$, we find the following expression of the matrix \mathbf{A} in the classical limit:

$$\mathbf{A} = \frac{1}{2} \mathbf{C}^{-1} \quad (\hbar \rightarrow 0). \quad (2.34)$$

Thus we recover the form that is expected for a general Gaussian probability measure. We note that in the classical case, for Gaussian white noise reservoirs, the correlation matrix \mathbf{C} can be explicitly determined for ordered harmonic lattices [3,4]. For arbitrary harmonic networks, they are given by the high temperature limit of Eq. (2.23), with appropriate choices of the bath spectral functions. Finding the inverse of the correlation matrix, however, presents a more difficult task.

III. WEAK-COUPLING LIMIT

In this section, we consider the special case of a weak coupling between the system and reservoirs. We note that it is essential that the weak-coupling limit is taken *after* the coupled system-reservoirs have evolved for an infinite time and thus reached the NESS. Generally, when the coupling

strength is weak, the density matrix can be expanded in terms of the coupling strength. In this case, the zeroth-order term in the coupling strength determines the overall structure of the electron density profile in the electron conduction case and the temperature profile in the case of phonon heat conduction. The higher-order terms of the expansion determine the amount of current flowing in the system. Therefore, although the coupling strengths must be finite for finite current, even the zeroth-order contribution in the expansion of the density matrix carries important information on the steady state. In this section, we focus on the zeroth-order contribution in the weak-coupling expansion of the steady-state density matrix, which we here refer to as the density matrix in the *weak-coupling limit*. We emphasize that at no instant do we switch off the coupling strength, which is always kept finite but small.

On decreasing the coupling strength, the current decreases; however, even in the limit of zero current, the steady-state density matrix is nontrivial and different from the equilibrium density matrix. In fact, we will find that the NESS is nonunique in the sense that it depends on the way the system-coupling strengths are made to vanish. For the case where the temperatures and chemical potentials of the two reservoirs are chosen equal one obtains, in the weak-coupling limit, the expected equilibrium grand-canonical (for the electron case) and canonical (for the phonon case) distributions.

A. Electron transport

We first note that the system's Hermitian Hamiltonian matrix \mathbf{H} has the eigenvalue equation $\sum_m \mathbf{H}_{l,m} \mathbf{V}_m(s) = \lambda_s \mathbf{V}_l(s)$, hence can be diagonalized by the unitary transformation \mathbf{V} as

$$\mathbf{V}^\dagger \mathbf{H} \mathbf{V} = \lambda, \quad \mathbf{V}^\dagger \mathbf{V} = \mathbf{I}. \quad (3.35)$$

Next we use the spectral decomposition:

$$\begin{aligned} \mathbf{G}^+ &= \mathbf{V} \mathbf{V}^{-1} [\hbar\omega - \mathbf{H} - \boldsymbol{\Sigma}_L^+ - \boldsymbol{\Sigma}_R^+]^{-1} [\mathbf{V}^\dagger]^{-1} \mathbf{V}^\dagger \\ &= \mathbf{V} [\hbar\omega - \lambda - \mathbf{V}^\dagger (\boldsymbol{\Sigma}_L^+ + \boldsymbol{\Sigma}_R^+) \mathbf{V}]^{-1} \mathbf{V}^\dagger. \end{aligned} \quad (3.36)$$

From this it follows that in the weak-coupling limit $\boldsymbol{\Sigma}_L^+, \boldsymbol{\Sigma}_R^+ \rightarrow 0$, the matrix element $\mathbf{G}_{l,m}^+$ is effectively given by

$$\mathbf{G}_{l,m}^+ = \sum_s \frac{\mathbf{V}_l(s) \mathbf{V}_m^*(s)}{\hbar\omega + \lambda_s - i \langle s | \boldsymbol{\Gamma} | s \rangle}, \quad (3.37)$$

where $\langle s | \boldsymbol{\Gamma} | s' \rangle = \sum_{l,m} \mathbf{V}_l^*(s) (\boldsymbol{\Gamma})_{l,m} \mathbf{V}_m(s')$ and $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}_L + \boldsymbol{\Gamma}_R$. It can be shown that the off-diagonal terms of the inverse matrix in Eq. (3.36) are of the order of the coupling strength. This contribution disappears, however, in the following calculation of the correlation function, given this weak-coupling limit. The real part of $\boldsymbol{\Sigma}_{L,R}^+$ is negligible compared to the remaining real parts and thus can be dropped. Hence we obtain

$$\begin{aligned} \langle c_m^\dagger c_l \rangle &= \int_{-\infty}^{\infty} d\omega \frac{\hbar}{\pi} \sum_{a=L,R} \sum_{j,k} \mathbf{G}_{l,k}^+(\boldsymbol{\Gamma}_a)_{k,j} \mathbf{G}_{j,m}^- f(\omega, \mu_a, T_a) \\ &= \int_{-\infty}^{\infty} d\omega \frac{\hbar}{\pi} \sum_{a=L,R} \sum_{s,s',j,k} \frac{\mathbf{V}_l(s) \mathbf{V}_k^*(s)}{\hbar\omega - \lambda_s - i \langle s | \boldsymbol{\Gamma} | s \rangle} [\boldsymbol{\Gamma}_a]_{k,j} \\ &\quad \times \frac{\mathbf{V}_j(s') \mathbf{V}_m^*(s')}{\hbar\omega - \lambda_{s'} + i \langle s' | \boldsymbol{\Gamma} | s' \rangle} f(\omega, \mu_a, T_a). \end{aligned}$$

A careful examination of the limit $\langle s | \boldsymbol{\Gamma}_a | s \rangle \rightarrow 0$ exhibits that only the terms $s = s'$ survive in the above summation, yielding

$$\begin{aligned} \langle c_m^\dagger c_l \rangle &= \int_{-\infty}^{\infty} d\omega \frac{\hbar}{\pi} \sum_{a=L,R} \\ &\quad \times \sum_s \frac{\mathbf{V}_l(s) \langle s | \boldsymbol{\Gamma}_a(\omega) | s \rangle \mathbf{V}_m^*(s)}{(\hbar\omega - \lambda_s)^2 + \langle s | \boldsymbol{\Gamma}(\omega) | s \rangle^2} f(\omega, \mu_a, T_a). \end{aligned}$$

Next, making use of the identity

$$\lim_{\epsilon \rightarrow 0} \frac{\epsilon}{(x-a)^2 + \epsilon^2} = \pi \delta(x-a),$$

we find

$$\langle c_m^\dagger c_l \rangle = \sum_s \mathbf{V}_l(s) \mathbf{V}_m^*(s) e_s,$$

where

$$\begin{aligned} e_s &= \sum_{a=L,R} \frac{\langle s | \boldsymbol{\Gamma}_a | s \rangle}{\langle s | \boldsymbol{\Gamma} | s \rangle} f(\lambda_s / \hbar, \mu_a, T_a) \\ &= \gamma_L f(\lambda_s / \hbar, \mu_L, T_L) + \gamma_R f(\lambda_s / \hbar, \mu_R, T_R), \end{aligned}$$

where

$$\gamma_L = \frac{\langle s | \boldsymbol{\Gamma}_L | s \rangle}{\langle s | \boldsymbol{\Gamma} | s \rangle}, \quad \gamma_R = \frac{\langle s | \boldsymbol{\Gamma}_R | s \rangle}{\langle s | \boldsymbol{\Gamma} | s \rangle} = 1 - \gamma_L.$$

Note that in the above expression, the limit $\langle s | \boldsymbol{\Gamma}_a | s \rangle \rightarrow 0$ is always implied, and it is then evident that the ratios γ_L, γ_R depend on the way the couplings $\rightarrow 0$. From the form above we can interpret e_s as an effective occupation probability of the energy level λ_s of the isolated system, and this probability depends on the temperatures and chemical potentials of the two reservoirs. Defining the diagonal matrix \mathbf{E} with elements e_s , we have $\mathbf{V}^\dagger \mathbf{C} \mathbf{V} = \mathbf{E}$. Comparing with Eq. (2.9), we see that the same unitary transformation that diagonalizes \mathbf{H} also diagonalizes the correlation matrix \mathbf{C} , and we have $\mathbf{U} = \mathbf{V}, \mathbf{D} = \mathbf{E}$.

Using the results in Eqs. (2.13) and (2.14), we then find $a_s = \ln(e_s^{-1} - 1)$ and $\mathbf{A} = \mathbf{V}^* \text{diag}(a_1, a_2, \dots, a_N) \mathbf{V}^T$, which in turn yields the steady-state density matrix in Eq. (2.13). For the equilibrium case $\mu_L = \mu_R = \mu$, $T_L = T_R = T$, we have $d_s = e_s = f(\lambda_s, \mu, T)$, hence $a_s = (\lambda_s - \mu)/(k_B T)$ and $\mathbf{A} = [\mathbf{H} - \mu \mathbf{I}]/(k_B T)$, as expected. Thus we obtain the nontrivial result that the density matrix of a system, weakly coupled to two reservoirs at the same temperatures and chemical potentials, is given by the grand-canonical distribution of the isolated system. Note that this is not the case for the case of strong coupling.

B. Phonon transport

For the harmonic model we first note that there exists a real normal mode transformation matrix \mathbf{V} , with elements $\mathbf{V}_l(s)$, which satisfies

$$\mathbf{V}^T \mathbf{M} \mathbf{V} = \mathbf{1}, \quad \mathbf{V}^T \mathbf{K} \mathbf{V} = \boldsymbol{\Omega}^2,$$

where $\boldsymbol{\Omega}$ is the diagonal matrix with elements as normal mode frequencies. It is easily verified that the matrix

$$\mathbf{S} = \begin{pmatrix} \mathbf{0} & -\boldsymbol{\Omega}^{-1/2} \mathbf{V}^T \\ \boldsymbol{\Omega}^{1/2} \mathbf{V}^T \mathbf{M} & \mathbf{0} \end{pmatrix} \quad (3.38)$$

is symplectic, i.e., $SS^T = \mathbf{J}$ and further has the following property:

$$\mathbf{S} \begin{pmatrix} \mathbf{K}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{M} \end{pmatrix} \mathbf{S}^T = \begin{pmatrix} \boldsymbol{\Omega}^{-1} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Omega}^{-1} \end{pmatrix}. \quad (3.39)$$

We now show that the correlations for the harmonic system in the weak-coupling limit are given by

$$\langle XX^T \rangle = \mathbf{V} \boldsymbol{\Omega}^{-1/2} \mathbf{E} \boldsymbol{\Omega}^{-1/2} \mathbf{V}^T, \quad (3.40)$$

$$\langle XP^T + [PX^T]^T \rangle = 0, \quad (3.41)$$

$$\langle PP^T \rangle = \mathbf{M} \mathbf{V} \boldsymbol{\Omega}^{1/2} \mathbf{E} \boldsymbol{\Omega}^{1/2} \mathbf{V}^T \mathbf{M}, \quad (3.42)$$

where we have defined the diagonal matrix \mathbf{E} whose elements are given by

$$\begin{aligned} e_s &= \frac{\hbar}{2} \sum_{a=L,R} \frac{\langle s|\boldsymbol{\Gamma}_a|s \rangle}{\langle s|\boldsymbol{\Gamma}|s \rangle} \coth \left[\frac{\hbar \boldsymbol{\Omega}_s}{2k_B T_a} \right]_{s=1,2,\dots,N} \\ &= \gamma_L \frac{\hbar}{2} \coth \left[\frac{\hbar \boldsymbol{\Omega}_s}{2k_B T_L} \right] + \gamma_R \frac{\hbar}{2} \coth \left[\frac{\hbar \boldsymbol{\Omega}_s}{2k_B T_R} \right], \end{aligned} \quad (3.43)$$

where

$$\gamma_L = \frac{\langle s|\boldsymbol{\Gamma}_L|s \rangle}{\langle s|\boldsymbol{\Gamma}|s \rangle}, \quad \gamma_R = \frac{\langle s|\boldsymbol{\Gamma}_R|s \rangle}{\langle s|\boldsymbol{\Gamma}|s \rangle} = 1 - \gamma_L.$$

Let us define the effective temperature \tilde{T}_s for each normal mode through the relation, reading

$$e_s = \frac{\hbar}{2} \coth \left[\frac{\hbar \boldsymbol{\Omega}_s}{2k_B \tilde{T}_s} \right], \quad (3.44)$$

giving

$$\frac{1}{\tilde{T}_s} = \frac{2k_B}{\hbar \boldsymbol{\Omega}_s} \coth^{-1} \left[\gamma_L \coth \left(\frac{\hbar \boldsymbol{\Omega}_s}{2k_B T_L} \right) + \gamma_R \coth \left(\frac{\hbar \boldsymbol{\Omega}_s}{2k_B T_R} \right) \right],$$

which notably depends on both temperatures T_L and T_R . We remark here again that in the above expressions the limit $\langle s|\boldsymbol{\Gamma}_a|s \rangle \rightarrow 0$ is implied; it is then clear that the ratios γ_L, γ_R depend on the way the couplings $\rightarrow 0$.

To prove the above results, Eqs. (3.40)–(3.43), we first introduce the following spectral decomposition:

$$\begin{aligned} \mathbf{G}^+(\omega) &= \mathbf{V} \mathbf{V}^{-1} [-\mathbf{M} \omega^2 + \mathbf{K} - \boldsymbol{\Sigma}_L^+ - \boldsymbol{\Sigma}_R^+]^{-1} [\mathbf{V}^T]^{-1} \mathbf{V}^T \\ &= \mathbf{V} [\mathbf{V}^T (-\mathbf{M} \omega^2 + \mathbf{K} - \boldsymbol{\Sigma}_L^+ - \boldsymbol{\Sigma}_R^+) \mathbf{V}]^{-1} \mathbf{V}^T \\ &= \mathbf{V} [-\omega^2 + \boldsymbol{\Omega}^2 - \mathbf{V}^T \boldsymbol{\Sigma}_L^+ \mathbf{V} - \mathbf{V}^T \boldsymbol{\Sigma}_R^+ \mathbf{V}]^{-1} \mathbf{V}^T. \end{aligned}$$

From this it follows that in the weak-coupling limit $\boldsymbol{\Sigma}_L^+, \boldsymbol{\Sigma}_R^+ \rightarrow 0$, the matrix element $\mathbf{G}_{l,m}^+$ is effectively given by

$$\mathbf{G}_{l,m}^+ = \sum_s \frac{\mathbf{V}_l(s) \mathbf{V}_m(s)}{-\omega^2 + \boldsymbol{\Omega}_s^2 - i \langle s|\boldsymbol{\Gamma}|s \rangle}, \quad (3.45)$$

where $\langle s|\boldsymbol{\Gamma}|s' \rangle = \sum_{l,m} \mathbf{V}_l(s) \boldsymbol{\Gamma}_{l,m} \mathbf{V}_m(s')$ and $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}_L + \boldsymbol{\Gamma}_R$. It can be shown that the off-diagonal terms $\langle s|\boldsymbol{\Gamma}|s' \rangle$ for $s \neq s'$, as well as the real part of $\boldsymbol{\Sigma}_{L,R}^+$, give lower-order contributions in the weak-coupling limit and can be dropped. Hence

we find

$$\begin{aligned} \langle x_l x_m \rangle &= \int_{-\infty}^{\infty} \frac{\hbar}{2\pi} \sum_{a=L,R} \sum_{j,k} \mathbf{G}_{l,k}^+ [\boldsymbol{\Gamma}_a]_{k,j} \mathbf{G}_{j,m}^- g(\omega, T_a) \\ &= \int_{-\infty}^{\infty} \frac{\hbar}{2\pi} \sum_{a=L,R} \sum_{s,s',j,k} \frac{\mathbf{V}_l(s) \mathbf{V}_k(s)}{-\omega^2 + \boldsymbol{\Omega}_s^2 - i \langle s|\boldsymbol{\Gamma}|s \rangle} [\boldsymbol{\Gamma}_a]_{k,j} \\ &\quad \times \frac{\mathbf{V}_j(s') \mathbf{V}_m(s')}{-\omega^2 + \boldsymbol{\Omega}_{s'}^2 + i \langle s'|\boldsymbol{\Gamma}|s' \rangle} g(\omega, T_a). \end{aligned}$$

A careful examination of the limit $\langle s|\boldsymbol{\Gamma}_a|s \rangle \rightarrow 0$ shows that only the terms $s = s'$ in the above summation survive, and we then obtain

$$\begin{aligned} \langle x_l x_m \rangle &= \int_{-\infty}^{\infty} \frac{\hbar}{2\pi} \sum_{a=L,R} \\ &\quad \times \sum_s \frac{\mathbf{V}_l(s) \langle s|\boldsymbol{\Gamma}_a(\omega)|s \rangle \mathbf{V}_m(s)}{(-\omega^2 + \boldsymbol{\Omega}_s^2)^2 + \langle s|\boldsymbol{\Gamma}(\omega)|s \rangle^2} g(\omega, T_a). \end{aligned}$$

Now we note the following identity:

$$\lim_{\epsilon \rightarrow 0} \frac{\epsilon}{(x^2 - a^2)^2 + \epsilon^2} = \frac{\pi}{2a} [\delta(x - a) + \delta(x + a)]. \quad (3.46)$$

Using this and the fact that $\boldsymbol{\Gamma}_a(\omega)$ and $g(\omega)$ are both odd functions of ω , one arrives at

$$\langle x_l x_m \rangle = \sum_s \frac{\hbar}{2} \mathbf{V}_l(s) \mathbf{V}_m(s) \sum_{a=L,R} \frac{\langle s|\boldsymbol{\Gamma}_a|s \rangle}{\langle s|\boldsymbol{\Gamma}|s \rangle} \frac{g(\boldsymbol{\Omega}_s, T_a)}{\boldsymbol{\Omega}_s}, \quad (3.47)$$

which proves Eq. (3.40). Similarly, we can evaluate other correlations and obtain Eqs. (3.41) and (3.42).

From the form of the correlations in Eqs. (3.40), (3.41), and (3.42), we deduce that the matrix \mathbf{S} given in Eq. (3.38) provides the required symplectic transformation in Eq. (2.25) with $\mathbf{D} = \mathbf{E}$. Therefore, using Eq. (2.31) and the definition in Eq. (3.44), we get $a_s = \boldsymbol{\Omega}_s / (2k_B \tilde{T}_s)$. Finally, Eq. (2.29) gives $\mathbf{A} = \mathbf{S}^T \boldsymbol{\Omega} \tilde{\mathbf{T}}^{-1} \mathbf{S} / (2k_B)$, and then from Eq. (2.28) we obtain ρ_S . This density matrix corresponds to each of the normal modes of the harmonic system being in equilibrium at an effective temperature \tilde{T}_s . For the equilibrium case $T_L = T_R = T$, we find, using Eq. (3.39), $\varphi^T \mathbf{A} \varphi = \mathcal{H}_S / (k_B T)$. This result is expected but nontrivial, and it is valid only in the weak-coupling limit.

IV. APPLICATION TO GENERIC SETUPS

A. Electron transport in a one-dimensional wire

1. System with single site

We consider the system plus reservoir to consist of a single site, such as, e.g., realized with a single-level quantum dot, that is connected to two one-dimensional reservoirs. The full Hamiltonian then reads

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{LS} + \mathcal{H}_{RS},$$

where

$$\mathcal{H}_S = \epsilon c_0^\dagger c_0,$$

$$\mathcal{H}_L = - \sum_{\alpha=1}^{\infty} t [c_\alpha^\dagger c_{\alpha+1} + c_{\alpha+1}^\dagger c_\alpha],$$

$$\mathcal{H}_R = - \sum_{\alpha'=1}^{\infty} t [c_{\alpha'}^{\dagger} c_{\alpha'+1} + c_{\alpha'+1}^{\dagger} c_{\alpha'}], \quad (4.48)$$

$$\mathcal{H}_{LS} = -t'_L [c_{\alpha=1}^{\dagger} c_0 + c_0^{\dagger} c_{\alpha=1}],$$

$$\mathcal{H}_{RS} = -t'_R [c_{\alpha'=1}^{\dagger} c_0 + c_0^{\dagger} c_{\alpha'=1}].$$

The self-energies can be expressed in terms of the Green functions of the uncoupled reservoir Hamiltonian $g_{L,R}^+$ and the coupling elements $t'_{L,R}$. Defining $\omega = -2t \cos q$, where $0 \leq q \leq \pi$, we find that for $|\omega| \leq 2t$:

$$\Sigma_L^+(\omega) = -\frac{t'^2_L}{t} e^{iq}, \quad \Sigma_R^+(\omega) = -\frac{t'^2_R}{t} e^{iq}, \quad (4.49)$$

$$\Gamma_L^+(\omega) = \frac{t'^2_L}{t} \sin q, \quad \Gamma_R^+(\omega) = \frac{t'^2_R}{t} \sin q.$$

Hence the system's Green function emerges to read

$$G^+(\omega) = \frac{1}{\hbar\omega - \epsilon - \Sigma_L^+(\omega) - \Sigma_R^+(\omega)}. \quad (4.50)$$

The correlation matrix element for the single-site problem is then readily obtained, given by:

$$d = \langle c_0^{\dagger} c_0 \rangle = \int_{-2t}^{2t} d\omega \frac{\hbar}{\pi} |G^+(\omega)|^2 [\Gamma_L(\omega) f(\omega, \mu_L, T_L) + \Gamma_R(\omega) f(\omega, \mu_R, T_R)]. \quad (4.51)$$

Consequently, we find for the steady-state nonequilibrium density matrix for this case the explicit result

$$\rho_S = \frac{\exp(-ac_0^{\dagger} c_0)}{1 + \exp(-a)}, \quad (4.52)$$

where

$$a = \ln(d^{-1} - 1).$$

2. System composed of two sites

We next consider a system where the reservoirs are identical to those in the previous section, while the system Hamiltonian and system-bath couplings are as follows:

$$\begin{aligned} \mathcal{H}_S &= \epsilon_1 c_1^{\dagger} c_1 + \epsilon_2 c_2^{\dagger} c_2 - t(c_1^{\dagger} c_2 + c_2^{\dagger} c_1), \\ \mathcal{H}_{LS} &= -t'_L [c_{\alpha=1}^{\dagger} c_1 + c_1^{\dagger} c_{\alpha=1}], \\ \mathcal{H}_{RS} &= -t'_R [c_{\alpha'=1}^{\dagger} c_2 + c_2^{\dagger} c_{\alpha'=1}]. \end{aligned} \quad (4.53)$$

The self-energies are again given by Eq. (4.49) and the system's Green function is then

$$G^+(\omega) = \begin{pmatrix} \hbar\omega - \epsilon_1 - \Sigma_L^+(\omega) & t \\ t & \hbar\omega - \epsilon_2 - \Sigma_R^+(\omega) \end{pmatrix}^{-1}. \quad (4.54)$$

In this case it is difficult to construct explicitly the required unitary matrix U though it is straightforward to evaluate it numerically and from that find the steady-state density matrix given by Eq. (2.11).

In what follows we present numerical precise results for this setup. In our numerics we use the following set of parameter values: $t = 1.0, t'_L = t'_R = 0.05, \epsilon_1 = 0.2, \epsilon_2 = 0.4, T_L = 0.25, T_R = 0.25$. The right reservoir chemical potential is fixed at $\mu_R = 0.0$ and we study the NESS for different values of $\Delta\mu = \mu_L - \mu_R$.

The Green function in Eq. (4.54) is first obtained and then all the elements of the correlation matrix given by Eqs. (2.8) are evaluated by numerical integration. As examples we give below the correlation matrices for the equilibrium case $\Delta\mu = 0$ and for $\Delta\mu = 2.0$:

$$\begin{aligned} C_S &= \begin{pmatrix} 0.519 & 0.465 \\ 0.465 & 0.427 \end{pmatrix} \quad \text{for } \Delta\mu = 0, \\ C_S &= \begin{pmatrix} 0.726 & 0.271 + i0.000473 \\ 0.271 - i0.000473 & 0.672 \end{pmatrix} \\ &\quad \text{for } \Delta\mu = 2.0. \end{aligned}$$

The electron current in the chain is given by $j_e = 2t \text{Im}[\langle c_1^{\dagger} c_2 \rangle]$, and in the above example $j_e = 0.000946$.

As discussed in Sec. II A, the NESS density matrix assumes the form

$$\rho_S = \frac{\exp(-c^{\dagger} A c)}{[1 + \exp(-a_1)][1 + \exp(-a_2)]}, \quad (4.55)$$

where $c = (c_1, c_2)^T$ and we numerically determined the coefficients a_1, a_2 and the matrix A . Finding the eigenvalues and eigenvectors of C yields the matrix D and the unitary matrix U , respectively. We evaluate $a_1 = \ln(d_1^{-1} - 1), a_2 = \ln(d_2^{-1} - 1)$ and numerically obtain the steady-state matrix

$$A = U^{\dagger} \text{diag}(a_1, a_2) U^T.$$

Note that for $\Delta\mu = 0$ ($\mu_L = \mu_R = 0$) and with a weak coupling to reservoirs, we expect the result $\rho_S = \rho_{\text{eq}} \sim e^{-\beta(\mathcal{H}_S - \mu N)}$, and hence

$$A_{\text{eq}} = \begin{pmatrix} 0.8 & -4.0 \\ -4.0 & 1.6 \end{pmatrix}.$$

In Fig. 1 we depict the matrix elements A_{11}, A_{22} , and $\text{Re}[A_{12}]$ as functions of the chemical potential difference $\Delta\mu$. In the inset we also evaluated the electron current; i.e., $j_e = 2\text{Im}[C_{12}]$ and show as well $\text{Im}[A_{12}]$.

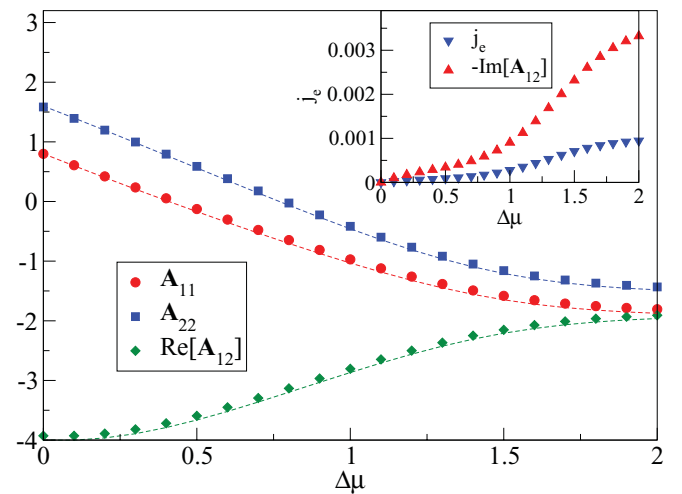


FIG. 1. (Color online) Plot of the NESS matrix elements A as a function of the chemical potential difference $\Delta\mu = \mu_L - \mu_R$ with fixed $\mu_R = 0.0$ and with the remaining parameters as given in the text. The dashed lines depict results obtained from the weak-coupling approximation. The inset shows the electron current $j_e = 2\text{Im}[C_{12}]$ together with $\text{Im}[A_{12}]$.

The matrix elements A_{11}, A_{22} and the real part of A_{12} can be obtained from our analytical weak-coupling results in Sec. III A. First we obtain the eigenvalues λ_s and eigenfunctions $V_l(s), s = 1, 2$, corresponding to the isolated system Hamiltonian \mathcal{H}_s . This provides the required unitary transformation that diagonalizes the matrix C . For the present two-site setup the corresponding eigenvalues, which determine the matrix elements of D , generally given by Eqs. (3.38), take on the following form:

$$d_s = \frac{t_L'^2 |V_1(s)|^2}{t_L'^2 |V_1(s)|^2 + t_R'^2 |V_2(s)|^2} \frac{1}{e^{(\lambda_s - \mu_L)/T_L} + 1} + \frac{t_R'^2 |V_2(s)|^2}{t_L'^2 |V_1(s)|^2 + t_R'^2 |V_2(s)|^2} \frac{1}{e^{(\lambda_s - \mu_R)/T_R} + 1}$$

for $s = 1, 2$. The weak-coupling results for A_{11}, A_{22} , and $\text{Re}[A_{12}]$ are depicted in Fig. 1 with dashed lines. We notice that these are in excellent agreement with the values obtained from exact numerics.

B. Phonon transport in one-dimensional oscillator chain

1. System consisting of a single oscillator

We consider our system plus reservoir to be described by the full Hamiltonian

$$\mathcal{H} = \frac{p^2}{2M} + \frac{k_o x^2}{2} + \sum_{\alpha=1}^N \frac{p_{\alpha}^2}{2m} + \frac{k(x_{\alpha} - x_{\alpha+1})^2}{2} + \frac{k'_L(x_{\alpha=1} - x)^2}{2} + \sum_{\alpha'=1}^N \frac{p_{\alpha'}^2}{2m} + \frac{k(x_{\alpha'} - x_{\alpha'+1})^2}{2} + \frac{k'_R(x_{\alpha'=1} - x)^2}{2},$$

where we assume $x_{\alpha=N+1} = x_{\alpha'=N+1} = 0$. The above Hamiltonian can be written in the canonical form:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{LS} + \mathcal{H}_{RS}, \quad (4.56)$$

where

$$\begin{aligned} \mathcal{H}_S &= \frac{p^2}{2M} + \frac{(k_o + k'_L + k'_R)x^2}{2}, \\ \mathcal{H}_L &= \sum_{\alpha=1}^N \frac{p_{\alpha}^2}{2m} + \frac{k(x_{\alpha} - x_{\alpha+1})^2}{2} + \frac{k'_L x_{\alpha=1}^2}{2}, \\ \mathcal{H}_R &= \sum_{\alpha'=1}^N \frac{p_{\alpha'}^2}{2m} + \frac{k(x_{\alpha'} - x_{\alpha'+1})^2}{2} + \frac{k'_R x_{\alpha'=1}^2}{2}, \\ \mathcal{H}_{LS} &= -k'_L x_{\alpha=1} x, \quad \mathcal{H}_{RS} = -k'_R x_{\alpha'=1} x. \end{aligned} \quad (4.57)$$

The self-energies can be expressed in terms of the Green functions of the uncoupled reservoir Hamiltonian $\mathbf{g}_{L,R}^+(\omega)$ and the coupling elements $k'_{L,R}$. We define $\omega^2 = (2k/m)(1 - \cos q)$, where $0 \leq q \leq \pi$. Then, we find that for $|\omega| < \omega_m = 2(k/m)^{1/2}$,

$$\begin{aligned} \Sigma_L^+(\omega) &= \frac{k_L'^2 \cos q - (1 - u_L) + i \sin q}{k} \frac{1}{2(1 - u_L)(1 - \cos q) + u_L^2}, \\ \Sigma_R^+(\omega) &= \frac{k_R'^2 \cos q - (1 - u_R) + i \sin q}{k} \frac{1}{2(1 - u_R)(1 - \cos q) + u_R^2}, \end{aligned}$$

$$\Gamma_L(\omega) = \frac{k_L'^2}{k} \frac{\sin q}{2(1 - u_L)(1 - \cos q) + u_L^2}, \quad (4.58)$$

$$\Gamma_R(\omega) = \frac{k_R'^2}{k} \frac{\sin q}{2(1 - u_R)(1 - \cos q) + u_R^2},$$

where $u_L = k'_L/k$ and $u_R = k'_R/k$. Hence the Green function is given by

$$G^+(\omega) = \frac{1}{-M\omega^2 + k_o + k'_L + k'_R - \Sigma_L^+(\omega) - \Sigma_R^+(\omega)}. \quad (4.59)$$

It is not difficult to verify that $\mathcal{T}(\omega) = 4\Gamma_L(\omega)\Gamma_R(\omega)|G^+(\omega)|^2$ gives the correct transmission coefficient as can be independently obtained by evaluating the transmission of plane waves from the left reservoir to the right one, across the intermediate system.

The correlation matrix elements for the single-particle problem are obtained as

$$\begin{aligned} c_1 = \langle x^2 \rangle &= \int_0^{\omega_m} d\omega \frac{\hbar}{\pi} |G^+(\omega)|^2 [\Gamma_L(\omega)g(\omega, T_L) \\ &\quad + \Gamma_R(\omega)g(\omega, T_R)], \\ c_2 = \langle p^2 \rangle &= \int_0^{\omega_m} d\omega \frac{\hbar M^2 \omega^2}{\pi} |G^+(\omega)|^2 [\Gamma_L(\omega)g(\omega, T_L) \\ &\quad + \Gamma_R(\omega)g(\omega, T_R)], \\ \langle xp + px \rangle &= 0, \end{aligned}$$

where $\omega_m = 2(k/m)^{1/2}$ and $g(\omega, T) = \coth(\beta\hbar\omega/2)$. Using the prescription in Sec. II B, we find that $d_1 = (c_1 c_2)^{1/2}$ and

$$S = \begin{pmatrix} 0 & -(c_1/c_2)^{1/4} \\ (c_2/c_1)^{1/4} & 0 \end{pmatrix}, \quad (4.60)$$

yielding the explicit NESS density matrix

$$\rho_S = \frac{e^{-[A_{11}x^2 + A_{22}p^2]}}{Z},$$

where

$$\begin{aligned} A_{11} &= \left(\frac{c_2}{c_1}\right)^{1/2} a, \quad A_{22} = \left(\frac{c_1}{c_2}\right)^{1/2} a, \\ a &= \hbar^{-1} \coth^{-1}[2\hbar^{-1}(c_1 c_2)^{1/2}], \\ Z &= [2 \sinh(\hbar a)]^{-1}. \end{aligned}$$

2. System composed of two coupled oscillators

In this case the baths have the same Hamiltonians as in the previous section while the system Hamiltonian and system-bath couplings are given by

$$\begin{aligned} \mathcal{H}_S &= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{(k_1 + k'_L)x_1^2}{2} \\ &\quad + \frac{k(x_1 - x_2)^2}{2} + \frac{(k_2 + k'_R)x_2^2}{2}, \\ \mathcal{H}_{LS} &= -k'_L x_{\alpha=1} x_1, \quad \mathcal{H}_{RS} = -k'_R x_{\alpha'=1} x_2. \end{aligned} \quad (4.61)$$

The self-energies are again given by Eq. (4.58) and the system's Green function is

$$\mathbf{G}^+(\omega) = \begin{pmatrix} -m_1\omega^2 + (k + k_1 + k'_L) - \Sigma_L^+(\omega) & & & \\ & -k & & \\ & & -m_2\omega^2 + (k + k_2 + k'_R) - \Sigma_R^+(\omega) & \\ & & & \end{pmatrix}^{-1}. \quad (4.62)$$

For this setup it again becomes difficult to evaluate explicitly the symplectic matrix \mathbf{S} for the general case though it is straightforward to evaluate it numerically to yield the steady-state density matrix given by Eq. (2.28).

We present some numerical results for this case. In our numerics we fix the following parameter values: $m_1 = 1.0, m_2 = 1.5, k = k_1 = k_2 = 1.0, k'_L = k'_R = 0.1$. Moreover, we keep the temperature of the right reservoir fixed at $T_R = 1.0$ and study the NESS for different values of $\Delta T = T_L - T_R$. We work in dimensionless units where $\hbar = k_B = 1$. The temperatures T_L, T_R are of the order of the normal mode frequencies, meaning that the system indeed operates in the quantum-mechanical regime.

The Green function in Eq. (4.62) is first obtained and then all the elements of the correlation matrix given by Eqs. (2.23) are evaluated by numerical integration. As examples, we detail below the symmetric parts of the correlation matrices for the equilibrium case $\Delta T = 0$ and for $\Delta T = 4.0$:

$$\mathbf{C}_S = \begin{pmatrix} 0.696 & 0.294 & 0 & 0 \\ 0.294 & 0.670 & 0 & 0 \\ 0 & 0 & 1.168 & -0.0788 \\ 0 & 0 & -0.0788 & 1.67 \end{pmatrix} \text{ for } \Delta T = 0,$$

$$\mathbf{C}_S = \begin{pmatrix} 1.851 & 1.331 & 0 & -0.0294 \\ 1.331 & 2.241 & 0.0196 & 0 \\ 0 & 0.0196 & 2.491 & 0.781 \\ -0.0294 & 0 & 0.781 & 4.558 \end{pmatrix} \text{ for } \Delta T = 4.$$

Note that the heat current across the chain is given by $j = k \langle x_1 p_2 \rangle / m_2 = -k \langle x_2 p_1 \rangle / m_1 = (k/m_2) \mathbf{C}_{14} = -(k/m_1) \mathbf{C}_{23}$. For the above example we obtain $j = 0.0196$.

As shown in Sec. II B, the NESS density matrix assumes the form

$$\rho_S = \frac{\exp(-\varphi^T \mathbf{A} \varphi)}{4 \sinh(a_1) \sinh(a_2)}, \quad (4.63)$$

where $\varphi^T = (x_1, x_2, p_1, p_2)$. We next numerically determine a_1, a_2 , and the matrix \mathbf{A} . To this end we need to construct the diagonal matrix \mathbf{D} and the symplectic matrix \mathbf{S} . The way of constructing these are described in the Appendix: It requires the following four numerical procedures:

(i) Find the eigenvalues and eigenfunctions of \mathbf{C}_S . Then construct the matrix $\mathbf{C}_S^{1/2}$.

(ii) Find the eigenvalues and eigenvectors of the matrix $i \mathbf{C}_S^{1/2} \mathbf{J} \mathbf{C}_S^{1/2}$. There are four eigenvectors that occur as complex conjugate pairs, $(\omega_1^+, \omega_1^-, \omega_2^+, \omega_2^-)$, with corresponding eigenvalues $(-d_1, d_1, -d_2, d_2)$.

(iii) Evaluate the vectors $v_1^\pm = \mathbf{C}_S^{1/2} \omega_1^\pm, v_2^\pm = \mathbf{C}_S^{1/2} \omega_2^\pm$ and use Eqs. (A4) and (A20) to obtain the matrix \mathbf{V} . The required symplectic transformation is then $\mathbf{S} = (\mathbf{J}\mathbf{V})^T$.

(iv) Evaluate $a_1 = \coth^{-1}(2d_1), a_2 = \coth^{-1}(2d_2)$ and the steady-state matrix

$$\mathbf{A} = \mathbf{S}^T \text{diag}(a_1, a_2, a_1, a_2) \mathbf{S}.$$

Note that for $\Delta T = 0$ ($T_L = T_R = 1$) and for weak-coupling with reservoirs, we expect $\rho_S = \rho_{\text{eq}} \sim e^{-\beta \mathcal{H}_S}$; hence

$$\mathbf{A}_{\text{eq}} = \begin{pmatrix} 1 & 0.5 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.33 \end{pmatrix}.$$

In Fig. 2 we depict the matrix elements $\mathbf{A}_{33}, \mathbf{A}_{44}$, and \mathbf{A}_{34} as functions of the temperature difference ΔT . In the inset we have plotted the element \mathbf{A}_{14} and the heat current $j = \mathbf{C}_{14}/m_2$.

The 2×2 diagonal blocks of the matrix \mathbf{A} , i.e., $\mathbf{A}_{11}, \mathbf{A}_{12}, \mathbf{A}_{21}, \mathbf{A}_{22}$ and $\mathbf{A}_{33}, \mathbf{A}_{34}, \mathbf{A}_{43}, \mathbf{A}_{44}$, can be obtained from the weak-coupling results in Sec. III B. First we obtain the normal mode eigenvalues Ω_s and eigenfunctions $\mathbf{V}_l(s)$, $s = 1, 2$, corresponding to the isolated system Hamiltonian \mathcal{H}_S . The symplectic transformation is constructed using Eq. (3.38). The matrix elements of \mathbf{D} , given generally by Eqs. (3.43) and (3.44), take the following form:

$$d_s = 12 \frac{k_L^2 \mathbf{V}_1^2(s)}{k_L^2 \mathbf{V}_1^2(s) + k_R'^2 \mathbf{V}_2^2(s)} \coth \left(\frac{\hbar \Omega_s}{2k_B T_L} \right) + \frac{1}{2} \frac{k_R'^2 \mathbf{V}_2^2(s)}{k_L'^2 \mathbf{V}_1^2(s) + k_R'^2 \mathbf{V}_2^2(s)} \coth \left(\frac{\hbar \Omega_s}{2k_B T_R} \right),$$

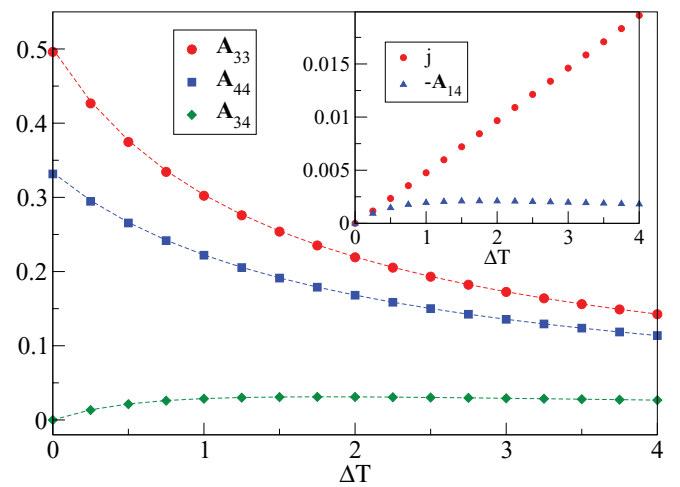


FIG. 2. (Color online) Plot of some relevant elements of the matrix \mathbf{A} as a function of the temperature difference $\Delta T = T_L - T_R$ with constant $T_R = 1.0$ while the other parameters are given in the text. The dashed lines depict results obtained from the analytical weak-coupling approximation. The inset shows both the matrix element $-\mathbf{A}_{14}$ and the linearly growing heat current j .

for $s = 1, 2$. The weak-coupling results for A_{33} , A_{44} , and A_{34} have been plotted in Fig. 2 (dashed lines), and we detect an excellent agreement with the values obtained from precise numerics.

V. CONCLUSIONS AND OUTLOOK

In summary, we have detailed the explicit construction of the reduced density matrix of the nonequilibrium steady states for two quantum transport problems: one involving noninteracting fermionic degrees of freedom and the other noninteracting bosonic degrees. The first setup concerns electron transport in a tight-binding lattice model composed of noninteracting electrons that are connected to noninteracting baths, while our second setup focuses on heat transport across an arbitrary harmonic oscillator network connected to harmonic oscillator baths. For both of these models the steady-state correlations are known exactly from various approaches and are usually expressed in terms of nonequilibrium Green functions. We have demonstrated that for the fermionic problem, the construction of the emerging time-independent steady-state density matrix requires that one evaluates a particular unitary matrix, while likewise, for the bosonic case, it requires finding an appropriate symplectic transformation.

For the limiting case of vanishingly weak coupling between intermediate system and reservoirs, we show that the required unitary and symplectic transformations can be explicitly found and the resulting density matrices assume simple forms whose explicit expressions depend on the way the coupling strengths are made to vanish. For the case where the two baths possess the same temperatures (and chemical potentials for electron case), the weak-coupling case yields a unique answer, which is the expected equilibrium canonical (grand canonical for electrons) distribution. This requires the assumption that the connecting reservoirs have sufficiently broad bandwidths [16,17].

The construction of the steady-state density matrices required one to use “diagonal” representations Eqs. (2.11) and (2.27), and these are analogous to the eigenmode or normal mode representation of the Hamiltonian. In the equilibrium case and for weak coupling, the density matrix is $\sim e^{-\beta\mathcal{H}}$, and then the eigenmode representation is useful in the computation of equilibrium averages of various physical observables. Similarly, we expect that the “diagonal” representations of the nonequilibrium density matrix is as useful for computing averages in the NESS. Thus, for example, the Von Neumann entropy of the nonequilibrium steady state, defined as $S = -\text{Tr}[\rho_S \ln \rho_S]$, can be readily obtained from our findings. In particular one finds that

$$S_{\text{fermion}} = - \sum_{s=1}^N (1 - d_s) \ln(1 - d_s) + d_s \ln d_s,$$

$$S_{\text{boson}} = - \sum_{s=1}^N (d_s/\hbar - 1/2) \ln(d_s/\hbar - 1/2) - (d_s/\hbar + 1/2) \ln(d_s/\hbar + 1/2), \quad (5.64)$$

where $\{d_s\}$ are the “diagonalized” correlations defined via Eqs. (2.9) and (2.25).

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APPENDIX: PROCEDURE TO FIND THE SYMPLECTIC MATRIX S

We here explain the general procedure to find the symplectic matrix S [24,25]. We first consider the eigenvalue problem for the matrices $iC_S^{\frac{1}{2}}JC_S^{\frac{1}{2}}$ and C_SJ . Note that the covariance matrix C_S is real-valued, symmetric, and positive definite. Positive definiteness is shown by $y^T C_S y = \langle (\varphi^T y)^2 \rangle_{ss} \geq 0$ for arbitrary real column vector y .

The matrix $iC_S^{\frac{1}{2}}JC_S^{\frac{1}{2}}$ is a Hermitian matrix. Therefore it possesses real eigenvalues as $iC_S^{\frac{1}{2}}JC_S^{\frac{1}{2}}\omega = d\omega$, where ω is the eigenvector. Taking the complex conjugate of both sides, we have the equation $iC_S^{\frac{1}{2}}JC_S^{\frac{1}{2}}\omega^* = -d\omega^*$. From this, if d is an eigenvalue, then $-d$ is also an eigenvalue.

Hence, we can start with the following equations:

$$iC_S^{\frac{1}{2}}JC_S^{\frac{1}{2}}\omega_k^{\pm} = \mp d_k \omega_k^{\pm}, \quad (A1)$$

where ω_k^{\pm} are eigenvectors ($\omega_k^- = \omega_k^{+*}$) which have real eigenvalues $\mp d_k$ ($d_k > 0$). These equations are equivalent to

$$C_S J v_k^{\pm} = \pm i d_k v_k^{\pm}, \quad (A2)$$

where the vectors v_k^{\pm} are defined as

$$v_k^{\pm} = C_S^{\frac{1}{2}} \omega_k^{\pm}. \quad (A3)$$

We divide the vector v_k^{\pm} into the real and imaginary parts as

$$v_k^{\pm} = v_k^R \pm i v_k^I. \quad (A4)$$

Then, Eq. (A2) implies the two relations

$$C_S J v_k^R = -v_k^I d_k, \quad (A5)$$

$$C_S J v_k^I = v_k^R d_k. \quad (A6)$$

Because the matrix $iC_S^{\frac{1}{2}}JC_S^{\frac{1}{2}}$ is Hermitian, we can normalize the vector ω_k^{\pm} as

$$(\omega_k^{\pm})^{\dagger} \omega_{k'}^{\pm} = 2d_k^{-1} \delta_{k,k'}, \quad (A7)$$

$$(\omega_k^{\pm})^{\dagger} \omega_{k'}^{\mp} = 0. \quad (A8)$$

From (A3), the vector ω_k^{\pm} is expressed with vectors $v_k^{R,I}$ as

$$\omega_k^{\pm} = C_S^{-\frac{1}{2}} (v_k^R \pm i v_k^I). \quad (A9)$$

Using this, Eqs. (A7) and (A8) are written as

$$\begin{aligned} & (v_k^R \mp i v_k^I)^T \mathbf{C}_S^{-\frac{1}{2}} \mathbf{C}_S^{-\frac{1}{2}} (v_{k'}^R \pm i v_{k'}^I) \\ &= (v_k^R)^T \mathbf{C}_S^{-1} v_{k'}^R + (v_k^I)^T \mathbf{C}_S^{-1} v_{k'}^I \\ & \mp i [(v_k^I)^T \mathbf{C}_S^{-1} v_{k'}^R - (v_k^R)^T \mathbf{C}_S^{-1} v_{k'}^I] = 2d_{k'}^{-1} \delta_{k,k'}, \end{aligned} \quad (\text{A10})$$

$$\begin{aligned} & (v_k^R \mp i v_k^I)^T \mathbf{C}_S^{-\frac{1}{2}} \mathbf{C}_S^{-\frac{1}{2}} (v_{k'}^R \mp i v_{k'}^I) \\ &= (v_k^R)^T \mathbf{C}_S^{-1} v_{k'}^R - (v_k^I)^T \mathbf{C}_S^{-1} v_{k'}^I \\ & \mp i [(v_k^I)^T \mathbf{C}_S^{-1} v_{k'}^R + (v_k^R)^T \mathbf{C}_S^{-1} v_{k'}^I] = 0. \end{aligned} \quad (\text{A11})$$

From this, we find the following set of relations:

$$(v_k^R)^T \mathbf{C}_S^{-1} v_{k'}^R = d_{k'}^{-1} \delta_{k,k'}, \quad (\text{A12})$$

$$(v_k^I)^T \mathbf{C}_S^{-1} v_{k'}^I = d_{k'}^{-1} \delta_{k,k'}, \quad (\text{A13})$$

$$(v_k^R)^T \mathbf{C}_S^{-1} v_{k'}^I = 0, \quad (\text{A14})$$

$$(v_k^I)^T \mathbf{C}_S^{-1} v_{k'}^R = 0. \quad (\text{A15})$$

Utilizing Eqs. (A5) and (A6), the above relations can be recast as

$$(v_k^R)^T \mathbf{J} v_{k'}^I = \delta_{k,k'}, \quad (\text{A16})$$

$$(v_k^I)^T \mathbf{J} v_{k'}^R = -\delta_{k,k'}, \quad (\text{A17})$$

$$(v_k^R)^T \mathbf{J} v_{k'}^R = 0, \quad (\text{A18})$$

$$(v_k^I)^T \mathbf{J} v_{k'}^I = 0. \quad (\text{A19})$$

We next define the $2N \times 2N$ matrix \mathcal{V} :

$$\mathcal{V} = (v_1^R, \dots, v_N^R, v_1^I, \dots, v_N^I). \quad (\text{A20})$$

Using the matrix \mathcal{V} , relations (A5) and (A6) can be simply written as

$$\mathbf{C}_S \mathbf{J} \mathcal{V} = \mathcal{V} \mathbf{J} \mathbf{D}, \quad (\text{A21})$$

where the matrix \mathbf{D} is a $2N \times 2N$ diagonal matrix:

$$\mathbf{D} = \text{diag}(d_1, \dots, d_N, d_1, \dots, d_N). \quad (\text{A22})$$

In addition, relations (A16)–(A19) can be written with the matrix \mathcal{V} as

$$\mathcal{V}^T \mathbf{J} \mathcal{V} = \mathbf{J}. \quad (\text{A23})$$

We now introduce the matrix \mathbf{S} as

$$\mathbf{S} = (\mathbf{J} \mathcal{V})^T. \quad (\text{A24})$$

One can prove that the matrix \mathbf{S} satisfies the symplectic relation, namely,

$$\begin{aligned} \mathbf{S} \mathbf{J} \mathbf{S}^T &= \mathcal{V}^T \mathbf{J}^T \mathbf{J} \mathcal{V} \\ &= -\mathcal{V}^T \mathbf{J}^T \mathcal{V} = \mathcal{V}^T \mathbf{J} \mathcal{V} = \mathbf{J}, \end{aligned} \quad (\text{A25})$$

$$\begin{aligned} \mathbf{S} \mathbf{C}_S \mathbf{S}^T &= \mathcal{V}^T \mathbf{J}^T \mathbf{C}_S \mathcal{V} \\ &= \mathcal{V}^T \mathbf{J}^T \mathcal{V} \mathbf{J} \mathbf{D} \\ &= -\mathcal{V}^T \mathbf{J} \mathcal{V} \mathbf{J} \mathbf{D} \\ &= -\mathbf{J}^2 \mathbf{D} = \mathbf{D}, \end{aligned} \quad (\text{A26})$$

where we used Eqs. (A21) and (A23).

To evaluate the symplectic matrix \mathbf{S} numerically, we first solve eigenvalue problem (A1) to obtain the eigenfunction ω_k^\pm . Next, we normalize them as in (A7), and find $v_k^{R,I}$. Finally, constructing the matrix \mathcal{V} as in (A20), one obtains the symplectic matrix as in (A24).

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