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Abstract

By revisiting previous definitions, we show that one can define an energy current operator that satisfies the continuity equation for a general Hamiltonian in one dimension. This expression is useful for studying electronic, phononic and photonic energy flow in linear systems and in hybrid structures. The definition allows us to deduce the necessary conditions that result in current conservation for general-statistics systems. The discrete form of the Fourier's law of heat conduction naturally emerges in the present definition.

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1. Introduction

The problem of energy transfer, electronic, phononic and photonic, in molecules and nanosystems has recently gained lots of interest [1–7]. In molecules, understanding energy flow is crucial for controlling reactivity, molecular dynamics and kinetics [8]. In nanosystems, energy transfer has recently attracted much attention with implications in thermal machinery [9–11], information processing and computation [12, 13], and molecular-based thermoelectricity [14–16]. Of special interest are hybrid structures, e.g. normal metal–superconductor junctions with applications in thermometry and refrigeration [17], and atom-radiation field systems, serving as a prototype for studying thermodynamics of quantum systems [18, 19].

From the theoretical point of view, systems of interest include collections of bosons, fermions, spins and mixed-statistics models [20]. For example, energy transfer from a dielectric solid into a molecule may be studied using a spin-boson model where the molecule is represented by a single anharmonic mode (spin) and the bulk includes a collection of harmonic modes (boson) [21]. In the analogous spin-fermion model an electronic excitation is transferred between two metals through a local mode, modeling a vibrating molecule. If

the central mode is harmonic, the model may further describe radiative heat transfer between electronic conductors [7, 22].

In order to perform first principle quantum-mechanical calculations of energy transfer in nanosystems it is necessary to consider a model-independent non-perturbative definition of the energy current. This expression should be applicable in non-stationary cases, as well as in steady-state situations. While there is no unique definition of the energy current operator in non-relativistic systems [23], the constructed expression should still fulfil a symmetry requirement, as we discuss below. We present here a consistent definition for the energy flux operator using a generic one-dimensional (1D) Hamiltonian. We show that this expression is useful for studying vibrational, electronic and spin-mediated energy transfer, and that it yields a non-perturbative expression for the energy current in hybrid systems, e.g. at a solid–molecule–solid interface represented by a two-bath spin-boson model.

Furthermore, the definition also brings in a useful physical insight: we derive a *necessary* condition for energy conservation in various systems, bosonic and electronic, by calculating the commutator of the total flux operator with H, the total Hamiltonian. If the current is a conserved quantity, the transport is ballistic, the conductivity diverges and Fourier's law of heat conduction cannot be fulfilled [24].

Derivation of the Fourier's law from fundamental principles, classical [24–27] or quantum [28–30], is a great challenge in theoretical physics. Model calculations manifested that the onset of diffusional behavior delicately depends on the details of the system. It is still not clear what necessary and sufficient conditions must the Hamiltonian fulfil for showing the Fourier's dynamics. Here we circumvent this challenge, and rather than test the applicability of the Fourier's law in specific systems, derive a general, *necessary* condition for current conservation. Systems that do not obey this condition may satisfy the Fourier's law. As an example, we verify that in systems of harmonic oscillators the total energy current is conserved, so that once prepared, a current in a closed loop system will never vanish.

Another implication of the proper definition of the energy current is the identification of a microscopic expression for the thermal conductivity in terms of Hamiltonian parameters. This expression might be useful for studying the thermal conduction properties of molecular wires and spin chains.

The paper is organized as follows. In section 2 we discuss the general definition of the energy flux operator in one dimension. Section 3 applies this expression to complex structures, e.g. the spin-boson model and the spin-fermion model, prototype models for studying energy transfer in hybrid systems. In section 4 we show that a current conservation condition naturally emerges from the energy flux definition for both bosonic and fermionic Hamiltonians. Section 5 further explores current conservation in general 1D systems. From the energy flux expression the discrete Fourier's law can be naturally identified, as shown in section 6. In section 7 we conclude.

2. Definition of the energy flux operator for a general Hamiltonian in one dimension

Defining an energy flux operator for a specific system such as phonons dates back to Hardy's early work [31]. The idea was applied to spin chains, see, e.g. [32–35], and other 1D systems, see, e.g. [29]. A general flux (current) operator may be obtained by assuming that there exists an operator continuity equation, for instance $\frac{\partial h(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0$ in one dimension, where $h(x,t)$ is the energy density operator and $j(x,t)$ is the energy flux operator. For an N-site chain with M states at each site, one can introduce a workable definition of the energy density operator, $h(x,t) = \sum_s h_s \delta(x - x_s)$, where h_s is a discrete energy density operator of the sth site. The total Hamiltonian of the chain is therefore given by $H = \int dx \, h(x,t) = \sum_s h_s$. Similarly, the

energy flux can be written as the sum of localized contributions $j(x, t) = \sum_s j_s \delta(x - x_s)$, so that the continuity equation can be written in a discrete form,

$$\frac{\mathrm{d}h_s}{\mathrm{d}t} = \frac{j_{s-1} - j_s}{a}, \tag{1}$$

where a is the lattice spacing and j_s/a is the current operator. The time evolution of h_s in the Heisenberg representation satisfies the Heisenberg equation of motion, $\frac{\mathrm{d}}{\mathrm{d}t}h_s = \mathrm{i}[H, h_s]$, assuming h_s does not depend on time in the Schrödinger representation ($\hbar \equiv 1$). This yields

$$\frac{\mathrm{d}h_s}{\mathrm{d}t} = \mathrm{i} \sum_k [h_k, h_s]. \tag{2}$$

In general, equation (2) cannot be expressed in terms of the difference of two operators at two sites as in (1), yet we can identify the currents j_s and j_{s-1} for a specific model Hamiltonian. We use here a generic 1D Hamiltonian with up to two-body nearest-neighbor interactions,

$$H = \sum_{s=1}^{N} \left(h_s^0 + V(s, s+1) \right), \tag{3}$$

where h_s^0 is the local Hamiltonian at site s. While the local energy density cannot be uniquely defined [23], one could make a reasonable separation of V, and assign mixed terms half to site s and half to $s + 1$. With this partition the energy density at the sth local site becomes

$$h_s = h_s^0 + \tfrac{1}{2}[V(s, s+1) + V(s-1, s)]. \tag{4}$$

This equation satisfies $H = \sum_{s=1}^{N} h_s$, as required, when one sets $V(N, N+1) = V(0, 1) = 0$. For this Hamiltonian, the energy flux operator can be identified as

$$j_s = j_{s \to s+1}^{(2)} + j_s^{(4)}, \tag{5}$$

where

$$j_{s \to s+1}^{(2)} = \frac{\mathrm{i}a}{2}\left[\left(h_s^0 - h_{s+1}^0\right), V(s, s+1)\right], \tag{6}$$

is a two-site contribution and

$$j_s^{(4)} = \frac{\mathrm{i}a}{2}\{[V(s, s+1), V(s+1, s+2)] + [V(s-1, s), V(s, s+1)]\} \tag{7}$$

is an operator connecting four sites, accounting for higher order inter-site interaction terms. As we show below, in some cases it is exactly zero. It is also noticeable that in our case (2) could be written in terms of the difference of operators at two neighbor sites. The definition also naturally classifies the perturbative orders with respect to the inter-site coupling V: the order of the flux operator (7) is higher than that of (6).

Definitions (5)–(7) possess significant symmetric features. For instance, $j_{s \to s+1}^{(2)}$ trivially shows the exchange symmetry $j_{s \to s+1}^{(2)} = -j_{s+1 \to s}^{(2)}$, assuming $V(s, s+1) = V(s+1, s)$. The exchange symmetry is an essential requirement when defining a current operator, since the current in opposite directions must have the same absolute value. The operators $j_s^{(4)}$ has a similar exchange property, but four sites are involved.

Definition (5) is state- and symmetry-independent unlike the expression recently utilized in [29, 36–38], $j_s = \mathrm{i}a[h_s^0, V(s, s+1)]$, which requires that the Hamiltonian fulfils the symmetric condition $[h_s^0 + h_{s+1}^0, V(s, s+1)] = 0$, see appendix A for details. In order to increase generality, [36] further suggests a 'symmetrized local flux' that has the same form as $j_{s \to s+1}^{(2)}$.

The energy flux operator was also extensively examined in 1D chains *in the absence of an on-site energy term* $(h_s^0 = 0)$, e.g. the Heisenberg model at zero magnetic field [39]. In this

case the energy at each site was defined as $h_s = V(s, s + 1)$, leading to the current operator $j_{s-1} = ia[V(s-1, s), V(s, s+1)]$. Since in this paper we are interested in the opposite limit, i.e. in structures where the inter-site interaction is considered as a perturbation to the local energy, e.g. impurity models, choice (4) for the local energy is more appropriate.

Note that we could have also defined a high-order local interaction term $U(s)$. For phononic systems U includes on-site interactions, incorporating harmonic and anharmonic contributions. For fermionic systems U may represent a local electron–electron repulsion. The potentials $V(s, s + 1)$ and $V(s, s + 1) + U(s) + U(s + 1)$ indeed produce different flux operators. We adopt here the convention that local s interactions (one-body and many-body) are all included within the potential h_s^0. Finally, one could consider next nearest-neighbor interactions and, by following the same procedure, identify the current j_s.

At this point we would like to comment that the separation of the energy change in a quantum system into its work and heat contributions is a fundamental question in physics. When the subsystem is coupled to a thermal bath, one refers to the energy exchange between the components as heat, while when the reservoir is mechanical, energy exchange is referred to as work. For an externally modulated system the heat flux and power can be standardly identified [19, 40]. However, for general modular systems the classification is not clear. In a recent work, Weimer *et al* [41] suggested to identify work and heat in quantum systems as changes in energy that do not alter the von Neumann entropy, and do change it, respectively. The focus of our work is the definition of the energy flow operator, valid in various modular-hybrid structures, and we do not discuss here its separation to the work and heat components.

3. Current operator in hybrid structures

Definition (5) can be applied to non-identical interacting systems which are spaciously connected. For example, we may consider an impurity spin coupled to two solids, and study the energy current at the contact. The bulk, serving as a thermal reservoir, may be composed of electrons (the Kondo problem) [42], collections of harmonic modes (the spin-boson model) [43] or spins [44, 45]. This impurity-bath scenario is the standard in molecular electronics and nanomechanical experiments, where the heat-transfer properties of a molecule connected to solid or liquid interfaces are investigated [2–5].

The generic impurity-bath Hamiltonian includes a central unit H_{spin}, two independent reservoirs H_ν^0 ($\nu = L, R$) maintained at different temperatures, and system–bath couplings V_ν. The energy flux operator, e.g. at the L contact is given by (5)–(7), disregarding for convenience the lattice constant a. Assuming that $[V_L, V_R] = 0$ we find that the heat current from the L contact into the junction is given by

$$j_L = \frac{\mathrm{i}}{2}\big[H_L^0 - H_{\text{spin}}, V_L\big]. \tag{8}$$

We then apply this result assuming either bosonic baths or electronic reservoirs.

Spin-boson model. A two-level system connected to two harmonic baths held at different temperatures serves as a prototype model for investigating phononic transfer in a nonlinear molecular junction. Calculations at the level of the Master equation, assuming weak system–bath couplings while ignoring coherence effects, have revealed interesting dynamics, e.g. thermal rectification [21], negative differential resistance [46] and pumping of heat [47]. It is of interest to derive a general expression for the heat current which is not limited to the weak coupling limit. Such an expression will open the door for non-perturbative calculations of

heat current in strongly coupled molecular systems. The multi-bath spin-boson Hamiltonian is given by

$$H_{\text{SB}} = \frac{B}{2}\sigma^z + \sum_{v,q} \omega_q b^\dagger_{v,q} b_{v,q} + \sigma^x \sum_{v,q} \lambda_{v,q}\left(b^\dagger_{v,q} + b_{v,q}\right). \tag{9}$$

Here, σ^i ($i = x, y, z$) are the Pauli matrices and B is the spin splitting. The reservoirs ($v = L, R$) include two infinite sets of harmonic oscillators (creation operators $b^\dagger_{v,q}$). Spin–bath interaction strength is denoted by $\lambda_{v,q}$, possibly different at the two ends.

Let H^0_v denotes the local Hamiltonian of the ensemble of harmonic oscillators at the v boundary, $H_{\text{spin}} = \frac{B}{2}\sigma^z$ be the Hamiltonian of the spin and $V_v = \sum_q \lambda_{v,q}\sigma^x\left(b^\dagger_{v,q} + b_{v,q}\right)$ be the interaction. Using (8), the energy flux from the L contact to the spin unit is given by

$$j_L = \frac{1}{2}\left[\mathrm{i}\sigma^x \sum_q \omega_q\lambda_{L,q}\left(b^\dagger_{L,q} - b_{L,q}\right) + B\sigma^y \sum_q \lambda_{L,q}\left(b^\dagger_{L,q} + b_{L,q}\right) \right], \tag{10}$$

or equivalently,

$$j_L = \tfrac{1}{2}[B\sigma^y X_L + \sigma^x P_L], \tag{11}$$

where $X_L = \sum_q \lambda_{L,q}\left(b^\dagger_{L,q} + b_{L,q}\right)$ and $P_L = \mathrm{i}\sum_q \lambda_{L,q}\omega_q\left(b^\dagger_{L,q} - b_{L,q}\right)$. An analogous expression exists at the R side. It can be shown that the flux operator (10) reduces to the stationary heat flux expression utilized in [21, 46, 47] when system–bath couplings are weak and the Markovian limit is assumed,

$$\langle j_L \rangle = -B\left[k^L_{u\to d}p_u - k^L_{d\to u}p_d\right]. \tag{12}$$

Here, $\langle j \rangle$ denotes the trace over system and bath degrees of freedom, p_u (p_d) is the steady-state population of the up (down) spin level and T_v is the temperature at the v contact. The rate constants satisfy the detailed balance relation, $k^v_{d\to u} = k^v_{u\to d}\,\mathrm{e}^{-B/T_v}$, where

$$
\begin{aligned}
k^v_{u\to d} &= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}B\tau}\langle X_v(\tau)X_v(0)\rangle\,\mathrm{d}\tau \\
&= 2\pi \sum_q \lambda^2_{v,q}\left[n^v_B(\omega_q) + 1\right]\delta(B - \omega_q).
\end{aligned} \tag{13}
$$

Here, $n^v_B(\omega_q) = [\mathrm{e}^{\omega_q/T_v} - 1]^{-1}$ is the Bose–Einstein distribution function with the Boltzmann constant $k_B \equiv 1$. Equation (12) describes energy current at the L contact as the balance between an energy extraction from the L reservoir into the spin, and an energy loss from the spin to the bath. Appendix B presents in detail the derivation of this perturbative result from the general operator expression (11).

Similarly, one may analyze the transport properties of the diagonally coupled spin-boson model with $V_v = \sigma^z \sum_q \kappa_{v,q}\left(b^\dagger_{v,q} + b_{v,q}\right)$ and $H_{\text{spin}} = \frac{B}{2}\sigma^z + \frac{\Delta}{2}\sigma^x$, leading to complicated behavior due to the non-separability of the two reservoirs [21].

Spin-fermion model. The spin-fermion model, where a spin impurity is coupled to two Fermi seas of different temperatures and/or chemical potentials, is another example of a hybrid structure, useful e.g. for studying electronic and radiative heat transfer between metals [22],

$$H_{\text{SF}} = \frac{B}{2}\sigma^z + \sum_{v,k} \epsilon_k c^\dagger_{v,k} c_{v,k} + \sigma^x \sum_{v,k,q} \alpha_{v,k,q} c^\dagger_{v,k} c_{v,q}. \tag{14}$$

The first term here accounts for spin splitting. The second term includes the two independent reservoirs (leads) of spinless electrons, creation operator $c^\dagger_{v,k}$ ($v = L, R$). We assume that the leads are kept (each) in thermal equilibrium at temperature T_v and chemical potential μ_v.

The last term in (14) describes spin–bath interactions, where we disregard charge tunneling between the metals and allow only for transfer of energy excitations. Utilizing (8), the heat current at the L contact is given by

$$j_L = \frac{\mathrm{i}}{2} \left[\sigma^x \sum_{k,q} \epsilon_k \alpha_{L,k,q} \big(c_{L,k}^\dagger c_{L,q} - c_{L,q}^\dagger c_{L,k} \big) - \mathrm{i} B \sigma^y \sum_{k,q} \alpha_{L,k,q} c_{L,k}^\dagger c_{L,q} \right]. \tag{15}$$

If the metals have a strictly linear dispersion relation, this result can be exactly mapped into a bosonized description [49] to yield the current (10). Deviations are expected when the metals have energy-dependent density of states [22]. Following the derivation sketched in appendix B, taking into account the fermionic nature of the operators, one can show that in second-order system–bath coupling, going into the Markovian limit, the stationary heat current is given by (12) with the rates

$$
\begin{aligned}
k_{d \to u}^\nu &= \int_{-\infty}^\infty \mathrm{e}^{-\mathrm{i} B \tau} \langle F_\nu(\tau) F_\nu(0) \rangle \, \mathrm{d}\tau \\
&= 2\pi \sum_{k,q} |\alpha_{\nu,k,q}|^2 n_F^\nu(\epsilon_k) \big[1 - n_F^\nu(\epsilon_q) \big] \delta(\epsilon_k - \epsilon_q - B) \\
k_{d \to u}^\nu &= k_{u \to d}^\nu \, \mathrm{e}^{-B/T_\nu},
\end{aligned}
\tag{16}
$$

where $F_\nu = \sum_{k,q} \alpha_{\nu,k,q} c_{\nu,k}^\dagger c_{\nu,q}$ and $n_F^\nu(\epsilon) = [\mathrm{e}^{(\epsilon-\mu_\nu)/T_\nu} + 1]^{-1}$ is the Fermi–Dirac distribution function of the ν bath.

The perturbative rate expression (12) also holds for mixed boson–fermion systems, e.g. when energy is directed from a phonon bath into an electronic excitation through a local impurity. One simply employs then expressions (13) and (16) for the phononic and electronic bath-induced transitions.

4. Current conservation conditions for bosonic and fermionic systems

With the help of the energy flux operator we can obtain general properties of specific quantum systems [39]. This is in contrast to standard calculations where one needs to make use of specific quantum states [33–35]. We then prove that linear harmonic systems and some special spin chains (XY, Ising) have zero thermal resistance using the operator form of the energy flux.

Bosons. We consider the quantized system used in [25], $h_s^0 = p_s^2/2 + U(x_s)$ and inter-site potential $V(s, s+1) = V(x_s, x_{s+1})$, where x_s and p_s are the coordinate and momentum of the particle at the s site. It is easy to show that $j_s^{(4)} = 0$, thus the flux operator is given by

$$j_s = \frac{a}{4} \left[\left\{ p_s, \frac{\partial V(s, s+1)}{\partial x_s} \right\}_+ - \left\{ p_{s+1}, \frac{\partial V(s, s+1)}{\partial x_{s+1}} \right\}_+ \right], \tag{17}$$

where $\{\}_+$ denotes the anticommutation relation. This is just the quantized form of the classical flux defined in [25]. For the quadratic interaction $(x_s - x_{s+1})^2$ we should exclude the local terms x_s^2 and x_{s+1}^2, or shift them into h_s^0 and h_{s+1}^0, respectively, as discussed in section 2. For a bilinear coupling model we thus consider the interaction $V(s, s+1) = \lambda x_s x_{s+1}$ with spring constant λ. The flux operator then reads

$$
\begin{aligned}
j_s &= a\lambda(p_s x_{s+1} - x_s p_{s+1})/2 \\
&= \mathrm{i} a\lambda \big(b_s^\dagger b_{s+1} - b_{s+1}^\dagger b_s \big)/2,
\end{aligned}
\tag{18}
$$

where the second line is the bosonic expression with the creation (annihilation) operator $b_s^\dagger$ (b_s). The commutation relation between the total Hamiltonian and the current operator is given by

$$[j_s, H] = i\frac{a\lambda}{2}\left(x_s\frac{\partial U(x_{s+1})}{\partial x_{s+1}} - x_{s+1}\frac{\partial U(x_s)}{\partial x_s}\right) + \widehat{O}(\lambda^2). \tag{19}$$

Therefore, if $\frac{\partial U(x)}{\partial x} = 0$, or $U \propto x^2$, $[j_s, H] = 0$ within first-order coupling. This implies that free particle motion and harmonic potentials pertain a constant current, or in other words, the energy current is conserved in these systems.

One can also calculate the higher order term in (19), $\widehat{O}(\lambda^2) = ia\lambda^2(x_s^2 + x_s x_{s+2} - x_{s-1}x_{s+1} - x_{s+1}^2)/2$. If the total flux is defined as $J = \sum_{s=1}^{N} j_s$, the commutation relation between the complete flux and the total Hamiltonian is given by $[J, H] = i\lambda^2\frac{a}{2}(x_1^2 - x_N^2)$ for the harmonic $U \propto x^2$ potential. Therefore, the Heisenberg equation of motion reads

$$dJ/dt = \frac{a\lambda^2}{2}(x_1^2 - x_N^2). \tag{20}$$

This result shows that the total flux depends only on the contacts properties: coupling strength and temperature (going into thermal averages). Furthermore, in closed loop systems, the complete current J is a constant operator. This conclusion is well established, however, we give here a simple proof of the operator form, without the need to go into the system's quantum states. It can be shown that the current is also conserved for *disordered* 1D harmonic systems. For example, assuming different force constants between sites $\lambda_{s,s+1}$, one gets $dJ/dt = \frac{a}{2}(\lambda_{1,2}^2 x_1^2 - \lambda_{N-1,N}^2 x_N^2)$.

Fermions: nearest-neighbor spin systems. We then consider a periodic spin chain of length N. The system can be mapped into a system of fermions using the Wigner–Jordan transformation, see, e.g. [50]. Let the on-site potential h_s^0 and the inter-site potential V be

$$h_s^0 = \frac{\epsilon}{2}\sigma_s^z, \qquad V(s, s+1) = \lambda(A\sigma_s^x\sigma_{s+1}^x + B\sigma_s^y\sigma_{s+1}^y + C\sigma_s^z\sigma_{s+1}^z), \tag{21}$$

where A, B, C are the interaction coefficients. It is easy to show that the first-order flux operator is given by

$$j_{s\to s+1}^{(2)} = a\epsilon\lambda\frac{A+B}{2}(\sigma_{s+1}^y\sigma_s^x - \sigma_s^y\sigma_{s+1}^x). \tag{22}$$

Using the Wigner–Jordan transformation, the current can also be rewritten as

$$j_{s\to s+1}^{(2)} = ia\epsilon\lambda(A+B)(c_{s+1}^\dagger c_s - c_s^\dagger c_{s+1}), \tag{23}$$

expressed in terms of spinless fermionic creation and annihilation operators $c_s^\dagger$ and c_s, respectively. The second-order contribution $j_s^{(4)} \propto \lambda^2$ is nonzero in general, but is too cumbersome to be included here.

The current operator $j_{s\to s+1}^{(2)}$ is essentially the standard spin current operator multiplied by the bias ϵ. This term reflects energy flow due to spin current, while $j_s^{(4)}$ is the current of interaction energy [39]. At weak inter-site coupling, $\lambda \ll \epsilon$, $j_{s\to s+1}^{(2)}$ dominates the energy current, while for zero magnetic fields only $j_s^{(4)}$ survives. Throughout the paper we always assume nonzero magnetic splitting ϵ, unless otherwise stated.

We continue and analyze current conservation in model (21),

$$[j_s, H] = [j_{s\to s+1}^{(2)}, h_s^0 + h_{s+1}^0] + [j_s^{(4)}, h_s^0 + h_{s+1}^0] + [j_{s\to s+1}^{(2)}, V(s-1, s)$$
$$+ V(s, s+1) + V(s+1, s+2)]. \tag{24}$$

To the first order in λ the commutator is therefore given by

$$\left[j^{(2)}_{s\to s+1}, h^0_s + h^0_{s+1}\right] = a\epsilon^2\lambda\frac{A + B}{4}\left[\sigma^y_{s+1}\sigma^x_s - \sigma^y_s\sigma^x_{s+1}, \sigma^z_s + \sigma^z_{s+1}\right] = 0. \tag{25}$$

Thus, for the periodic spin chains considered here, only high-order terms in λ may lead to current decay. We then discuss some special cases: (i) $A = -B$, corresponding to the antiferromagnetic phase. Here $j^{(2)}_{s\to s+1} = 0$, implying that there is no current in the antiferromagnetic phase in the first-order approximation. (ii) The Heisenberg model, $A = B = C$. In this case, the flux operator (6) agrees with the definition of [29], see also appendix A, since $\left[(\sigma^z_s + \sigma^z_{s+1}), V(s, s + 1)\right] = 0$. This system was extensively investigated in [29, 38]. (iii) The *XY* model, $A = B$ and $C = 0$. We calculate here the high-order contribution to the current and find

$$j^{(4)}_s = \mathrm{i}\frac{a\lambda^2 A^2}{2}\left(c^\dagger_s c_{s+2} - c^\dagger_{s+2}c_s + c^\dagger_{s-1}c_{s+1} - c^\dagger_{s+1}c_{s-1}\right). \tag{26}$$

Combining (23) with (26) we get that $[j_s, H] = 0 + \widehat{O}(\lambda^2)$ in the *XY* model. The current operator is therefore a constant in the first-order approximation, while the total current $J = \sum_s j_s$ exactly becomes

$$\mathrm{d}J/\mathrm{d}t = 8a\epsilon\lambda^2 A^2(n_1 - n_N), \tag{27}$$

in analogy with equation (20) for the bosonic Hamiltonian. Here, $n_s = c^\dagger_s c_s$ is the number operator. We conclude that the total current across the systems depends only on the properties of the chain's ends. Thus, in closed loop systems the total current J is a constant operator.

As a final case (iv) we consider the transverse Ising model, $B = C = 0$. Here, $j^{(2)}_{s\to s+1} = \frac{\lambda\epsilon A}{2}\left(\sigma^x_s\sigma^y_{s+1} - \sigma^y_s\sigma^x_{s+1}\right)$, $j^{(4)}_s = 0$. The commutator $[j_s, H]$ is zero in the first order of λ while the second-order contribution, resulting from the commutator $\left[j^{(2)}_{s\to s+1}, V(s - 1, s) + V(s, s + 1) + V(s + 1, s + 2)\right]$, leads to

$$\mathrm{d}J/\mathrm{d}t = 4a\epsilon\lambda^2 A^2(n_1 - n_N). \tag{28}$$

We can summarize our observations as follows: if a Hamiltonian is written by a linear combination of bilinear operators, a bosonic set $\{b^\dagger_s b_t, b^\dagger_s b^\dagger_t, b_s b_t\}$ and a fermionic set $\{c^\dagger_s c_t, c^\dagger_s c^\dagger_t, c_s c_t\}$, it can always be expressed in terms of quasiparticle operators γ_q, where $H = \sum_{q=1}^N \epsilon_q \gamma^\dagger_q \gamma_q$ (see, e.g. [51]). Since there is no interaction between the quasiparticles, the systems behaves like a collection of free particles. The harmonic oscillator chain with linear couplings is an example of bosonic Hamiltonian. The *XY* models are examples for independent fermions. Both systems yield ballistic motion with no thermal resistance. In contrast, the Heisenberg model with nonzero magnetic field does not belong to such systems because it contains an on-site interaction $c^\dagger_s c_s c^\dagger_t c_t$ when C is not zero [20].

5. Necessary condition for current conservation for a general one-dimensional system

We consider a chain of length N with M levels at each site. The commutation relation between the total Hamiltonian and the flux operator can be written as

$$[j_s, H] = F(\lambda) + \widehat{O}(\lambda^2), \tag{29}$$

where $F(\lambda)$ is the first-order term and $\widehat{O}(\lambda^2)$ contains higher order terms in λ. The necessary condition for current conservation is $F(\lambda) \equiv 0$. We emphasize that this is only a *necessary* condition. If $F(\lambda) \neq 0$ the system potentially shows a diffusive dynamics.

The most general Hamiltonian for this system can be generated by M^2 generator set $g = \{\overrightarrow{h}, E^{\overrightarrow{\alpha}}\}$, where $\overrightarrow{h} = (n^1, n^2, \dots, n^M)$ is the vector operator with $n^i = |i\rangle\langle i|$ and

$E^{\vec{\alpha}}$ denotes $M^2 - M$ operators $|i\rangle \langle j|$ where $i \neq j$. The vectors $\vec{\alpha}$'s are M-dimensional and are usually referred to as roots [52]. The commutation relation between $\vec{h}$ and $E^{\vec{\alpha}}$ is $[\vec{h}, E^{\vec{\alpha}}] = \vec{\alpha} E^{\vec{\alpha}}$, where the vector $\vec{\alpha}$ can be considered as an eigenvalue of the vector operator $\vec{h}$. For instance, in the two-level system ($M = 2$), $\vec{h} = (|1\rangle \langle 1|, |2\rangle \langle 2|)$, $E^{\vec{\alpha}} = (|1\rangle \langle 2|, |2\rangle \langle 1|)$ and there are two roots $\vec{\alpha_1} = (1, -1)$ and $\vec{\alpha_2} = (-1, 1)$, corresponding to $E^{\vec{\alpha_1}} = |1\rangle \langle 2|$ and $E^{\vec{\alpha_2}} = |2\rangle \langle 1|$. Appendix C presents the $M = 3$ case.

Using this notation, the most general Hamiltonian up to a two-body interaction can be written as

$$H = \sum_s \vec{\epsilon} \cdot \vec{h_s} + \lambda \sum_s [V_{\vec{\alpha}, \vec{\beta}} E_s^{\vec{\alpha}} E_{s+1}^{\vec{\beta}} + V_d(s, s+1)], \tag{30}$$

where the vector $\vec{\epsilon} = (\epsilon_1, \epsilon_2, \ldots, \epsilon_M)$, ϵ_i is the i state energy level and $V_{\vec{\alpha}, \vec{\beta}}$ are inter-site coupling parameters. The units are assumed to have identical spectra and we use constant nearest-neighbor interactions along the chain. The last term in (30) includes many-body interactions $V_d(s, s+1) = \sum U_{i,j} n_s^i n_{s+1}^j$. It is easy to show that the commutator of the current with H yields

$$F(\lambda) = -\frac{ia\lambda}{2} \sum V_{\vec{\alpha}, \vec{\beta}} [(\vec{\epsilon} \cdot \vec{\alpha})^2 - (\vec{\epsilon} \cdot \vec{\beta})^2] E_s^{\vec{\alpha}} E_{s+1}^{\vec{\beta}}. \tag{31}$$

The necessary condition for current conservation, $F(\lambda) \equiv 0$, therefore implies

$$\vec{\epsilon} \cdot \vec{\alpha} = \pm \vec{\epsilon} \cdot \vec{\beta} \tag{32}$$

for nonzero coupling parameters $V_{\vec{\alpha}, \vec{\beta}}$. This condition (with the plus sign) is naturally fulfilled for harmonic systems, since $(\epsilon_{j-1} - \epsilon_j) = (\epsilon_{k-1} - \epsilon_k)$ for any j, k. For fermionic models $M = 2$ and the $\vec{\epsilon} \cdot \vec{\beta} = -\vec{\epsilon} \cdot \vec{\alpha}$ condition is trivially conformed. Both systems indeed lead to current conservation (see section 4).

For a system with an arbitrary spectra this condition translates into $\vec{\alpha} = \pm \vec{\beta}$, implying that the interaction contains only the following terms: $E_s^{\vec{\alpha}} E_{s+1}^{\vec{\alpha}}$, $E_s^{\vec{\alpha}} E_{s+1}^{-\vec{\alpha}}$ and $V_d(s, s+1)$.[1] The corresponding current operator is

$$j_{s \to s+1}^{(2)} = ia \sum V_{\vec{\alpha}, -\vec{\alpha}} (\vec{\epsilon} \cdot \vec{\alpha}) E_s^{\vec{\alpha}} E_{s+1}^{-\vec{\alpha}}. \tag{33}$$

This expression reduces into the fermionic limit (section 4) when $M = 2$. The $M = 3$ case is exemplified in appendix C.

The necessary condition (32) is an imperative step toward identifying normal transport (Fourier) systems, as it helps us to pinpoint current conserved systems directly, without detailed numerical calculations. If the system satisfies $\vec{\epsilon} \cdot \vec{\alpha} \neq \pm \vec{\epsilon} \cdot \vec{\beta}$, one can directly deduce that the thermal current is not conserved. Note that in the Heisenberg model $F(\lambda) = 0$, and only the next term in equation (29) is finite, accounting for the dissipation of energy[2].

6. Formal Fourier's law

Recently, there are several ideas of how to approach Fourier's law from fundamental principles [26–30]. Here we will show that the appropriately defined flux operator naturally leads to the discrete form of the law. The derivation yields the conductivity coefficient for a general 1D

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[1] For a two-level system $E^{\vec{\alpha}} = \sigma^{\pm}$, thus $F(\lambda) = 0$ when the inter-site interaction includes the following terms: $\sigma_s^+ \sigma_{s+1}^-, \sigma_s^+ \sigma_{s+1}^+$ and $\sigma_s^- \sigma_{s+1}^-$.

[2] In first order of λ the commutator $[j_s, H] = [j_{s \to s+1}^{(2)}, h_s^0 + h_{s+1}^0]$, where $j_{s \to s+1}^{(2)} \propto [h_s^0 - h_{s+1}^0, V(s, s+1)]$. Since $V_d \propto U n_s^i n_{s+1}^j$ commutes with $h_s^0 \propto n_s^i$, the many-body V_d term does not destroy current conservation in the lowest approximation.

system in terms of the Hamiltonian parameters. We begin with a generic nearest-neighbor Hamiltonian

$$H = \sum_s \left(h_s^0 + V(s, s+1) \right), \tag{34}$$

including local interactions and inter-site couplings. In our definition (6), the average flux, $\overline{j} = \text{Tr}\{\rho j\}$, at weak interactions reads

$$\overline{j}_{s \to s+1}^{(2)} = -\frac{ia}{2} \text{Tr}\left\{ \rho \left[\left(h_{s+1}^0 - h_s^0 \right), V(s, s+1) \right] \right\}$$

$$= -\frac{a}{2} \text{Tr}\left\{ \Delta h_s^0 \Gamma(t) \right\}, \tag{35}$$

using the cyclic property of the trace. Here, ρ is the total density matrix, $\Delta h_s^0 = h_{s+1}^0 - h_s^0$ is the difference between local energies at neighboring sites and $\Gamma(t) = i[V(s, s+1), \rho(t)]$ is Hermitian. We can also write this expression explicitly in terms of local s functions,

$$\overline{j}_{s \to s+1}^{(2)} = -\frac{a}{2} (\overline{g}_{s+1} - \overline{g}_s), \tag{36}$$

where $\overline{g}_s = \text{Tr}\{h_s^0 \Gamma(t)\}$. If we can define a local temperature T_s at each site, we can then relate the current between sites with the temperature difference $\Delta T_s = T_{s+1} - T_s$,

$$\overline{j}_{s \to s+1}^{(2)} = -\left(a^2 \frac{\Delta \overline{g}_s}{\Delta \overline{h}_s^0} C_s \right) \frac{\Delta T_s}{a}, \tag{37}$$

where $\Delta \overline{g}_s = \overline{g}_{s+1} - \overline{g}_s$, and $C_s = \frac{\Delta \overline{h}_s^0}{\Delta T_s}$ is the specific heat. This is the discrete Fourier's law [29, 38]. We can identify the microscopic-local thermal conductivity as $\kappa_s = a^2 \frac{\Delta \overline{g}_s}{\Delta \overline{h}_s^0} C_s$, as long as $\overline{g}_s$ can be uniquely defined (see discussion below) and the ratio $\frac{\Delta \overline{g}_s}{\Delta \overline{h}_s^0}$ is finite.

As an example we consider a three-spin system. For the *XY* model, if the initial state is $|0\rangle_1 |1\rangle_2 |0\rangle_3$, it is easy to show that $\frac{\Delta \overline{g}_2}{\Delta \overline{h}_2^0} = 2\sqrt{2}\lambda \frac{\sin 2\sqrt{2}\lambda t}{3 \cos 2\sqrt{2}\lambda t + 1}$. For weak coupling, $\lambda t < 1$, $\frac{\Delta \overline{g}_2}{\Delta \overline{h}_2^0} \to 2\lambda^2 t$ holds. The thermal conductivity is then given by $\kappa = 2\lambda^2 t C_s$, in agreement with our recent calculation [30]. It also shows that although the total current of the *XY* model is conserved, the partial current between two sites may have the form of the Fourier's law before thermal equilibrium sets [24].

We then explain how to define $\overline{g}_s$ uniquely. Although we could formally write equation (37), $\overline{g}_s$ may not be uniquely defined because $\Gamma(t)$ depends on the index s: $\Gamma(t)$ could be either defined as $i[V(s, s+1), \rho(t)]$ or $i[V(s, s-1), \rho(t)]$. Therefore, the condition for $\overline{g}_s$ to be exclusively defined is

$$\text{Tr}_s\{[V(s, s+1), \rho(t)]\} = \text{Tr}_s\{[V(s, s-1), \rho(t)]\}. \tag{38}$$

The trace Tr_s runs over all sites except site s. It is easy to show that $P_{s-1,s+1}\rho(t)P_{s-1,s+1} = \rho(t)$ is a sufficient condition for satisfying equation (38), where $P_{s-1,s+1}$ is the exchange operator between sites $s-1$ and $s+1$. If the total Hamiltonian is invariant under $P_{s-1,s+1}$, as it is in many physical cases, the last condition translates into a condition on the system preparation,

$$P_{s-1,s+1}\rho(0)P_{s-1,s+1} = \rho(0). \tag{39}$$

This is a sufficient (but not necessary) condition for attaining a unique expression for $\overline{g}_s$. Once $\overline{g}_s$ is carefully defined, we can proceed and calculate the thermal conductivity using equation (37). In the above example the initial state was set to $|0\rangle_1 |1\rangle_2 |0\rangle_3$, which is indeed invariant under the exchange $P_{1,3}$. Note that since the validity of the Fourier's law is independent of initial conditions, the requirement to fulfil equation (39) is solely meant for distinctively identifying the conductivity.

7. Conclusion

In this paper, we present and re-examine the energy flux operator that exactly satisfies the continuity equation for a general Hamiltonian in one dimension. Based on the definition, we deduce the necessary conditions on the inter-site interaction that result in current conservation. This analysis sets the first step toward the exploration of the validity of Fourier's law of heat conduction in Hamiltonian systems: systems that conserve energy have diverging conductivity. As an example, using a simple operator algebra, we prove that independent bosons and fermions conduct energy ballistically. We further apply the definition to various impurity models, relevant for understanding energy flow in nanojunctions, and obtain a non-perturbative non-stationary expression for the heat current between interfaces. The microscopic heat conductivity coefficient naturally emerges in the present definition.

While previous works have typically relied on specific quantum states, calculating only expectation values, see for example [34–38], the results presented here essentially depend only on operator calculations. Possible extensions include generalization of the energy current definition to time-dependent situations, and exploration of the necessary condition for the applicability of the Fourier's law of heat conduction in 1D chains [30].

Acknowledgments

Appendix A. An alternative, symmetry-limited, definition for the energy current

We follow here a symmetry-limited definition of the energy flux operator often adopted in the literature [29, 36, 37]. The generic 1D Hamiltonian includes local potentials and inter-site interactions

$$H = \sum_s \left(h_s^0 + V(s, s+1) \right). \tag{A.1}$$

The energy flow operator is defined by considering the time evolution of the *local, non-interacting* energy operator,

$$\frac{dh_s^0}{dt} = i \left[H, h_s^0 \right]$$
$$= -i \left[h_s^0, V(s, s-1) \right] - i \left[h_s^0, V(s, s+1) \right]. \tag{A.2}$$

We next assume that a continuity equation for h_s^0 holds, based on the approximation that the local energy is conserved [36]

$$\frac{dh_s^0}{dt} = \frac{(j_{s-1} - j_s)}{a}. \tag{A.3}$$

By comparing equation (A.2) with (A.3) one can identify the current between sites as

$$j_s = ia \left[h_s^0, V(s, s+1) \right]; \qquad j_{s-1} = -ia \left[h_s^0, V(s, s-1) \right]. \tag{A.4}$$

However, the second equality above produces $j_s = -ia \left[h_{s+1}^0, V(s+1, s) \right]$ when shifted to site s. This can be consistent with the first equality of equation (A.4) only if the condition

$$\left[h_s^0 + h_{s+1}^0, V(s, s+1) \right] = 0 \tag{A.5}$$

is satisfied. Definition (A.4) is thus restricted to a limited class of Hamiltonians that satisfy (A.5). It is not satisfied, for example, in phononic systems $\left[h_s^0 = \left(x_s^2 + p_s^2 \right) / 2; \; V(s, s+1) = \right.$

$V(x_s, x_{s+1})\big]$ *irrespective of the coupling strength*. Therefore, the formulation in [36–38], utilizing this definition, cannot lead to expressions (17)–(21), as it is limited to a small class of spin models. The Heisenberg spin-$\frac{1}{2}$ model, $h_s^0 = \frac{\epsilon}{2}\sigma_s^z$, $V(s, s+1) = \lambda\big(\sigma_s^x\sigma_{s+1}^x + \sigma_s^y\sigma_{s+1}^y + \sigma_s^z\sigma_{s+1}^z\big)$, is an example of a system obeying (A.5).

  We emphasize again that the energy current is defined here by studying *local, non-interacting* energy changes. In contrast, equation (5) defines the energy current by studying the total energy at a site, incorporating inter-site interactions, see equation (4).

Appendix B. Spin-boson model: derivation of the weak coupling expression for the energy current

We derive here a weak-coupling expression for the steady-state energy current in the spin-boson model using the non-perturbative definition (10). The two-bath ($\nu = L, R$) spin-boson Hamiltonian is given by

$$H_{SB} = H_{spin} + \sum_\nu H_\nu^0 + \sum_\nu V_\nu, \tag{B.1}$$

where

$$H_{spin} = \frac{B}{2}\sigma^z; \qquad H_\nu^0 = \sum_q \omega_q b_{\nu,q}^\dagger b_{\nu,q}; \qquad V_\nu = \sigma^x X_\nu. \tag{B.2}$$

Here, B is the spin splitting, $b_{\nu,q}^\dagger$ is a creation operator satisfying the bosonic statistics and V_ν includes system–bath interactions at each contact, $X_\nu = \sum_q \lambda_{\nu,q}\big(b_{\nu,q}^\dagger + b_{\nu,q}\big)$. There is no direct coupling between the two harmonic baths (temperature T_ν), as they are coupled only through the central spin.

  The general expression for the current operator is given by equation (6), $j_L = \frac{i}{2}\big[H_L^0 - H_{spin}, V_L\big]$, disregarding for convenience the factor a. Note that $j^{(4)} = 0$, see equation (7), since $[V_L, V_R] = 0$. In the present model the current operator from the L interface to the spin is given by

$$j_L = \tfrac{1}{2}[B\sigma^y X_L + \sigma^x P_L], \tag{B.3}$$

where $P_L = i\sum_q \lambda_{L,q}\omega_q\big(b_{L,q}^\dagger - b_{L,q}\big)$ denotes the sum of the momenta of the harmonic oscillators at the left boundary. This expression is valid in the non-perturbative regime and for non-stationary situations. In steady state the expectation value of the interaction is zero, e.g. at the L contact,

$$\left\langle \frac{\partial V_L}{\partial t} \right\rangle = \langle \dot{\sigma}^x X_L + \sigma^x \dot{X}_L \rangle = 0. \tag{B.4}$$

Since $\dot{\sigma}^x = -B\sigma^y$ and $\dot{X}_L = P_L$, we find that $\langle \sigma^x P_L \rangle = \langle B\sigma^y X_L \rangle$. The stationary heat current is therefore given by

$$\langle j_L \rangle = \mathrm{Tr}\{\rho j_L\} = B\,\mathrm{Tr}\{\rho\sigma^y X_L\}, \tag{B.5}$$

where ρ is the total density matrix. Using the energy representation, $\sigma^z = |u\rangle\langle u| - |d\rangle\langle d|$, $\sigma^x = |d\rangle\langle u| + |u\rangle\langle d|$, $\sigma^y = -i|u\rangle\langle d| + i|d\rangle\langle u|$, we can write the heat current as

$$\langle j_L \rangle = iB\,\mathrm{Tr}_B\{(\rho_{u,d} - \rho_{d,u})X_L\}, \tag{B.6}$$

where Tr_B denotes the trace over the thermal baths (L and R) states only. This expression can be evaluated by solving the Liouville equation, written here explicitly for the nondiagonal matrix element

$$\dot{\rho}_{d,u}(t) = iB\rho_{d,u}(t) - iX(t)\rho_{u,u}(t) + i\rho_{d,d}(t)X(t), \tag{B.7}$$

with $X = X_L + X_R$, $X(t) = e^{iH_B t} X e^{-iH_B t}$. Formal integration of this differential equation yields

$$\rho_{d,u}(t) = \int_0^t e^{iB(t-\tau)}[-iX(\tau)\rho_{u,u}(\tau) + i\rho_{d,d}(\tau)X(\tau)]\,d\tau. \tag{B.8}$$

We then evaluate the term $\text{Tr}_B\{\rho_{d,u}X_L\}$ under the following approximations: (i) weak system–bath coupling, neglecting higher order correlation functions, (ii) Markovian limit, assuming the spin's relaxation timescale is longer than that of the bath fluctuations, and (iii) initial factorized condition, where ρ is well approximated by the product $\rho(t=0) = \rho_{\text{spin}}(t=0)\rho_L\rho_R$. Here, $\rho_\nu = e^{-H_\nu^0/T_\nu}/\text{Tr}\{e^{-H_\nu^0/T_\nu}\}$ are the density operators of the thermal baths. These assumptions are compatible with the Redfield approximation [53]. Using (B.8) we get

$$\text{Tr}_B\{\rho_{d,u}X_L\} = -ip_u(t)\int_0^\infty e^{iB\tau}\langle X_L(\tau)X_L(0)\rangle\,d\tau + ip_d(t)\int_0^\infty e^{iB\tau}\langle X_L(0)X_L(\tau)\rangle\,d\tau, \tag{B.9}$$

where $p_u = \text{Tr}_B\{\rho_{u,u}\}$ denotes the population of the spin-up state and p_d is the spin-down population. Note that terms of the form $\langle X_L(t)X_R(\tau)\rangle$ disappear, since the two reservoirs are not correlated. Following the same procedure for the second term in equation (B.6) we obtain

$$\text{Tr}_B\{\rho_{u,d}X_L\} = ip_u(t)\int_{-\infty}^0 e^{iB\tau}\langle X_L(\tau)X_L(0)\rangle\,d\tau - ip_d(t)\int_{-\infty}^0 e^{iB\tau}\langle X_L(0)X_L(\tau)\rangle\,d\tau. \tag{B.10}$$

Combining equations (B.9) and (B.10) provides us with the stationary thermal current under weak-coupling and Markovian approximations,

$$\langle j_L\rangle = -B[p_u k_{u\to d}^L - p_d k_{d\to u}^L], \tag{B.11}$$

with the relaxation rates

$$k_{u\to d}^L = \int_{-\infty}^\infty e^{iB\tau}\langle X_L(\tau)X_L(0)\rangle\,d\tau, \qquad k_{d\to u}^\nu = \int_{-\infty}^\infty e^{-iB\tau}\langle X_L(\tau)X_L(0)\rangle\,d\tau. \tag{B.12}$$

Equation (B.11) describes energy current through the junction, calculated, e.g. at the L contact, as the balance between an energy gain from the reservoir to the spin and an energy loss from the spin to the L bath.

The diagonal elements of the density matrix, p_d and p_u, can be further calculated under the same set of approximations, to yield the quantum Master equation,

$$\dot{p}_u = -p_u(t)\sum_\nu k_{u\to d}^\nu + p_d(t)\sum_\nu k_{d\to u}^\nu; \qquad p_u(t) + p_d(t) = 1. \tag{B.13}$$

In steady state ($\dot{p} = 0$) the spin occupations are

$$p_u = \frac{k_{d\to u}^L + k_{d\to u}^R}{k_{d\to u}^L + k_{d\to u}^R + k_{u\to d}^R + k_{u\to d}^R}; \qquad p_u + p_d = 1. \tag{B.14}$$

Plugging equation (B.14) into (B.12) leads to an explicit expression for the current

$$\langle j_L\rangle = B\frac{k_{u\to d}^L k_{u\to d}^R (e^{-B/T_L} - e^{-B/T_R})}{k_{u\to d}^R + k_{u\to d}^L + k_{d\to u}^R + k_{d\to u}^L}. \tag{B.15}$$

An analogous expression holds at the R contact. This is the well-established quantum Master-equation limit, used in various applications [21, 22, 46, 47, 54–56].

We can also extend the calculations to non-stationary situations. In this case one needs to evaluate the extra term $\text{Tr}\{\sigma^x P_L\} = \text{Tr}_B\{(\rho_{u,d} + \rho_{d,u})P_L\}$ in equation (B.3), resulting in

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momentum–position correlation functions of the form, $\langle P_L(t) X_L(\tau)\rangle$ in second-order system–bath couplings.

Note that $\left[H_L^0 + H_{\text{spin}}, V_L\right] \neq 0$ for the spin-boson Hamiltonian. Therefore, we cannot use in general the definition of appendix A, $j_L = \text{i}[H_{\text{spin}}, V_L]$. This limited expression is still applicable in a steady-state situation since $\langle \partial V_L / \partial t\rangle = 0$, translating into $\langle[H_{\text{SB}}, V_L]\rangle = \left\langle\left[H_L^0 + H_{\text{spin}}, V_L\right]\right\rangle = 0$; see equation (A.5).

Appendix C. Current conservation in an $M = 3$ states model

We clarify the notation and the results of section 5 using an $M = 3$ level system. According to our notation, the diagonal operators are

$$\overrightarrow{h} = (|1\rangle\langle1|, |2\rangle\langle2|, |3\rangle\langle3|). \tag{C.1}$$

The six nondiagonal operators with their respective roots are

$$
\begin{aligned}
E^{\overrightarrow{\alpha_1}} &= |1\rangle\langle2|, & \overrightarrow{\alpha_1} &= (1, -1, 0)\\
E^{\overrightarrow{\alpha_2}} &= |2\rangle\langle1|, & \overrightarrow{\alpha_2} &= (-1, 1, 0)\\
E^{\overrightarrow{\alpha_3}} &= |1\rangle\langle3|, & \overrightarrow{\alpha_3} &= (1, 0, -1)\\
E^{\overrightarrow{\alpha_4}} &= |3\rangle\langle1|, & \overrightarrow{\alpha_4} &= (-1, 0, 1)\\
E^{\overrightarrow{\alpha_5}} &= |2\rangle\langle3|, & \overrightarrow{\alpha_5} &= (0, 1, -1)\\
E^{\overrightarrow{\alpha_6}} &= |3\rangle\langle2|, & \overrightarrow{\alpha_6} &= (0, -1, 1),
\end{aligned}
\tag{C.2}
$$

where the energies at each site are $\overrightarrow{\epsilon} = (\epsilon_1, \epsilon_2, \epsilon_3)$. If the system conserves current (i.e., it fulfils (32)), the site–site interaction can include only the following terms: $E_s^{\overrightarrow{\alpha_n}} E_{s+1}^{\overrightarrow{\alpha_n}}$ ($n = 1, \ldots, 6$) and the pairs $E_s^{\overrightarrow{\alpha_1}} E_{s\pm1}^{\overrightarrow{\alpha_2}}$, $E_s^{\overrightarrow{\alpha_3}} E_{s\pm1}^{\overrightarrow{\alpha_4}}$, $E_s^{\overrightarrow{\alpha_5}} E_{s\pm1}^{\overrightarrow{\alpha_6}}$. The current operator in this model is given by equation (33),

$$
\begin{aligned}
j_{s\to s+1}^{(2)} = \text{i}a\Big\{ &V_{\overrightarrow{\alpha_1},\overrightarrow{\alpha_2}}(\epsilon_1 - \epsilon_2)\big(E_s^{\overrightarrow{\alpha_1}} E_{s+1}^{\overrightarrow{\alpha_2}} - E_s^{\overrightarrow{\alpha_2}} E_{s+1}^{\overrightarrow{\alpha_1}}\big)\\
&+ V_{\overrightarrow{\alpha_3},\overrightarrow{\alpha_4}}(\epsilon_1 - \epsilon_3)\big(E_s^{\overrightarrow{\alpha_3}} E_{s+1}^{\overrightarrow{\alpha_4}} - E_s^{\overrightarrow{\alpha_4}} E_{s+1}^{\overrightarrow{\alpha_3}}\big)\\
&+ V_{\overrightarrow{\alpha_5},\overrightarrow{\alpha_6}}(\epsilon_2 - \epsilon_3)\big(E_s^{\overrightarrow{\alpha_5}} E_{s+1}^{\overrightarrow{\alpha_6}} - E_s^{\overrightarrow{\alpha_6}} E_{s+1}^{\overrightarrow{\alpha_5}}\big)\Big\},
\end{aligned}
\tag{C.3}
$$

a generalization of the spin chain result (22).

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