A LETTERS JOURNAL EXPLORING
THE FRONTIERS OF PHYSICS

OFFPRINT

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EPL, **92** (2010) 30003

A Letters Journal Exploring the Frontiers of Physics

November 2010

EPL, **92** (2010) 30003
doi: 10.1209/0295-5075/92/30003

www.epljournal.org

Kubo formula for open finite-size systems

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received 16 July 2010; accepted in final form 14 October 2010
published online 19 November 2010

PACS 05.60.Gg – Quantum transport
PACS 05.70.Ln – Nonequilibrium and irreversible thermodynamics

Abstract – We derive a Kubo-type formula that describes proper non-equilibrium stationary states for finite-size systems. We first argue that the usual Kubo formula considers only equilibrium states of the perturbed system, which are inappropriate to describe transport properties. Moreover, we show that the standard Kubo formula for the *dc* conductance is only appropriate in the thermodynamic limit. We demonstrate that taking into consideration explicitly the coupling to the leads/baths solves both problems. This approach results in well-behaved response functions, without the singular contributions from degenerate states encountered when Kubo formulae for infinite-size systems are inappropriately used for finite-size systems. We also derive a second, more efficient formulation which is valid only for a set of special physical quantities, which includes the charge current density operator.

Introduction. – In this letter, we consider a finite-size one-dimensional system whose ends are coupled to two baths/reservoirs which are held at different temperatures T and/or chemical potentials μ, leading to flow of charge or thermal currents through the system. The question of interest to us is how can one find the stationary state that is reached after a long enough time, in order to characterize the steady-state currents flowing through the system and thus the *dc* charge/thermal conductances of the finite-size system. Note that we focus on a simple 1D system coupled to only two baths for simplicity; our results can be straightforwardly generalized to finite-size systems with any topology and connected to any number of baths.

Different physical pictures have been used to describe this problem and different calculation schemes have been proposed. Here, we use the system-bath scenario as the physical picture and present a Kubo-like formula as the calculation scheme to find the steady-state currents in the perturbational limit of a very small difference in the parameters of the two baths. We start with a brief review of commonly used physical pictures and calculation schemes.

We begin by discussing charge currents. There are two types of "driving forces" responsible for a steady-state charge current flow. The first is the applied electric field, which gives rise to an additional term V to be included in the total Hamiltonian $H = H_0 + V$ of the system, where H_0 describes the system without the field. The second is the imbalance in the chemical potentials and/or temperatures of the two baths, which results in a non-equilibrium distribution function ρ. Only if the baths have the same μ and T, does this distribution equal the thermal equilibrium distribution $\rho_{eq}(H) = \frac{1}{Z} e^{-\beta(H-\mu N)}$. However, this is not true when the two baths are biased.

The steady-state expectation value of the current is $\langle J \rangle = \mathrm{Tr}(\hat{J}\rho_\infty)$, where $\rho_\infty = \rho(t \to \infty)$ is the steady-state distribution for the non-equilibrium stationary state (NESS) established in the system a sufficiently long time after it was connected to the biased baths. For large systems in the linear-response regime it is customary to *assume* that $\rho_\infty \approx \rho_{eq}(H)$ and use the later to calculate the current [1]. Details regarding the baths and their coupling to the system are totally irrelevant.

The situation is different for thermal currents, since here there is only one driving force: the non-equilibrium distribution. There is no thermal equivalent for the electric potential. A calculation of the proper ρ_∞ therefore seems to be necessary. However, in fact it is still possible to introduce either the assumption of local equilibrium [2] or use gravitational potentials [3] to generate an artificial potential V which is added to H_0 and then one uses $\rho_{eq}(H)$ instead of the proper ρ_∞, in direct analogy with the usual approach for charge currents. In the following, we will refer to this approach as the standard Kubo formula (SKF). Again the baths play no explicit role in this approach, and therefore their existence is ignored.

The SKF has been widely used for both infinite [4] and finite-size systems [5], usually with periodic boundary

conditions. Open boundary conditions have also been used, leading to qualitatively different results [6]. In spite of this, it is a widely held belief that when the size of the systems approaches infinity, the difference between different boundary conditions should disappear and both should converge to the results for infinite systems [6].

For finite-size systems, it has also been suggested that they could be coupled to baths through infinitely long, perfectly conducting leads [7] so that the resulting total system of lead-system-lead becomes infinite and can be studied with the SKF. For non-interacting systems, this has been shown to be equivalent to the Landauer formula where ρ_∞ is replaced by the assumption that the distributions for states injected from the two leads are the thermal distributions of their respective baths. However, the vast majority of studies of conductances via the SKF are for infinite homogeneous systems [4], or extrapolations for $N\to\infty$ from results on finite-size systems [5]. For the latter, once the eigenstates $H_0|m\rangle=\epsilon_m|m\rangle$ are found, the SKF can be used to calculate physical quantities. For example, the well-known Drude weight [4–6]:

$$D=\frac{\pi\beta}{L}\sum_{\substack{m,n\\ \epsilon_m=\epsilon_n}}\frac{e^{-\beta\epsilon_m}}{Z}|\langle m|\hat{J}|n\rangle|^2 \tag{1}$$

is used often when discussing charge or thermal transport.

The first goal of this work is to show that the SKF does not give correct results for finite-size systems coupled to baths, which is the relevant experimental set-up. The second task, therefore, is to find a proper solution and hopefully also an efficient way to implement it.

A very different physical picture used to study transport is based on quantum master equations derived under various assumptions for a system explicitly coupled to baths. The most common are the Redfield equation (RE) [8–10] and the local-operator Lindblad equation (LOLE) [11–17]. LOLEs are easier to solve, for technical reasons. Systems with $N\sim 100$ were studied with a method based on density matrix renormalization [15], which does not apply to REs. Stochastic wave function methods have also been used for systems with $N\sim 20$ [13,18,19], comparable to what direct diagonalization can handle. However, the LOLEs' derivation has additional approximations to the REs' [16], and qualitative differences between their results have been reported [10,13,15]. In particular, while REs predict the correct $\rho_\infty=\rho_{eq}(H)$ for unbiased baths [16], LOLEs do not. Their use to describe weakly biased baths, on which we focus here, is therefore questionable.

Consequently, we use the RE in this work[1]. The downside is the significant computational cost which allows only systems of size $N\sim 10$ to be solved by direct means [9,10]. The stochastic wave function methods are also believed to work for REs [16]. We present here another technique for the linear-response limit of a weak bias, which requires only the diagonalization of the Hamiltonian and therefore works up to $N\sim 20$. However, this more efficient approach is valid only for certain response functions.

Limitations of the standard Kubo formula. – The Liouville-von Neumann equation of motion for the density matrix $\rho(t)$ of a *closed* system is ($\hbar=1$):

$$\frac{\partial\rho(t)}{\partial t}=L_H\rho(t)=-i[H,\rho], \tag{2}$$

where H is its Hamiltonian. Stationary solutions of this equation are not unique. They include the equilibrium distributions $\rho_{eq}(H)=\frac{1}{Z}e^{-\beta H}$ for any $\beta=1/k_BT$.

If $H=H_0+V$, where V is a static weak coupling to an external field, one can use perturbation theory to find $\rho(t)=\rho_0+\delta\rho(t)$ near a state ρ_0 of the isolated system, $L_{H_0}\rho_0=0$. Neglecting $L_V\delta\rho(t)$ in eq. (2), we integrate for $\delta\rho(t)$ to obtain the $t\to\infty$, steady-state solution:

$$\delta\rho=\int_0^\infty \mathrm{d}t e^{L_0t-\eta t}L_V\rho_0, \tag{3}$$

where $\eta\to 0^+$ and $L_0=L_{H_0}$. If $\rho_0=\rho_{eq}(H_0)$, this gives the standard Kubo formula (SKF) [1,3]:

$$\delta\rho=-i\int_0^\infty \mathrm{d}t e^{-\eta t}\left[V(-t),\frac{e^{-\beta H_0}}{Z}\right], \tag{4}$$

where $V(t)=e^{iH_0t}Ve^{-iH_0t}$. We can use the identity $[V(-t),e^{-\beta H_0}]=-ie^{-\beta H_0}\int_0^\beta \mathrm{d}\tau\dot{V}(-t-i\tau)$ to rewrite

$$\delta\rho=-\int_0^\infty \mathrm{d}t e^{-\eta t}\int_0^\beta \mathrm{d}\tau\rho_0\dot{V}(-t-i\tau). \tag{5}$$

In terms of the eigenvectors of H_0, $\langle m|\dot{V}(t)|n\rangle=i(\epsilon_m-\epsilon_n)V_{mn}e^{i(\epsilon_m-\epsilon_n)t}$ leading to:

$$\delta\rho=\sum_{\substack{m,n\\ \epsilon_m\neq\epsilon_n}}\frac{e^{-\beta\epsilon_m}-e^{-\beta\epsilon_n}}{Z}\frac{V_{mn}}{\epsilon_m-\epsilon_n-i\eta}|m\rangle\langle n|. \tag{6}$$

Incidentally, note that there is no contribution from states with $\epsilon_n=\epsilon_m$, for which $\langle m|\dot{V}(t)|n\rangle=0$. This also follows directly from eq. (4); if we write $V=V_0+V_\perp$, where $V_0=\sum_{\epsilon_m=\epsilon_n}V_{mn}|m\rangle\langle n|$ commutes with H_0, then $[V(-t),\rho_0]=[V_\perp(-t),\rho_0]$. The "diagonal" part V_0 of V does not contribute to $\delta\rho$ and thus to transport properties. We return to this important point below.

However, first we prove our claim that the resulting $\tilde{\rho}=\rho_{eq}(H_0)+\delta\rho$ is the first-order perturbational expansion of $\rho_{eq}(H)$, not of a NESS. We assume $\langle m|V|n\rangle=0$ if $\epsilon_m=\epsilon_n$. If it is not, we simply remove the "diagonal" part $V_0=\sum_{\epsilon_m=\epsilon_n}V_{mn}|m\rangle\langle n|$ from V and add it to H_0. Consider then the eigenstates of the full Hamiltonian, $H|\tilde{n}\rangle=\tilde{\epsilon}_n|\tilde{n}\rangle$, to first-order perturbation in V. Since $\langle m|V|n\rangle=0$ for all $\epsilon_m=\epsilon_n$, we can apply perturbation theory for non-degenerate states to all the states, whether degenerate or not, to find $\tilde{\epsilon}_n=\epsilon_n+\mathcal{O}(V^2)$ and

$$|\tilde{n}\rangle=|n\rangle+\sum_{m,\epsilon_m\neq\epsilon_n}\frac{\langle m|V|n\rangle}{\epsilon_n-\epsilon_m}|m\rangle+\mathcal{O}(V^2). \tag{7}$$

[1] We note that while the RE in principle can predict non-positive density operators, we have not encountered such problems in any of our simulations.

This leads to $\rho_{eq}(H) = \sum_n \frac{1}{Z} e^{-\beta\tilde{\epsilon}_n} |\tilde{n}\rangle\langle\tilde{n}| = \rho_{eq}(H_0) + \delta\rho + \mathcal{O}(V^2)$, where $\delta\rho$ is given by eq. (6).

This verifies that indeed, the SKF predicts $\rho_\infty \to \rho_{eq}(H)$. This is rather problematic because normally, if invariance to time reversal symmetry is not broken, no currents are generated in a thermal equilibrium state and therefore no steady-state transport through the closed finite system can be described by this approach. However, because we only keep the first-order perturbational correction, the situation is less clear cut. In principle, it is not impossible for $\delta\rho$ of eq. (6) to also be a first-order approximation to the true NESS, $\rho_\infty - \rho_{eq}(H_0)$, as well, or at least to capture a sizable part from it. This issue needs to be investigated in more detail.

Before doing so, however, we point to an even more serious problem with the SKF as used in literature, for example for the Drude weight of eq. (1), and which is only naturally resolved for infinite systems or for finite-size systems with periodic boundary conditions. A cursory comparison of eqs. (1) and (6) shows that while the former has contributions only from degenerate states with $\epsilon_n = \epsilon_m$, the latter has no contributions from such states.

To understand the reason for this difference, consider the derivation of eq. (1) from eq. (5), *e.g.* for spinless fermions in a one-dimensional chain (lattice constant $a = 1$), described by

$$H_0 = -t \sum_l \left(c_l^\dagger c_{l+1} + \text{h.c.} \right) + V_0 \sum_l n_l n_{l+1}, \tag{8}$$

where $n_l = c_l^\dagger c_l$, plus a static electric potential

$$V = \sum_l V_l n_l \tag{9}$$

induced by a homogeneous electric field $E = -\nabla V$. From the continuity equation,

$$\dot{V}(t) = \sum_l V_l \frac{\mathrm{d}}{\mathrm{d}t} n_l(t) = -\sum_l V_l [J_{l+1}(t) - J_l(t)], \tag{10}$$

where $J_l = it(c_{l+1}^+ c_l - c_l^+ c_{l+1})$ is the local current operator. This can be changed to

$$-\sum_l [V_{l-1} J_l(t) - V_l J_l(t)] = -EJ(t), \tag{11}$$

where $J(t) = \sum_l J_l(t)$ is the total current operator. Using $\dot{V}(t) = -EJ(t)$ in eq. (5) gives

$$\delta\rho = E \int_0^\infty \mathrm{d}t e^{-\eta t} \int_0^\beta \mathrm{d}\tau \rho_0 J(-t - i\tau). \tag{12}$$

The *dc* conductivity is then

$$\sigma = \int_0^\infty \mathrm{d}t e^{-\eta t} \int_0^\beta \mathrm{d}\tau \langle J(-t - i\tau) J \rangle, \tag{13}$$

where $\langle O \rangle = \mathrm{Tr}[\rho_{eq}(H_0) O]$. This expression can be further simplified to arrive at eq. (1).

The only questionable step in this derivation, and the one responsible for going from a result with no contributions from states with $\epsilon_n = \epsilon_m$ to one with contributions only from these states, is the change

$$\sum_l V_l J_{l+1}(t) \to \sum_l V_{l-1} J_l(t). \tag{14}$$

This is only justified for an infinite system (where boundary terms are presumed to be negligible), or a system with periodic boundary conditions and *an external field with the same periodicity*. This latter condition can only be achieved for a charge current in a finite system with periodic boundary conditions driven by a varying magnetic flux through the area enclosed by the system. For a finite-size system (even one with periodic boundary conditions) in a static applied electric field this approach will certainly fail. The same is true for thermal transport, which cannot experimentally be induced in a system with periodic boundary conditions. In both cases, the physical relevance of the results of eq. (1) are hard to fathom.

That the use of eq. (1) and its equivalents for finite-size systems is problematic can also be seen from the following technical considerations. The spectrum of a finite-size system is always discrete. As a result, any pair of degenerate eigenstates $\epsilon_m = \epsilon_n$ gives a δ-function contribution to the response functions. Such a singular response is unphysical for finite-size systems. Various techniques have been proposed to smooth out these singular contributions in order to extract some finite values, such as use of imaginary frequencies [20] or averaging σ over a small range of frequencies $\delta\omega$ and then taking $\delta\omega \to 0$ [21]. These different approaches may lead to different results. Moreover, the order in which the various limits are approached, *e.g.*, taking $\eta \to 0$ before $N \to \infty$ or vice versa, also make a difference [21]. All of these subtleties of the SKF are related to the potential divergence whenever $\epsilon_m = \epsilon_n$.

To summarize, using the SKF for finite-size systems is fraught with both conceptual and technical problems. *We conclude that in order to describe a NESS with a steady-state current flow in a finite-size system, one needs to go beyond viewing the system as a closed system, and to explicitly consider its connection to leads/baths.*

Kubo formula for open finite-size systems. – Transport through finite-size systems coupled to baths has been considered previously in the literature, for example in refs. [12,15–19,22]. In particular, ref. [22] derived a Kubo-like formula by taking into consideration currents flowing between the system and the baths in a stochastic manner. Here we present an alternative deterministic formulation that explicitly considers the effects of coupling to leads (for charge transport) or thermal baths (for heat transport) on the state of the system. It is based on the Redfield equation (RE) [23] which describes the evolution of the projected density matrix for the central system of interest. This is obtained from the Liouville-von Neumann equation for the total

density matrix describing the system+baths after using the projection technique [24] to trace out the baths.

For concreteness, let us assume coupling to thermal baths kept at temperatures $T_{L/R} = T \pm \frac{\Delta T}{2}$ and investigate the transport in the resulting steady state. If $\Delta T \ll T$, this will lead to a Kubo-like formula which replaces eq. (5). This approach can be generalized straightforwardly to derive a Kubo-like formula for charge transport.

The Redfield equation has the general form [8,10,16,24]:

$$\frac{\partial \rho(t)}{\partial t} = [L_H + L_L(T_L) + L_R(T_R)]\,\rho(t), \tag{15}$$

where $L_H \rho = -i[H, \rho]$, just like for an isolated system, while $L_{L/R}$ are additional terms that describe the effects of the left/right thermal baths (assumed to be in equilibrium at their corresponding temperatures $T_{L/R}$) on the evolution of the system. The expressions for $L_{L/R}$ depend on the Hamiltonian H of the system and on its coupling to the baths (an example is provided below).

If $\Delta T \ll T$, we can Taylor expand $L_{L/R}$ and re-arrange the Redfield equation to read

$$\frac{\partial \rho(t)}{\partial t} = [L_{H_0} + L_B(T) + L_P(\Delta T)]\,\rho(t) = L\rho(t), \tag{16}$$

where $L_B(T) = L_R(T) + L_L(T)$ is the contribution from the thermal baths if both are kept at the same temperature, while $L_P(\Delta T)$ collects the terms proportional to ΔT. Here we assume that $H = H_0$, *i.e.* that the thermal coupling does not induce a potential V in the system. For charge transport such a term appears, and its Liouvillian L_V should be grouped together with L_P.

We are interested in the $t \to \infty$, stationary state solution ρ_∞ of the above equation, which satisfies

$$L\rho_\infty = 0 \tag{17}$$

and which we assume to be unique for any value of ΔT. This means that L has a non-degenerate zero eigenvalue, and that all its other (transient) eigenvalues have a negative real part. Note that $L|_{\Delta T=0} = L_{H_0} + L_B(T)$ indeed has this property. In fact, it can be shown that in this case the $t \to \infty$ solution converges to the expected thermal equilibrium for the system held at temperature T, $\rho_\infty = \rho_{eq}(H_0)$ [24].

For small systems, eq. (17) can be solved numerically to find this eigenstate corresponding to the zero eigenvalue. We call this solution ρ_{ex} and we use it to validate the solutions of various approximation schemes. A Kubo-like formula, which is potentially more efficient, can be obtained using the linear-response theory. The first step is to separate the Liouvillian L of eq. (16) into a "large" plus a "small" part. There are two possible choices:

$$\begin{cases} L_0^{(1)} = L_{H_0} + L_B(T), \\ \Delta L^{(1)} = L_P(\Delta T), \end{cases} \tag{18}$$

or

$$\begin{cases} L_0^{(2)} = L_{H_0}, \\ \Delta L^{(2)} = L_B(T) + L_P(\Delta T). \end{cases} \tag{19}$$

We begin with the first choice. Assume that $L_0^{(1)}$ has eigenvalues $\{L_{0,\mu}^{(1)}\}$ and left/right eigenvectors $\{|\mathcal{L}_\mu)\}$, $\{|\mathcal{R}_\mu)\}$. As discussed, the unique (zero order in perturbation theory) steady-state solution of $L_0^{(1)}\rho_0 = 0$ is $\rho_0 = \rho_{eq}(H_0)$. The deviation $\delta\rho_K^{(1)}$ due to the perturbation $\Delta L^{(1)}$ is obtained like in eq. (3):

$$\delta\rho_K^{(1)} = \sum_\mu \int_0^\infty \mathrm{d}t e^{L_{0,\mu}^{(1)} t - \eta t} \,|\mathcal{R}_\mu)\,(\mathcal{L}_\mu|\,\Delta L^{(1)}\rho_0 = \\ -\sum_\mu \frac{|\mathcal{R}_\mu)\,(\mathcal{L}_\mu|}{L_{0,\mu}^{(1)} - \eta}\Delta L^{(1)}\rho_0 = -\sum_{\mu>0} \frac{|\mathcal{R}_\mu)\,(\mathcal{L}_\mu|}{L_{0,\mu}^{(1)}}\Delta L^{(1)}\rho_0. \tag{20}$$

Note that the only divergent term, due to $L_{0,0}^{(1)} = 0$, disappears because $(\mathcal{L}_0|\,\Delta L^{(1)}\rho_0 = (\rho_0|\,\Delta L^{(1)}\rho_0 = 0$. To see why, we start from eq. (17), $L(\rho_0 + \delta\rho) = 0$, project it on $(\rho_0|$ and keep terms only to the first order, to find $0 = (\rho_0|(L_0^{(1)} + \Delta L^{(1)})(\rho_0 + \delta\rho) = (\rho_0|\Delta L^{(1)}\rho_0$ since $L_0^{(1)}\rho_0 = 0$. As a result, eq. (20) has only regular contributions. A similar approach has been suggested in ref. [12], but for the LOLE [11] instead of the RE.

However, eq. (20) is difficult to use in practice: finding all eigenstates of $L_0^{(1)}$ is a hard task unless the system has an extremely small Hilbert space. A computationally simpler solution is obtained if we combine the eigenequation $L\rho_\infty = 0$ with the constraint $\mathrm{Tr}(\rho_\infty) = 1$ into a regular system of coupled equations $\bar{L}\rho_\infty = \nu$, where, in matrix terms, $\bar{L}$ is defined by replacing the first row of the equation $L\rho_\infty = 0$ by $\mathrm{Tr}(\rho_\infty) = 1$, so that ν is a vector whose first element is 1, all remaining ones being 0. As a result $\det(\bar{L}) \neq 0$ while $\det(L) = 0$. If solved numerically, $\bar{L}\bar{\rho}_\infty = \nu$ produces the expected exact solution ρ_{ex}.

We can also solve it to obtain a Kubo-like formula by dividing $\bar{L} = \bar{L}_0^{(1)} + \Delta\bar{L}^{(1)}$. Again, the overbar shows that in matrix terms, $\bar{L}_0^{(1)}$ is obtained from $L_0^{(1)}$ by replacing its first row with $\mathrm{Tr}(\rho_\infty) = 1$, while $\Delta\bar{L}^{(1)}$ is obtained from $\Delta L^{(1)}$ by replacing its first row with zeros. We find

$$\delta\bar{\rho}^{(1)} = -[\bar{L}_0^{(1)}]^{-1}\Delta\bar{L}^{(1)}\rho_0. \tag{21}$$

This is more convenient because inverting the non-singular matrix $\bar{L}_0^{(1)}$ is simpler than finding all eigenstates of $L_0^{(1)}$, and works for up to $N \sim 10$. We have verified that both schemes produce identical results for small N where both can be performed. We denote $\rho_0 + \delta\bar{\rho}^{(1)} = \rho_\infty^{(1)}$.

The second option is to take $L_0^{(2)} = L_{H_0}$ and $\Delta L^{(2)} = L_B(T) + L_P(\Delta T)$. In this case, we can still *choose* the stationary solution associated with $L_0^{(2)}$ to be the thermal equilibrium state at T, $\rho_0 = \rho_{eq}(H_0)$. However, this solution is no longer unique, since any matrix ρ_0 that commutes with H_0 satisfies $L_0^{(2)}\rho_0 = 0$. Expanding the corresponding analogue of eq. (4) in the eigenbasis of H_0, we now find

$$\delta\rho^{(2)} = -i\sum_{n,m} \frac{\langle m|\Delta L^{(2)}\rho_0|n\rangle}{\epsilon_m - \epsilon_n - i\eta}|m\rangle\langle n|. \tag{22}$$

We call $\rho_0 + \delta\rho^{(2)} = \rho_\infty^{(2)}$. This expansion can be performed as long as all eigenstates of H_0 can be found, thus this can be applied to systems up to $N \sim 20$. Note that unlike $\rho^{(1)}$ of eq. (21), this solution has divergent contributions from states with $\epsilon_n = \epsilon_m$. As such, it is analogous to the SKF for infinite systems. This is not an accident. As discussed, the SKF for infinite systems always ignores the coupling to the leads. It also takes $L_0 = L_{H_0}$ and assumes that $\rho_0 = \rho_{eq}(H_0)$. Moreover, the driving force for transport is only the potential V added to H_0, so that $\Delta L \to L_V$. With these assumptions, eq. (22) maps straightforwardly into the SKF of eq. (6).

Results and discussion. – To see which of these two solutions —the regular solution $\rho_\infty^{(1)}$ or the singular solution $\rho_\infty^{(2)}$— gives a proper density matrix, we compare them against the exact numerical solution ρ_{ex} of eq. (17) in the limit $\Delta T \ll T$.

We do this for an N-site chain of spinless fermions

$$\mathcal{H}_0 = -t \sum_{l=1}^{N-1} \left(c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l \right) + V_0 \sum_{l=1}^{N-1} c_{l+1}^\dagger c_{l+1} c_l^\dagger c_l. \tag{23}$$

coupled to two heat baths, modeled as collections of fermions:

$$\mathcal{H}_B = \sum_{k,\alpha=L,R} \omega_{k,\alpha} b_{k,\alpha}^\dagger b_{k,\alpha}, \tag{24}$$

where α indexes the left- and right-side baths and we set $\hbar = 1, k_B = 1$, the lattice constant $a = 1$, and hopping $t = 1$. The system-baths coupling is chosen as:

$$V_{SB} = \lambda \sum_{k,\alpha} V_k^\alpha \left(c_\alpha^\dagger b_{k,\alpha} + c_\alpha b_{k,\alpha}^\dagger \right), \tag{25}$$

where the left (right) bath is coupled to the first (last) site: $c_L = c_1$ and $c_R = c_N$. Bath parameters, including temperature and chemical potential, are chosen to be (T_L, μ) and (T_R, μ) with $T_{L/R} = T \pm \frac{\Delta T}{2}$.

The corresponding Redfield equation reads [8,10,24],

$$\frac{\partial \rho(t)}{\partial t} = -i[\mathcal{H}_0, \rho(t)] - \lambda^2 \sum_{\alpha=L,R} \Big\{ \big[c_\alpha^\dagger, \hat{m}_\alpha \rho(t)\big] + \big[c_\alpha, \hat{\bar{m}}_\alpha \rho(t)\big] + \text{h.c.} \Big\}, \tag{26}$$

where operators $\hat{m}_\alpha$ and $\hat{\bar{m}}_\alpha$ are defined as

$$\hat{m}_\alpha = \pi \sum_{m,n} |m\rangle\langle n| \langle m|c_\alpha|n\rangle \left(1 - n_\alpha(\Omega_{nm})\right), \tag{27a}$$

$$\hat{\bar{m}}_\alpha = \pi \sum_{m,n} |m\rangle\langle n| \langle m|c_\alpha^\dagger|n\rangle n_\alpha(\Omega_{mn}), \tag{27b}$$

where $\Omega_{mn} = E_m - E_n = -\Omega_{nm}$ and $n_\alpha(\Omega_{mn})$ is the Fermi-Dirac distribution at temperature T_α. We have furthermore assumed V_k^α and the densities of states of the baths to be constants and absorbed them into λ^2.

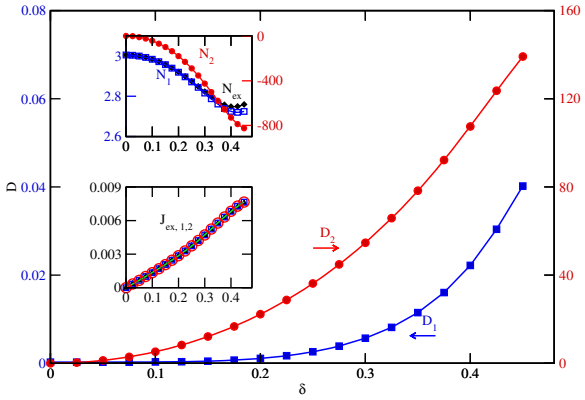

Fig. 1: (Color online) D_1 (squares) and D_2 (circles) of eq. (28) *vs.* $\delta = \Delta T/2T$, for $N = 8$, $t = 1.0$, $V_0 = 0.2$, $T = 2.0$, $\mu = -1.0$, $\lambda = 0.1$, $\eta = 0.00001$. The upper (lower) inset shows the steady-state particle number (electric current) calculated with ρ_{ex} (triangles) and $\rho_\infty^{(1,2)}$ (squares and circles).

Equation (26) is an example of the general eq. (15). Since $T_{L/R}$ enters only in the Fermi-Dirac distributions, it is easy to expand when $T_{L/R} = T \pm \frac{\Delta T}{2}$, $\Delta T \ll T$ to identify $L_B(T)$ and $L_P(\Delta T)$ needed in eqs. (21) and (22).

We characterize the distance between the exact numerical solution ρ_{ex} and the two possible Kubo solutions $\rho_\infty^{(i)}$, $i = 1, 2$ by calculating the norm

$$D_i = \sqrt{\sum_{n,m} \left| \langle n|\rho_{ex} - \rho_\infty^{(i)}|m\rangle \right|^2}. \tag{28}$$

For the proper solution, this difference should be small but finite due to higher-order perturbation terms.

Results typical of those found in all the cases we investigated are shown for $N = 8, V_0 = 0.2, \lambda = 0.1, \eta = 10^{-5}$ in fig. 1, where we plot $D_{1,2}$ *vs.* $\delta = \Delta T/2T$. This small N value is used so that we can calculate ρ_{ex} reasonably fast. We see that D_2 (circles, axis on the right) is very large. In fact, because of the singular contributions from $\epsilon_n = \epsilon_m$ states, D_2 is divergent, with a magnitude controlled by the cutoff η. In contrast, D_1 (squares, left axis) is small and independent of η. The insets show the total number of particles (N) and electric current (J) calculated with ρ_{ex}, $\rho_\infty^{(1)}$ and $\rho_\infty^{(2)}$ (triangles, squares, respectively circles). Both N_1 and J_1 are very close to the exact values N_{ex}, J_{ex}. However, N_2 is very different from N_{ex} while J_2 is close to J_{ex}. These results confirm that $\rho_\infty^{(1)}$ of eq. (21) is the proper perturbational solution. They also show that $\rho_\infty^{(2)}$ can also be used, but only for quantities A for which $\langle m|A|n\rangle = 0$ whenever $\epsilon_m = \epsilon_n$, so that the divergences in eq. (22) disappear. This explains the previous success of this formula to be somewhat of an accident. Note that for eq. (22) only the eigenstates of H_0 are needed, so when valid it is computationally more efficient.

Figure 2 shows the same quantities as fig. 1, at a fixed bias ΔT as a function of the strength of the system-bath

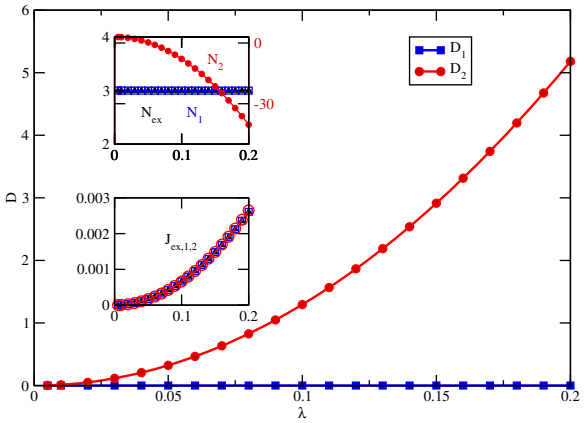

Fig. 2: (Color online) D_1 (squares) and D_2 (circles) of eq. (28) *vs.* λ, for $N=8$, $t=1.0$, $V_0=0.2$, $T=2.0$, $\mu=-1.0$, $\delta=0.1$, $\eta=0.00001$. The upper (lower) inset shows the steady-state particle number (electric current) calculated with ρ_{ex} (triangles) and $\rho_K^{(1,2)}$ (squares and circles).

coupling λ. It confirms again that $\rho_\infty^{(1)}$ is the proper approximation of ρ_{ex}, but that for the charge current $\rho_\infty^{(2)}$ works well too. It also shows that the NESSs depend on coupling strength λ. This is not surprising for a finite-size system: the intrinsic conductance of the system is added to comparable "contact" contributions from the interfaces between the system and the baths, and experiments measure the total conductance. It follows that quantitative modeling of transport in finite systems will require a careful consideration of the entire experimental set-up.

Conclusion. – In summary, we demonstrated that the SKF fails to provide an approximation of NESSs. Instead it gives the first-order correction to the equilibrium state corresponding to the full Hamiltonian. Moreover, applying the standard Kubo formula to finite systems generically leads to unphysical divergences. We then showed that taking explicitly into consideration the coupling to baths solves both problems and leads to a well-behaved Kubo-like formula, that can be used on systems with up to $N\sim 10$. This is still a very low value, therefore more efficient methods like those of ref. [15] need to be extended to the RE equation. Some progress in that direction has recently been reported in ref. [25]. Finally, we argued that the more numerically efficient but improper solution similar to those used in literature can give correct values for up to $N\sim 20$, but only for certain physical quantities.

While elements of this work have similarities with work published elsewhere —for example a similar formula to our OKF has already been proposed for the LOLE [12], and discussions about differences between SKF and LOLE results are pursued in refs. [14,17–19]— to our knowledge this is the first time when it is shown explicitly why the SKF does not work for finite-size systems. Using methods which explicitly consider the coupling to baths is thus no longer just a possible alternative, but a necessary step when dealing with transport through small open quantum systems.

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We thank I. Affleck for many discussions and suggestions. This work was supported by NSERC and CIFAR.

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