## Kubo formula for finite size systems

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We demonstrate that the proper calculation of the linear response for finite-size systems can only be performed if the coupling to the leads/baths is explicitly taken into consideration. We exemplify this by obtaining a Kubo-type formula for heat transport in a finite-size system coupled to two thermal baths, kept at different temperatures. We show that the proper calculation results in a well-behaved response, without the singular contributions from degenerate states encountered when Kubo formulae for infinite-size systems are inappropriately used for finite-size systems.

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The Liouville-von Neumann equation of motion for the density matrix  $\rho(t)$  of a closed system is  $(\hbar = 1)$ :

$$\frac{\partial \rho(t)}{\partial t} = L_H \rho(t) = -i[H, \rho], \tag{1}$$

where H is the Hamiltonian describing the evolution of the system. If  $H = H_0 + V$ , where V is a static weak coupling to an external field, one can use perturbation theory to find a solution  $\rho(t) = \rho_0 + \delta \rho(t)$  near a state  $\rho_0$  of the unperturbed system,  $L_{H_0}\rho_0 = 0$ . Neglecting  $L_V \delta \rho(t)$  in Eq. (1), we integrate the resulting equation for  $\delta \rho(t)$  to obtain the  $t \to \infty$ , steady-state solution:

$$\delta \rho = \int_0^\infty dt e^{L_0 t - \eta t} L_V \rho_0, \tag{2}$$

where  $\eta \to 0^+$ . If  $\rho_0 = \frac{1}{Z}e^{-\beta H_0}$  describes the unperturbed system in equilibrium at temperature  $k_BT = 1/\beta$ , then this is known as the Kubo formula [1, 2]:

$$\delta \rho = -i \int_{0}^{\infty} dt e^{-\eta t} \left[ V(-t), \frac{e^{-\beta H_0}}{Z} \right], \quad (3)$$

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

$$\delta \rho = -\int_0^\infty dt e^{-\eta t} \int_0^\beta d\tau \rho_0 \dot{V} \left( -t - i\tau \right). \tag{4}$$

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

$$\delta \rho = \sum_{\substack{m,n\\\epsilon_m \neq \epsilon_n}} \frac{e^{-\beta \epsilon_m} - e^{-\beta \epsilon_n}}{Z} \frac{V_{mn}}{\epsilon_m - \epsilon_n - i\eta} |m\rangle\langle n|. \quad (5)$$

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. (3); 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 consequently has no influence on the static response functions.

The lack of contributions from eigenstates with  $\epsilon_n = \epsilon_m$  is, however, puzzling, because the well-known Drude weight derived directly from the Kubo formula is [3]:

$$D = \frac{\pi \beta}{L} \sum_{\substack{m,n \\ \epsilon_m = \epsilon_n}} \frac{e^{-\beta \epsilon_m}}{Z} |\langle m|\hat{J}|n\rangle|^2, \tag{6}$$

i.e. it has contributions only from these eigenstates.

To understand the reason for this difference, consider the derivation of Eq. (6) from Eq. (4), for simplicity for a one-dimensional chain described by  $H_0 = -t \sum_l \left(c_l^\dagger c_{l+1} + h.c.\right) + V_0 \sum_l n_l n_{l+1}$ , where  $n_l = c_l^\dagger c_l$ , plus a static potential  $V = \sum_l V_l n_l$  induced by a homogeneous electric field  $E = -\nabla V$ . From the continuity equation,  $\dot{V}(t) = \sum_l V_l \frac{d}{dt} n_l(t) = -\frac{1}{a} \sum_l V_l [J_{l+1}(t) - J_l(t)]$ , where  $J_l = it \left(c_{l+1}^+ c_l - c_l^+ c_{l+1}\right)$  is the local current operator. This can be changed to  $-\frac{1}{a} \sum_l [V_{l-1} J_l(t) - V_l J_l(t)] = \nabla V \sum_l J_l(t) = -EJ(t)$ , where J(t) is the total current operator. Using  $\dot{V}(t) = -EJ(t)$  in Eq. (4) gives  $\delta \rho = E \int_0^\infty dt e^{-\eta t} \int_0^\beta d\tau \rho_0 J\left(-t - i\tau\right)$ . The dc conductivity is then  $\sigma = \int_0^\infty dt e^{-\eta t} \int_0^\beta d\tau \left\langle J\left(-t - i\tau\right) J\right\rangle$ , where  $\langle O\rangle = Tr[\rho_0 O]$ , from which Eq. (6) follows.

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  $\sum_l V_l J_{l+1}(t) \rightarrow \sum_l V_{l-1} J_l(t)$ . This is only justified for an infinite system (where boundary terms are negligible), or a system with periodic boundary conditions and an external electric potential with the same periodicity [4]. It is certainly not valid for a finite size system connected to external leads, which break this symmetry. In such cases, the use of formulae like Eq. (6) is simply not appropriate [5].

The solution, however, is not the use of Eqs. (4) or (5), derived for a finite size, closed system. Instead, one needs to derive their analogue for an open system coupled to leads. The reason is that  $\tilde{\rho} = \rho_0 + \delta \rho$  of Eq. (5) does not describe a non-equilibrium stationary state (NESS), in which transport of charge or heat through the system is possible. Instead,  $\tilde{\rho}$  is a first-order approximation of the thermal equilibrium state  $\tilde{\rho}_{th} = e^{-\beta H}/\tilde{Z}$  of the

full Hamiltonian  $H = H_0 + V$ . Normally (for example 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 finite system can be described by this approach [6].

To prove the above statement relating  $\tilde{\rho}$  to  $\tilde{\rho}_{th}$ , we take  $\langle m | V | n \rangle = 0$  if  $\epsilon_m = \epsilon_n$ , since as already discussed, the "diagonal" part  $V_0$  of V does not contribute to transport. Consider then the eigenbasis  $H | \tilde{n} \rangle = \tilde{\epsilon}_n | \tilde{n} \rangle$ , to first order perturbation in V. Since  $\langle m | V | n \rangle = 0$  for all  $\epsilon_m = \epsilon_n$ , we can apply the first order 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  $|\tilde{n}\rangle = |n\rangle + \sum_{m,\epsilon_m \neq \epsilon_n} \frac{\langle m | V | n \rangle}{\epsilon_n - \epsilon_m} |m\rangle + \mathcal{O}(V^2)$ . This immediately leads to  $\tilde{\rho}_{th} = \sum_n \frac{1}{Z} e^{-\beta \tilde{\epsilon}_n} |\tilde{n}\rangle \langle \tilde{n} | = \rho_0 + \delta \rho + \mathcal{O}(V^2)$ , where  $\delta \rho$  is indeed given by Eq. (5).

Therefore, we conclude that in order to describe an NESS with current flow, one needs to go beyond viewing the finite size system of interest as a closed system, and to explicitly consider its connection to leads. We note that the effects of boundary conditions have been considered previously, eg in Refs. [7, 8]. In particular, Ref. [8] derived a Kubo-like formula that takes into consideration cross-boundary currents in a stochastic approach.

In this Letter 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 [9] which describes the evolution of the projected density matrix for the central system of interest, obtained if we start from the Liouvillevon Neumann equation for the total density matrix describing the system+leads/baths and use the projection technique [10] to trace out the leads/baths.

For simplicity, we assume coupling to thermal baths kept at temperatures  $T_{L/R} = T \pm \frac{\Delta T}{2}$  and investigate the heat transport in the resulting steady state. If  $\Delta T \ll T$ , this leads to a Kubo-like formula which replaces Eq. (4). This approach can be generalized straightforwardly to derive a Kubo-like formula for charge transport.

The Redfield equation has the general form [10–12]:

$$\frac{\partial \rho(t)}{\partial t} = \left[ L_H + L_L(T_L) + L_R(T_R) \right] \rho(t), \tag{7}$$

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:

$$\frac{\partial \rho(t)}{\partial t} = \left[ L_{H_0} + L_B(T) + L_P(\Delta T) \right] \rho(t) = L\rho(t), \quad (8)$$

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  $\Delta T$ . Here we assume that  $H = H_0$ , i.e. that the thermal coupling does not induce an interaction V in the system. For charge transport such a term appears, and its Liouvillian  $L_V$  should be grouped together with  $L_P$ .

Again, we are interested in the  $t \to \infty$ , stationary state solution  $\rho$  of the above equation, *i.e.* 

$$L\rho = 0 \tag{9}$$

which we assume to be unique for any value of  $\Delta T$ . This means that L has a single zero eigenvalue, and all its other (transient) eigenvalues have a negative real part. Note that  $L|_{\Delta T=0}=L_{H_0}+L_B(T)$  has this property. In fact, one can show that in this case the  $t\to\infty$  solution converges to the expected thermal equilibrium for the system held at temperature T,  $\rho_0 = \frac{1}{Z}e^{-\beta H_0}$  [10].

Eq. (9) can be solved numerically to find this eigenstate. We call this solution  $\rho_{ex}$ . However, our goal is to obtain a Kubo-like formula. This can be done by analogy with the calculation for the closed system discussed in the beginning of this work. The first step is to separate the Liouvillian L of Eq. (8) into a "large" plus a "small" part. There are two possible choices: either take the "large" part to be  $L_0^{(1)} = L_{H_0} + L_B(T)$  with the perturbation  $\Delta L^{(1)} = L_P(\Delta T)$ , or take  $L_0^{(2)} = L_{H_0}$  and let  $\Delta L^{(2)} = L_B(T) + L_P(\Delta T)$  be the perturbation.

We begin with the first choice.  $L_0^{(1)} = L_{H_0} + L_B(T)$  has eigenvalues  $\left\{L_{0,\mu}^{(1)}\right\}$  and left/right eigenvectors  $\{|\mathcal{L}_{\mu})\}$ ,  $\{|\mathcal{R}_{\mu})\}$ . As discussed, the unique steady-state solution of  $L_0^{(1)}\rho_0 = 0$  is  $\rho_0 = \frac{1}{Z}e^{-\beta H_0}$ . The deviation  $\delta\rho_K^{(1)}$  due to the perturbation  $\Delta L^{(1)}$  is obtained like in Eq. (2):

$$\delta \rho_K^{(1)} = \sum_{\mu} \int_0^{\infty} dt e^{L_{0,\mu}^{(1)} t - \eta t} |\mathcal{R}_{\mu}| (\mathcal{L}_{\mu}| \Delta L^{(1)} \rho_0)$$

$$= -\sum_{\mu} \frac{|\mathcal{R}_{\mu}| (\mathcal{L}_{\mu}|}{L_{0,\mu}^{(1)} - \eta} \Delta L^{(1)} \rho_0 = -\sum_{\mu > 0} \frac{|\mathcal{R}_{\mu}| (\mathcal{L}_{\mu}|}{L_{0,\mu}^{(1)}} \Delta L^{(1)} \rho_0.$$
(10)

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. (9),  $L(\rho_0+\delta\rho)=0$ , project it on  $(\rho_0|$  and keep terms only to first order, to find  $0=(\rho_0|\left(L_0^{(1)}+\Delta L^{(1)}\right)(\rho_0+\delta\rho)=(\rho_0|\Delta L^{(1)}\rho_0)$  since  $L_0^{(1)}\rho_0=0$ . As a result, Eq. (10) has only regular contributions. We denote  $\rho_0+\delta\rho_K^{(1)}=\rho_K^{(1)}$ . A similar approach using the eigenvalues and eigenvectors of  $L_{H_0}+L_B(T)$  has been suggested in Ref. [13], but for the Lindblad equation [14] instead of the Redfield equation.

However, Eq. (10) 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  $L\rho=0$  with the constraint  $Tr\rho=1$  into a regular system of coupled equations  $\bar{L}\bar{\rho}=\nu$ , where, in matrix terms,  $\bar{L}$  is defined by replacing the first row of the equation  $L\rho=0$  by  $Tr(\rho)=1$ , so that  $\nu$  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,  $\bar{L}\bar{\rho}=\nu$  produces the expected solution  $\rho_{ex}$ .

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  $Tr\rho = 1$ , while  $\Delta \bar{L}^{(1)}$  is obtained from  $\Delta L^{(1)}$  by replacing its first row with zeros. Then:

$$\delta \bar{\rho}_K^{(1)} = -[\bar{L}_0^{(1)}]^{-1} \Delta \bar{L}^{(1)} \rho_0. \tag{11}$$

This is much more convenient because inverting the non-singular matrix  $\bar{L}_0^{(1)}$  is a much simpler task than finding all the eigenvalues and eigenvectors of  $L_0^{(1)}$ . We have verified that both schemes produce identical results.

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,  $\rho_0 = \frac{1}{Z}e^{-\beta H_0}$ . However, this solution is no longer unique, in particular the thermal equilibrium state corresponding to any other temperature satisfies  $L_0^{(2)}\rho_0 = 0$ . Expanding the analogue of Eq. (3) in the eigenbasis of  $H_0$ , we find:

$$\delta \rho_K^{(2)} = -i \sum_{n,m} \frac{\langle m | \Delta L^{(2)} \rho_0 | n \rangle}{\epsilon_m - \epsilon_n - i\eta} | m \rangle \langle n |.$$
 (12)

We call  $\rho_0 + \delta \rho_K^{(2)} = \rho_K^{(2)}$ . Note that unlike  $\rho_K^{(1)}$  of Eq. (10), this solution has divergent contributions from states with  $\epsilon_n = \epsilon_m$ . As such, it is analogous to the Kubo formulae for infinite systems.

This similarity is not accidental. Kubo formulae for infinite systems always ignore the coupling to the leads, taking  $L_0 = L_{H_0}$  and assuming that  $\rho_0 = e^{-\beta H_0}/Z$ , where the temperature is arbitrarily chosen. Moreover, the driving force leading to transport is not a term  $L_P(\Delta T)$ , since the leads are ignored, but rather the addition of some potential V to  $H_0$  leading to  $\Delta L = L_V$ . Using only such a V is rather questionable even for charge transport, because of the previously mentioned problems with the periodic boundary conditions, which may be negligible for infinite size systems but are certainly not for finite-size systems. For heat transport, using a V to describe a variation in the gravitational potential [2] is rather contrived, besides having the same boundary conditions issues. Nevertheless, with these assumptions, Eq. (12) maps into the usual Kubo formula for an infinite system. Thus, we can think of Eq. (12) with  $L_P(\Delta T)$ included in  $\Delta L$  as being a finite-size analog of the usual infinite-size Kubo formulae. (As discussed, for a finite size system  $L_P(\Delta T)$  cannot be entirely replaced by an  $L_V$ , if steady-state transport is to be established).

To see which of these two solutions – the regular solution  $\rho_K^{(1)}$  or the singular solution  $\rho_K^{(2)}$  which is analogous to formulae for infinite systems – is the proper one, we compare them against the exact numerical solution  $\rho_{ex}$  of Eq. (9) in the limit  $\Delta T \ll T$ .

We do this for a chain of N spins  $\frac{1}{2}$  coupled by nearest-neighbour exchange and placed in a magnetic field:

$$\mathcal{H}_0 = \sum_{i=1}^{N-1} J \vec{s}_i \cdot \vec{s}_{i+1} - B_z \sum_{i=1}^{N} s_i^z$$

while the heat baths are collections of bosonic modes,

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

where  $\alpha = R, L$  indexes the right/left-side baths. The system-baths coupling is chosen as:

$$V_{int} = \lambda \sum_{k,\alpha} V_k^{(\alpha)} s_{i_{\alpha}}^y \left( b_{k,\alpha}^{\dagger} + b_{k,\alpha} \right)$$

where  $i_L = 1$ ,  $i_R = N$ , *i.e.* the left/right bath is coupled to the first/last spin and can induce its spin-flipping.

Using the projector technique [11, 12], the equation of evolution for  $\rho(t) = Tr_B \rho_t(t)$ , where  $\rho_t$  is the total density of states for the system+baths, is found to second-order perturbation theory in  $V_{int}$ , to be:

$$\frac{\partial \rho(t)}{\partial t} = -i[\mathcal{H}_0, \rho(t)] - \lambda^2 \sum_{\alpha = L, R} \left( \left[ s_{i_\alpha}^y, \hat{m}_\alpha \rho(t) \right] + h.c. \right)$$
(13)

where  $\hat{m}_{\alpha} = s_{i_{\alpha}}^{y} \cdot \hat{\Sigma}_{\alpha}$ . Here, (·) refers to the element-wise product of two matrices,  $\langle n|\hat{a}\cdot\hat{b}|m\rangle = \langle n|\hat{a}|m\rangle\langle n|\hat{b}|m\rangle$ . The bath matrices  $\hat{\Sigma}_{L,R}$  are defined in terms of the eigenstates of the system's Hamiltonian  $\mathcal{H}_{0}|n\rangle = \epsilon_{n}|n\rangle$  as:

$$\begin{split} \hat{\Sigma}_{\alpha} &= \pi \sum_{m,n} |m\rangle \langle n| \left[ \Theta\left(\Omega_{mn}\right) n_{\alpha}\left(\Omega_{mn}\right) D_{\alpha}\left(\Omega_{mn}\right) |V_{k_{mn}}^{(\alpha)}|^{2} \right. \\ &\left. + \Theta\left(\Omega_{nm}\right) \left(1 + n_{\alpha}\left(\Omega_{nm}\right)\right) D_{\alpha}\left(\Omega_{nm}\right) |V_{k_{nm}}^{(\alpha)}|^{2} \right] \end{split}$$

where  $\Omega_{mn} = \epsilon_m - \epsilon_n = -\Omega_{nm}$  and  $k_{mn}$  is defined by  $\omega_{k_{mn},\alpha} = \Omega_{mn}$ , i.e. is a bath mode resonant with this transition. Furthermore,  $\Theta(x)$  is the Heaviside function,  $n_{\alpha}(\Omega) = \left[e^{\beta_{\alpha}\Omega} - 1\right]^{-1}$  is the Bose-Einstein equilibrium distribution for the bosonic modes of energy  $\Omega$  at the bath temperature  $T_{\alpha} = 1/\beta_{\alpha}$ , and  $D_{\alpha}(\Omega)$  is the bath's density of states. The product  $D_{\alpha}(\Omega_{mn}) |V_{k_{mn}}^{(\alpha)}|^2$  is the bath's spectral density function. For simplicity, we take it to be a constant independent of m and n.

Eq. (13) is thus a particular example of the general Eq. (7), with the last two terms coming from the coupling

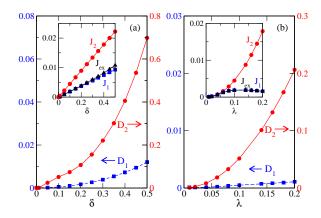


FIG. 1: (color online)  $D_1$  (squares) and  $D_2$  (circles) of Eq. (14) (a) vs.  $\delta = \Delta T/2T$  at a fixed  $\lambda = 0.1$ , and (b) vs.  $\lambda$  at a fixed  $\delta = 0.1$ , for  $N = 8, J = 0.1, B_z = 1$ . The insets show the steady-state thermal current calculated with  $\rho_{ex}$  (triangles) and  $\rho_K^{(1,2)}$  (squares and circles). See text for more details.

to the two thermal baths. Since the temperatures  $T_{L/R}$  enter only in the Bose-Einstein occupation numbers, it is straightforward to expand them when  $T_{L/R} = T \pm \frac{\Delta T}{2}$ ,  $\Delta T \ll T$  and so to identify  $L_B(T)$  and  $L_P(\Delta T)$ .

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

$$D_i = \sqrt{\sum_{n,m} \left| \langle n | \rho_{ex} - \rho_K^{(i)} | m \rangle \right|^2}.$$
 (14)

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 in Fig. 1 for  $N = 8, J = 0.1, B_z = 1.0$ . In Fig. 1(a), we plot  $D_{1,2}$  vs.  $\delta = \Delta T/2T$  for a fixed system-baths coupling  $\lambda = 0.1$ , while in Fig. 1(b) we show them vs.  $\lambda$ , for  $\delta T = 0.1$ . In both cases,  $D_2$  (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, its magnitude being controlled by the cutoff  $\eta$ used ( $\eta = 10^{-5}$  here). In contrast,  $D_1$  (squares, left axis) has a small value independent of  $\eta \to 0$ , showing that the regular  $\rho_K^{(1)}$  is the proper Kubo solution. The insets show the thermal current calculated with  $\rho_{ex}$ ,  $\rho_{K}^{(1)}$  and  $\rho_K^{(2)}$  (triangles, squares, respectively circles).  $J_2$  becomes independent of  $\eta$  as  $\eta \to 0$ , however, unlike  $J_1$  it is quite different from the exact solution. This again confirms that  $\rho_K^{(1)}$  is the proper Kubo solution. Fig. 1(b) also shows that the answer depends on the

Fig. 1(b) also shows that the answer depends on the details of the coupling to the baths. 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 fi-

nite systems will require a careful consideration of the entire experimental set-up.

To conclude, we make two claims regarding the proper Kubo formulae to be used for finite-size systems. The first is that the coupling to leads/baths simply cannot be ignored, as is usually done for infinite-size systems. Instead, it has to be considered explicitly if steady-state transport is to be established in the system. Secondly, we showed that the proper way to derive a Kubo-like formula in such cases leads to a well-behaved result. This is to be contrasted with the formulae typically used in literature, similar to those valid for infinite-size systems, and which have singular contributions from eigenstates with  $\epsilon_n = \epsilon_m$ . In infinite systems this is not a problem because the spectrum is continuous and the final result is still well-behaved. However, for finite-size systems the spectrum is discrete and the singularities cannot be avoided. This is clearly unphysical: a finite-size system cannot have singular response functions. Of course, in reality the "eigenstates" of the open system are no longer sharp, instead they acquire a finite lifetime due to tunneling of charge/heat into and out of the leads/baths. The need to properly consider the effects of the leads/baths on the system is therefore unavoidable.

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- [5] The fact that one should not sum over  $\epsilon_n = \epsilon_m$  states in the Kubo formula for finite systems can also be verified explicitly for toy models, eg.  $H_0 = \frac{1}{2} \left( p^2 + x^2 \right)$  and  $V = \frac{\lambda}{2} x^2$ , which are exactly solvable. It is easy to check that Eq. (5) gives the correct answer to  $\mathcal{O}(\lambda^2)$ , while inclusion of  $\epsilon_m = \epsilon_n$  terms gives wrong results.
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