LETTER

The Green–Kubo formula for heat conduction in open systems

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Abstract. We obtain an exact Green–Kubo type linear response result for the heat current in an open system. The result is derived for classical Hamiltonian systems coupled to heat baths. Both lattice models and fluid systems are studied and several commonly used implementations of heat baths, stochastic as well as deterministic, are considered. The results are valid in arbitrary dimensions and for any system sizes. Our results are useful for obtaining the linear response transport properties of mesoscopic systems. Also we point out that for systems with anomalous heat transport, as is the case in low-dimensional systems, the use of the standard Green–Kubo formula is problematic and the open system formula should be used.

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The Green–Kubo formula [1, 2] is a cornerstone of the study of transport phenomena. For a system governed by Hamiltonian dynamics, the currents that flow in response to small applied fields can be related to the equilibrium correlation functions of the currents. For the case of heat transport the Green–Kubo formula (in the classical limit, which this paper is restricted to) gives

$$\kappa = \lim_{\tau \to \infty} \lim_{L \to \infty} \frac{1}{k_{\mathrm{B}} T^2 L^d} \int_0^{\tau} \mathrm{d}t \, \langle J(t) J(0) \rangle, \tag{1}$$

where κ is the thermal conductivity of a d-dimensional system of linear dimension L at temperature T. The autocorrelation function on the right-hand side is evaluated at equilibrium, without a temperature gradient. The total heat current in the system is $J(t) = \int j(\mathbf{x}, t) \, \mathrm{d}\mathbf{x}$, where $j(\mathbf{x}, t)$ as the heat flux density. The order of the limits in equation (1) is important. With the correct order of limits, one can calculate the correlation functions with arbitrary boundary conditions and apply equation (1) to obtain the response of an open system with reservoirs at the ends. There have been a number of derivations of equation (1) by various authors [1]–[3].

There are several situations where the Green–Kubo formula in equation (1) is not applicable. For example, for the small structures that are studied in mesoscopic physics, the thermodynamic limit is meaningless, and one is interested in the conductance of a specific finite system. Secondly, in many low-dimensional systems, heat transport is anomalous and the thermal conductivity diverges [4]. In such cases it is impossible to take the limits as in equation (1); one is there interested in the thermal conductance as a function of L instead of an L-independent thermal conductivity. The usual procedure that has been followed in the heat conduction literature is to put a cut-off at $t_{\mathrm{c}} \sim L$, in the upper limit in the Green–Kubo integral [4]. There is no rigorous justification for this assumption. A related case is that of integrable systems, where the infinite time limit of the correlation function in equation (1) is non-zero. Another way of using the Green–Kubo formula for finite systems is to include the infinite reservoirs also while applying the formula and this was done, for example, by Allen and Ford [5] for heat transport and by Fisher and Lee [6] for electron transport. Both of these cases are for non-interacting systems and the final expression for conductance is what one also obtains from the nonequilibrium Green's function approach, a formalism of transport commonly used in the mesoscopic literature. More recently, it has been shown that Green–Kubo like expressions for finite open systems can be derived rigorously by using the steady state fluctuation theorem (SSFT) [7]–[10].

In this letter, we derive a Green–Kubo like formula for open systems, without invoking the SSFT. Our proof applies to all classical systems, of arbitrary size and dimensionality, with a variety of commonly used implementations of heat baths. The proof consists in first solving the equation of motion for the phase space probability distribution to find the $\mathcal{O}(\Delta T)$ correction to the equilibrium distribution function. The average current at this order can then be expressed in terms of the equilibrium correlation $\langle J(t) J_{\mathrm{fp}}(0) \rangle$, where J_{fp} is a specified current operator. Secondly we use the energy continuity equations to relate two different current–current correlation functions, namely $\langle J(0) J(t) \rangle$ and $\langle J(0) J_{\mathrm{b}}(t) \rangle$ where J_{b} is an instantaneous current operator involving heat flux from the baths. Finally one relates $\langle J(0) J_{\mathrm{b}}(t) \rangle$ to $\langle J(0) J_{\mathrm{fp}}(t) \rangle$ and then, using time-reversal invariance, to $\langle J(t) J_{\mathrm{fp}}(0) \rangle$. For baths with stochastic dynamics, time-reversal invariance follows from the detailed balance principle, which is an essential requirement of our proof.

We first give a proof of our linear response result for a 1D lattice model with white noise Langevin baths. We consider the following general Hamiltonian:

$$H = \sum_{l=1}^{N} \left[\frac{m_l v_l^2}{2} + V(x_l) \right] + \sum_{l=1}^{N-1} U(x_l - x_{l+1}),$$ (2)

where $\mathbf{x} = \{x_l\}$, $\mathbf{v} = \{v_l\}$ with $l = 1, 2, \ldots, N$ denotes displacements of the particles about their equilibrium positions and their velocities, and $\{m_l\}$ denotes their masses. The particles at the ends are connected to two white noise heat baths of temperatures T_{L} and T_{R} respectively. The equations of motion of the system are given by

$$m_l \dot{v}_l = f_l - \delta_{l,1}[\gamma^{\mathrm{L}} v_1 - \eta^{\mathrm{L}}] - \delta_{l,N}[\gamma^{\mathrm{R}} v_N - \eta^{\mathrm{R}}],$$ (3)

where $f_l = -\partial H/\partial x_l$, and $\eta^{\mathrm{L,R}}(t)$ are Gaussian noise terms with zero mean and satisfying the fluctuation-dissipation relations: $\langle \eta^{\mathrm{L,R}}(t) \eta^{\mathrm{L,R}}(t') \rangle = 2\gamma^{\mathrm{L,R}} k_{\mathrm{B}} T_{\mathrm{L,R}} \delta(t - t')$.

In the first part of the proof we obtain an expression for the nonequilibrium steady state average $\langle J \rangle_{\Delta T}$, at linear order in ΔT, and then we will relate this to the equilibrium correlation function $\langle J(t) J(0) \rangle$.[3] Corresponding to the stochastic Langevin equations in equation (3), one has a Fokker–Planck (FP) equation for the phase space distribution $P(\mathbf{x}, \mathbf{v}, t)$. Setting $T_{\mathrm{L}} = T + \Delta T/2$ and $T_{\mathrm{R}} = T - \Delta T/2$ we write the FP equation in the following form:

$$\frac{\partial P(\mathbf{x}, \mathbf{v}, t)}{\partial t} = \hat{L} P(\mathbf{x}, \mathbf{v}, t) + \hat{L}^{\Delta T} P(\mathbf{x}, \mathbf{v}, t),$$ (4)

where

$$\hat{L}(\mathbf{x}, \mathbf{v}) = \hat{L}^H + \sum_{l=1,N} \frac{\gamma^l}{m_l} \frac{\partial}{\partial v_l} \left(v_l + \frac{k_{\mathrm{B}} T}{m_l} \frac{\partial}{\partial v_l} \right),$$
$$\hat{L}^{\Delta T}(\mathbf{v}) = \frac{k_{\mathrm{B}} \Delta T}{2} \left(\frac{\gamma^{\mathrm{L}}}{m_1^2} \frac{\partial^2}{\partial v_1^2} - \frac{\gamma^{\mathrm{R}}}{m_N^2} \frac{\partial^2}{\partial v_N^2} \right),$$ (5)

where $\hat{L}^H = -\sum_l [v_l \partial/\partial x_l + (f_l/m_l) \partial/\partial v_l]$ is the Hamiltonian Liouville operator and $\gamma^1 = \gamma^{\mathrm{L}}, \gamma^N = \gamma^{\mathrm{R}}$. For $\Delta T = 0$ the steady state solution of the FP equation is known and is just the usual equilibrium Boltzmann distribution $P_0 = \mathrm{e}^{-\beta H}/Z$, where $Z = \int \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{v} \, \mathrm{e}^{-\beta H}$ is the canonical partition function $[\beta = (k_{\mathrm{B}} T)^{-1}]$. It is easily verified that $\hat{L} P_0 = 0$. For $\Delta T \neq 0$, we solve equation (4) using perturbation theory, starting from the equilibrium solution at time $t = -\infty$. Writing $P(\mathbf{x}, \mathbf{v}, t) = P_0 + p(\mathbf{x}, \mathbf{v}, t)$, we obtain the following solution at $\mathcal{O}(\Delta T)$:

$$p(\mathbf{x}, \mathbf{v}, t) = \int_{-\infty}^{t} \mathrm{d}t' \, \mathrm{e}^{\hat{L}(t-t')} \hat{L}^{\Delta T} P_0(\mathbf{x}, \mathbf{v}) = \Delta\beta \int_{-\infty}^{t} \mathrm{d}t' \, \mathrm{e}^{\hat{L}(t-t')} J_{\mathrm{fp}}(\mathbf{v}) P_0(\mathbf{x}, \mathbf{v}),$$

$$\text{with } J_{\mathrm{fp}}(\mathbf{v}) = (\Delta\beta P_0)^{-1} \hat{L}^{\Delta T} P_0 = -\frac{\gamma^{\mathrm{L}}}{2} \left[v_1^2 - \frac{k_{\mathrm{B}} T}{m_1} \right] + \frac{\gamma^{\mathrm{R}}}{2} \left[v_N^2 - \frac{k_{\mathrm{B}} T}{m_N} \right]. \quad (6)$$

[3] The $\langle \cdots \rangle$ denotes a thermal equilibrium average. Time-dependent equilibrium correlation functions require an averaging over initial conditions as well as one over paths. In the Fokker–Planck representation this can be obtained using the time-evolution operator, while in the Langevin representation, thermal noise occurs explicitly and has to be averaged over.

To define the current operator, one first defines the local energy density at the lth site: $\epsilon_l = m_l v_l^2/2 + V(x_l) + \frac{1}{2}[U(x_{l-1} - x_l) + U(x_l - x_{l+1})]$. Taking a time derivative gives the energy continuity equation

$$d\epsilon_l/dt + j_{l+1,l} - j_{l,l-1} = j_{1,\mathrm{L}}\delta_{l,1} + j_{N,\mathrm{R}}\delta_{l,N}, \qquad \text{where } j_{l+1,l} = \tfrac{1}{2}(v_l + v_{l+1})f_{l+1,l} \tag{7}$$

gives the current from the lth to the $l + 1$th site ($f_{l+1,l}$ is the force on $l + 1$th particle due to the lth particle). We define the total current flowing through the system as $J = \sum_{l=1}^{N-1} j_{l+1,l}$. The expectation value of the total current is then given by

$$
\begin{aligned}
\langle J \rangle_{\Delta T} &= \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\, J p(\mathbf{x}, \mathbf{v}) \\
&= \Delta\beta \int_0^\infty \mathrm{d}t \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\, J e^{\hat{L}t} J_{\mathrm{fp}} P_0 \\
&= \Delta\beta \int_0^\infty \mathrm{d}t \langle J(t) J_{\mathrm{fp}}(0)\rangle.
\end{aligned}
\tag{8}
$$

There are two parts of the proof remaining. Let us define the current variable J_{b} as the mean of the instantaneous heat currents flowing into the system from the left reservoir and flowing out of the system to the right reservoir. Thus we have

$$J_{\mathrm{b}}(t) = \tfrac{1}{2}(j_{1,\mathrm{L}} - j_{N,\mathrm{R}}), \tag{9}$$

where

$$j_{1,\mathrm{L}}(t) = -\gamma^{\mathrm{L}} v_1^2(t) + \eta^{\mathrm{L}}(t) v_1(t), \qquad j_{N,\mathrm{R}}(t) = -\gamma^{\mathrm{R}} v_N^2(t) + \eta^{\mathrm{R}}(t) v_N(t). \tag{10}$$

The two remaining steps then consist of proving the relations

$$
\begin{aligned}
\langle J(0) J_{\mathrm{b}}(t)\rangle &= \langle J(0) J_{\mathrm{fp}}(t)\rangle \\
&= -\langle J(t) J_{\mathrm{fp}}(0)\rangle,
\end{aligned}
\tag{11}
$$

and

$$\int_0^\infty \mathrm{d}t \langle J(t) J(0)\rangle = (N - 1) \int_0^\infty \mathrm{d}t \langle J(0) J_{\mathrm{b}}(t)\rangle. \tag{12}$$

The first line in equation (11) follows from $\langle J(0)\rangle = 0$ and the result

$$\langle J(0) \eta^{\mathrm{L}}(t) v_1(t)\rangle = \langle J(0) \eta^{\mathrm{R}}(t) v_N(t)\rangle = 0, \tag{13}$$

which can be proved by making use of Novikov's theorem [11][4]. The second line in equation (11) is a statement of time-reversal symmetry. To prove this we write $\langle J_{\mathrm{fp}}(t) J(0)\rangle = \int \mathrm{d}q \int \mathrm{d}q' J_{\mathrm{fp}}(q) J(q') P_0(q') W(q, t | q', 0)$ where $W(q, t | q', 0)$ denotes the transition probability from $q' = (\mathbf{x}', \mathbf{v}')$ to $q = (\mathbf{x}, \mathbf{v})$ in time t. Then, using the detailed balance principle $W(\mathbf{x}, \mathbf{v}, t | \mathbf{x}', \mathbf{v}', 0) P_0(\mathbf{x}', \mathbf{v}') = W(\mathbf{x}', -\mathbf{v}', t | \mathbf{x}, -\mathbf{v}, 0) P_0(\mathbf{x}, -\mathbf{v})$

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[4] Novikov's theorem: let $\{\eta_i\}$ be a set of arbitrary Gaussian noise variables with $\langle \eta_i(t) \eta_j(t')\rangle = K_{ij}(t, t')$ and let $H[\eta]$ be a functional of the noise variables. Then

$$\langle \eta_i(t) H[\eta]\rangle = \sum_j \int \langle \eta_i(t) \eta_j(t')\rangle \left\langle \frac{\delta H[\eta]}{\delta \eta_j(t')}\right\rangle \mathrm{d}t',$$

where $\delta H[\eta]/\delta \eta_j(t')$ represents a functional derivative of $H[\eta]$ with respect to η.

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(see [12]–[14]) and the fact that J is odd in the velocities while $J_{\rm fp}$ is even, one gets $\langle J_{\rm fp}(t)J(0)\rangle = -\langle J_{\rm fp}(0)J(t)\rangle$. A more direct but equivalent proof is given in a footnote[5].

We next prove the relation given by equation (12). Let us define $D_l(t) = \sum_{k=1}^{l} \epsilon_k - \sum_{k=l+1}^{N} \epsilon_k$ for $l = 1, 2, \ldots, N-1$. Then from the continuity equation (7) one can show that

$$\mathrm{d}D_l/\mathrm{d}t = -2j_{l+1,l}(t) + 2J_{\rm b}(t). \tag{14}$$

We multiply this equation by $J(0)$, take a steady state average, and integrate over time from $t = 0$ to ∞. Since $D_l J$ has an odd power of velocity we therefore get $\langle D_l(0)J(0)\rangle = 0$. Also $\langle D_l(\infty)J(0)\rangle = \langle D_l(\infty)\rangle\langle J(0)\rangle = 0$ and using these we immediately get $\int_0^\infty \mathrm{d}t\langle j_{l+1,l}(t)J(0)\rangle = \int_0^\infty \mathrm{d}t\langle J_{\rm b}(t)J(0)\rangle$. Summing over all bonds thus proves equation (12). With a temperature difference ΔT between the reservoirs, the steady state current between the reservoirs and the system $\langle I\rangle_{\Delta T}$ is equal to $\langle\overline{j}\rangle$ where $\overline{j} = J/(N-1)$. Using equations (8), (11), (12), the conductance is given by

$$G = \lim_{\Delta T\to 0}\frac{\langle\overline{j}\rangle_{\Delta T}}{\Delta T} = \frac{1}{k_{\rm B}T^2}\int_0^\infty \mathrm{d}t\langle\overline{j}(t)\overline{j}(0)\rangle, \tag{15}$$

which is the central result of this letter.

The above proof can be extended to the case where the noise from the baths is exponentially correlated in time [15]. Here we will outline the proof for two other models: a deterministic bath model coupled to a lattice Hamiltonian and another model where Maxwell baths are coupled to a fluid system.

Nose–Hoover baths. In this case the equations of motion are given by: $m_l\dot{v}_l = f_l - \delta_{l,1}\zeta_{\rm L}v_1 - \delta_{l,N}\zeta_{\rm R}v_N$ where $\zeta_{\rm L,R}$ are themselves dynamically evolving as given by the equations

$$\dot{\zeta_{\rm L}} = (\beta_{\rm L}m_1 v_1^2 - 1)/\theta_{\rm L} \qquad \dot{\zeta_{\rm R}} = (\beta_{\rm R}m_N v_N^2 - 1)/\theta_{\rm R}.$$

For small ΔT, we then write an equation of motion for the extended distribution function $P(\mathbf{x},\mathbf{v},\zeta_{\rm L},\zeta_{\rm R},t)$ and find that this has the same form as equation (4) but now with

$$\hat{L}^{\Delta T} = \frac{\Delta T}{2k_{\rm B}T^2}\left(\frac{m_1 v_1^2}{\theta_{\rm L}}\frac{\partial}{\partial\zeta_{\rm L}} - \frac{m_N v_N^2}{\theta_{\rm R}}\frac{\partial}{\partial\zeta_{\rm R}}\right). \tag{16}$$

If $T_{\rm L} = T_{\rm R} = T$, one can verify that the equilibrium phase space density is given by $\hat{P}_0 = cP_0(\mathbf{x},\mathbf{v})\exp[-\theta_{\rm L}\zeta_{\rm L}^2/2m_1 - \theta_{\rm R}\zeta_{\rm R}^2/2m_N]$, where c is a normalization constant (independent of $T_{\rm L,R}$), and we assume convergence to this distribution. Acting with $\hat{L}^{\Delta T}$ on this, we then obtain

$$J_{\rm fp} = \tfrac{1}{2}(v_1^2\zeta_{\rm L} - v_N^2\zeta_{\rm R}). \tag{17}$$

On the other hand, since $-\zeta_{\rm L}v_1$ is the force from the left reservoir on the first particle, hence $j_{1,\rm L} = -\zeta_{\rm L}v_1^2$ and similarly, $j_{N,\rm R} = -\zeta_{\rm R}v_{\rm R}^2$. Hence from the definition of $J_{\rm b}$ in

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[5] An integration by parts followed by the transformation $\mathbf{v} \to -\mathbf{v}$ yields: $\langle J(t)J_{\rm fp}(0)\rangle = \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\,Je^{\hat{L}t}J_{\rm fp}P_0 = \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\,J_{\rm fp}P_0 e^{\bar{\hat{L}}t}J = -\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\,J_{\rm fp}P_0 e^{\hat{L}^\dagger t}J$ where $\hat{T}\bar{\hat{L}} = \hat{L}^\dagger = \hat{L}^H - \sum_{l=1,N}[v_l - (\beta m_l)^{-1}\partial_{v_l}](\gamma^l/m_l)\partial_{v_l}$ and $\hat{T}$ denotes time reversal. We now note the operator identities $\hat{L}P_0 = P_0\hat{L}^\dagger$ and consequently $e^{\hat{L}t}P_0 = P_0 e^{\hat{L}^\dagger t}$ which can be proved using the form of P_0. Using this in the above equation immediately gives: $\langle J(t)J_{\rm fp}(0)\rangle = -\int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\,J_{\rm fp}e^{\hat{L}t}JP_0 = -\langle J(0)J_{\rm fp}(t)\rangle$.

equation (9), we obtain $J_{\mathrm{fp}} = -J_{\mathrm{b}}$. The rest of the proof is similar to that for the previous case, except that there is a minus sign in the right-hand side of the first line of equation (11). This minus sign is not reversed in the second line of equation (11) since under time reversal $(x, v, \zeta) \to (x, -v, -\zeta)$ and therefore both J and J_{fp} change their signs (see arguments given after equation (13)). Hence we finally get the same linear response result, that of equation (15).

The generalization to arbitrary dimensions is straightforward and we outline the white noise case. We consider a d-dimensional hypercubic lattice with points represented by $\mathbf{l} = (l_1, l_2, \ldots, l_d)$ where $l_\alpha = 1, 2, \ldots, N$ with $\alpha = 1, 2, \ldots, d$. Let $\mathbf{x_l}$ and $\mathbf{v_l}$ be the d-dimensional displacement and velocity vectors, respectively, of the particle at $\mathbf{l}$. Heat conduction is assumed to take place in the $\alpha = \nu$ direction because of heat baths at temperature T_{L} and T_{R} that are attached to all lattice points on the two hypersurfaces $l_\nu = 1$ and $l_\nu = N$. The corresponding Langevin equations of motion are

$$m_{\mathbf{l}} \dot{\mathbf{v}}_{\mathbf{l}} = \mathbf{f_l} + \delta_{l_\nu,1}[\boldsymbol{\eta}_{\mathbf{l'}}^{\mathrm{L}} - \gamma_{\mathbf{l'}}^{\mathrm{L}} \mathbf{v_l}] + \delta_{l_\nu,\mathrm{L}}[\boldsymbol{\eta}_{\mathbf{l'}}^{\mathrm{R}} - \gamma_{\mathbf{l'}}^{\mathrm{L}} \mathbf{v_{l'}}], \tag{18}$$

where $\mathbf{l} = (l_\nu, \mathbf{l'})$, so $\mathbf{l'}$ denotes points on a constant l_ν hypersurface. The noise terms at different lattice points and in different directions are assumed to be uncorrelated, and satisfy the usual fluctuation-dissipation relations.

Defining the layer energy $\epsilon_{l_\nu} = \sum_{\mathbf{l'}} \epsilon_{\mathbf{l}}$ and the interlayer current $j_{l_\nu+1,l_\nu}^\nu$ we find, following the same steps as in the 1D case, the analogue of equation (12) with J replaced by $J^\nu = \sum_{l_\nu=1}^{N-1} j_{l_\nu+1,l_\nu}^\nu$ and J_{b} replaced by

$$J_{\mathrm{b}}^\nu = (j_{1\mathrm{L}}^\nu - j_{N\mathrm{R}}^\nu)/2 = \tfrac{1}{2} \sum_{\mathbf{l'}} \left\{ -\left[\gamma_{\mathbf{l'}}^{\mathrm{L}} \mathbf{v}_{(1,\mathbf{l})}^2 - \boldsymbol{\eta}_{\mathbf{l'}}^{\mathrm{L}} \cdot \mathbf{v}_{(1,\mathbf{l'})}\right] + \left[\gamma_{\mathbf{l'}}^{\mathrm{R}} \mathbf{v}_{(N,\mathbf{l'})}^2 - \boldsymbol{\eta}_{\mathbf{l'}}^{\mathrm{R}} \cdot \mathbf{v}_{(N,\mathbf{l'})}\right] \right\}. \tag{19}$$

Writing the FP equation and acting with $\hat{L}^{\Delta T}$ on the equilibrium distribution gives

$$J_{\mathrm{fp}}^\nu = \sum_{\mathbf{l'}} \frac{-\gamma_{\mathbf{l'}}^{\mathrm{L}}}{2} \left[\mathbf{v}_{(1,\mathbf{l})}^2 - \frac{\mathrm{d}k_{\mathrm{B}} T}{m_{(1,\mathbf{l'})}}\right] + \frac{\gamma_{\mathbf{l'}}^{\mathrm{R}}}{2} \left[\mathbf{v}_{(N,\mathbf{l'})}^2 - \frac{\mathrm{d}k_{\mathrm{B}} T}{m_{(N,\mathbf{l'})}}\right].$$

From the forms of J_{b}^ν and J_{fp}^ν, it is clear that we can repeat the arguments for the 1D case which led to equations (8), (11). Hence we get equation (15) with $\bar{j}$ replaced by $\bar{j}^\nu = J^\nu/(N-1)$.

Fluid systems coupled to Maxwell baths. We first consider a 1D system of particles in a box of length L. The end particles (1 and N) interact with baths at temperatures T_{L} and T_{R} respectively. Whenever the first particle hits the left wall it is reflected back with a random velocity chosen from the distribution: $\Pi(v) = m_1 \beta_{\mathrm{L}} \theta(v) v \exp[-\beta_{\mathrm{L}} m_1 v^2/2]$, with a similar rule at the right end. Otherwise the dynamics is Hamiltonian.

We find the FP current by noting that $J_{\mathrm{fp}} = (\Delta\beta)^{-1}[\partial_t P/P]_{P=P_0}$. There are two parts to the evolution of the phase space density: the Hamiltonian dynamics inside the system, and the effect of the heat baths. After a small time interval ϵ, the phase space

density $P(\mathbf{x}; \mathbf{v}; t + \epsilon)$ is

$$= \beta_{\mathrm{L}} m_1 \mathrm{e}^{-(1/2)\beta_{\mathrm{L}} m_1 v_1^2} \int_0^\infty P(0, \mathbf{x}' - \mathbf{v}'\epsilon; -v_0, \mathbf{v}' - \mathbf{a}'\epsilon; t) v_0 \, \mathrm{d}v_0$$

$$\text{for } x_1 < v_1 \epsilon$$

$$= \beta_{\mathrm{R}} m_N \mathrm{e}^{-(1/2)\beta_{\mathrm{R}} m_N v_N^2} \int_0^\infty P(\mathbf{x}' - \mathbf{v}'\epsilon, L; \mathbf{v}' - \mathbf{a}'\epsilon, v_0; t) v_0 \, \mathrm{d}v_0 \qquad (20)$$

$$\text{for } x_N > L + v_N \epsilon$$

$$= P(\mathbf{x} - \mathbf{v}\epsilon, \mathbf{v} - \mathbf{a}\epsilon, t) \qquad \text{otherwise}$$

where the primed variables in the first and second lines leave out particles 1 and N respectively. (Note that since $0 < x_1$ and $x_N < L$, the conditions in the second and third lines imply $v_1 > 0$ and $v_N < 0$.)

If $T_{\mathrm{L}} = T_{\mathrm{R}} = T$, and $P(\mathbf{x}, \mathbf{v}, t) = P_0$, the equilibrium phase space density for the temperature T, then the phase space density at time $t + \epsilon$ is the same. Now if $T_{\mathrm{L,R}} = T \pm \Delta T/2$, with $P(\mathbf{x}, \mathbf{v}, t)$ still equal to P_0, then

$$P(\mathbf{x}; \mathbf{v}; t + \epsilon) = P_0 + \frac{\Delta T}{2T} \left[\left(\frac{1}{2} \beta m_1 v_1^2 - 1 \right) \theta(v_1 \epsilon - x_1) \right.$$

$$\left. - \left(\tfrac{1}{2} \beta m_N v_N^2 - 1 \right) \theta(x_N - L - v_N \epsilon) \right] P_0.$$

Dividing by ϵ throughout and taking $\epsilon \to 0$, we see that

$$J_{\mathrm{fp}} = -\tfrac{1}{2} (\tfrac{1}{2} m_1 v_1^2 - k_{\mathrm{B}} T) v_1 \delta(x_1) \theta(v_1) - \tfrac{1}{2} (\tfrac{1}{2} m_N v_N^2 - k_{\mathrm{B}} T) v_N \delta(x_N - L) \theta(-v_N). \qquad (21)$$

We have to use continuum energy density $\epsilon(x, t)$ and current $j(x, t)$, and the total heat current is now $J = \int j(x) \, \mathrm{d}x$ instead of $\sum j_{i+1,i}$. The continuity equation is still valid, and defining $D(x, t) = \int_0^x \mathrm{d}x' \epsilon(x', t) - \int_x^L \epsilon(x', t)$ and $A(t) = \int_0^L \mathrm{d}x \, D(x)$, we get the analogue of equation (12):

$$\int_0^\infty \langle J(t) J(0) \rangle \mathrm{d}t = L \int_0^\infty \langle J_{\mathrm{b}}(t) J(0) \rangle \mathrm{d}t. \qquad (22)$$

Here $J_{\mathrm{b}} = \frac{1}{2}[j_{1,\mathrm{L}} - j_{N,\mathrm{R}}]$ as before, and

$$j_{1,\mathrm{L}} = \tfrac{1}{2} m_1 v_1 (v_{1,\mathrm{L}}^2 - v_1^2) \delta(x_1) \theta(-v_1) \qquad j_{N,\mathrm{R}} = \tfrac{1}{2} m_N v_N (v_{N,\mathrm{L}}^2 - v_{\mathrm{L}}^2) \delta(x_N - L) \theta(v_N).$$

The δ-functions enforce the condition that the particle is colliding with the bath, and $v_{1,\mathrm{L}}$ and $v_{N,\mathrm{R}}$ are the random velocities with which they emerge from the collision. Invoking detailed balance, using the explicit forms of J_{fp} and J_{b}, and the fact that $J(0)$ is uncorrelated with $v_{1,\mathrm{L}}, v_{N,\mathrm{R}}$ we can show that $\langle J(0) J_{\mathrm{b}}(t) \rangle = -\langle J(t) J_{\mathrm{fp}}(0) \rangle$. With equations (22) and (8), we obtain equation (15) with $(N - 1)$ replaced with L. The generalization to a d-dimensional system is straightforward. First, any particle can interact with the baths at the ends if it reaches $x = 0$ or L. Including the effect of the components of the velocity transverse to the heat flow direction, the derivation of equation (21) gets modified and gives

$$J_{\mathrm{fp}} = \sum_l -\tfrac{1}{2} (\tfrac{1}{2} m_l \mathbf{v}_l^2 - \tfrac{1}{2}(d + 1) k_{\mathrm{B}} T) v_l^\nu \delta(x_l^\nu) \theta(v_l^\nu)$$

$$- \tfrac{1}{2} (\tfrac{1}{2} m_l \mathbf{v}_l^2 - \tfrac{1}{2}(d + 1) k_{\mathrm{B}} T) v_l^\nu \delta(x_l^\nu - L) \theta(-v_l^\nu).$$

The expression for J_b changes similarly, so that the final result of the previous paragraph is still valid.

Conclusions. In this letter we have derived an exact expression for the linear response conductance in a system connected to heat baths. Our results are valid in arbitrary dimensions and have been derived for a solid where particles execute small displacements about fixed lattice positions as well as for a fluid system where the motion of particles is unrestricted, and various heat bath models have been considered.

The important differences from the usual Green–Kubo formula are worth noting. In the present formula, one does not need to first take the limit of infinite system size; the result is valid for finite systems. The fact that a sensible answer is obtained even for a finite system (unlike the case for the usual Green–Kubo formula) is because here we are dealing with an open system. Secondly the correlation function here has to be evaluated *not* with Hamiltonian dynamics, but for an open system evolving with heat bath dynamics. Finally we note that unlike the usual derivation of the Green–Kubo formula where the assumption of local thermal equilibrium is crucial, the present derivation requires no such assumption. The results are thus valid even for integrable Hamiltonian models, the only requirement being that they should attain thermal equilibrium when coupled to one or more heat reservoirs all at the same temperature.

Our derivation here is based on using the microscopic equations of motion and also the equation for the phase space distribution. The broad class of systems and heat baths for which we have obtained our results strongly suggests that they are valid whenever detailed balance is satisfied.

References

[1] Green M S, 1954 *J. Chem. Phys.* **22** 398
[2] Kubo R, Yokota M and Nakajima S, 1957 *J. Phys. Soc. Japan* **12** 1203
[3] Mori H, 1958 *Phys. Rev.* **112** 1829
    Green M S, 1960 *Phys. Rev.* **119** 829
    Kadanoff L P and Martin P C, 1963 *Ann. Phys.* **24** 419
    Luttinger J M, 1964 *Phys. Rev.* **135** A1505
    Visscher W M, 1974 *Phys. Rev. A* **10** 2461
[4] Lepri S, Livi R and Politi A, 2003 *Phys. Rep.* **377** 1
    Dhar A, 2008 *Adv. Phys.* **57** 457
[5] Allen K R and Ford J, 1968 *Phys. Rev.* **176** 1046
[6] Fisher D S and Lee P A, 1981 *Phys. Rev. B* **23** 6851
[7] Gallavotti G, 1996 *Phys. Rev. Lett.* **77** 4334
[8] Lebowitz J L and Spohn H, 1999 *J. Stat. Phys.* **95** 333
[9] Rey-Bellet L and Thomas L E, 2002 *Ann. Inst. Henri Poincare* **3** 483
    Rey-Bellet L, 2005 *14th Int. Cong. on Mathematical Physics* (Hackensack, NJ: World Scientific) pp 447–54
[10] Andrieux D and Gaspard P, 2007 *J. Stat. Mech.* P02006
[11] Novikov E A, 1964 *Zh. Eksp. Teor. Fiz.* **47** 1919
    Novikov E A, 1965 *Sov. Phys. JETP* **20** 1290 (translation)
    Konotop V V and Vazquez L, 1994 *Nonlinear Random Waves* (Singapore: World Scientific) pp 14–15
[12] Haken H, 1975 *Rev. Mod. Phys.* **47** 67
[13] Risken H, 1989 *The Fokker–Planck Equation: Methods of Solutions and Applications* 2nd edn
        (Berlin: Springer)
[14] Kurchan J, 2009 arXiv:0901.1271
[15] Kundu A, Dhar A and Narayan O, 2009 in preparation