

Exact evaluation of the Kubo formula for boundary resistance

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The Kubo formula for the thermal resistance at the boundary between two dissimilar harmonic solids is evaluated exactly. Little's result is then recovered in a more rigorous manner, without resorting to the neglect of phases. The formalism illustrates how dissipation arises in a quantum system and in particular emphasizes the role of coarse graining.

I. INTRODUCTION

It has long been known that the boundary between two dissimilar materials presents a thermal resistance to the flow of phonons.¹ At low temperatures T , the umklapp contribution vanishes exponentially,² so that the boundary resistance, going roughly as T^{-3} , is often an important source of resistance, e.g., for the contact between liquid helium and a solid sample,¹ for semicrystalline materials,³ for composites,⁴ and for samples of finite size.⁵ A theory was first developed by Little,⁶ who considered the scattering and transmission of phonons at the interface.

In this paper we evaluate the boundary resistance from the Kubo formula;⁷ both the formula itself and the evaluation are exact. Such a calculation is interesting from several points of view: (a) the theory of boundary resistance itself, or of thermal conductivity in general, (b) the Kubo formula as an exact, nonperturbative expression, and (c) in the wider perspective of dissipation in a quantum system.

Little's theory is based on the scattering of plane waves (or implicitly, wave packets), which are eigenstates only for a uniform medium. However, for two harmonic solids in contact, certain linear combinations of plane waves form exact eigenstates of the whole system and hence do not undergo scattering. Thus the concept of boundary scattering is basis dependent and best avoided. Secondly, the heat current $J(\mathbf{r})$ at point \mathbf{r} is not diagonal in the phonon-number representation (although for a uniform medium its integral over all space is diagonal). Therefore thermal conduction should involve off-diagonal quantities such as $\langle a_i^\dagger a_j \rangle$, where a_i^\dagger, a_i are the phonon creation and annihilation operators for mode i . [For example, see (26) below.] In Little's theory, only the phonon number $n_i = \langle a_i^\dagger a_i \rangle$ is considered, which corresponds to the neglect of interference between different modes, or equivalently, a random-phase approximation (RPA). While the RPA is physically sensible, it does not expose clearly how dissipation creeps into a Hamiltonian system, which is a generic problem; even the usual proofs of the Boltzmann H theorem⁸ rely on the assumption of randomness before each collision—a clear example of inserting irreversibility by hand.

Quantum-mechanical master equations⁹ or transport equations² are often derived “intuitively” or through the RPA, although recent works have exercised greater care.¹⁰ Nevertheless, for a system described by a quadratic Hamiltonian, the boundary resistance can be evaluated without approximations, so that the origin of dissipation becomes unambiguous. In this sense this paper resembles the exact solution for the relaxation of a central harmonic oscillator coupled to a bath of other oscillators,¹¹ which answers a similar question about the origin of irreversibility.

The Kubo formula expresses the surface conductance K exactly as an integral over the correlation function $\langle J_i(\mathbf{r}, t) J_j(\mathbf{r}', t') \rangle$, for the heat current. However, it is known that the formula does not make sense if evaluated perturbatively to finite order. Nonperturbative (but nevertheless approximate) evaluations for thermal or electrical conductivity include summing an infinite subset of diagrams¹² or proving equivalence to a master equation.¹³ The exact evaluation of the Kubo formula for a nontrivial model system is therefore interesting.

The use of master equations for dissipative systems emphasizes the evolution of the expectation value of the number operator, or quantities such as $q^2(t)$ and $p^2(t)$, where q and p are the coordinates and momenta. A large body of works, starting with Ullersma,¹¹ discuss a central system coupled to a bath of oscillators, either by solving an integrable model explicitly,¹¹ through the use of influence functionals¹⁴ or response functions,¹⁵ or by going to a Markovian description,¹⁶ and have enjoyed renewed attention in the context of macroscopic quantum tunneling.¹⁷ These works emphasize the relaxation of quantities such as $q(t)$, which by linear-response theory is related to correlation functions such as $\langle q(t)q(t') \rangle$. In contrast, the heat current is of the form $J \sim qp$, and its evolution is governed by a slightly more complicated quantity of the form $\langle J(t)J(t') \rangle \sim \langle (q(t)p(t)q(t')p(t')) \rangle$.

The rest of the paper is organized as follows. Section II outlines the derivation of the Kubo formula for the case of response to a temperature step in a medium consisting of two dissimilar solids. Section III presents the exact evaluation of the formula, first of all in a one-dimensional case, and then generalizing to three dimen-

sions. The treatment refers to an infinite medium (so that outgoing waves are not reflected) and standard finite-temperature Green's-function techniques¹⁸ will be used. In Section IV we consider a finite medium, from which the origin of dissipation is most clearly seen.

II. KUBO FORMULA FOR BOUNDARY RESISTANCE

Consider an infinite medium consisting of two solids: solid 1 (2) in the region $z < 0$ ($z > 0$). It will be useful to calculate the average heat flux \mathcal{J} at time t and position z_2 in response to an initial temperature step ΔT imposed at position z_1 . We define the ratio

$$K(z_1, z_2, t) = \mathcal{J}(z_2, t) / \Delta T(z_1). \quad (1)$$

The surface conductance K (the inverse of the surface resistance R) is obtained by setting $z_1 = z_2 = 0$ and $t \rightarrow \infty$. In other words, the temperature step is imposed across the interface, and the heat flux is also measured across the interface when steady state is reached.

The temperature step at $t = 0$ is described by an initial density matrix

$$\rho(0) = N^{-1} \exp \left[- \int d^3r \beta(\mathbf{r}) \mathcal{H}(\mathbf{r}) \right], \quad (2)$$

where \mathcal{H} is the Hamiltonian density and N a normalization constant. The local inverse temperature β represents a small step at z_1 : $\beta(\mathbf{r}) = [T + \Delta T \varepsilon(\mathbf{r}, z_1)]^{-1}$, where $\varepsilon(\mathbf{r}, z_1) = +\frac{1}{2}$ ($-\frac{1}{2}$) for $z > z_1$ ($z < z_1$). The density matrix $\rho(t)$ for later times is obtained by solving $\partial\rho/\partial t = -i[H, \rho(t)]$, where H is the Hamiltonian. Now the average energy current is given by

$$\mathcal{J}(z_2, t) = - \frac{1}{\mathcal{A}} \int d^3r [\text{tr} \mathbf{J}(\mathbf{r}) \rho(t)] \cdot \nabla \varepsilon(\mathbf{r}, z_2), \quad (3)$$

in which $\nabla \varepsilon(\mathbf{r}, z_2) = -\hat{n} \delta(z - z_2)$ and \hat{n} is the normal to the interface, \mathcal{A} is the transverse area of the sample, and the energy-current operator $\mathbf{J}(\mathbf{r})$ satisfies $\partial \mathcal{H}' / \partial t + \nabla \cdot \mathbf{J}' = 0$, where the prime denotes the corresponding Heisenberg operators.

It is then straightforward to show, as in the usual case of response to a temperature gradient, that

$$K(z, z', t) = \frac{2i}{\mathcal{A}T} \int_0^t d\tau \tau \int d^2r_1 d^2r'_1 \times \langle J_3(\mathbf{r}', \tau) J_3(\mathbf{r}, 0) \rangle_{\text{odd}}, \quad (4)$$

where we have changed the notation $z_1, z_2 \rightarrow z, z'$, $\mathbf{r} = (\mathbf{r}_\perp, z)$, etc., and only the part of the correlation function odd in τ is to be taken. For values of t so large that steady state prevails, energy conservation implies $\partial \mathcal{J}(z', t) / \partial z' = 0$, so (4) can be evaluated at any z' . Moreover, because of symmetry under $z \leftrightarrow z'$, z is likewise arbitrary. This freedom will be exploited to simplify by averaging over z and z' . The only condition for the Kubo formula (4) is that terms of more than first order in ΔT have been discarded; this restriction is intrinsic to the definition of thermal conductivity.

III. EVALUATION OF KUBO FORMULA

A. One-dimensional system

We first consider a one-dimensional system (a "string") with coordinate $\phi(z)$ and a position-dependent density $\rho(z)$ and modulus $M(z)$, described by the Lagrangian density

$$\mathcal{L} = \frac{1}{2} \rho(z) \left[\frac{\partial \phi}{\partial t} \right]^2 - \frac{1}{2} M(z) \left[\frac{\partial \phi}{\partial z} \right]^2. \quad (5)$$

Eventually we want $\rho(z) = \rho_1$ (ρ_2), $M(z) = M_1$ (M_2) for $z < 0$ ($z > 0$). It is straightforward to evaluate the Hamiltonian density and the energy current

$$\mathcal{H} = \frac{\pi(z)^2}{2\rho(z)} + \frac{1}{2} M(z) \left[\frac{\partial \phi}{\partial z} \right]^2, \quad (6)$$

$$\mathbf{J} = - \frac{M(z)}{\rho(z)} \pi(z) \frac{\partial \phi}{\partial z}, \quad (7)$$

where $\pi = \rho \dot{\phi}$ is the conjugate momentum and normal ordering is everywhere understood. When (7) is inserted into (4), the correlation involves four operators at two different times, schematically

$$\begin{aligned} \langle J(z', \tau) J(z, 0) \rangle &\sim \langle \pi(z', \tau) \phi(z', \tau) \pi(z, 0) \phi(z, 0) \rangle \\ &\sim \langle \pi(z', \tau) \pi(z, 0) \rangle \langle \phi(z', \tau) \phi(z, 0) \rangle \\ &\quad + \langle \pi(z', \tau) \phi(z, 0) \rangle \langle \phi(z', \tau) \pi(z, 0) \rangle, \end{aligned}$$

by Wick's theorem. The other contraction does not contribute, since each J is normal ordered and there is no connected four-point function since the Hamiltonian is quadratic. All results can thus be expressed in terms of the correlation function $F(z, z', t) = \langle \phi(z, t) \phi(z', 0) \rangle$ and some algebra leads to

$$K = \frac{-2iM(z)M(z')}{T} \int_0^\infty dt t \left[\frac{\partial^2 F}{\partial t^2} \frac{\partial^2 F}{\partial z \partial z'} + \frac{\partial^2 F}{\partial t \partial z'} \frac{\partial^2 F}{\partial t \partial z} \right]_{\text{odd}}. \quad (8)$$

Since we wish to calculate \mathcal{J} in (3) when steady state is achieved, the time integral has been extended to infinity and for one dimension, \mathcal{A} has been set to 1.

The freedom to choose z and z' allows us to average over these positions, e.g., by $(1/L) \int_0^L dz$. For convenience we shall restrict $z > 0$ and $z' < 0$, so $M(z) = M_2$, $M(z') = M_1$ are constants in the average. Since z, z' , and t are now all under the integral sign, we may freely integrate by parts; a little arithmetic then shows that the second term in (8) makes the same contribution as the first.

Secondly we introduce the Fourier transform

$$F(z, z', t) = \int \frac{d\omega}{2\pi} \tilde{F}(z, z', \omega) e^{-i\omega t}, \quad (9)$$

which is related to the retarded Green's function

$$G(z, z', t) = -i\Theta(t) \langle [\phi(z, t), \phi(z', 0)] \rangle \quad (10)$$

by¹⁸

$$\bar{F}(z, z', \omega) = \frac{-2}{1 - e^{-\beta\omega}} \text{Im} \bar{G}(z, z', \omega). \quad (11)$$

Inserting these into (8) then gives

$$K = -\frac{8M_1M_2}{T^2} \int_0^\infty \frac{d\omega}{2\pi} \frac{\omega^2 e^{-\beta\omega}}{(1 - e^{-\beta\omega})^2} H(\omega), \quad (12)$$

where

$$H(\omega) = \text{Im} \frac{\partial}{\partial z} \bar{G}(z, z', \omega) \text{Im} \frac{\partial}{\partial z'} \bar{G}(z, z', \omega), \quad (13)$$

and the right-hand side is understood to be averaged over z, z' . Note that in (13), the two factors of \bar{G} are forced to the same frequency by the infinite time integral in (8).

The Green's function can be evaluated from the defining equation, written in the frequency domain as

$$\left[-\rho(z)\omega^2 - \frac{\partial}{\partial z} M(z) \frac{\partial}{\partial z} \right] \bar{G}(z, z', \omega) = -\delta(z - z'). \quad (14)$$

The function G has the interpretation of being a wave produced by a harmonic point source at z' (< 0) and observed at the point z (> 0). The solution to (14) is just plane waves in each region with a gradient discontinuity at $z = z'$. The wave vectors for the plane waves are $k_i = \omega/v_i$ in the two regions $i = 1, 2$, and $v_i = \sqrt{M_i/\rho_i}$. The retarded nature selects outgoing waves at infinity. The amplitudes of the plane waves are obtained by matching \bar{G} across the three regions ($z < z'$, $z' < z < 0$, $0 < z$) and the result is best expressed in terms of the impedances $Z_i = \rho_i v_i$ and the amplitude reflection coefficient $r = (Z_1 - Z_2)/(Z_1 + Z_2)$. Then it is easily shown that

$$H = -\frac{1}{8} \frac{1 - r^2}{M_1 M_2}. \quad (15)$$

The factor $1 - r^2$ is just the energy transmission coefficient \mathcal{T} . We then obtain

$$K = \frac{1}{T^2} \int_0^\infty \frac{d\omega}{2\pi} \frac{\omega^2 e^{-\beta\omega}}{(1 - e^{-\beta\omega})^2} \mathcal{T}, \quad (16)$$

which gives (in units with $k_B = \hbar = 1$)

$$K = \frac{\pi}{6} \mathcal{T} T, \quad (17)$$

linear in the temperature T and agreeing with Little's theory for such a one-dimensional system. Since boundary resistance is important only for low temperatures, there is no need for a Debye cutoff.

The one-dimensional case is sufficiently simple that there is in fact no need to average over z and z' . In this way we have verified explicitly that (4) is indeed independent of z and z' .

B. Three-dimensional solid

A three-dimensional solid with displacement field $\mathbf{u}(\mathbf{r}, t)$ is described by the Lagrangian density

$$\mathcal{L} = \frac{1}{2} \rho(\mathbf{r}) \frac{\partial \mathbf{u}_i}{\partial t} \frac{\partial \mathbf{u}_i}{\partial t} - \frac{1}{2} c_{ij,kl}(\mathbf{r}) \partial_j \mathbf{u}_i \partial_l \mathbf{u}_k, \quad (18)$$

where the stiffness tensor is

$$c_{ij,kl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (19)$$

and $\lambda = \lambda_1$ (λ_2), $\mu = \mu_1$ (μ_2) for $z < 0$ ($z > 0$). The calculation now involves the correlation $F_{ij}(\mathbf{r}, \mathbf{r}', t) = \langle \mathbf{u}_i(\mathbf{r}, t) \mathbf{u}_j(\mathbf{r}', 0) \rangle$ and the corresponding retarded Green's functions. While the details of the calculation are in general complicated (but rendered manageable by the freedom to average over z and z'), the result is simple and easily made plausible. First let $\mu_1 = \mu_2 = 0$, so that there are only compressional waves. Since the system retains translational invariance in the x and y directions, one of the transverse integrals in (4), say $d^2 r_\perp$, is trivial and cancels the factor \mathcal{A} , while the other, say $d^2 r'_\perp$, can be written in terms of the corresponding transverse wave vector \mathbf{q} . Since \mathbf{q} is a good quantum number, different \mathbf{q} 's contribute to the heat flux independently. It is then not surprising to find, in analogy to (16), that

$$K = \frac{1}{T^2} \int_0^\infty \frac{d\omega}{2\pi} \frac{\omega^2 e^{-\beta\omega}}{(1 - e^{-\beta\omega})^2} \int \frac{d^2 q}{(2\pi)^2} \mathcal{T}(\omega, \mathbf{q}), \quad (20)$$

where the energy transmission coefficient \mathcal{T} is now dependent on frequency and transverse wave number.

Moreover, \mathcal{T} is still given by the same formulas as before, since at fixed ω and \mathbf{q} , wave propagation is a one-dimensional phenomenon along z . However, the wave velocity in each medium is $c_i = \sqrt{\lambda_i/\rho_i}$, but the remaining wave number in the z direction is given by $k_i = (\omega^2/c_i^2 - q^2)^{1/2}$, so the phase velocity in the z direction, namely $v_i = \omega/k_i$, is now no longer a constant. The q integral in (20) is restricted to values such that k_1 and k_2 are both real. Physically imaginary k represents total internal reflection and hence zero energy transmission. Mathematically this restriction may be seen from the freedom to choose z and z' arbitrarily: if they are far from the interface and on opposite sides, waves with imaginary k will not propagate from r and r' and hence the Green's function vanishes.

When the integrals in (20) are evaluated, we find that K agrees with the result given by Little,⁶ in particular $K \propto T^3$:

$$K = \frac{4}{15} \pi^2 \frac{T^3}{c_2^2} \int_0^{\pi/2} d\theta_2 \sin\theta_2 \cos\theta_2 \times \left[\frac{Z_1 \cos\theta_1}{Z_2 \cos\theta_2} \right] / \left[\frac{Z_1}{Z_2} + \frac{\cos\theta_1}{\cos\theta_2} \right]^2, \quad (21)$$

where θ_1 (θ_2) are the angles of incidence (refraction) in the two media, related by Snell's law in the usual way, and in (21) we have assumed $c_1 < c_2$.

When the shear modulus is not zero, a similar calculation shows that $\mathcal{T}(\omega, \mathbf{q})$ in (20) is replaced by

$$\mathcal{T}(\omega, \mathbf{q}) \rightarrow \sum_{\alpha, \beta} \mathcal{T}_{\alpha\beta}(\omega, \mathbf{q}),$$

where $\mathcal{T}_{\alpha\beta}$ is the energy transmission coefficient for po-

larization α striking the interface and transmitted to the other side as polarization β . For the same physical reason, the different transverse momenta contribute independently to K . Again $K \propto T^3$ and the result agrees with Little.⁶ Our expressions [e.g., (20)], written in terms of the conserved quantity q rather than angles θ_1 and θ_2 , are more physically obvious by virtue of the analogy to (16) and moreover exhibit manifest symmetry between the two solids.

IV. FINITE SOLID

The origin of dissipation becomes even clearer if we consider a finite solid and express the calculation in terms of normal modes. It suffices to illustrate the idea by the one-dimensional model defined by (5), whose normal modes satisfy

$$-\omega_n^2 \rho(z) \phi_n(z) = \frac{\partial}{\partial z} \left[M(z) \frac{\partial}{\partial z} \phi_n(z) \right] \quad (22)$$

with normalization

$$\int dz \rho(z) \phi_n(z) \phi_m(z) = \delta_{nm} . \quad (23)$$

Introduce normal coordinates q_n by

$$\phi(z, t) = \sum_n q_n(t) \phi_n(z) \quad (24)$$

and the corresponding momenta $p_n = \partial L / \partial \dot{q}_n$ where $L = \int dz \mathcal{L}$ with \mathcal{L} given in (5). Then the Hamiltonian and the energy current are

$$H = \sum_n \frac{1}{2} (p_n^2 + \omega_n^2 q_n^2) , \quad (25)$$

$$J(z) = \sum_{m,n} p_m q_n Q_{mn}(z) , \quad (26)$$

where normal ordering is implied, and the c -number function Q_{mn} is

$$Q_{mn}(z) = -\phi_m(z) M(z) \frac{\partial}{\partial z} \phi_n(z) , \quad (27)$$

which is continuous across the interface.

When these are put into (4), we find

$$K = \frac{2i}{T} \sum_{m,n,r,s} Q_{mn} Q_{rs} \int_0^t d\tau \tau \langle p_m(\tau) q_n(\tau) p_r(0) q_s(0) \rangle_{\text{odd}} . \quad (28)$$

In (28) we have kept t finite; without the assumption of steady state, z and z' are no longer arbitrary, so Q_{mn} and Q_{rs} must be evaluated at the origin (say $z=0^-$). The correlation in (28) can be broken into

$$\langle p_m(\tau) p_r \rangle \langle q_n(\tau) q_s \rangle + \langle p_m(\tau) q_s \rangle \langle q_n(\tau) p_r \rangle ,$$

where $p_r = p_r(0)$, etc., are the Schrödinger operators. The τ dependence is now explicit, e.g.,

$$q_m(\tau) = q_m \cos(\omega_m \tau) + \frac{1}{\omega_m} p_m \sin(\omega_m \tau) . \quad (29)$$

The ensemble averages over the Schrödinger operators are

$$\begin{aligned} \omega_m^2 \langle q_m q_n \rangle &= \langle p_m p_n \rangle = \omega_m N(\omega_m) \delta_{mn} , \\ \langle q_m p_n \rangle &= -\langle p_m q_n \rangle = \frac{i}{2} \delta_{mn} \end{aligned} \quad (30)$$

and $N(\omega) = [\exp(\beta\omega) - 1]^{-1}$ is the Bose-Einstein occupation number. When these are put into (28), the τ integral leads to

$$\begin{aligned} K &= -\frac{\pi}{2T} \sum_{m,n} \left[Q_{mn}^2 \frac{\omega_m}{\omega_n} - Q_{mn} Q_{nm} \right] [N(\omega_n) - N(\omega_m)] \\ &\quad \times \frac{\partial}{\partial \omega_m} \Delta_t(\omega_m - \omega_n) , \end{aligned} \quad (31)$$

where $\Delta_t(\alpha) = (1/\pi) \sin(\alpha t) / \alpha$ may be thought of as a δ function given a width of $\sim 1/t$.

Now on account of the first two factors in the summation in (31), the $m=n$ term clearly does not contribute, so $|\omega_m - \omega_n| \gtrsim c/L$, where L is the size of the solid and c is a typical phonon speed. On the other hand, $\Delta_t(\omega_m - \omega_n) \rightarrow 0$ if $|\omega_m - \omega_n| > 1/t$. (An exception will be noted below.) Thus $K \rightarrow 0$ if $t \gg L/c$, so that the literal interpretation of (4) with $t \rightarrow \infty$ is incorrect. The physical reason is obvious: phonons are reflected at the ends of the finite solid after a time $\sim L/c$, so that the heat flow caused by the original temperature step quenches itself. (In a more realistic model with three-phonon scattering, phonons should diffuse rather than propagate, and the heat flow quenches on a time scale proportional to L^2 rather than to L .)

Thus we are led to consider (31) with finite t , in particular

$$\frac{L}{c} \gg t \gg \frac{1}{T} . \quad (32)$$

By virtue of these inequalities, the large parentheses in (31) can be averaged over several neighboring modes, and moreover $\omega_m / \omega_n \approx 1$. This is just the process of energy coarse graining¹⁹ known to be necessary for deriving dissipative behavior. For example, a similar step is necessary in the work of Ullersma¹¹ to convert poles in the frequency plane into a cut, thereby endowing the relevant Green's function with an imaginary part. Coarse graining is here justified mathematically by restricting attention to the time domain (32). Secondly, since ω_m and ω_n are restricted to $\sim 1/t$ of each other and $N(\omega)$ varies slowly on this scale,

$$N(\omega_n) - N(\omega_m) \approx (\omega_n - \omega_m) \frac{\partial}{\partial \omega_m} N(\omega_m) .$$

We then obtain

$$K = -\frac{\pi}{2T} \int d\omega \sigma^2 \Gamma(\omega) \frac{\partial n}{\partial \omega}(\omega) , \quad (33)$$

where $\omega_m \rightarrow \omega$, $\omega_n \rightarrow \omega'$, the sums have been converted to integrals using the density of states σ , $\sum_m = \int d\omega \sigma(\omega)$, and

$$\Gamma(\omega) = \overline{Q_{mn}^2} - \overline{Q_{mn} Q_{nm}} , \quad (34)$$

in which the long overbar denotes averaging over several

neighboring modes and the ω' integral has been canceled against Δ_i , which can now be regarded as a δ function. Only when (32) is satisfied can we eliminate off-diagonal terms and hence justify RPA. In particular, one would not expect RPA to hold for the heat current at short times.

In order to evaluate $\Gamma(\omega)$, consider a "string" extending from $-L_1$ to $+L_2$, with $L_1/c_1=L_2/c_2=X$; this choice merely simplifies the arithmetic and is not essential. The m th eigenfunction is

$$\begin{aligned}\phi_m(z) &= A_m \sin[k_{1m}(L_1+z)], \quad z < 0 \\ &= B_m \sin[k_{2m}(z-L_2)], \quad z > 0,\end{aligned}$$

where $k_{im}=\omega_m/c_i$, $i=1,2$. Matching the two solutions gives

$$\begin{aligned}A_m^2 &= B_m^2 = 2(\rho_1 L_1 + \rho_2 L_2)^{-1}, \quad m \text{ odd} \\ Z_1^2 A_m^2 &= Z_2^2 B_m^2 = 2(\rho_1 L_1 Z_1^{-2} + \rho_2 L_2 Z_2^{-2})^{-1}, \quad m \text{ even}\end{aligned}$$

and

$$Q_{mn} = -\frac{M_1}{c_1} \omega_n A_m A_n \sin(m\pi/2) \cos(n\pi/2), \quad (35)$$

which is zero unless m is odd and n is even. These results lead to

$$\Gamma(\omega) = \frac{\omega^2}{4X^2} \mathcal{T}, \quad (36)$$

where $\mathcal{T}=4Z_1 Z_2/(Z_1+Z_2)^2$ is the energy transmission coefficient as before. The density of states in this case is $\sigma=2X/\pi$ and (33) finally gives

$$K = -\frac{1}{T} \int \frac{d\omega}{2\pi} \omega^2 \frac{\partial N}{\partial \omega} \mathcal{T} \quad (37)$$

in agreement with (16).

The present choice of L_1 and L_2 causes the eigenfre-

quencies to be evenly spaced by $\Delta\omega=1/\sigma$, a condition which will not be true in general. In this case $\Delta_i(\omega_m-\omega_n)$ and hence K in (31) becomes periodic in t with period $2\pi\sigma=4X$. This is a trivial example of Poincaré recurrence²⁰ and clearly in the Kubo formula one must send the size of the system to infinity before $t \rightarrow \infty$ in order to avoid such recurrence.

V. DISCUSSION

It is generally believed that dissipation (or irreversibility) requires, first of all, that suitable initial conditions (as opposed to final conditions) are chosen, thus introducing an arrow of time. However, finite systems will recur over a long but finite time.²⁰ If the system is harmonic and the frequency spacing $\Delta\omega$ is uniform, then this time is simply $2\pi/\Delta\omega$; otherwise the recurrence time could be extremely long, but still finite. When the state of the system recurs, i.e., when the initial state is recovered (or nearly recovered), there will be "antidissipation," and to avoid this requires that attention be restricted to a suitable time interval. This in turn permits coarse graining in the frequency domain, which is mathematically the same as setting $\Delta\omega \rightarrow 0$ or considering an infinite system with only outgoing waves. The present work then constitutes an explicit demonstration of this widely held belief in a simple, exactly soluble model.

In closing it should be remarked that the result for boundary resistance is unphysical in the limit of two identical solids, for which one would expect the boundary resistance to vanish. This has already been discussed by Little,⁶ and is attributed to the neglect of three-phonon scattering in the Hamiltonian—which must become the dominant mechanism when the boundary mismatch is sufficiently small, and which defines the mean free path as the scale below which a local temperature is meaningless.

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