Temperature relaxation and the Kapitza boundary resistance paradox

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Abstract

The calculation of the Kapitza boundary resistance between dissimilar harmonic solids has since long (Little [Can. J. Phys. 37, 334 (1959)]) suffered from a paradox: this resistance erroneously tends to a finite value in the limit of identical solids. We resolve this paradox by calculating temperature differences in the final heat-transporting state, rather than with respect to the initial state of local equilibrium. For a one-dimensional model we thus derive an exact, paradox-free formula for the boundary resistance. The analogy to ballistic electron transport is explained.

05.60.+w, 44.30.+v, 67.40.Pm, 72.10.-d
I. INTRODUCTION

The occurrence of a thermal resistance at an interface between two materials, also known as Kapitza resistance, is a well-known phenomenon, in particular in low-temperature physics. In fact, the present work has been prompted in the course of an investigation of non-isothermal stochastic processes in Josephson junction devices. The basic physical mechanism is partial reflection of the phonons transporting the heat current. For the low temperatures (in comparison with the Debye temperature) at which the boundary contributes significantly to the total thermal resistance of a typical sample, phonon wavelengths are much larger than the lattice spacing and a continuum description of the materials should be adequate. In this case the reflection process becomes a standard problem in elasticity theory, and using semi-classical arguments to determine phonon densities and fluxes the Kapitza resistance was calculated along these lines in a classic paper by Little.

For an ideal interface between the two elastic media and an infinitesimal temperature difference between them so as to allow the use of linear response theory, a fully quantum statistical calculation of the transport process was given by Leung and Young. Besides confirming the intuitive expectation that for this idealized system the semi-classical result should be exact, the calculation is of interest in its own right as a non-perturbative evaluation of a Kubo formula. In addition, for a sample of finite size the dissipative behaviour implicit in the term ‘resistance’ was explicitly shown to hold only up to times at which Poincaré recurrence sets in.

In Refs. 3 and 4 the authors noted their result for the Kapitza resistance to be paradoxical in the limit of identical media: it tends to a finite value instead of vanishing. They attributed this artifact to the neglect of three-phonon scattering (which would take over as the dominant origin of resistance in this case), arguing that without such scattering the phonon mean free path is infinite so that it would become problematic to describe the system in terms of local temperatures. This explanation is unsatisfactory for the following reasons. First of all, three-phonon scattering is effective as a cause of heat resistance and thermalization only when Umklapp processes are possible. Thus, one would have to endow the model with a lattice structure as well. However, as mentioned above, this should not be relevant. Secondly, the phonon mean free path is infinite for all values of the energy transmission coefficient $T$, and the authors of Refs. 3 and 4 rightly do not suspect their results in the case of small $T$. Thirdly, the vanishing of the boundary resistance for a homogeneous medium is a matter of principle, and should not depend on the relative magnitude of other resistance contributions.

In this article we show that the aforementioned paradox is resolved in a simple manner by calculating temperature differences in the final, heat-transporting state of the system, and not with respect to the initial state of local equilibrium. For clarity of exposition we limit ourselves here to one space dimension. A report on the technically more involved three-dimensional case is currently in preparation. In section II the corrected formula will be obtained by a semi-classical consideration in the spirit of Ref. 3. In Sec. III this new result will be derived in the Kubo formalism. Apart from solving the Kapitza resistance paradox (for which Leung and Young’s Kubo formula itself needs to be amended) the work of Ref. 4 will be extended by giving the full space and time dependence of the heat current. In the one-dimensional case the relaxation to a stationary non-equilibrium state is thus
shown to be degenerate, namely jump-wise. Also, one will see that the semi-classical result holds without the necessity of coarse-graining, partly because the problem has no length scale apart from $\beta \bar{\hbar}c$ (where $c$ is the sound velocity). The issue discussed in this paper has a striking analogy\[7\] in ballistic electron transport\[8\]. This analogy is the subject of Sec. [V]. Some concluding remarks are made in Sec. [V].

II. SEMI-CLASSICAL ANALYSIS OF TEMPERATURE RELAXATION

Consider two semi-infinite harmonic strings,\[4\] joined at $x = 0$, with sound velocities $c_l (c_r)$ for $x < 0 (x > 0)$. For this system the boundary conductance $K$ was defined in Ref. [4] as
\[K \equiv \frac{J}{\Delta T},\]
where $J$ is the energy current in the stationary state which is reached after the system has started at time $t = 0$ in a state of local equilibrium with temperatures $T_r$ for $x > 0$ and $T_l = T_r + \Delta T$ for $x < 0$. Their result (Eq. (17)) is
\[K = \frac{\pi}{6\bar{\hbar}c},\]
with $T$ given in (A2). The ensuing value for $K$ in the case of identical strings (i.e., $T = 1$) is easily understood using a semi-classical picture (Ref. [3]) in which energy-carrying fields propagate according to the wave equation. In view of the absence of an interface, excess energy at $x < 0$ will then be radiated half to $x = -\infty$, half to positive $x$. One thus arrives at
\[K = \frac{1}{2}cC,\]
where $C$ is the heat capacitance per unit length $C = \pi T/3\bar{\hbar}c$. This indeed gives the finite value $K = \frac{\pi}{6\bar{\hbar}c}$, in contrast with the expected result $K = \infty$. The finite heat current is a consequence of the finite specific heat of the quantum string, combined with the finite speed of propagation (as opposed to diffusive transport).

Now consider the general case of unequal strings, with initial thermal energy density $\varepsilon_l (\varepsilon_r) (\equiv \langle H_l (r) \rangle$, where $\langle H \rangle$ is the expectation value of the Hamiltonian density; see Sec. [II]) for $x < 0 (x > 0)$ at time $t = 0$. At any $t = t_1 > 0$ the situation is as in Fig. [II]. Properly accounting for left- and right-going radiation, the expression for the steady state value of the energy density $\varepsilon_i'$ ($i = l, r$) is obtained by considering the history of an energy packet $\varepsilon_i \delta x_i$ and noticing that $\delta x_r/\delta x_l = c_r/c_l$. The result reads:
\[\varepsilon_l' = \frac{\varepsilon_l + R \varepsilon_l + T \varepsilon_l c_l/c_r}{2}, \quad \varepsilon_r' = \frac{\varepsilon_r + R \varepsilon_r + T \varepsilon_r c_r/c_l}{2},\]
with $R = 1 - T$. Again putting $T_l = T_r + \Delta T$ ($\Delta T \ll T_i$), $\varepsilon_i (T_i) = \pi T_i^{(2)}/6\bar{\hbar}c_i$ —where we have used the specific heat as given above—, one gets
\[\begin{align*}
T_l' &= T_r + (1 - T/2) \Delta T \\
T_l' &= T_r + (T/2) \Delta T
\end{align*}\]
\[\Rightarrow \Delta T' = R \Delta T.\]

With the boundary conductance defined as the ratio of the stationary heat flux and the stationary temperature jump, one now finds
\[K = \frac{J}{\Delta T'} = \frac{J}{\Delta T} \frac{\Delta T}{\Delta T'} = \frac{\pi}{6\bar{\hbar}c} \frac{T}{R},\]
which indeed diverges for $T \to 1$.  

\[3\]
III. TEMPERATURE RELAXATION IN THE KUBO FORMALISM

The result (3) can also be calculated in the Kubo formalism. That calculation (Sec. III B), however, requires a nontrivial correction of the Kubo formula used in Ref. 4. In both Secs. III A and III B we set \( \hbar = 1 \).

A. The Kubo formula

At \( t = 0 \), to within first order in the temperature nonuniformity, the local equilibrium density matrix is

\[
\rho_{\text{loc}} = \rho_0 \left\{ 1 - \beta^{-1} \int_0^\beta d\tau \int dx' \delta \beta(x') \left( \mathcal{H}(x', -i\tau) - \langle \mathcal{H}(x', -i\tau) \rangle_0 \right) \right\},
\]

(4)

where \( \beta^{-1} \) is the equilibrium temperature, \( \rho_0 = \exp(-\beta H) \) is the equilibrium density matrix (\( H \) is the full Hamiltonian), \( \mathcal{H} \) is again the Hamiltonian density and \( \langle \cdot \rangle_0 \) indicates an equilibrium average. Note that (4) is not restricted to the one-dimensional situation. When calculating the energy current \( \langle \mathcal{J}(x, t) \rangle_{\text{loc}} \), the first and third term of \( \rho_{\text{loc}} \) do not contribute, and one obtains

\[
\langle \mathcal{J}(x, t) \rangle_{\text{loc}} = T^{-1} \int_0^\beta d\tau \int dx' \delta T(x') \langle \mathcal{H}(x', -i\tau) \mathcal{J}(x, t) \rangle_0
\]

\[
= \langle \mathcal{J}(x, 0) \rangle_{\text{loc}} + \frac{i}{T} \int dx' \delta T(x') \int_0^t dt' \text{Tr} \left\{ \rho_0 \int_0^\beta d\tau e^{iH\tau} [\mathcal{H}(x'), H] e^{-iH\tau} \mathcal{J}(x, t') \right\}.
\]

(5)

To begin with, \( \langle \mathcal{J}(x, 0) \rangle_{\text{loc}} \) vanishes because of time reversal invariance. In the second term, the trace can be taken as a single correlation function; one would then get \( \langle \mathcal{J}(x, t) \rangle_{\text{loc}} \propto \int_0^t dt' \langle \rho_0^0 \delta T(x') \mathcal{J}(x, t') \rangle_0 \) without an additional \( t' \) in the integrand. However, in order to relate \( \langle \mathcal{J} \rangle_{\text{loc}} \) to \( \langle \mathcal{J} \mathcal{J} \rangle_{\text{odd}} \) we proceed differently and apply the Kubo identity:

\[
\langle \mathcal{J}(x, t) \rangle_{\text{loc}} = \frac{i}{T} \int dx' \delta T(x') \int_0^t dt' \text{Tr} \left\{ [\rho_0, \mathcal{H}(x')] \mathcal{J}(x, t') \right\}
\]

\[
= \frac{i}{T} \int dx' \delta T(x') \int_0^t dt' \left\{ \left[ \mathcal{H}(x') + \int_0^{t'} dt'' e^{-iHt''} \nabla \mathcal{J}(x') e^{iHt''}, \mathcal{J}(x) \right] \right\}_0,
\]

(6)

where the step taken on the second line of Eq. (5) has been repeated. Integration by parts over \( x' \) and combining the \( t' \)- and \( t'' \)-integrals now yields

\[
\langle \mathcal{J}(x, t) \rangle_{\text{loc}} = \frac{i}{T} \int dx' \nabla T(x') \int_0^t dt' (t - t') \langle [\mathcal{J}(x, t'), \mathcal{J}(x', 0)] \rangle_0 +
\]

\[
\frac{it}{T} \int dx' \delta T(x') \langle [\mathcal{H}(x'), \mathcal{J}(x)] \rangle_0
\]

\[
= 2\frac{i}{T} \int dx' \nabla T(x') \int_0^t dt' (t - t') \langle \mathcal{J}(x, t'), \mathcal{J}(x', 0) \rangle_{\text{odd}} +
\]

\[
\frac{it}{T} \int dx' \delta T(x') \langle [\mathcal{H}(x'), \mathcal{J}(x)] \rangle_0.
\]

(7)
This Kubo formula will be crucial in Sec. III B. Apart from the boundary term, it differs from the one used in Ref. 1 in that the integrand presently involves \( t' - t \) instead of \( t' \).

To be sure, this modification does not affect the value of the stationary current. This follows from the explicit form for \( \langle JJ \rangle_{\text{odd}} \) calculated in the Appendix:

\[
\langle J(x, t)J(x', 0) \rangle_{\text{odd}} = \frac{T}{i} \left\{ \frac{1}{48\pi} \delta'''(t - \alpha) - \frac{\pi}{12\beta^2} \delta'(t - \alpha) \right\} + (\alpha \leftrightarrow -\alpha),
\]

where \( x > 0, \ x' < 0, \ \alpha \equiv x/c_r - x'/c_l, \) and where we returned to the one-dimensional case. Because the distributions \( \delta''' \) and \( \delta' \) are odd functions of their arguments, \( \int_0^\infty dt' \langle J(t')J \rangle_{\text{odd}} \) is seen to vanish.

In the boundary term of the Kubo formula (7), the commutator \( [\mathcal{H}, J] \) will be localized at \( x' = x \). As will be shown explicitly in a simple case, this boundary term compensates a second unphysical term arising from the lower limit of the \( t' \)-integration in the first part of Eq. (7). In this first part, \( \langle J(x, t)J(x', 0) \rangle_{\text{odd}} \) vanishes outside the ‘sound cone’. Thus, for \( t' \downarrow 0 \) only the point \( x' = x \) contributes in the \( x' \)-integration. In the calculation of the energy drop in Sec. III B, \( \delta T(x') \) vanishes identically near \( x' = x > 0 \) and hence both unphysical contributions to the current are absent. To show their cancellation for arbitrary \( \delta T(x') \) one needs the full space dependence of \( \langle JJ \rangle_{\text{odd}} \). Therefore, we will temporarily restrict ourselves to the case \( T = 1 \), where—by symmetry—formula (8) does hold for any \( t \) and \( \alpha \). The equal-time commutator \( \langle [\mathcal{H}, J] \rangle \) can be calculated using Wick’s theorem or, equivalently, by expanding the fields in creation and annihilation operators. The answer is:

\[
\langle [\mathcal{H}(x'), J(x)] \rangle_0 = -\frac{i}{c} \left\{ \frac{\delta''(\alpha)}{12\pi} - \frac{\pi \delta'(\alpha)}{3\beta^2} \right\}.
\]

Inserting this in the second term of (9), and evaluating the first term of that formula to be

\[
\frac{1}{T} \int dx' \nabla T(x') \left\{ \frac{\delta'(t - \alpha)}{24\pi} - \frac{\pi}{6\beta^2} \theta(t - \alpha) - \theta(-\alpha) \right\} - t \left( \frac{\delta''(\alpha)}{24\pi} - \frac{\pi \delta'(\alpha)}{6\beta^2} \right) + (\alpha \leftrightarrow -\alpha),
\]

the unphysical terms which grow linearly in \( t \) are seen to cancel.

B. The energy drop

For the case of arbitrary \( T \), the drop in energy density \( \Delta \langle \mathcal{H} \rangle_{\text{loc}} \) can be calculated from (8) by using the detailed form of (8). However, only a few general properties of this correlation function will actually be needed (thereby suggesting the validity of the present analysis beyond the case of the 1D elastic continuum). Namely, by inspection of the defining integrals it is easy to verify that for \( t, \alpha > 0 \), \( \langle JJ \rangle_{\text{odd}} \) is an odd function \( f(s \equiv t - \alpha) \), which is localized at \( s = 0 \). As mentioned after Eq. (8), this immediately shows that the additional \( t \)-term in the Kubo relation (8) gives a vanishing contribution to the current, except at \( t = \alpha \).

On the other hand, omission of this term would lead to a \( \Delta \langle \mathcal{H} \rangle_{\text{loc}} \) which is a factor two too large compared to the correct value obtained below in Eq. (11).
Let us now finally give a microscopic calculation of the change in energy density. Again choosing \( x > 0 \), one has
\[
\Delta \langle H(x) \rangle_{\text{loc}} = \int_0^\infty dt \partial_t \langle H(x,t) \rangle_{\text{loc}} = -\frac{1}{c_r} \int_0^\infty dt \partial_\alpha \langle J(\alpha,t) \rangle_{\text{loc}}
\]
\[
= \lim_{\tau \to \infty} \frac{\text{Const}}{c_r} \int_0^\tau dt \int_0^t dt' (t - t') \partial_\alpha f(t' - \alpha)
\]
\[
= \lim_{\tau \to \infty} \frac{\text{Const}}{c_r} \int_0^\tau dt \left[ tf(-\alpha) - \int_0^t dt' f(t' - \alpha) \right]
\]
\[
= \lim_{\tau \to \infty} \frac{\text{Const}}{c_r} \int_0^\tau dt (\tau - t) f(t - \alpha)
\]
\[
= \frac{1}{c_r} \langle J(x,t = \infty) \rangle_{\text{loc}}.
\]
(11)

In the fourth and fifth line the first term vanishes because of the properties of \( f \) mentioned above. With \( \langle J \rangle_{\text{loc}} = \frac{\pi}{6} T \Delta T \), the value of \( \Delta \langle H \rangle_{\text{loc}} \) according to Eq. (11) coincides with the one obtained in the semi-classical analysis of Sec. II, leading to our result (3).

IV. ANALOGY WITH BALLISTIC ELECTRON TRANSPORT

The analysis of electric current in a one-dimensional conductor as a scattering problem was pioneered by Landauer. Consider two well-separated reservoirs at electrochemical potentials \( \mu_l = \varepsilon_F + eV \) and \( \mu_r = \varepsilon_F \), respectively. Let the reservoirs be connected by a one-dimensional lead, interrupted by a barrier (at \( x = 0 \), say) with transmission coefficient \( T \). Using the 1D density of states \( 1/hv_F \) (\( v_F \) being the Fermi velocity), at zero temperature the current per spin direction is obtained as \( I = T(ev_F)(eV/hv_F) = \frac{e^2}{h} TV \). This leads to a conductance \( G = \frac{e^2}{h} T \) in the case of a voltage measurement at the reservoirs.

Near the barrier, however, the conductor is not well characterized by the reservoir potentials \( \mu_{l,r} \). For energies between \( \mu_l \) and \( \mu_r \), at a position \( x < 0 \) all left-going states are occupied, but only a fraction \( \mathcal{R} \) of the right-going states is filled. This leads to an effective electrochemical potential \( \mu'_l = \varepsilon_F + eV(1 + \mathcal{R})/2 \). Similarly, for \( x > 0 \) one gets \( \mu'_r = \varepsilon_F + eV/2 \). Calculating the conductivity using \( (\mu'_l - \mu'_r)/e = \mathcal{R} V \) as the relevant voltage difference for a measurement near the barrier, one finds the Landauer formula
\[
G = \frac{e^2}{h} \mathcal{R}.
\]
(12)

If one measures the voltage difference between the reservoirs, the finite upper limit of \( G = \frac{e^2}{h} T \) as \( T \uparrow 1 \) makes perfect sense physically. The resulting \( G^{-1} = \frac{h}{e^2} \) has the significance of a purely geometric contact resistance between the reservoirs. On the other hand, \( G \) in Eq. (12) is the quantity which describes the intrinsic properties of the barrier.

The analogy to the heat transport problem is now easily seen: the role of the electric current is played by the heat current, the electron densities from which the electrochemical potentials are determined are the analogue of the energy densities considered in Secs. II and III, and the effective electrochemical potentials translate into local temperatures.
The appropriate definition of $\mu_i'$ is not trivial: one could argue that local chemical potentials are only defined up to the difference in potential pertaining to left- and right-going states separately. This leads to a conceptual uncertainty $(\Delta G)/G \approx 2T$, and would therefore allow a thermodynamic description of the current transport only if $T \ll 1$. In that case the distinction between the two formulas for $G$ obviously loses its meaning. The analogous caveat holds for heat transport. However, the potentials $\mu_{l,r}'$ leading to Eq. (12) are defined in such a way that, if the system would have been in local equilibrium at these potentials, the electron density would be the same as the actual density. This guarantees that the conductance (12) trivially satisfies the Einstein relation $G = e^2 \partial_{\mu} n_p D$, where the diffusivity $D$ relates the particle current $J_p$ to the particle density jump across the barrier $\Delta n_p$ by $J_p = D \Delta n_p$. Moreover, this definition is the correct one in the following sense: if one couples two additional reservoirs infinitesimally weakly to the left and right of the barrier, the condition that no current will flow is that they must be at the potential $\mu_l'$ and $\mu_r'$, respectively (see Ref. 9 for the precise statement). In our case one could—at least in principle—probe local temperatures by weakly coupling additional heat baths in a similar way.

In the system described in Secs. II and III, the role of the reservoirs is played by the infinite leads themselves. For electron transport, this way of modeling the reservoirs was introduced earlier in Ref. 10. The criterion for a good reservoir is that it should only re-emit electrons (phonons) after complete thermalization and loss of phase memory. The leads satisfy this condition by never re-emitting any particle. Violation of this condition, for example by taking finite leads, will lead to different results, as mentioned already in the Introduction.

The absolute temperature, which enters as a prefactor in our formula for the boundary conductance, has no counterpart in the current transport problem. Its presence is a consequence of the Bose statistics obeyed by the phonons (see also the denominator in (A1)), as opposed to the Fermi statistics of electrons.

V. CONCLUDING REMARKS

The reasoning leading to the paradox-free formula (Eq. (3)) for the Kapitza boundary conductance $K$ calculated in this article is not invalidated by the presence of a thermalization mechanism like the weak three-phonon scattering contemplated in Refs. 3 and 4. On the contrary, such a mechanism rather brings the local energy distribution closer to a thermal one (under the condition that there should be a heat current $J$), and thus only strengthens the case for $\varepsilon_1'$ as the energy from which stationary temperatures should be calculated.

In conclusion: using the model of coupled harmonic strings, we have solved the Kapitza boundary resistance paradox (Little’s formula) by means of an exact calculation of the properties of the interface in the final steady state, leading to the new formula Eq. (3). Besides, we have explained the analogy between local temperature measurements in the heat transport problem and voltage measurements in ballistic electron transport (Landauer’s formula).
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APPENDIX: THE CURRENT-CURRENT CORRELATION FUNCTION

We calculate (8) along the lines of Ref. 4. With the Hamiltonian density $\mathcal{H} = \frac{1}{2p} \pi^2 + \frac{M}{2} (\nabla \phi)^2$ (where $\phi$ is the field operator, $\pi$ is its conjugate momentum, $\rho$ is the mass density, and $M$ is the modulus of elasticity), local energy conservation implies $J = -\frac{M}{2\rho} \{\pi, \nabla \phi\}$ for the energy current. Using this expression for $J$, $\langle JJ \rangle_{\text{odd}}$ can be expanded in terms of field-field correlation functions using Wick’s theorem. By a KMS-relation, the field-field correlation functions can be obtained from the field-field commutators only, and these in turn follow from the classical wave equation. Carrying out this procedure leads to

$$\langle J(x, t) J(x', 0) \rangle_{\text{odd}} = \frac{T}{2i} \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \frac{\omega \omega' \sin[(\omega + \omega')(t - \alpha)]}{(1 - e^{-\beta \omega})(1 - e^{-\beta \omega'})} + (\alpha \leftrightarrow -\alpha), \quad (A1)$$

where $T$ is defined in terms of the impedances $Z_i \equiv \rho_i c_i$ as

$$T = \frac{4Z_l Z_r}{(Z_l + Z_r)^2}, \quad (A2)$$

and $x > 0$, $x' < 0$ as in the main text. The infrared divergence present in the field-field correlation functions because the energy of an oscillation vanishes in the long-wavelength limit, is seen to be absent in the current-current correlation function as such long-wavelength excitations hardly contribute to the energy transport. On the other hand, the ultraviolet divergence caused by taking the continuum limit for the string must be dealt with, e.g., by regularizing $\langle J J \rangle_{\text{odd}}$ using a spatial smoothing. Taking a Lorentzian for that purpose leads to a cutoff $e^{-\eta |\omega + \omega'|}$ in the integral in $(A1)$. However, since the integrand vanishes as $\sim e^{-\beta |\omega'|}$ in the half plane $\omega + \omega' < 0$ one may as well use the cutoff $e^{-\eta |\omega + \omega'|}$. The integral then factorizes and the ensuing single integrals can be done exactly. With $\beta = 1$, this yields

$$\int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \frac{\omega \omega' \sin[(\omega + \omega)t] e^{-\eta(\omega + \omega')}}{(1 - e^{-\omega})(1 - e^{-\omega'})} = \text{Im} \left[ \frac{\pi}{2 \sin^2(\pi(\eta - it))} \right]^2$$

$$= \left\{ \frac{1}{6} \delta_t - \frac{1}{24\pi^2} \delta^3 \right\} \text{Im} \frac{1}{t + i\eta} + \text{Im} \left[ O \left( (t + i\eta)^0 \right) \right]$$

$$= \frac{1}{24\pi} \delta'''(t) - \frac{\pi}{6} \delta(t) \quad \text{for} \quad \eta \downarrow 0. \quad (A3)$$

Scaling back to $\beta \neq 1$ and inserting this result into $(A1)$, one obtains $\langle J J \rangle_{\text{odd}}$ as given in Eq. (8).
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15 In the fourth line below Eq. (2) of Ref. 4, the labels $z > z_1$ and $z < z_1$ should be interchanged. Apart from this, all signs are consistent.
16 A calculation like $[\mathcal{H}(x'), \mathcal{J}(x)] = \left[ \frac{\pi(x')^2}{2\beta} + \frac{M}{\rho} (\partial_x \phi(x'))^2, -\frac{M}{\rho} \{\pi(x), \partial_x \phi(x)\}\right]$ (by repeated use of $[\phi(x), \pi(x')] = i \delta(x-x')$) is incorrect, because the Hamiltonian densities arising at the end of this exercise are not normally ordered (even if one would start with $:\mathcal{H}:$, since $\mathcal{H} - \mathcal{H} : \propto 1$, which commutes with $\mathcal{J}$). This means that in the above formula one is multiplying delta functions with an infinite object, which can only be done reliably by means of the more elaborate method of the main text. The additional, temperature-independent contribution which is found there (and the analogous one for $\langle \mathcal{J}\mathcal{J}\rangle_{\text{odd}}$ in Eq. (8)) is known as a Schwinger term. See, e.g., C. Itzykson, J.-B. Zuber, Quantum Field Theory (McGraw-Hill, Singapore, 1988).
17 Because the prefactor $t - t'$ multiplying $\langle \mathcal{J}\mathcal{J}\rangle_{\text{odd}}$ in Eq. (8) has a first order zero at $t' = t = \alpha$, $\langle \mathcal{J}\rangle_{\text{loc}}$ as obtained from Eq. (8) is less singular than it would have been without the $t$-term: it contains $\delta'(t - \alpha)$ (see also Eq. (11)) but not $\delta''(t - \alpha)$.
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19 This subtlety is absent in the study of bulk transport, where one can unambiguously define local quantities by averaging over a spatial region which is much larger than a thermalization length. See also the Introduction.
20 Notice that the unsymmetrized Eq. (7) from Ref. 4 would incorrectly imply that $\mathcal{J}$ is not hermitian.
FIGURES

FIG. 1. Two harmonic strings (with an interface at $x = 0$) at a time $t = t_1$ after the system started in a different local equilibrium on either side of $x = 0$. 