Kapitza resistance between electron and phonon gases in the 1D case

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Received July 7, 2012; Accepted October 30, 2012; Published January 1, 2013

This study addresses the exact behavior of electrons and phonons in semi-infinite 1D systems with due allowance for the local interaction between them. The spectral functions of electrons and phonons in such a system have been derived and analyzed in an analytical form. The paper considers, in particular, the problems involved in the hardening and softening of phonon modes and renormalization of the electron–phonon interaction constant. The results obtained have been employed in calculation of the thermal resistance constant at the boundary separating the electron from the phonon systems and in an analysis of its dependence on the renormalized electron–phonon interaction constant. All the results were obtained in the adiabatic limit for several cases of special significance, such as a half-filled and an empty conduction band at temperatures both higher and lower than the characteristic phonon frequencies. Significantly, the problem was treated exactly for an arbitrary electron–phonon interaction constant, in both the weak and the strong limits. It has been demonstrated that thermal resistance decreases with increasing electron–phonon interaction coefficient and/or temperature; at large values of these parameters, thermal resistance at the boundary no longer depends on these quantities.

Subject Index I11,I30,I53

1. Introduction

In recent years, we have witnessed a growth of interest in the investigation of the processes involved in heat transfer in solid, including composite, materials. This can be traced both to present-day trends in miniaturization of electronic devices and to an ever-increasing density of electronic components per chip and impressive progress in molecular and thin-film electronics. It is these areas that provide stimuli for a search for an appropriate material to reject heat in modern electronics. Indeed, all the above systems contain in their structure nanosized regions with a high fraction of surface-bound atoms. Therefore, heat transfer in such systems differs essentially from that observed in a macroscopic case. It is known that any surface represents an obstacle to heat flow and acts as an energy barrier, which accounts for the formation of thermal resistance at the boundary between any two materials, first observed by Kapitza [1]. Reducing this resistance becomes a problem of ever-more increasing importance for nanosized systems. Recourse to high thermal-conductivity materials such as diamond, carbon nanotubes, or graphene can only alleviate but not remove the problem altogether, because the surfaces separating different components of a device always interfere with heat flow.

It thus comes as no surprise that thermal resistance is currently being actively studied in different systems, among them superlattices [2–4] and composites based both on classical semiconductors such as arsenides or nitrides [5,6] and on nanotubes [7] and nanodiamonds [8]; surface contacts between specific materials also generate interest [9–11].
Fig. 1. Schematic visualization of a semi-infinite electron system, in which the overlap integral for neighboring atoms is $t$, and a semi-infinite phonon system, in which elastic coupling between neighboring atoms is characterized by the elastic constant $k$. At site 0, local electron–phonon interaction is operative, and the electron–phonon subsystem coupling energy is $\gamma$.

Thermal resistance attracts interest not only from experimenters but from theoreticians as well. Significantly, however, all the studies reported so far have involved only the phonon flow between two bodies, the so-called acoustic mismatch and diffuse mismatch models [12–14], even in cases where the molecular dynamics approach was invoked [15,16]. At the same time, the case of most interest, to wit, the metal–dielectric contact, where heat is transferred between the electron gas in a metal and the phonon gas in a dielectric, has not thus far been enjoying adequate attention. This gap appears essential, because electrons are the major carriers of heat in metals, and phonons, those in a dielectric. Thus, for heat transfer to be efficient, such a mechanism should provide a major contribution to heat transfer between a dielectric and a metal [17].

Furthermore, earlier works on heat flow through a metal–dielectric surface were primarily focused on discussing a specific mechanism of interaction between electrons and phonons in a system. To cite just a few examples, analysis has been made of an interaction involving the deformation-potential interaction [18–20] or the mechanism based on the image potential of ions of the metal surface [21]. Significantly, the thermal resistance coefficient was calculated for small electron–phonon interaction coefficients only. The results obtained in these studies were only to be expected, namely, that thermal resistance decreases with increasing electron–phonon interaction coefficient. It should be stressed that the cases treated were always those of the metal–dielectric contact, while the studies attracting ever-increasing interest currently involve thermal resistance of dielectrics with nanotubes [7], which are actually semimetals.

The phenomenon itself of thermal resistance actually remains unexplored. One could consider a case, for instance, of two materials separated by an interlayer with a preset electron–phonon interaction coefficient, and ask the question of whether one could reach a low thermal resistance for large enough values of this coefficient? Another question—could one realize a situation with a large enough value of this coefficient in which the electron and the phonon would be localized close to the interface by strong mutual interaction, so that the heat would not propagate at all? Would the thermal resistance coefficient under these conditions reach saturation or would it increase with increasing electron–phonon interaction coefficient?

To determine the thermal resistance coefficient at the boundary separating the electron from the phonon subsystems, we have considered in this work a semi-infinite electronic system coupled to the phonon subsystem at one point only (Fig. 1). In our subsequent calculations, we are going to restrict ourselves to the adiabatic case, in which the phonon frequency is assumed to be substantially smaller than the hopping integral. Nevertheless, our model is applicable to consideration of thermal current in a broad class of objects, in particular, to carbon nanotubes coated by nanodiamonds [22], as well
as to Pandey chains on the surface of nanodiamonds [23, 24]. Although we treat 1D chains in this work, our findings form the basis for higher-dimensional applications in which the results are more complicated; we will present them elsewhere. Formulated in this way, the problem overlaps with another area that has been enjoying considerable interest in recent years, namely, electron–phonon interaction in thin films and nanostructures [25] and their interaction in a local region [26–29], an approach in which Holstein’s model has been widely employed [30–32]. In the studies cited above, however, the results obtained were either limited to small electron–phonon interaction constants or were applicable to metals only.

All this suggests that one should consider the problem of the behavior of electrons and phonons with due allowance for local interaction between them, and the process of energy transfer between the electron and phonon gases.

2. Model

We are going to consider here a 1D problem in which the electron and phonon gases interact at one point only. The system to be studied is shown schematically in Fig. 1.

By analogy with Holstein’s Hamiltonian, we write the Hamiltonian of our system with due allowance for the fact that electrons can interact with phonons at one point only, at the boundary between the electron and phonon subsystems.

\[
\hat{H} = t \sum_{i=-\infty}^{0} \left( \hat{c}_{i+1}^+ \hat{c}_{i} + \hat{c}_{i}^+ \hat{c}_{i+1} \right) + \frac{\omega_0}{2} \sum_{i=0}^{\infty} \left( p_i^2 + \frac{1}{2} (\hat{x}_i - \hat{x}_{i+1})^2 \right) + \frac{\omega_0}{4} \hat{n}_0^2 + \gamma \hat{n}_0 \hat{x}_0. \tag{1}
\]

where the following notation is introduced: \( \hat{c}_{i}^+ \), \( \hat{c}_{i} \) are the operators of creation and annihilation of an electron at the \( i \)th site. The particle number operator at the 0th site is \( \hat{n}_0 = \hat{c}_{0}^+ \hat{c}_0 \). \( \hat{p}_i, \hat{x}_i \) are the operators of the momentum and displacement of the \( i \)th atom expressed in terms of the operators of creation \( \hat{a}_{i}^+ \) and annihilation \( \hat{a}_{i} \) of phonons: \( \hat{p}_i = i (\hat{a}_{i}^+ - \hat{a}_{i}) \), \( \hat{x}_i = (\hat{a}_{i}^+ + \hat{a}_{i}) \). \( \omega_0 \) is the vibration frequency of atoms, and \( \gamma \) is the coefficient of interaction between an electron and displacement at the 0th site. We are going to assume in what follows that \( \hbar = 1 \). Although we are going to disregard in what follows spin degrees of freedom and direct interaction among electrons, it can be assumed in the first approximation that this will result only in a decrease of the electron–phonon interaction constant \( \gamma \) [33].

Our major problem lies in finding the Green’s function for electrons and phonons \( G_{ij} = -\langle T_r \hat{c}_i(\tau) \hat{c}_j^+(0) \rangle \), \( D_{ij} = -\langle T_r \hat{x}_i(\tau) \hat{x}_j(0) \rangle \), and the corresponding spectral functions \( A_{ij}(\omega) = -2\Im G_{ij}(i\omega), B_{ij}(\omega) = -2\Im D_{ij}(i\omega) \).

To calculate the spectral functions \( A \) and \( B \), we shall need to derive a system of equations for the \( \hat{x}, \hat{c} \) operators, which can be readily obtained from the equation of motion \( \partial \hat{c}/\partial \tau = [\hat{K}, \hat{c}] \):

\[
\frac{\partial \hat{c}_i}{\partial \tau} = \mu \hat{c}_0 - \delta_{i,0} \gamma \hat{x}_0 \hat{n}_0 - t (\hat{c}_{i+1} + \hat{c}_{i-1})
\]

\[
\frac{2 \omega_0^2}{\omega_0} \frac{\partial^2 \hat{x}_i}{\partial \tau^2} = \frac{2 \gamma}{\omega_0} \hat{n}_0 \delta_{i,0} + 2 \gamma \hat{x}_i - (\hat{x}_{i+1} + \hat{x}_{i-1}). \tag{2}
\]

where \( \hat{K} = \hat{H} - \mu \hat{N} \), \( \mu \) is the chemical potential, and \( \hat{N} \) is the operator of the number of particles. \( \hat{c}_1 = \hat{x}_{-1} = 0 \) are the boundary conditions for this system of equations.
2.1. Noninteracting case

The qualitative solution of Eq. (1) for $\gamma = 0$ is well known. The electron spectrum will depend on the wave vector $k$ and the distances between neighboring atoms $\varepsilon(k) = 2t \cos(ka)$, with energy reckoned from the band center. Thus for the width of the electron band we obtain $4t$. The phonon spectrum is given by the relation $\omega(k) = \sqrt{2\omega_0 \sin(ka)}$. In addition to the conventional, bulk states, the solution provides surface states as well for both the electrons and phonons. In the $\gamma = 0$ case, a set of equations (2) allows an easy solution:

$$G_{ij}^0 = -\frac{1}{t} F_{ij} \left( -\frac{i\omega + \mu}{t} \right),$$
$$D_{ij}^0 = \frac{1}{\omega_0} F_{ij} \left( \frac{2}{\omega_0} \left( \frac{i\omega}{\omega_0} \right)^2 - 2 \right),$$

where

$$F_{ij}(\Omega) = \frac{1}{\pi} \int_{-\pi}^{\pi} dx \frac{\sin(j + 1)x \sin(i + 1)x}{\Omega + 2 \cos(x) + i0},$$

which can be readily verified by straightforward substitution. We are going to resort frequently in what follows to the use of this function for the values $i, j = 0$, in which case the expression for $F$ reduces to $F_{00} = \exp[i \arccos(\Omega/2)]$.

To the parameters of the problem introduced earlier, $t, \omega_0, \mu, \gamma$, we may add $T$, the temperature in the system. As pointed out in the Introduction, we shall restrict ourselves to the most important cases, namely, we shall assume that $T, \omega_0 \ll t$ is the signature of the adiabatic case for temperatures low compared with the band width. Also, we shall consider below only two cases, called conventionally here “metallic”, when the free electron concentration in a system is high, and the chemical potential is at the band center $\mu = 0$, and “semimetallic”, if the free electron concentration is low, and the chemical potential level is at the band bottom $\mu = -2t$. Significantly, in the case under consideration, the chemical potential $\mu$ does not depend on the interaction parameter $\gamma$, because the infinite electron and phonon subsystems interact at one point only. This point interaction cannot affect the chemical potential of the infinite electron system. Treated in this way, chemical potential is a specified external parameter that is the same for all points of the electron subsystem.

We turn now to an analysis of the Green’s functions for electrons and phonons assuming point interaction.

2.2. Electron Green’s function

To find the electron Green’s function, we shall use the recursive method developed by Cini [34], which was demonstrated [31,35,36] to be applicable to calculation of the Green’s function of the electron engaged in point interaction with phonons.

We diagonalize Hamiltonian (1) over the phonon variables:

$$\hat{H} = t \sum_{i=0}^{\infty} \varepsilon_i \hat{c}_i^+ \hat{c}_i + \omega_0 \sum_{i=0}^{\infty} \omega_i \hat{a}_i^+ \hat{a}_i + \sum_{j=0}^{\infty} \gamma_j \hat{n}_0 \hat{x}_j,$$

Here $\omega_i$ specifies the phonon spectrum in half-space $\gamma_j = \gamma U_{0,j}$ and $U_{0j}$ is the eigenvector for the matrix of transition from representation (1) to (5); as we shall see further on, its actual form is of no significance to us here.
Consider the probability amplitude for the transition from site $i$ to site $j$ accompanied by emission of $k$ phonons:

$$
\Psi_{ij}(k; i\omega) = \sum_k \gamma_0 \cdots \gamma_{mk} \left( \prod_k a_k^{m_k} \hat{c}_i \frac{1}{i\omega - \hat{H}} \hat{c}^+_j \right). \tag{6}
$$

The summation here is run over all possible combinations of phonon variables, with their total number $k$. We readily see that the electron Green’s function is directly connected with this quantity: $G_{ij}(i\omega) = \Psi_{ij}(0; i\omega)$.

We now have to identify in Hamiltonian (5) the terms accounting for the noninteracting phonons and electrons $\hat{H}_0$ and their interaction $\hat{H}_1$: $\hat{H} = \hat{H}_0 + \hat{H}_1$. This opens the way to deriving recurrence relations for the quantities $\Psi_{ij}(k; i\omega)$ by averaging the operator identity:

$$
\frac{1}{\omega - \hat{H}} = \frac{1}{\omega - \hat{H}_0} + \frac{1}{\omega - \hat{H}_0} \hat{H}_1 \frac{1}{\omega - \hat{H}}.
$$

Significantly, at this point, an essential simplification is introduced in Cini’s method; more specifically, dispersion is assumed to be absent: $\omega_j = \omega_0$. This approach is justified not only for the optical but for acoustic phonons as well. This can be partially assigned to the fact that in this way one does not neglect spatial dispersion for the coupling constant $\gamma'$. It was shown [37] that this method can be generalized by including spatial dispersion of frequencies. In this case, for the Green’s function, one obtains a perturbation theory series, but it will not differ qualitatively from the results derived in the above approximation.

One can write in the above approximations the following recurrence relations for the $\Psi_{ij}(k; i\omega)$ functions:

$$
\Psi_{ij}(k; i\omega) = G_{ij}^0 \delta_{k,0} + G_{ij}^0 (i\omega - k\omega_0) [\Psi_{0j}(k + 1; i\omega) + \gamma^2 k \Psi_{0j}(k - 1; i\omega)]. \tag{7}
$$

Significantly, here $\gamma^2 = \sum \gamma_j^2$, a consequence of $U_{ij}$ being a unitary transition matrix.

The solution of this system of recurrence relations for the Green’s function $G_{ij}(i\omega) = \Psi_{ij}(0; i\omega)$ can be written as

$$
G_{ij} = G_{ij}(i\omega) + \frac{G_{i0}^0(i\omega)G_{0j}^0(i\omega)}{G_{00}^0(i\omega)} (C_{el}(i\omega) - 1), \tag{8}
$$

where

$$
C_{el}(i\omega) = \frac{1}{1 - \frac{\gamma^2 G_{00}^0(i\omega - \omega_0) G_{00}^0(i\omega)}{1 - 2 \gamma^2 G_{00}^0(i\omega - 2\omega_0) G_{00}^0(i\omega - \omega_0)}} \cdots \tag{9}
$$

For small $\omega_0$, we can expand the $C_{el}$ function in a Taylor series. As is evident from the form of expression (9), as well as of Green’s function $G^0$ (3), the only small dimensionless parameter in this function is $\gamma^2 2\omega_0/\hbar^2$, so that $C_{el}(i\omega, \omega_0) = C_{el}(i\omega, 0) + O(\gamma^2 2\omega_0/\hbar^2)$.

But then the expression for $C_{el}$ allows significant simplification. It can readily be shown that by comparing the expression for $C_{el}$ written for $\omega_0 = 0$ with that for the complementary error function erfc expressed in the form of continued fractions [38,39] one can obtain an exact analytical expression for $\omega_0/\hbar \to 0$. In fact, this is a main result of this paper:

$$
C_{el} = \frac{i \sqrt{\pi}}{\sqrt{2 \gamma^2 G_{00}^0(i\omega)}} w \left( \frac{1}{\sqrt{2 \gamma^2 G_{00}^0(i\omega)}} \right), \tag{10}
$$

where $w$ is the normalized complementary error function.
Fig. 2. Spectral functions for an electron (a) $A_{00}$, (b) $A_{0,-1}$, (c) $A_{-1,-1}$ plotted versus its energy $\omega$ for different parameters of interaction $\gamma$ between electrons and phonons at site 0.

where $w = \exp(-x^2)\text{erfc}(-ix)$ is the Faddeeva function. We note that the Faddeeva function $w(1/x) \sim ix/\sqrt{\pi}$ for $x \to 0$ [40]. Thus, for $\gamma \to 0$, $C_{\text{el}} \to 1$ and $G(i\omega) \to G^0(i\omega)$.

As already mentioned, the simplification accepted in this method, namely, neglect of the spatial dispersion of phonons, can hardly affect seriously the final results. This effect can obviously be neglected altogether in the $\omega_0 \ll t$ approximation. Indeed, for $\omega_0 \to 0$ we also have $\omega_i < \sqrt{2}\omega_0 \to 0$. This brings us to the exact solution for the Green’s function allowing for dispersion in the form $G_{\text{disp}}(i\omega, \omega_0, \omega_2, \ldots) = G_{\text{disp}}(i\omega, 0, 0, \ldots) + O(\omega_0/t)$. But $G_{\text{disp}}(i\omega, 0, 0, \ldots) = G_{ij}(i\omega, \omega_0 = 0)$. In other words, spatial dispersion of phonons would become manifest only in the next order of the smallness parameter $\omega_0/t$.

Figure 2 plots the spectral functions at different sites $A_{00}$, $A_{0,-1}$, $A_{-1,-1}$ versus electron energy, as well as versus the electron–phonon interaction energy. The graphs relate to the metallic case, where the major fraction of electrons reside close to the band center. The spectral functions for the semimetallic case can be obtained by displacing the points from which the energy is reckoned to the left by $2t$. Significantly, the spectral function $A_{00}$ at the band center (at the $\omega = 0$ point) is larger than $A_{-1,-1}$, which implies the existence of a bound state on the surface. As $\gamma$ increases, states with energies both lower than $-2t$ and higher than $2t$ appear in the density of states $A_{00}$ at site 0. This is a direct consequence of an electron now acquiring a probability of both emitting and absorbing a phonon. As the interaction energy $\gamma$ continues to increase still more, the density at site 0 progressively approaches the Gaussian form. This correlates with the independent boson models, because at high $\gamma$ the interaction between the 0th and $-1$th sites becomes inessential, and electrons at the 0th site behave independently. At the same time, the $-1$th site actually becomes the boundary of the electron subsystem, with the result that, with increasing $\gamma$, the density $A_{-1,-1}$ approaches the density $A_{00}$ at low $\gamma$.

2.3. Phonon Green’s function

We turn now to a consideration of the behavior of phonons in a system with local electron–phonon interaction. Equations (2) for the phonon Green’s function can be solved using standard techniques. But, in contrast to the uniform case [41], in the case of point interaction one can obtain an exact solution:

$$D_{ij}(i\omega) = D^0_{ij} + \gamma^2 D^0_{ij} \Pi(i\omega) D^0_{ij}. \quad (11)$$

It should be pointed out that, while this equation resembles in its form the solution of Dyson for small interaction parameters, the present solution was obtained without using the condition of
smallness of the coefficient \( \gamma \); indeed, the smallness parameter here acted the size of the interaction region.

We shall write here only the spectral part of the polarization operator \( C = -2 \Re \Pi \) because, as follows from the Lehmann relation

\[
\Pi(i\omega_n) = \int \frac{d\omega}{2\pi} \frac{C(\omega)}{i\omega_n - \omega},
\]

if one knows it, reconstruction of the polarization operator should not present any difficulties:

\[
C(\omega) = 2\int d\omega' A_{00}(\omega') A_{00}(\omega' + \omega)(n_F(\omega') - n_F(\omega' + \omega)).
\]

This function can be readily calculated as soon as we find the electron spectral function at the zero site \( A_{00} \). In the low-temperature case of interest to us here, one can invoke Eqs. (10) and (8) to rewrite Eq. (13) in the form

\[
C(\omega) = \frac{2}{\gamma^2} \int_{-\omega}^{\omega} d\omega' \Re w \left( \frac{1}{G^0_{00}(\omega')\gamma\sqrt{2}} \right) \Re w \left( \frac{1}{G^0_{00}(\omega' + \omega)\gamma\sqrt{2}} \right).
\]

2.4. Renormalization of the interaction constant

Prior to continuing the discussion of the phonon properties and thermal resistance, we should first renormalize the electron–phonon interaction constant. To do this, we write the potential of effective interaction between the electron and the phonons in the form:

\[
V_{\text{ep}} = \gamma^2 D^0_{00} = \lambda^2 D_{00},
\]

where \( \lambda \) is the normalized interaction constant.

Electron–phonon interaction in a local region (close to the boundary) exerts the strongest effect on phonons with small wavelengths, i.e., with high energies. Therefore the relation for \( \lambda \) will be given here for phonon energies of about \( \sqrt{2}\omega_0 \):

\[
\lambda = \frac{\gamma}{\sqrt{1 + \frac{\gamma^2}{\omega_0^2}\Re \Pi(\sqrt{2}\omega_0)}}.
\]

In the “metallic” case, where the electron concentration is high \( \mu = 0 \), they reshape the phonon spectrum strongly; in these conditions, the effect of phonons on electrons may be safely neglected. Therefore, calculation of Eq. (14) may be performed, in the first approximation, under the assumption of \( \gamma \rightarrow 0 \). Recalling that \( \omega_0 \ll t \), one may also assume that \( \Re \Pi(\omega) \approx \Re \Pi(0) \). With these simplifications we come to \( \Pi(0) \approx -0.9/t \), from which it follows immediately that for \( \gamma \) equal to \( \gamma_c = 1.1\sqrt{\omega_0 t} \) the effective electron–phonon interaction constant grows strongly.

It is known [33] that \( \lambda \) relates the renormalized frequencies \( \omega \) with the “bare” ones \( \omega_0 \): \( \lambda \approx \gamma^2 \omega_0^2 / \omega^2 \). Therefore, an increase of \( \lambda \) can be identified with mode “softening”, i.e., decrease of phonon frequency. Thus, in the metallic case, we meet with softening of high-energy phonons.

In contrast, for low-energy phonons \( \Re D_{00} < 0 \), which translates into reversal of the sign of \( \gamma^2 / \omega_0 \) in Eq. (16). Thus low-energy phonons “harden” with increasing \( \lambda \), i.e., their frequency increases.

The dependence of the effective electron–phonon interaction constant on the \( \lambda \) parameter is presented in graphical form in Fig. 3(a). Figure 3(b) visualizes the behavior of the phonon spectral function at the zero site.
Fig. 3. (a) Normalized constant of electron–phonon interaction $\lambda$ plotted versus $\gamma$ for the metallic case ($\mu = 0$). Close to $\gamma_c$, this dependence follows a strongly nonlinear pattern. (b) Spectral function of phonons at site 0 $D_{00}$ in the metallic case drawn for different $\gamma$. Arrows identify hardening of low-energy phonons and softening of the high-energy ones. (c) Variation of the normalized electron–phonon interaction constant $\lambda$ with $\gamma$ in the semimetallic case ($\mu = -2$). (d) Spectral function of phonons at site 0 in the semimetallic case drawn for different $\gamma$. The $\omega_0/t$ parameter was chosen equal to 0.01.

As seen from Eq. (15), whether low-energy phonons soften or harden can also be inferred readily from the derivative of the spectral function with respect to energy. The latter can be derived from (11):

$$\frac{\partial B}{\partial \omega} \bigg|_{0} = \frac{2}{\omega_0^2} \left( \sqrt{2} - \frac{2\sqrt{2}\gamma^2}{\omega_0} \Re \Pi(0) + \frac{\gamma^2}{2\pi} A^2(0) \right).$$  \hspace{1cm} (17)

We immediately see that, in the metallic case, an increase of $\gamma$ initiates accordingly growth of the derivative, i.e. hardening of low-energy phonons, the situation shown in Fig. 3(b).

Consider now the empty band case, i.e. the case of semimetals $\mu = -2t$. In this case, $\Re \Pi$ exhibits a more complex, nonlinear pattern of variation with $\gamma$. At small $\gamma$, $\Re \Pi$ is close to zero, because at small interaction coefficients the number of electrons at the Fermi level is small. At high interaction energies, however, as is evident from Fig. 2(a), the density of states at energies $-2t$ increases significantly. The electron concentration and hence $\Re \Pi$ grows with increasing $\gamma$. At large $\gamma$ parameters, when the number of electrons at the Fermi level becomes large, we actually come to the metallic case, with $\Re \Pi$ saturating.

The dependence of the electron–phonon interaction constant on $\gamma$ for semimetals is shown in graphic form in Fig. 3(c). Figure 3(d) visualizes the behavior of the spectral function for phonons at site 0. Just as in the metallic case, we observe here softening of the high-energy phonons and hardening of the low-energy phonons.

3. Kubo formula for Kapitza resistance

Thermal resistance at the boundary separating the electron from the phonon system can be calculated in terms of the Kubo formalism. Incidentally, while in practical calculations it is quite often more
we obtain in the steady state case the surface that separates the electron from the phonon gas can be readily specified by presenting $z$ where the integrals are over the whole infinite plane at $t = 0$. We calculate the average heat flux being trivial, we are going to refer in what follows to thermal surface conductance only.

We shall follow a path largely similar to that chosen in the works dealing with calculation of the resistance for phonon systems \cite{42,43}. We calculate the average heat flux $\mathcal{J}$ at point $z_2$ at time $t$ resulting from application of a temperature jump $\Delta T$ at point $z_1$ at time zero. We first define the ratio

$$ K(z_1, z_2, t) = \frac{\mathcal{J}(z_2, t)}{\Delta T(z_1)}, \quad (18) $$

The surface conductance $K$ can be found by setting $z_1 = z_2 = 0$ for $t \to \infty$. In other words, we are interested in the dependence of the heat flux crossing the boundary on the applied temperature difference in the steady state. The average flux can be expressed in terms of the density matrix $\rho(t)$:

$$ \mathcal{J}(z_2, t) = \frac{1}{S} \int dr \text{Tr} \rho(t) \hat{J}(r, t) \delta(z - z_2) n, \quad (19) $$

where $n$ is a vector normal to the surface, $S$ is the surface area, and $\hat{J}(r, t)$ is the heat current operator.

$$ \rho(t) = \frac{1}{N} \exp \left( - \int dr \beta(r) \hat{H}(r) \right). \quad (20) $$

Here $\hat{H}$ is the Hamiltonian density, and $N$ is the normalization constant. The local inverse temperature $\beta(r)$ identifies the temperature jump at point $z_1$: $\beta(r) = 1/\left[T + \Delta T \Theta(z - z_1)\right]$ The expression for the Hamiltonian density $\hat{H}$ will be presented later. It is pertinent to note here that it does not depend on temperature and is related to the current operator through the equation of continuity: $\partial \hat{H}/\partial t + \nabla \hat{J} = 0$.

In the first order in temperature nonuniformity $\delta \beta(r) = -\beta^2 \Delta T \Theta(z - z_1)$ we obtain:

$$ \rho(t) = \rho_0 \left( 1 - \frac{1}{\beta} \int_0^\beta d\tau \int d\tau' \delta \beta(r') \left[ \hat{H}(r', -i\tau) - \langle \hat{H}(r', -i\tau) \rangle_0 \right] \right), \quad (21) $$

where $\rho_0 = \exp(-\beta \hat{H})/\text{Tr} \exp(-\beta \hat{H})$, and $\langle \cdots \rangle_0$ specifies averaging over the equilibrium state.

In calculation of the average current (19), the first and last terms of the expression for $\rho(t)$ do not contribute; using the equation of continuity for the current operator, one comes to:

$$ \mathcal{J}(z_2, t) = \frac{1}{S} \int d r d r' \text{Tr} \rho_0 \frac{1}{\beta} \int_0^\beta d\tau \int_0^t d\tau' \delta \beta(r') \nabla \hat{J}(r', -i\tau') \hat{J}(r, t) \delta(z - z_2) n. \quad (22) $$

After integrating by parts integral $r'$ and substituting the expression thus found in expression (18), we obtain in the steady state case $t \to \infty$ and close to the boundary $z_1, z_2 \to 0$:

$$ K = \frac{1}{T} \left. \pi(i\omega) \right|_{\omega \to 0} \quad (23) $$

where $\pi$ is the correlator of the heat currents incident on the surface $n\hat{J}$:

$$ \pi(i\omega) = \frac{1}{S} \int d^2 r d^2 r' \int_0^\beta d\tau e^{i\omega \tau} \langle T_r n\hat{J}(r, \tau) n\hat{J}(0, r') \rangle, \quad (24) $$

where the integrals are over the whole infinite plane at $z = 0$. The density of heat flow passing through the surface that separates the electron from the phonon gas can be readily specified by presenting
Hamiltonian (1) as a sum of the energy operators at a site \( \hat{h}_i \), i.e., the Hamiltonian density \( \hat{H} = \sum \hat{h}_i \), where

\[
\hat{h}_i = \begin{cases} 
  t/2 (\hat{c}_{i+1}^+ \hat{c}_i + \hat{c}_i^+ \hat{c}_{i+1}) & i < 0 \\
  t/2 (\hat{c}_{i-1}^+ \hat{c}_i + \hat{c}_i^+ \hat{c}_{i-1}) + \gamma \hat{n}_0 \hat{c}_i + \omega_0/2(p_i^2 + x_i^2) - \omega_0/4x_0x_1 & i = 0 \\
  \omega_0/2(p_i^2 + x_i^2) - \omega_0/4(x_i x_{i+1} + x_{i-1} x_i) & i > 0
\end{cases}
\] (25)

In this case, the heat current operator \( \hat{J} = i \sum_{lm} \mathbf{R}_l [\hat{h}_m; \hat{h}_l] - \mu \mathbf{J}_e \), where \( \mathbf{R}_l \) are the site position and \( \mathbf{J}_e \) are the electron current operator (see Ref. [44]). The only term proportional to the energy of interaction between the electrons and phonons \( \gamma \) specifies the heat flow passing through the boundary:

\[
\mathbf{nJ} = i \frac{1}{2} \gamma t (\hat{c}_{i-1}^+ \hat{c}_0 - \hat{c}_0^+ \hat{c}_{i-1}) x_0.
\] (26)

Substituting the expression for the energy current operator into the correlation function (24) and averaging using Wick’s theorem, we come to

\[
\pi(i\omega) = \frac{1}{4} \gamma^2 t^2 a^2 \int_0^\beta d\tau e^{i\omega t} \mathcal{D}_{00}(\tau) (\mathcal{G}_{00}(\tau)\mathcal{G}_{11}(-\tau) + \mathcal{G}_{11}(\tau)\mathcal{G}_{00}(-\tau) - 2\mathcal{G}_{01}(\tau)\mathcal{G}_{10}(-\tau)).
\] (27)

One can readily demonstrate the validity of the following relation

\[
\int_0^\beta d\tau e^{i\omega t} \mathcal{G}_a(\tau)\mathcal{G}_b(-\tau)\mathcal{D}_\gamma(\tau) = \int \frac{d\varepsilon_a}{2\pi} \frac{d\varepsilon_\beta}{2\pi} A_a(\varepsilon_a) A_\beta(\varepsilon_\beta) \mathcal{B}_\gamma(\omega') \times n_F(\varepsilon_\beta - \omega') - n_F(\varepsilon_a)(n_B(\omega') + n_F(\varepsilon_\beta)),
\] (28)

where \( n_F, n_B \) are the Fermi–Dirac and Bose–Einstein distribution functions. Expressing correlator (27) through the spectral functions and substituting it into expression (23) leads us to:

\[
K = -\frac{\pi}{4T} \gamma^2 t^2 a^2 \int \frac{d\omega'}{2\pi} B_{00}(\omega') \int \frac{d\varepsilon_\beta}{2\pi} \frac{\partial n_F(\varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon - \omega} (n_B(\omega') + n_F(\varepsilon_\beta)) \times \left[A_{00}(\varepsilon_\beta - \omega') A_{-1,-1}(\varepsilon_\beta) + A_{-1,-1}(\varepsilon_\beta - \omega') A_{00}(\varepsilon_\beta) - 2A_{-1,0}(\varepsilon_\beta - \omega') A_{-1,0}(\varepsilon_\beta)\right].
\] (29)

Figure 4 displays graphically this dependence of surface conductance on temperature for various interaction parameters \( \gamma \), for both the metallic and semimetallic cases. This relation becomes substantially simplified in the cases under consideration here.

We first note that \( d n_F(x)/dx = -\delta(x) \), and also \( n_B(x) + n_F(x) = 1/\sinh(\beta x) \). In turn, for \( \beta \to \infty \) this function behaves as \( -\pi^2/2\beta^2 \delta(x)/dx \), and for \( \beta \to 0 \), as \( 1/\beta x \). We may also note that \( B_{00} \) is nonzero within a narrow interval of frequencies close to \( \omega_0 \); therefore \( A(\omega) \approx A(0) \), because \( \omega_0 \ll T \). This means that terms containing \( A \) can be factored out from underneath the integral sign.

We shall now consider two limiting cases: low temperatures \( \omega_0 \gg T \), for which the expression for surface conductance (29) assumes the form

\[
K = \frac{\pi}{16} \gamma^2 t^2 a^2 T \left[A_{00}(0)A_{-1,-1}(0) - A_{-1,0}^2(0)\right] \frac{\partial B_{00}(\omega)}{\partial \omega}\bigg|_0,
\] (30)

and high temperatures \( T \gg \omega_0 \):

\[
K = \frac{1}{4} \gamma^2 t^2 a^2 \left[A_{00}(0)A_{-1,1}(0) - A_{-1,0}^2(0)\right] \int \frac{d\omega}{2\pi} \frac{B_{00}(\omega)}{\omega}.
\] (31)
Fig. 4. The surface conductance \( K \) plotted versus temperature \( T \) for various electron–phonon interaction parameters \( \gamma \) for the (a) metallic and (b) semimetallic cases. The graphs are drawn in units of \( K' = \gamma^2 a^2 / (4\omega_0) \), \( \omega_0/t = 0.01 \).

As seen from the above expressions for the surface conductance, in the cases of both the metal–dielectric and semimetal–dielectric contacts the relation is linear at low temperatures and saturates at high temperatures, as observed in Fig. 4. This holds for any values of the electron–phonon interaction constants close to the boundary. For weak electron–phonon interactions, this conclusion correlates well with available experimental data [45–47] and coincides with the theoretical result obtained for metals [21].

The expression obtained earlier for the derivative (17) can be complemented with another one for the integral of the phonon spectral function:

\[
\int \frac{d\omega}{2\pi} \frac{B_{00}(\omega)}{\omega} = \frac{1}{\omega_0} \left( 1 - \frac{\gamma^2}{\omega_0} \Re \Pi(0) - \frac{2\sqrt{2}}{15\pi} \gamma^2 A^2(0) \right). \tag{32}
\]

Thus, the system of equations produced [(8), (14), (17), (30)–(32)] provides a complete solution to the problem of the dependence of thermal resistance on the electron–phonon interaction constant.

The above approach permits one to calculate readily the dependence of thermal resistance on the effective electron–phonon interaction constant in the metallic and semimetallic cases, at temperatures both higher and lower than the characteristic phonon frequencies \( \omega_0 \).

Figures 5(a) and 5(b) plot these dependences for low and high temperatures, accordingly, for the metallic case. We see immediately that they follow practically the same pattern. This was only to be expected, because the dependences on \( \lambda \) of the relations (32) and (17) are practically identical.

While for small interaction coefficients the thermal conductivity scales as \( \approx \lambda^2 \), at large \( \lambda \) it reaches saturation. The explanation for the latter feature lies in the fact that at large interaction parameters electrons and phonons find it energetically preferable to reside close to the interaction region.

Figures 5(c) and 5(d) plot surface conductance for the semimetallic case in the low- and high-temperature domains, respectively. These curves are seen to practically coincide, for the same reasons as in the metallic case. For small parameters of interaction among electrons and phonons, the surface conductance varies in an essentially nonlinear pattern, more specifically, as \( \approx \exp(-t^2/\lambda^2) \), while at large \( \lambda \) it saturates, as it does in the metallic case. Apart from the essentially different behavior at zero, the semimetallic case differs from the metallic one in the values of the \( \lambda \) parameter at which the transition to saturation becomes evident. We readily see that in the semimetallic case saturation is
Fig. 5. The surface conductance $K$ of the metal–dielectric boundary in the (a) low- and (b) high-temperature cases plotted versus the renormalized electron–phonon interaction constant $\lambda$, and the surface conductance $K$ of the semimetal–dielectric boundary in the (c) low- and (d) high-temperature cases plotted versus the renormalized electron–phonon interaction constant $\lambda$. The graphs are drawn in units of $K_0 = (\pi/8)(t^2a^2/\omega_0)T/\omega_0$, $K_1 = t^2a^2/(4\omega_0)$, $\omega_0/t = 0.01$.

approached at large values of $\lambda$. This should be assigned to the fact that only at $\lambda \approx t$ does electron–phonon coupling become strong enough to result in a high enough electron concentration comparable to that in the metallic case.

4. Conclusion

Thus we have succeeded in “summing up” for the adiabatic case the solution for the electron Green’s function derived by Cini’s method. We have obtained an analytic expression for the density of states of electrons and phonons in a 1D system for the case of local electron–phonon interaction.

A careful analysis of the phonon density of states suggests a firm conclusion that in the metallic and semimetal cases, as the local electron–phonon interaction constant increases, the low-energy phonon modes harden, and the high-energy phonon modes soften. These effects should become manifest, as has been demonstrated, for instance, in Ref. [48], in the Raman spectra of such systems.

Basically, the approach proposed for the calculation of thermal resistance at the boundary between the electron and phonon subsystems is applicable for arbitrary parameters of a system, in both the adiabatic and nonadiabatic cases.

The exact solution obtained in the adiabatic case for Green’s function for electrons and phonons made it possible to derive the relation for thermal conductance of the boundary, which covered a broad range of temperatures and electron–phonon interaction parameters, both in the metallic and semimetallic cases. This offers the possibility of answering a number of questions not treated in earlier publications [18–21], which considered only the case of weak electron–phonon interaction at the metal–dielectric boundary.

We have shown that the behavior with temperature of the thermal conductance does not qualitatively depend on the electron–phonon interaction constant. At high electron–phonon interaction
Table 1. Main results.

| Parameters             | Semimetal \((\mu = -2t)\) | Metal \((\mu = 0)\) |
|------------------------|-----------------------------|---------------------|
| \(\gamma_c/\sqrt{\omega_0 t}\) | 5.4                         | 1.1                 |

- **phonons**
  - low frequency hardening
  - high frequency softening

- **\(K\)**
  - \(T \to 0\) saturation at \(T \gtrsim 0.5\omega_0\)
  - \(T \to \infty\) \(\sim T\)
  - \(\lambda \to 0\) \(\exp(-\lambda^2/t^2)\)
  - \(\lambda \to \infty\) saturation at \(\lambda \gtrsim t\)

constants, just as at low ones, thermal conductance grows with increasing temperature, to reach saturation at temperatures on the order of the characteristic phonon energies (see Table 1).

Earlier publications [18–21] seemed to suggest that thermal conductance should grow indefinitely with increasing electron–phonon interaction constant. We have shown that, at a strong electron–phonon interaction, thermal conductance should reach saturation.

In addition, in contrast to earlier publications, we have studied the dependence of thermal conductance on the electron–phonon interaction coefficient for both the metallic and semimetallic cases. These two cases should reveal a significant difference both in the strong dependence of thermal conductance on the electron–phonon interaction coefficient—indeed, at coefficients in excess of the critical level, thermal conductance grows sharply—and in the characteristic magnitude of this conductance.

**Acknowledgments**

The author owes sincere gratitude to A. Ya. Vul’ for helpful advice and assistance provided in the course of the work. Financial support from the Dynasty Foundation, RFBR (No. 12-02-31518, No. 12-08-00174), and the Ministry of Education and Science of Russia (project number 8621) is gratefully acknowledged.

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