Transfer of Heat between Electrons and Phonons in Metallic Nanostructures

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Abstract— It is demonstrated explicitly on an example relevant for nano- and micro-scale sensors, bolometric and microcaloric devices how the nano-scale confinement of electron and phonon subsystems affects their coupling and heat exchange. The temperature dependence of the transferred power, \( P(T) \), is considered for a layered metal-insulator structure. It is shown that below the phonon crossover temperature \( T^* \) the heat transfer is strongly enhanced while its \( T \)-dependence becomes weaker than in the bulk material. The phonon modes responsible for this enhancement are identified and the analytic form of \( P(T) \) is derived, which suggests ways of controlling the heat flux. Quantitative accuracy is confirmed by comparing to the results of recent experiments.

Keywords— Enter up to five keywords and separate them by commas.

I. INTRODUCTION

Coupling of electrons to oscillations of the ion lattice, \( He_p \), in nanodevices is an area of active research for both practical and fundamental reasons [1]. For example, nanosensors serve various medicinal purposes or as gateways to building other nanoproducts, such as computer chips that work at the nanoscale, e.g. nanorobots. Electronic and thermal properties of all such devices are qualitatively different from their macroscopic analogs. The fundamental reason is that excitation spectra of electrons and phonons, as well as their coupling differ significantly from the bulk material and understanding this modification remains an open issue. Of particular interest is a non-equilibrium situation, commonly realized in nanoelectronic cooling or sensing devices [2] with a typical setup including a metallic element (e.g. a copper nanostrip) mounted on an insulating support element (e.g. a silicone-nitride thin film).

When a current is injected into a metallic strip, the main electron energy dissipation mechanism consists in emission and absorption of phonons. In a stationary regime each of the subsystems is characterized by its own temperature, \( T_e \) and \( T_p \), and the heat flux is proportional to their difference. The key characteristics of the heat balance is the temperature dependent power \( P(T) \) transferred from the heated electron gas to the lattice. In earlier studies, [3], this process has been described theoretically for a bulk metal, resulting in the following expression:

\[
P_{3D} = \Sigma_{3D} V_e (T_e - T_p)^5,
\]

where \( V_e \) is the volume of the sample and \( \Sigma_{3D} \) is determined by the deformation potential coupling which relates the mass density \( \rho \) fluctuations to variation of the Fermi energy \( E_F \):

\[
\Sigma_{3D} = 0.01 \cdot k_F^4 \cdot k_B^5 / (\hbar^3 c_\perp^4 \rho).
\]

Here \( k_F \) is the length of the Fermi wavevector, \( k_B \) – the Boltzmann constant, \( c_\perp \) - longitudinal sound velocity. The temperature dependence (1) fits well the experimentally observed behavior, however the predicted values of \( \Sigma \) are an order of magnitude smaller than in real metals, \( \sim 10^{-8} W K^{-5} m^{-3} \). In [4] an experimentally more realistic situation has been considered, when a thin metallic film is deposited on a bulky insulating substrate. Although the interface introduces a thermal (Kapitza) resistance, this can be neglected at the low temperatures considered, when the dominating thermal phonon wavelength is much longer than the width of the metallic film. More importantly, the phonon spectrum itself is strongly modified: for a semi-infinite medium geometry there exist 5 types of eigen-modes, of which the Rayleigh surface waves become most important. As a result the authors have found a dependence \( \sim T^x \), where \( x > 5 \) in Eq. (1), a behavior which was also observed in some experiments with a thick insulating support layer. Nevertheless, the large discrepancy for the magnitude of the heat flux, i.e. still a too small value of \( \Sigma \), remains unexplained suggesting existence of an additional scattering mechanism.

On the other hand, a non-integer exponent \( x < 5 \) has been reported, see e.g. [5, 6], for thinner layered structures with an overall thickness \( L \) below 100 nm (we have reserved “d” for the metal film). It can be seen that the latter enters the range of the thermal phonon wavelength at a crossover temperature,

\[
T^* \simeq \tau v_A \hbar / (k_B L) \sim 1 K,
\]

where the phonon sub-system becomes quasi two-dimensional. Respectively, for layers thinner than 10 nm this temperature can reach some dozens of Kelvin. The phonon spectrum is then drastically modified by scattering and reflection from the boundaries as known from the theory of elastic plates [1]. Such nanoscopic systems have been investigated in the context of semiconductor heterostructures [7], e.g. Ge/SiGe, where due to confinement also the charge
carriers show a quasi two-dimensional behavior: a quantum well (QW) state. It has been shown that \( H_{ep} \) essentially involves only the Lamb vibrational modes and of these just the flexural ones account for the electron scattering rate, \( \tau^{-1} \).

This theory is based on the outstanding feature of the scattering acoustic Lamb waves of having quadratic (instead of standard linear) low energy dispersion. This ensures a high density of states, which, in turn, provides an enhanced coupling to electron excitations. But how does the scattering rate translate into the actual heat transfer, i.e. \( P(T) \) behavior, remains unknown. This is an important question since excitations which actually count at low temperatures are those with long wavelength and the phonons with quadratic dispersion have a vanishing group velocity.

Moreover, for metallic nanostructures electron coupling to the Lamb modes has not been considered so far, i.e. both qualitative and quantitative understanding is missing. For instance, unlike semiconductors, the QW state is very rare in metals and has actually been observed only in ultrathin films. Because of the much shorter Fermi wavelength, i.e. \( \hbar k_F >> 1 \), a more common situation in metals corresponds to the 3D Fermi gas (FG). One of the consequences is that electrons can now be scattered also in the direction transverse to the propagation of Lamb waves, i.e. into the thickness of the layer. We will therefore mainly focus our discussion to the 3D FG case.

II. NORMALIZATION AND ELECTRON–PHONON COUPLING

The Hamiltonian describing our system is

\[
H = \sum_k E(k) c_k^\dagger c_k + \sum_q \hbar \omega(q) a_q^\dagger a_q + H_{ep},
\]

where electron \( (c_k) \) and phonon \( (a_q) \) annihilation operators with respective wave-vectors, \( k \) and \( q \), and dispersions \( E(k) \) and \( \omega(q) \) – solutions of the Schrödinger and continuum elasticity equations subject to the considered boundary conditions, see details in [7,9]. Since the transverse size of our system is comparable to thermal phonon wavelength, a single phonon distribution may be assumed for the whole sample viewed as a single elastic plate of volume \( L \cdot A \) and mass \( M \), where \( A \) is the surface of the plate. The electron wave function \( \Psi \) is normalized over the volume \( V_{el} = dA \) and coupling to phonons is:

\[
H_{ep} = \frac{2}{3} E_F \int_{V_{el}} d^3r \, \Psi^\dagger(r) \psi(r) \nabla \cdot u(r).
\]

The displacement field \( u(r) \) has only \((x,z)\) components and is expanded in eigenmodes, \( \xi \), with in-plane \((x,y)\) momentum \( q_\parallel \):

\[
u(r,t) = \sum_{\xi \parallel} \sqrt{\frac{\hbar}{2 M \omega(q_\parallel)}} \left[ u_{\xi}(t) + i a_{\xi}^\dagger(t) \right] u_{\xi}(q_\parallel, z) \exp \left( i (q_\parallel r - i \omega t) \right). \tag{6}
\]

Proper normalization is crucial for transport phenomena and in (6) it is fixed by orthonormality of the amplitudes \( u_{\xi}(q,z) \) on \( z = [-L / 2, L / 2] \). With this choice the flexural eigenmodes are antisymmetric \((\alpha)\) upon reflection with respect to the \( z = 0 \) plane while dilatational modes are symmetric \((\sigma)\) (explicit expressions to be given elsewhere).

The respective solutions of the Lamb eigenenergy equations

\[
\frac{4q^2 p_{\parallel}^2}{(q^2 - q_\parallel^2)^2} = \tan(\pi L / 2) \tan(\pi L / 2), \quad \frac{4q^2 p_{\parallel}^2}{(q^2 + p_{\parallel}^2)^2} = \tan(\pi L / 2) \tan(\pi L / 2), \tag{7}
\]

depend on the auxiliary parameters \( q \) and \( p_{\parallel} \) determined by (7) and which also appear in the dispersion relation

\[
\omega(q) = c_\| \sqrt{q^2 - p_{\parallel}^2} = c_\| \sqrt{q^2 + p_{\parallel}^2},
\]

where \( c_\parallel \) are the longitudinal and transverse sound velocities with the ratio \( v = (c_\| / c_\|)^2 < 0.5 \). Fortunately, from the whole sophisticated set of solutions of (7) we can separate analytically the acoustic branches to account for the low temperature properties of the system:

\[
\begin{align*}
\omega_\sigma &\approx 2q c_\| \sqrt{1 - \nu}, \quad q_\parallel^2 \approx q \sqrt{3 - 4 \nu}, \quad p_{\parallel}^2 \approx q (1 - 2 \nu); \\
\omega_\sigma &\approx q^2 L c_\| \sqrt{(1 - \nu) / 3}, \\
p_{\parallel}^3 &\approx -q + q^3 L^2 (1 - \nu) / 6, \quad p_{\parallel}^3 \approx -q + q^3 L^2 (1 - \nu) / 6.
\end{align*}
\]

The electron-phonon matrix element of the \( H_{ep} \) (4) describing emission and absorption of such a phonon with electron scattering from an initial state \( \Psi_n \) to a final state \( \Psi_m \) is given by

\[
|g_{m,n}^{\alpha,\beta}|^2 = \frac{8 \pi \hbar E_F^2}{9 M \omega_\xi}, \tag{9}
\]

where \( F_{\xi} \) have absorbed the normalization factors:

\[
F_\xi = \sqrt{\int \left( q^3 - p_{\parallel}^2 \right)^2 \cos^2 (L q_\parallel / 2) / \sqrt{16 q^6 (3 - 4 \nu) (1 - \nu)^3}}, \\
F_\parallel = 6 | \int \sin^2 (L p_{\parallel} / 2) / (q^2 L^3 (1 - \nu)).
\]

The \( S \) - function in (8) is the overlap integral between the \( z \)-components of the electron wave functions modulated by the phonon displacement field:

\[
S(m, n, \xi, \nu) = \int_{L / 2}^{L / 2} \phi_\sigma(z) \phi_\sigma(z) \left| \begin{array}{c}
\cos \left( \frac{\pi L}{2} \right) \xi \sinh (z) \\
\sin \left( \frac{\pi L}{2} \right) \xi \sinh (z)
\end{array} \right| dz^2.
\]

The wave function \( \phi(z) \) for the 3D Fermi gas is a plane wave.