Effect of electronic disorder on phonon-drag thermopower

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Using the quantum-transport equation and Keldysh diagrammatic technique, we investigate the phonon-drag thermopower in a disordered conductor. We consider phonon drag of three-dimensional electrons, which interact with longitudinal phonons via the deformation potential. The scattering potential of impurities, boundaries, and defects is modeled by quasistatic scatterers and vibrating scatterers, which move in the same way as host atoms. In thin films and nanostructures the phonons relax mainly in a substrate, and the phonon-drag thermopower substantially depends on the character of electron scatterers. Vibrating scatterers decrease thermopower, while static scatterers, such as rigid boundaries and heavy impurities, increase it. These changes in thermopower correlate to the disorder-induced modification of the electron-phonon relaxation rate. In bulk conductors, phonon-electron scattering dominates in the phonon relaxation, and the phonon-drag thermopower just slightly varies with electron mean free path.

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I. INTRODUCTION

Quantum transport in disordered systems has been studied for many years, yet many open problems remain. One focus of these investigations is the disorder-induced modification of the electron-electron and electron-phonon interactions.[1–5] Quantum interference of scattering processes violates the Mathiessen rule, according to which the contributions to transport coefficients due to a random potential and phonons are additive.[2,6] The quantum transport equation based on the Keldysh technique has been quite successful in describing transport phenomena, such as the electron relaxation/dephasing and temperature-dependent conductivity.[2–4,6–8]

The electron-phonon interaction is drastically modified in disordered conductors. In processes of ''pure'' electron-phonon scattering the transferred momentum is of the order of the wave vector of a thermal phonon, $q_T=T/u$ (u is the sound velocity), and the region of the interaction is $\sim 1/q_T$. Elastic electron scattering confines an electron to the interaction region. Diffusive electron motion increases the electron-phonon interaction time to $\sim Dq^2$ (D is the diffusion coefficient) and enhances the interaction. Electron scattering from vibrating impurities and boundaries generates another channel of the electron-phonon interaction in a disordered conductor. Various scattering processes interfere with one another, and the interference results in nontrivial changes of kinetic and transport coefficients. If impurities and boundaries vibrate in the same way as the host lattice, the electron-phonon relaxation rate is decreased by a factor of $q_T l$ ($q_T l \ll 1$, l is the electron mean free path) compared with the rate in a pure bulk material.[1,3,9] This statement is well known as Pippard ineffectiveness condition.[10] On the contrary, in the presence of a quasistatic scattering potential of rigid boundaries or heavy impurities, the relaxation rate is enhanced by the same factor.[2,8] Even in the pure limit, $q_T l \gg 1$, electron scattering from static or vibrating potentials changes the temperature-dependent resistivity from T^5 to T^2, and the T^2 term is proportional to the residual resistivity.[2,6,11] Effects of the electronic disorder cannot be described in terms of the effective electron-phonon matrix element. The quantum-transport equation or Kubo method can be employed to take into account the interference of scattering processes in disordered conductors.

The purpose of this paper is to investigate the effect of the elastic electron scattering on the phonon-drag thermopower. In the pure case, $q_T l \gg 1$, the thermoelectric coefficient, $\eta = -J_e/\nabla T$, is given by[12–14] (for details see Sec. III)

$$\eta_0 = -\frac{b_n}{3\pi}\frac{e\beta\tau\tau_{\rm ph}(T)T^4}{p_F u^2}, \tag{1}$$

where τ is the electron momentum relaxation time, the $\tau_{\rm ph}$ is the lifetime of a thermal phonon with frequency $\omega_q = T$, β is the dimensionless electron-phonon coupling constant, p_F is the Fermi momentum, n the exponent in the frequency dependence of the phonon relaxation rate ($\tau_{\rm ph}^{-1} \propto \omega_q^n$), and b_n is the numeric coefficient

$$b_n = \int_0^\infty dx\, x^{5-n}\frac{\partial N(x)}{\partial x}, \tag{2}$$

$N(x) = [\exp(x)-1]^{-1}$. In a degenerate conductor, the electron-phonon coupling constant is given by

$$\beta = \left(\frac{2\epsilon_F}{3}\right)^2 \frac{\nu}{2\rho u^2}, \tag{3}$$

where ϵ_F is the Fermi energy, ν is the electron density of states at the Fermi surface, and ρ is the density.

The measured transport coefficient is the phonon-drag thermopower, $S = -\eta/\sigma$, where σ is the electrical conductivity. Considering the phonon drag in disordered systems, we accept that the main mechanism of the electron momentum relaxation is scattering from boundaries and impurities. The electrical conductivity is given by Drude formula, $\sigma = e^2 \nu v_F l/3$, where v_F is the Fermi velocity. Thus, in the pure limit, $q_T l \gg 1$, the phonon-drag thermopower is independent of the electron mean free path

$$S_0^{\rm dr} = \frac{\pi b_n \beta \tau_{\rm ph}(T) T^4}{2e\epsilon_F (p_F u)^2}. \tag{4}$$

In the pure limit, $q_T l \gg 1$, the phonon-electron scattering time is[9]

$$\tau_{\text{ph-}e}(T) = \frac{v_F}{\pi \beta u T}, \tag{5}$$

and $b_1 = 4\pi^4/15$.

Thus, if the phonon-electron scattering dominates in the phonon relaxation, $\tau_{\text{ph}} = \tau_{\text{ph-e}}$, the thermoelectric coefficient is given by the well-known Gurevitch formula[12–14]

$$\eta_0^{\text{ph-e}} = -\frac{2\pi^2}{45}\frac{eT^3 l}{p_F u^3}, \tag{6}$$

and thermopower is independent of electron-phonon coupling

$$S_0^{\text{ph-e}} = -\frac{\eta_0}{\sigma} = \frac{2\pi^4}{15}\frac{T^3}{e(p_F u)^3}. \tag{7}$$

In the current paper we calculate the phonon-drag thermopower in a disordered conductor. We consider three-dimensional (3D) electrons interacting with longitudinal phonons via the deformation potential, which is renormalized by elastic electron scattering. We study the effects of quasistatic and vibrating scattering potentials. The quasistatic potential models rigid boundaries and heavy impurities. The vibrating potential that moves in the same way as host atoms corresponds to the Pippard model. Note, that in the pure limit, $q_T l \ll 1$, correction to the thermopower due to inelastic electron-impurity scattering has been calculated in Ref. 15. Here we take into account all processes of the electron-phonon-impurity/boundary interference at an arbitrary concentration of electron scatterers.

To solve this problem we use the following methods. First, we employ the quantum-transport equation. The transport equation deals only with electron self-energy diagrams, while the linear-response methods require more complicated diagrams to be considered.[6] Second, to find the phonon-drag thermoelectric coefficient, we will calculate the electric current of electrons as a response to the temperature gradient in the phonon subsystems. Note, that the symmetric problem of the phonon thermal flux due to the electric field turns out to be significantly more difficult, because one should take into account specific terms in the form of Poisson brackets.[2,6] According to the Onsager relation, both approaches give the same result for the thermoelectric coefficient. Third, in considering the vibrating potential, we will employ the Tsuneto transformation,[16] which allows one to simplify the electron-phonon-impurity Hamiltonian.[1]

The outline of this paper is as follows. In the following section we obtain the quantum-transport equation, which will be used to calculate the electric current under the phonon temperature gradient. In Sec. III we investigate the effect of static scatterers on the drag thermopower. In Sec. IV we study the effect of vibrating scatterers. Discussion of our main results is presented in Sec. V.

II. TRANSPORT EQUATION

To find the phonon-drag thermoelectric coefficient η^{dr} we will calculate the electric current as a response to the temperature gradient in the phonon subsystems ∇T_{ph}

$$\mathbf{J}_e = \sigma \mathbf{E} + \eta^{\text{dr}} \nabla T_{\text{ph}} + \eta^{\text{df}} \nabla T_e. \tag{8}$$

The last term with the electronic diffusion thermoelectric coefficient η^{df} describes the response to the temperature gradient in the electron subsystem ∇T_e.

We use the quantum-transport equation method developed in Ref. 2 (for review see Ref. 4) and then generalized in Ref. 17 for thermoelectric phenomena (details may be found in Refs. 18 and 19). This method is based on the Keldysh diagrammatic technique for nonequilibrium processes. In the Keldysh technique the phonon and electron Green functions, $\hat{D}$ and $\hat{G}$, and the electron self-energy $\hat{\Sigma}$ are represented by matrices

$$\hat{D} = \begin{pmatrix} 0 & D^A \\ D^R & D^C \end{pmatrix}, \quad \hat{\Sigma} = \begin{pmatrix} \Sigma^C & \Sigma^R \\ \Sigma^A & 0 \end{pmatrix}. \tag{9}$$

Every matrix consists of three nonzero components: retarded (R), advanced (A) and kinetic (C) functions.

Assuming that the phonon spectrum ω_q has been renormalized due to the electron-phonon interaction, we may present the retarded component of the phonon Green functions as

$$D^R(\mathbf{q},\omega) = (\omega - \omega_{\mathbf{q}} + i0)^{-1} - (\omega + \omega_{\mathbf{q}} + i0)^{-1}. \tag{10}$$

In the presence of the temperature gradient the kinetic-phonon Green function is given by

$$D^C(\mathbf{q},\omega) = 2iF(\mathbf{q},\omega)\,\text{Im}\,D^R(\mathbf{q},\omega) + \delta D^C(\mathbf{q},\omega) \tag{11}$$

The second term in Eq. (11) has the form of the Poisson bracket

$$\delta D^C(\mathbf{q},\omega) = \frac{i}{2}\{\text{Re}\,D^R(\mathbf{q},\omega), F(\omega, T(r))\}, \tag{12}$$

$$\{A,B\} = \nabla T\left(\frac{\partial A}{\partial T}\frac{\partial B}{\partial \mathbf{q}} - \frac{\partial B}{\partial T}\frac{\partial A}{\partial \mathbf{q}}\right). \tag{13}$$

Thus, $\delta D^C(\mathbf{q},\omega)$ is proportional to $(D^{R,A})^2$ and may be neglected.

The phonon distribution function is given by

$$F(\mathbf{q},\omega) = F_0(\omega) + F_1(\mathbf{q},\omega), \tag{14}$$

$$F_0(\omega) = 2N_\omega + 1 = \coth(\omega/2T), \tag{15}$$

$$F_1(\mathbf{q},\omega) = \frac{\omega}{T}\frac{\partial(2N_\omega+1)}{\partial\omega}\tau_{\text{ph}}\mathbf{u}\nabla T_{\text{ph}}, \tag{16}$$

where $F_0(\omega)$ is the equilibrium distribution function, $F_1(\mathbf{q},\omega)$ is the nonequilibrium function, which is proportional to ∇T_{ph},[12,13] and τ_{ph} is the phonon momentum relaxation time.

Our aim is to calculate the electric current initiated by the temperature gradient in the phonon system

$$\mathbf{J}_e = \sigma^{\mathrm{dr}} \boldsymbol{\nabla} T = 2e \int \frac{d\mathbf{p}\, d\epsilon}{(2\pi)^4} \mathbf{v} S(\mathbf{p},\epsilon) \mathrm{Im}\, G^A(\mathbf{p},\epsilon), \quad (17)$$

where $\mathbf{v}$ is the electron velocity, and $S(\mathbf{p},\epsilon)$ is the electron distribution function, which will be found from the quantum-transport equation.

The retarded (advanced) component of the electron Green function, taking into account the elastic electron scattering, is given by

$$G_0^R(\mathbf{p},\epsilon)[G_0^A(\mathbf{p},\epsilon)]^* = (\epsilon - \xi_p + i/2\tau)^{-1}, \quad (18)$$

where $\xi_p = (p^2 - p_F^2)/2m$. The momentum relaxation rate $1/\tau$ is determined by electron scattering from impurities, defects, and boundaries.

In equilibrium, the electron distribution function is $S_0(\epsilon) = -\tanh(\epsilon/T)$. In the presence of the temperature gradient, the electron distribution function $S(\mathbf{p},\epsilon)$ is determined from the transport equation

$$-(\mathbf{v}\cdot\boldsymbol{\nabla} T_e)\frac{\epsilon}{T}\frac{\partial S}{\partial \epsilon} = I_{\text{e-imp}}[S] + I_{\text{e-ph-imp}}[S,F], \quad (19)$$

where $I_{\text{e-imp}}$ and $I_{\text{e-ph-imp}}$ are the collision integrals: $I_{\text{e-imp}}$ describes the electron-impurity (boundary) scattering, and $I_{\text{e-ph-imp}}$ takes into account electron-phonon scattering and all interference processes. As we discussed above, the electronic diffusion thermopower is conditioned by the temperature gradient in the electron subsystem ($\boldsymbol{\nabla} T_e$), while the phonon drag thermopower arises due to the temperature gradient in the phonon subsystem. In the kinetic equation for electron distribution function, the phonon temperature appears only in the collision integral $I_{\text{e-ph-imp}}[S,F(T_{\text{ph}})]$. Assuming that the elastic electron scattering from impurities, boundaries, and defects dominates in the electron momentum relaxation, one can linearize the transport equation in the following way:

$$I_{\text{e-imp}}[\phi] + I_{\text{e-ph-imp}}[S_0 F_1] = 0, \quad (20)$$

where $\phi(\mathbf{p},\epsilon)$ is the nonequilibrium electron distribution function. Employing τ approximation for electron-impurity scattering, we get

$$\phi(\mathbf{p},\epsilon) = \tau I_{\text{e-ph-imp}}[S_0, F_1]. \quad (21)$$

The collision integral is expressed through the electron self-energy as

$$I_{\text{e-ph-imp}} = -i[\Sigma^C - S(\Sigma^A - \Sigma^R)]. \quad (22)$$

The nonequilibrium corrections in the form of the Poisson bracket between Σ and G are absent, because we consider response to the temperature gradient in the phonon subsystem. Using powerful arsenal of the Keldysh diagrammatic technique, we calculate the corresponding electron self-energies and find $\phi(\mathbf{p},\epsilon)$ in the following sections.

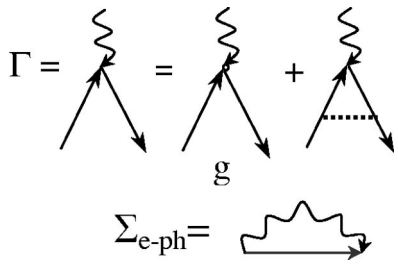

FIG. 1. Renormalization of the electron-phonon vertex due to elastic electron scattering. Electron self-energy diagram.

III. STATIC ELECTRON SCATTERERS

Heavy impurities and rigid boundaries may be considered as quasistatic electron scatterers. In the model with static scatterers the electron-phonon interaction is renormalized via elastic scattering in the same way as the electron-electron interaction.[2,5,8] We consider the Hamiltonian, which includes electron-phonon interaction and electron scattering from static potential

$$H_{\text{int}} = \sum_{p,q} g(\mathbf{q}) c^\dagger_{\mathbf{p}+\mathbf{q}} c_{\mathbf{p}} (b_{\mathbf{q},n} + b^+_{-\mathbf{q},n}) + \sum_{\mathbf{p},\mathbf{k}\cdot\mathbf{R}_\alpha} V(\mathbf{k}) c^\dagger_{\mathbf{p}+\mathbf{k}} c_{\mathbf{p}} \exp(-i\mathbf{k}\cdot\mathbf{R}_\alpha), \quad (23)$$

where $c^\dagger_{\mathbf{p}}$ is the electron creation operator, $b^\dagger_{\mathbf{q},n}$ is the creation operator of a phonon with a wave vector $\mathbf{q}$ and polarization index n, $V(\mathbf{k})$ is the scattering potential, and $\mathbf{R}_\alpha$ are the positions of static scatterers.

The vertex of the electron-phonon interaction is given by

$$g = \frac{2\epsilon_F}{3}\frac{\mathbf{q}\cdot\mathbf{e}_n}{(2\rho\omega)^{1/2}} K^k_{ij}, \quad (24)$$

where ϵ_F is the Fermi energy, $\mathbf{e}_n$ is the phonon polarization vector, and ρ is the density.

In the Keldysh technique, vertices are tensors with an upper phonon index and lower electron indices in the Keldysh space. The vertex $\hat{g}$ is given by

$$\hat{g} = g K^k_{ij}, \quad (25)$$

where $K^1_{ij} = \delta_{ij}/\sqrt{2}$, and $K^2_{ij} = (\sigma_x)_{ij}/\sqrt{2}$. In what follows, we will present vertex components with phonon index $k=2$, because only these components give a term with $D_{22} = D^C$, which is proportional to the phonon distribution function, i.e., to the phonon temperature gradient.

The vertex of elastic electron scattering may be expressed through the corresponding momentum relaxation rate

$$\tau^{-1} = \pi \nu N_{\text{sc}} V^2, \quad (26)$$

where N_{sc} is the concentration of short-range scatterers.

Diffusion enhancement of the electron-phonon interaction is described by the vertex dressed by ''impurity'' ladder (see Fig. 1). The dressed vertex is given by

$$\Gamma^2_{22}=0, \quad \Gamma^2_{12}=\Gamma^2_{12}=ig/\sqrt{2},$$

$$\Gamma^2_{11}=\frac{ig}{\sqrt{2}}\frac{1}{1-\zeta_0^*}[S_0(\epsilon+\omega)-S_0(\epsilon)]. \tag{27}$$

Here we introduce the following notations for integrals of electrons Green functions

$$\zeta_n=\frac{1}{\pi\nu\tau}\int\frac{d\mathbf{p}}{(2\pi)^3}y^n G^A(\mathbf{p},\epsilon)G^R(\mathbf{p}+\mathbf{q},\epsilon+\omega), \tag{28}$$

where $y=\mathbf{pq}/(pq)$. The particle-hole asymmetry is described by the parameter $q/(2p_F)$. In the first order in $q/(2p_F)$ the integrals ζ_n are given by

$$\zeta_n=\int_{-1}^{1}dy\frac{y^n}{1+iql(y-q/2p_F)}\left(1-\frac{qy}{2p_F}\right). \tag{29}$$

The factor $(1-qy/2p_F)$ is due to the energy dependence of the electron density of states.

The vertex Γ^2_{11} consists of a factor $1/(1-\zeta_0^*)$, its asymptotic behavior is given by

$$\mathrm{Re}(1-\zeta_0^*)^{-1}=\begin{cases}1+\pi/(2x), & x\gg 1\\ 3/x^2, & x\ll 1,\end{cases} \tag{30}$$

$$\mathrm{Im}(1-\zeta_0^*)^{-1}=\frac{q}{2p_F}\begin{cases}\pi/(2x^2), & x\gg 1\\ 6/x^3, & x\ll 1,\end{cases} \tag{31}$$

where $x=ql$.

The electron self-energy diagram with vertices Γ is shown in Fig. 1. Calculating the electron self-energy with the nonequilibrium phonon distribution function $F_1(\mathbf{q},\omega)$ [Eq. (14)], we get

$$\mathrm{Im}\,\Sigma^A(\mathbf{p},\epsilon)=-\int\frac{d\mathbf{q}\,d\omega}{(2\pi)^4}g^2F_1(\mathbf{q},\omega)\mathrm{Im}\,D^R(\mathbf{q},\omega)\times\mathrm{Im}\,G^A(\mathbf{p}+\mathbf{q},\epsilon+\omega), \tag{32}$$

$$\Sigma^C(\mathbf{p},\epsilon)=-2i\int\frac{d\mathbf{q}\,d\omega}{(2\pi)^4}g^2F_1(\mathbf{q},\omega)\mathrm{Im}\,D^R(\mathbf{q},\omega)\times\mathrm{Im}\frac{G^A(\mathbf{p}+\mathbf{q},\epsilon+\omega)[S_0(\epsilon+\omega)-\zeta^*S_0(\epsilon)]}{(1-\zeta^*)}. \tag{33}$$

Using Eqs. (32) and (33), we find the corresponding collision integral [Eq. (22)] and determine the nonequilibrium electron distribution function [Eq. (21)]

$$\phi_{\mathrm{st}}(\mathbf{p},\epsilon)=-2\tau\int\frac{d\mathbf{q}\,d\omega}{(2\pi)^4}g^2F_1(\mathbf{q},\omega)[S_0(\epsilon+\omega)-S_0(\epsilon)]\times\mathrm{Im}\,D^R(\mathbf{q},\omega)\mathrm{Im}[(1-\zeta^*)^{-1}G^A(\mathbf{p}+\mathbf{q},\epsilon+\omega)]. \tag{34}$$

Calculating the electric current [Eq. (17)], we find the thermoelectric coefficient

$$\eta_{\mathrm{st}}\boldsymbol{\nabla}T=2e\tau\int\frac{d\mathbf{p}\,d\mathbf{q}\,d\epsilon\,d\omega}{(2\pi)^8}\mathbf{v}F_1(\mathbf{q},\omega)[S_0(\epsilon+\omega)-S_0(\epsilon)]\times g^2\,\mathrm{Im}\,D^R(\mathbf{q},\omega)\mathrm{Re}[(1-\zeta)^{-1}G^A(\mathbf{p})G^R(\mathbf{p}+\mathbf{q})]. \tag{35}$$

Integrating the electron Green functions, we get

$$\eta_{\mathrm{st}}=\frac{e\beta_l\tau}{6\pi p_F u^2 T}\int d\omega_q\omega_q^5\frac{\partial N(\omega_q)}{\partial\omega_q}\tau_{\mathrm{ph}}(\omega_q)W_{\mathrm{st}}(ql), \tag{36}$$

where

$$W_{\mathrm{st}}(x)=\frac{2}{\pi}\frac{(x^2-1)\arctan(x)+x}{x(x-\arctan[x])}. \tag{37}$$

In the limiting cases this function is given by

$$W_{\mathrm{st}}=\begin{cases}1+\pi/(2x), & x\gg 1\\ 8/(\pi x), & x\ll 1.\end{cases} \tag{38}$$

Therefore, in the pure limit, $q_Tl\gg 1$, the correction to the thermoelectric coefficient due to elastic electron scattering is

$$\frac{\eta_{\mathrm{st}}-\eta_0}{\eta_0}=\frac{\pi}{2}\frac{b_{n-1}}{b_n}\frac{u}{Tl}. \tag{39}$$

where numeric coefficients b_n are given by Eq. (2). For $n=0$, the ratio b_{-1}/b_0 is 5.89.

In the impure limit, $q_Tl\ll 1$, the thermoelectric coefficient is given by

$$\frac{\eta_{\mathrm{st}}}{\eta_0}=\frac{8}{\pi}\frac{b_{n-1}}{b_n}\frac{u}{Tl}. \tag{40}$$

Thus, the phonon-drag thermopower in a disordered conductor with static scatterers is

$$S_{\mathrm{st}}^{\mathrm{dr}}=\frac{2b_{n-1}\beta\tau_{\mathrm{ph}}T^3}{e\tau\epsilon_F^2p_Fu}. \tag{41}$$

If phonon relaxation is determined by the phonon-electron scattering, the phonon-electron scattering time is given by[20]

$$\frac{1}{\tau_{\text{ph-}e}}=2\beta\omega_q\frac{u_l}{v_F}\frac{ql\arctan(ql)}{ql-\arctan(ql)}. \tag{42}$$

In this case the thermoelectric coefficient is

$$\eta_{\mathrm{st}}^{\text{ph-}e}=\frac{e\tau v_FT^3}{6\pi^2p_Fu^3}\int dx\,x^4\frac{\partial N(x)}{\partial x}W_{\mathrm{st}}^{\text{ph-e}}(q_Tlx), \tag{43}$$

where

$$W'_{\mathrm{st}}(y)=\frac{(y^2-1)\arctan(y)+y}{y^2\arctan(y)}. \tag{44}$$

The function $W_{\mathrm{st}}^{\text{ph-e}}(q_Tl)$ is shown in Fig. 2. As seen, it weakly depends on the electronic disorder.

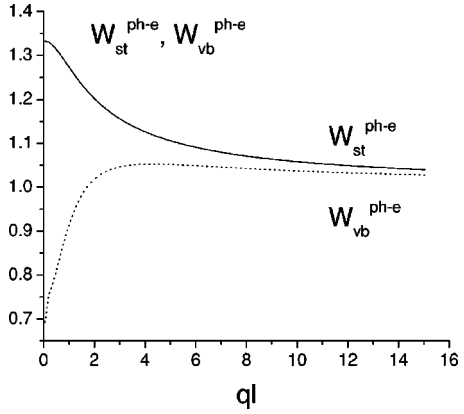

FIG. 2. Functions $W_{\rm sb}^{\rm ph\text{-}e}(ql)$ [Eqs. (43) and (44)] and $W_{\rm vb}^{\rm ph\text{-}e}(ql)$ [Eq. (61)] which describe corrections to the Gurevitch formula [Eq. (6)].

IV. VIBRATING ELECTRON SCATTERERS

Vibrating in the same way as a host lattice, electron scatterers (boundaries and impurities) weaken the electron-phonon interaction. The phonon-electron scattering rate is given by the Pippard formula[1,3,9,20]

$$\frac{1}{\tau_{\rm ph\text{-}e}}=2\beta\omega_q\frac{u_l}{v_F}\left(\frac{ql\arctan(ql)}{ql-\arctan(ql)}-\frac{3}{ql}\right). \tag{45}$$

To take into account vibrations of electron scatterers, one should define $\mathbf{R}_\alpha$ in Hamiltonian $H_{\rm int}$ [Eq. (23)] as equilibrium positions of scatterers. Also, one should add the additional term corresponding to electron scattering from the potential shifted from $\mathbf{R}_\alpha$ (Refs. 3 and 8)

$$H_{vb}=\sum_{\mathbf{p},\mathbf{k},\mathbf{q},n,\mathbf{R}_0}-iV\frac{\mathbf{k}\cdot\mathbf{e}_n}{(2\rho\omega)^{1/2}}c_{\mathbf{p}}^{\dagger}c_{\mathbf{p}-\mathbf{k}}(b_{\mathbf{q},n}+b_{-\mathbf{q},n}^{\dagger})\times\exp[-i(\mathbf{k}-\mathbf{q})\mathbf{R}_0]. \tag{46}$$

Thus, the Hamiltonian consists of three terms, which describe interactions in the electron-phonon-impurity system. This gives rise to a very complex interference picture.[3,8,20] Considering the vibrating potential, it is convenient to treat the electron-phonon interaction in the frame of reference, which moves locally with the lattice. As suggested by Tsuneto,[16] the transformation of electron coordinates is defined according to

$$r_i\rightarrow r_i+u(r_i), \tag{47}$$

where $u(r_i)$ is the displacement of the ion with a coordinate r_i. After this transformation, electron scatterers are motionless and the Hamiltonian is significantly simplified[1]

$$H_{\rm int}=\sum_{\mathbf{p},\mathbf{q}}\Gamma_0(\mathbf{q})c_{\mathbf{p}}^{\dagger}c_{\mathbf{p}-\mathbf{q}}(b_{\mathbf{q},n}+b_{-\mathbf{q},n}^{\dagger})+\sum_{\mathbf{p},\mathbf{k}\cdot\mathbf{R}_\alpha}V_{\rm sc}(\mathbf{k})c_{\mathbf{p}}^{\dagger}c_{\mathbf{p}-\mathbf{k}}\exp(-i\mathbf{k}\cdot\mathbf{R}_\alpha), \tag{48}$$

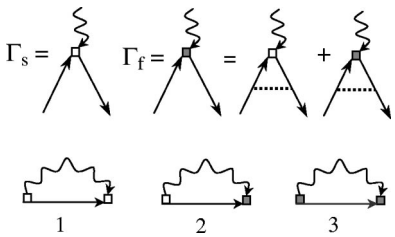

FIG. 3. Vertices and self-energy diagrams describing electron-phonon scattering in the presence of the vibrating potential of boundaries and impurities.

where Γ_0 is the vertex at which an electron is scattered from $\mathbf{p}$ to $\mathbf{p}+\mathbf{q}$,

$$\hat{\Gamma}_0=\frac{[(2\mathbf{p}+\mathbf{q})\cdot\mathbf{q}][(2\mathbf{p}+\mathbf{q})\cdot\mathbf{e}_n]}{4\rho^{1/2}\omega_q}K_{ij}^k. \tag{49}$$

Screening of the vertex Γ_0 results in the vertex[1]

$$\hat{\Gamma}_s=\hat{g}+\hat{\Gamma}_0. \tag{50}$$

As we already mentioned, after the transformation given by Eq. (47) all phonon scatterers are motionless. Therefore, the effect of elastic electron scattering is reduced to the renormalization of the vertex Γ_s by the impurity ladder, as it is shown in Fig. 3. The renormalized vertex is given by

$$(\Gamma_f)_{12}^2=(\Gamma_f)_{12}^2=(\Gamma_f)_{12}^20, \tag{51}$$

$$(\Gamma_f)_{11}^2=\frac{ig}{\sqrt{2}}\left(\tilde{\zeta}_0^*-3\tilde{\zeta}_2^*+\frac{3q}{p_F}\zeta_1^*\right)\frac{S_0(\epsilon+\omega)-S_0(\epsilon)}{1-\zeta_0^*}. \tag{52}$$

Compared to functions ζ_n [Eq. (29)], functions $\tilde{\zeta}_n$ consist of an additional factor $(1-q/p_F)$ via the energy dependence of Γ_0.

Three possible electron self-energy diagrams with vertices Γ_s and Γ_f are shown in Fig. 1. The contribution of the third diagram is zero due to the structure of $\hat{\Gamma}_f$ in the Keldysh space [see Eq. (51)].

The nonequilibrium electron distribution function [Eq. (21)] corresponding to the first diagram is given by

$$\phi_1(\mathbf{p},\epsilon)=-2\tau\int\frac{d\mathbf{q}\,d\omega}{(2\pi)^4}\Gamma_0^2F_1(\mathbf{q},\omega)[S_0(\epsilon+\omega)-S_0(\epsilon)]\times\mathrm{Im}\,D^R(\mathbf{q},\omega)\mathrm{Im}[G^A(\mathbf{p}+\mathbf{q},\epsilon+\omega)]. \tag{53}$$

The contribution of the second diagram is

$$\phi_2(\mathbf{p},\epsilon)=-2\tau\int\frac{d\mathbf{q}\,d\omega}{(2\pi)^4}g^2F_1(\mathbf{q},\omega)[S_0(\epsilon+\omega)-S_0(\epsilon)]\times\mathrm{Im}\,D^R(\mathbf{q},\omega)\mathrm{Im}\left[\frac{\tilde{\zeta}_0^*-3\tilde{\zeta}_0^*+6(q/2p_F)\zeta_1^*}{1-\zeta_0^*}\times G^A(\mathbf{p}+\mathbf{q})\right]. \tag{54}$$

Substituting the nonequilibrium distribution function, $\phi_{\rm vb}=\phi_1+\phi_2$, in Eq. (17) and integrating the electron Green functions we get

$$\eta_{\rm vb}=\frac{\epsilon\beta\tau}{6\pi p_F u^2 T}\int d\omega_q \omega_q^5 \frac{\partial N(\omega_q)}{\partial\omega_q}\tau_{\rm ph}(\omega_q)W_{\rm vb}(ql), \tag{55}$$

where

$$W_{\rm vb}(x)=2[(-5x^6-11x^4+39x^2+15)[\arctan(x)]^2 +(5x^7+17x^5-78x^3-90x)\arctan(x)-11x^6 +39x^4+45x^2]/[\pi x^3(1+x^2)\{x-\arctan(x)\}^2]. \tag{56}$$

In the limiting cases this function is given by

$$W_{\rm vb}=\begin{cases}1+[\pi/2-32/(5\pi)]/x, & x\gg 1\\ 104x/(\pi 175), & x\ll 1\end{cases}. \tag{57}$$

In the pure limit, $q_T l\gg 1$, the correction to the thermoelectric coefficient due to elastic electron scattering is

$$\frac{\eta_{\rm vb}-\eta_0}{\eta_0}=\left(\frac{\pi}{2}-\frac{32}{5\pi}\right)\frac{b_{n-1}}{b_n}\frac{u}{Tl}, \tag{58}$$

where numeric coefficients b_n are given by Eq. (2). For $n=0$, the ratio b_{-1}/b_0 is 5.89.

In the impure limit, $q_T l\ll 1$, the thermoelectric coefficient is

$$\frac{\eta_{\rm vb}}{\eta_0}=\frac{104}{175\pi}\frac{b_{n+1}}{b_n}\frac{Tl}{u}. \tag{59}$$

Thus, the phonon-drag thermopower in the impure limit is

$$S_{\rm vb}^{\rm dr}=\frac{104 b_{n+1}\beta\tau_{\rm ph}\tau T^5}{175 e(p_F u)^3}. \tag{60}$$

If phonon relaxation is determined by the phonon-electron scattering and the phonon-electron relaxation time is given by Eq. (45), the thermoelectric coefficient may be presented as

$$\eta_{\rm vb}^{\rm ph\text{-}e}=\frac{e\tau v_F T^3}{6\pi^2 p_F u^3}\int dx\, x^4\frac{\partial N(x)}{\partial x}W_{\rm vb}^{\rm ph\text{-}e}(q_T l x). \tag{61}$$

The function $W_{\rm vb}^{\rm ph\text{-}e}(ql)$ is shown in Fig. 2. As seen, corrections to the Gurevitch formula [Eq. (6)] due to electron scattering from the vibrating potential are small.

V. CONCLUSIONS

The electron-phonon interaction determines the electron-energy loss rate and also manifests itself in the electron transport. In a pure conductor, the electron-energy and momentum-relaxation rates are described by the same matrix element of the electron-phonon interaction. In a disordered conductor, the inter-relation of inelastic and elastic scattering processes is complicated by the interference of scattering mechanisms. This requires consistent quantum description of energy loss and transport phenomena.

Electron-energy loss and temperature-dependent resistivity in disordered metallic films have been studied in Refs. 11,21, and 22. By fitting experimental data to the theory,[1,3,6] the coupling constants independently determined from resistivity and hot-electron measurements have been found to be in a good agreement.

Very recently it has been realized that study of the phonon-drag thermopower is also a convenient way to determine electron-phonon coupling.[23,24] Coupling of a two-dimensional electron gas in a Si metal-oxide-semiconductor field-effect transistor in the temperature range 0.3–4 K has been investigated using the phonon-drag thermopower and energy loss rate. On the basis of this well-developed theory, good agreement has been found at the temperature range $T>1.5\,{\rm K}$, which corresponds to the pure limit, $q_T l\gg 1$. At lower temperatures, where $q_T l\leqslant 1$, the available theory ignoring the interference of interactions does not provide a consistent description of both phenomena. The paper in Ref. 23 has raised a number of issues about the role of electron-phonon-impurity/boundary interference in the phonon-drag and energy loss phenomena.

The current work is concerned with effects of elastic electron scattering on the phonon-drag thermopower in 3D degenerate conductors. The quantum-transport equation is extended to study phonon-drag effects. The electric current is calculated as a response of electrons to the temperature gradient in the phonon subsystem. This approach allows one to avoid complex diagrams in the Kubo method and numerous Poisson bracket corrections, if response to the electric field is calculated.[18,19] The developed method is also convenient to study drag effects in coupled electron systems (for a recent review see Ref. 25).

Note that, as all other thermoelectric coefficients, the phonon-drag thermopower is proportional to the particle-hole asymmetry, i.e., to the difference between parameters of electron states inside $\mathbf{p}$ and outside $\tilde{\mathbf{p}}$ the Fermi surface. In the pure limit, $q_T l\gg 1$, the phonon-drag thermopower originates only due to asymmetry in the electron energy, $\xi_{\mathbf{p}}\neq\xi_{\tilde{\mathbf{p}}}$ (if $\xi_{\mathbf{p}}=\xi_{\tilde{\mathbf{p}}}=v_F|p-p_F|$, the phonon-drag thermopower is absent). In our isotropic model with quadratic electron spectrum, the asymmetry is given by $(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})/\xi_{\mathbf{p}}\sim q_T/p_F\sim T/\theta_D$, where θ_D is the Debye temperature. Calculating drag effects in the impure limit, one should take into account particle-hole asymmetry in all other electron characteristics, such as density of states [Eq. (29)] and the velocity. For this reason thermopower in a disordered conductor is more sensitive to peculiarities of electron parameters.

We demonstrate that in bulk samples, where phonon-electron scattering dominates in the phonon relaxation, the phonon-drag thermopower is just slightly modified due to elastic scattering [Eqs. (43) and (61)]. Thus, Gurevitch formula [Eq. (6)] provides the adequate description of the phonon-drag thermopower even in disordered bulk conductors.

In thin film structures phonons mainly scatter in a substrate, and thermopower is strongly affected by elastic electron scattering from boundaries, impurities, and defects. The vibrating electron scattering potential substantially decreases

the thermopower. In the impure limit, $Tl/u \ll 1$, the phonon-drag thermopower is of the order of $(Tl/u)S_0^{\mathrm{dr}}$ [Eq. (60)]. On the contrary, static scatterers, such as rigid boundaries and heavy impurities, increase the thermopower by a factor of $u/(Tl)$ [Eq. (41)]. Such modification correlates to the effect of elastic electron scattering on the electron-phonon relaxation.[1–3,8]

While our results are not directly applicable to the electron-phonon interaction via the piezoelectric potential, we may evaluate the disorder-induced modification of the thermopower in the following way. According to Refs. 26 and 27, the renormalization of the piezoelectric vertex by elastic electron scattering is exactly the same as the renormalization of the deformation-potential vertex by static scatterers [Eq. (27)]. Diffusion enhancement of the piezoelectric interaction increases the energy loss rate by the factor $u/(Tl)$.[26,27] The results of Sec. III show that the phonon-drag thermopower is also increased by the same factor. Thus, correlated disorder-induced changes in the energy loss and in thermopower are also expected for the piezoelectric potential. Very recently the effect of elastic scattering on the energy loss rate has been observed in gated GaAS/$Ga_{1-x}Al_x$ δ-doped quantum wells.[28] It would be interesting to investigate the phonon-drag thermopower in these structures.

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