Theory of nonlinear electron transport for solids in a strong electric field

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The nonlinear transport for interacting electrons with phonons and impurities is studied in the presence of a strong electric field E. By separating the center-of-mass motion from the relative motion of electrons we are able to obtain force- and energy-balance equations in steady states, from which the electron temperature and current density can be determined self-consistently as a function of E.

To invent a tractable method of calculating nonlinear electron transport in solids has been an outstanding problem for a long time.[1-6] So far the phenomenological Boltzmann equation seems to be the only tool for practical calculations.[7-9] In this Brief Report we shall introduce a different approach to this problem. The essential idea is to separate the center-of-mass motion from the relative motion of electrons in Hamiltonian and in density matrix, by which a force balance equation and a energy-balance equation are obtained for steady states in the presence of electric fields. Thus both frictional and heating effects are included in a natural way.

We consider a model electron-phonon-impurity system in the presence of a uniform electric field E, which consists of N interacting electrons, n_i randomly distributed impurities, and phonons. The electrons interact with phonons and are scattered by impurities. The conventional expression of the Hamiltonian for this system is well known. In order to calculate the transport properties we find it is more convenient to write this Hamiltonian in terms of the center-of-mass (c.m.) variables and the electron variables in the relative coordinates[10]

$$H = H_{\text{c.m.}} + H_e + H_{\text{ph}} + H_{e\text{ph}} + H_{ei} \ , \tag{1}$$

$$H_{\text{c.m.}} = \frac{\vec{\mathrm{P}}^2}{2Nm} - Ne\vec{\mathrm{E}}\cdot\vec{\mathrm{R}} \ ,$$

$$H_e = \sum_i \frac{(\vec{\mathrm{p}}_i'^2)}{2m} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0|\vec{\mathrm{r}}_i' - \vec{\mathrm{r}}_j'|} \ , \tag{2}$$

$$H_{\text{ph}} = \sum_{\vec{q},\lambda} \Omega_{\vec{q}\lambda} b^\dagger_{\vec{q}\lambda} b_{\vec{q}\lambda} \ , \tag{3}$$

$$H_{e\text{ph}} = \sum_{\vec{q},\lambda} M(\vec{q},\lambda)(b^\dagger_{\vec{q}\lambda} + b_{-\vec{q}\lambda})\exp(i\vec{q}\cdot\vec{\mathrm{R}})\rho_{\vec{q}} \ , \tag{4}$$

$$H_{ei} = \sum_{\vec{q},a} u(\vec{q})\exp[i\vec{q}(\vec{\mathrm{R}} - \vec{\mathrm{R}}_a)]\rho_{\vec{q}} \ . \tag{5}$$

Here $\vec{\mathrm{P}}$ and $\vec{\mathrm{R}}$ are, respectively, the momentum and coordinate of the center of mass, $\vec{\mathrm{p}}_i'$ and $\vec{\mathrm{r}}_i'$ are, respectively, the momentum and coordinate of ith electron relative to the center of mass, e and m are the charge and mass of an electron, and $\rho_{\vec{q}} = \sum_j \exp[i\vec{q}\cdot\vec{\mathrm{r}}_j']$ is the electron density operator in the relative coordinates. In Eqs. (3) and (4), $b^\dagger_{\vec{q}\lambda}$ ($b_{\vec{q}\lambda}$) are the phonon creation (annihilation) operators in branch λ with wave vector $\vec{q}$ and frequency $\Omega_{\vec{q}\lambda}$, and $M(\vec{q},\lambda)$ is the electron-phonon interaction matrix element. In Eq. (5) $\vec{\mathrm{R}}_a$ and $u(\vec{q})$, respectively, represent the ath impurity position and the electron-impurity interaction in momentum space. From Eq. (1) we can see that the electric field E acts directly on the center-of-mass variables. The center-of-mass motion couples to the electrons in the relative coordinates only through the electron-impurity and electron-phonon interactions. The center-of-mass system behaves like a single particle with mass $M = Nm$ and is expected to be described by the classical equation of motion. The statistical properties of the electrons in relative coordinates and the phonons can be described by a density matrix $\hat{\rho}$. In the absence of electron-impurity and electron-phonon interactions, the electrons in relative coordinates and the phonons are two decoupled and isolated equilibrium systems with their own temperatures T_e (electron) and T (lattice or phonon). Then the density matrix takes the form

$$\hat{\rho}_0 = \frac{1}{Z_e} e^{-H_e/T_e} \frac{1}{Z_{\text{ph}}} e^{-H_{\text{ph}}/T} = \frac{1}{Z} e^{-H_0/T_e} \ , \tag{6}$$

with $H_0 = H_e + \alpha H_{\text{ph}} (\alpha = T_e/T)$ and $Z = Z_e Z_{\text{ph}}$. The physical meaning of the electronic temperature T_e will be discussed later. If the interaction $H_I = H_{e\text{ph}} + H_{ei}$ and the electric field are turned on adiabatically from $t = -\infty$, the density matrix $\hat{\rho}$ satisfies the Liouville equation[11]

$$i\frac{\partial\hat{\rho}}{\partial t} = (H_e + H_{\text{ph}} + H_{It}, \hat{\rho}) \tag{7}$$

with the initial condition

$$\hat{\rho}|_{t=-\infty} = \hat{\rho}_0 \ . \tag{8}$$

Here H_{It} is $H_{e\text{ph}} + H_{ei}$ of Eqs. (4) and (5) with $\vec{\mathrm{R}}$ replaced by its expectation value $\vec{\mathrm{R}}(t)$. The statistical average of a dynamical variable A_t at time t is $\langle A_t\rangle = \mathrm{Tr}(\hat{\rho}A_t)$. If $\hat{\rho}$ is solved to the first order in H_{It}, we obtain

$$\langle A_t\rangle = \langle A_t\rangle_0 - i\int_{-\infty}^{\infty}\Theta(t-t')\langle[A_t^{(\alpha-1)(t'-t)}(t),H_{It'}(t')]\rangle_0 dt' \ . \tag{9}$$

Here

$$A_t^{(\alpha-1)\tau}(t') = \exp[i(\alpha-1)H_{\rm ph}\tau]A_t(t')\exp[-i(\alpha-1)H_{\rm ph}\tau] \ ,$$

with $A_t(t')=\exp(iH_0t')A_t\exp(-iH_0t')$ and $\langle(\cdots)\rangle_0=\mathrm{Tr}[\hat\rho_0(\cdots)]$. In steady state, the center of mass moves with a constant speed v_d along the field direction $\vec R(t)-\vec R(t')=v_d(t-t')\hat i$ (we assume E is in x direction) and the total force acting on the center of mass must be zero: $\langle\dot P_x\rangle=-\langle i[P_x,H]\rangle=0$. From this we obtain the following momentum balance equation:

$$NeE = -n_i\sum_{\vec q}[u(\vec q)]^2q_x\hat\Pi_2(\vec q,\omega_0) - 2\sum_{\vec q,\lambda}[M(\vec q,\lambda)]^2q_x\hat\Pi_2(\vec q,\omega_0+\Omega_{\vec q\lambda})\left[n\left(\frac{\Omega_{\vec q\lambda}}{T}\right)-n\left(\frac{\omega_0+\Omega_{\vec q\lambda}}{\alpha T}\right)\right] \ , \tag{10}$$

in which $\omega_0=q_xv_d$, $n(x/T)=(e^{x/T}-1)^{-1}$ and $\Pi_2(\vec q,\omega)$ is the imaginary part of the electron density-density correlation function $\hat\Pi(\vec q,\omega)$ calculated at electron temperature T_e, which can be represented by the shaded bubble in Fig. 1. Under random-phase approximation [Fig. 1(c)] we have[12]

$$\hat\Pi(\vec q,\omega)=\frac{\Pi(\vec q,\omega)}{1-v_C(\vec q)\Pi(\vec q,\omega)} \ , \tag{11}$$

where $v_C(\vec q)=e^2/\epsilon_0\vec q^2$ and $\Pi(\vec q,\omega)$ is the density-density correlation function without Coulomb interaction:

$$\Pi(\vec q,\omega)=2\sum_{\vec k}\frac{f(\epsilon_{\vec k+\vec q},T_e)-f(\epsilon_{\vec k},T_e)}{\omega+\epsilon_{\vec k+\vec q}-\epsilon_{\vec k}+i\delta} \ . \tag{12}$$

Here $f(\epsilon_{\vec k},T_e)=\{\exp[(\epsilon_{\vec k}-\epsilon_F)/T_e]+1\}^{-1}$ is Fermi function at T_e and ϵ_F is the chemical potential. The first and second terms on the right-hand side (RHS) of Eq. (10) are, respectively, the frictional forces due to impurities and due to phonons, experienced by the center of mass when it moves. They can be described by Figs. 1(a) and 1(b), respectively. The dotted vertices in these graphs denote momenta along x direction. We can obtain the energy transfer rate from electrons to phonons by calculating $\langle\dot H_{\rm ph}\rangle=-i\langle[H_{\rm ph},H]\rangle$. In steady states the power fed to the system by the electric field JE should be equal to energy transfer rate. From $\langle\dot H_{\rm ph}\rangle=JE$ and together with Eq. (10) we obtain the following energy-balance equation:

$$0 = -n_iv_d\sum_{\vec q,\lambda}[u(\vec q)]^2q_x\hat\Pi_2(\vec q,\omega_0) - 2\sum_{\vec q,\lambda}[M(\vec q,\lambda)]^2(\omega_0+\Omega_{\vec q\lambda})\hat\Pi_2(\vec q,\omega_0+\Omega_{\vec q\lambda})\left[n\left(\frac{\Omega_{\vec q\lambda}}{T}\right)-n\left(\frac{\omega_0+\Omega_{\vec q\lambda}}{\alpha T}\right)\right] \ , \tag{13}$$

with $\omega_0=q_xv_d$. The above equation can also be obtained by requiring that the energy of relative electrons is a constant in steady states: $\langle\dot H_e\rangle=-i\langle[H_e,H]\rangle=0$. The second part of the second term on the RHS of Eq. (13) is the energy-transfer rate from electrons to phonons, which can also be represented by Fig. 1(b) if the dotted vertex is understood as phonon energy.

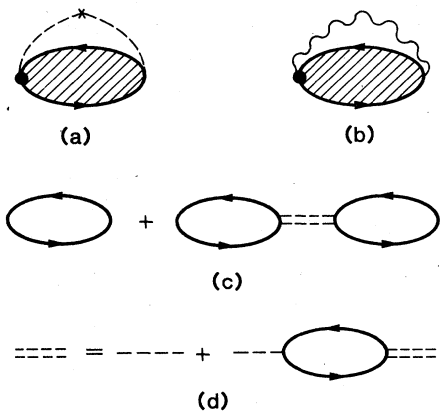

FIG. 1. (a) and (b) represent the lowest-order diagrams for the frictional forces due to impurities and due to phonons, respectively. The dashed line with a cross represents impurity and the wavy line represents the phonon Green's function. The shaded bubble is the electron density-density correlation function, which can be represented by (c) under the random-phase approximation (RPA). The double dashed line in (c) is dynamically screened Coulomb interaction, which satisfies the Dyson equation (d).

Equations (10) and (13) are our main results, from which the temperature ratio $\alpha=T_e/T$ and the current density $J=Nev_d$ can be determined self-consistently. The total resistivity ρ_T is defined as the ratio of the electric field to the current density $\rho_T=E/J$. The resistivities due to phonon ρ and impurities ρ_I, according to Eq. (10), are additive: $\rho_T=\rho+\rho_I$. If $\Pi_2(\vec q,\omega_0)$ is expanded to the lowest order in $\omega_0(=q_xv_d)$, the results of the linear-response theory are recovered for both ρ and ρ_I.[13]

One of the outstanding features in our balance equations is that the drift velocity v_d (therefore electric field) enters the electron density-density correlation function dynamically, so that electric field has a significant influence on the screening. For large v_d (therefore high field) in most cases the denominator of the RHS of Eq. (11) would reduce almost to 1, as if high electric field may act to break up the screening. This is consistent with the high-field descreening effect discussed by Barker.[14]

In the following we shall apply the above approach to study two different problems. The first one is for simple metals at relatively low temperatures such that $T_e\ll\epsilon_F$ and the primary scattering mechanisms are electron-acoustic phonon and electron-impurity interactions. By the use of Debye spectrum for acoustic phonon, deformation potential for electron-phonon interaction and short-range potential for electron-impurity scattering, we obtain the solutions to Eqs. (10) and (13). In zero-field limit $\alpha=T_e/T\to 1$ and the phonon-induced resistivity reduces to the well-known

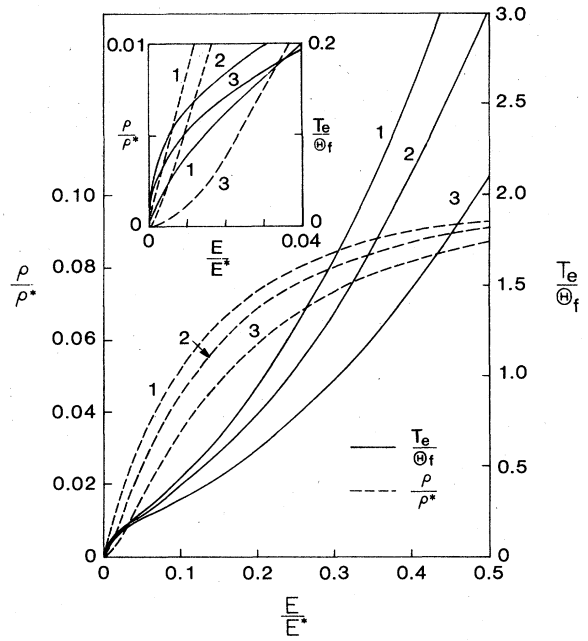

FIG. 2. The electron temperature T_e and phonon resistivity ρ in the limit of $T \to 0$ are shown as functions of dimensionless electric field E/E^* for several different impurity resistivities in a degenerate electron system with acoustic phonon and impurity scatterings. $\rho_{i0}/\rho^* = 0$, 0.03, and 0.1 for curves 1, 2, and 3, respectively.

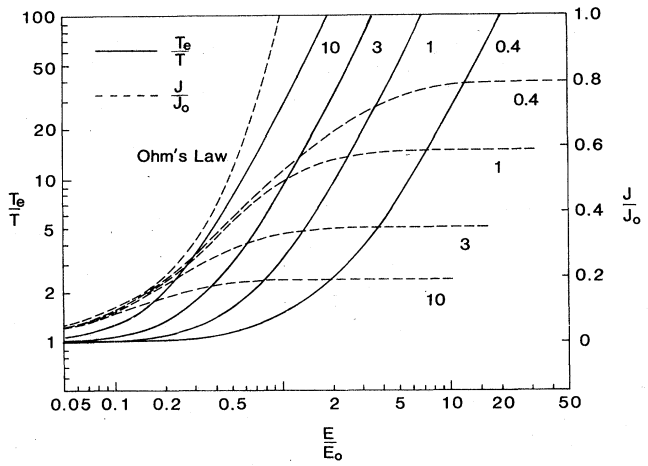

FIG. 3. Dimensionless current density J/J_0 and temperature ratio $\alpha = T_e/T$ are shown as functions of dimensionless electric field E/E_0 for an electron system obeying the Maxwell-Boltzmann distribution at several different T. The scattering mechanism here is entirely due to optical phonons. The numbers near the curves are the values of T/Θ_0. $\Theta_0 = \Omega_0/k_B$; k_B is the Boltzmann constant.

Bloch-Grüneisen formula[15]

$$\rho(E=0) = \rho_B = \rho^* g\left(\frac{T}{\Theta_F}\right) . \tag{14}$$

Here ρ^* is a constant,

$$g(t) = \frac{1}{t}\int_0^1 \frac{y^5 dy}{(e^{y/t}-1)(1-e^{-y/t})} ,$$

and $\Theta_F = 2k_F\Theta_D/q_D$, with Θ_D for Debye temperature, k_F and q_D for Fermi and Debye wave vectors, respectively. It is interesting to see what happens at very low lattice temperatures and finite field. From Eq. (13) we find that when $T \to 0$ the electron temperature T_e approaches a finite, field, and impurity-dependent value T^*. The calculated T^* and the phonon part of the resisitvity are shown in Fig. 2 as a function of dimensionless electric field E/E^* for several values of ρ_{i0}/ρ^*, where $E^* = \rho^* N e v_s$, v_s is sound speed, and ρ_{i0} is the impurity-induced resistivity in zero-field limit at $T_e = 0$ K. For impure sample at relatively low field our results can be reduced to

$$\frac{T^*}{\Theta_F} = 0.422\left(\frac{\rho^*}{\rho_{i0}}\right)^{1/5}\left(\frac{E}{E^*}\right)^{2/5} , \tag{15}$$

which is in agreement with the result obtained recently by Arai[16] from phenomenological Boltzmann equation. However, Eq. (15) is valid only for $\rho_{i0}/\rho^* > 0.01$ and $E/E^* < 0.01$. For higher field or cleaner sample, our curves show great deviation from $E^{2/5}$. It is also worth mentioning that in high field the phonon contribution to resistivity will not vanish at $T = 0$ K in our model.

The second problem is for semiconductors at relative high temperatures, where the equilibrium electrons obey the Maxwell-Boltzmann distribution and electron-optical-phonon scattering is expected to play a major role. We plot in Fig. 3 the temperature ratio $\alpha = T_e/T$ and dimensionless current density J/J_0 as a function of dimensionless electric field E/E_0 at several different lattice temperatures. Here $J_0 = Ne v_0$ and $E_0 = J_0\rho_0$. ρ_0 is the zero-field resistivity due to optical phonons with frequency Ω_0 and $v_0 = (\Omega_0/m)^{1/2}$. The outstanding characteristics of J-E curves are the saturation of the current density at high field and the value of the saturation current decreases as T increases. These features seem in agreement with experimental results of Ryder[17] on n-Ge.

In summary, we have introduced a self-consistent approach to nonlinear electron transport for solids in a static electric field, in which electron-electron interaction, electron-phonon interaction, and electron-impurity scattering are assumed to exist. The electron heating effect has been taken into full consideration by the introduction of electron temperature T_e and by the energy balance equation. The physical meaning of T_e can be understood as follows. If we turn off the electron-phonon and electron-impurity interaction at a certain instant after the system has already reached the steady state, the electrons in relative coordinates will decouple themselves from the center-of-mass and phonons. They will become thermalized and will approach to an equilibrium state. The thermodynamical temperature of this equilibrium state is defined as T_e. The most important aspect of the present approach is its simplicity in mathematical structure, so that the numerical labor involved is kept minimal. Moreover, many-body effects can be taken into account microscopically by diagrammatic methods. At present moment we have performed calculation only to the lowest order in scattering potentials; the higher-order process can, in principle, also be included.

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