Residual resistance and Joule heat generation in bulk samples and nanostructures

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The Joule heat generation under residual resistance conditions in bulk samples of metals and degenerate semiconductors is discussed. We assume that the conductance of the system is determined by elastic scattering of conduction electrons and consider Ohmic regime. We come to conclusion that the amount of Joule heat generated in such a system is determined by the residual resistance provided the length of phase coherence of the electron wave functions is smaller than the dimensions of the sample. For a quantum well this condition is imposed on its lateral dimensions and does not concern its width. It is indicated that this is only a sufficient condition that can be relaxed by further investigations.

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The purpose of the present paper is to discuss the physics of heat generation under residual resistance conditions in bulk samples of metals and degenerate semiconductors. In a way, this might be considered as the simplest example of heat generation. This case is particularly instructive as one can sometimes find in the physical literature statements that only inelastic electron collisions can result in generation of heat as the collisions with impurities conserve the electron energy. We will describe a mechanism of the heat generation where the amount of heat is determined by the residual resistance, i. e. by elastic electron–impurity collisions. We will demonstrate that such a mechanism of heat generation is effective provided it is accompanied by a sort of inelastic electron scattering. Yet it is remarkable that this scattering need not result in an energy transfer but rather in destruction of the phase coherence of electron wave functions over some length L_φ smaller than the sample dimensions.

The formulation of the problem is similar to that discussed in Ref. [1]. Namely, we will consider an isolated physical system consisting of a capacitor discharging through the conductor in consideration. The current is assumed to be almost stationary. In such a case the rate of heat generation is given by (see Landau and Lifshitz [2], §13)

$$\frac{d\mathcal{Q}}{dt} = T\,\frac{d\hat{\mathcal{S}}}{dt} = T\int d^3r\left[\frac{dS}{dt}\right]_{\rm coll}, \tag{1}$$

where T is the temperature (we set $k_{\rm B}\equiv 1$ and assume that the Ohm's law is valid, so the electron distribution is only slightly shifted from equilibrium under the action of electric field), $\hat{\mathcal{S}}$ is the total entropy of the electron system, S is the entropy density, and the integrand on the right-hand side of Eq. (1) describes its variation due to collisions. In our case these are collisions of the conduction electrons with defects of crystal lattice, i. e. with impurities.

The scattering potential of randomly distributed impurities is

$$\mathscr{V}(\mathbf{r}) = \sum_n V(\mathbf{r}-\mathbf{r}_n), \tag{2}$$

where $\mathbf{r}_n$ is the position of the nth impurity.

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The electron scattering amplitude in the Born approximation is given by

$$\langle \mathbf{p}'|\mathscr{V}||\mathbf{p}\rangle = \sum_n \int d^3r\,\psi^*_{\mathbf{p}'}(\mathbf{r})\psi_{\mathbf{p}}(\mathbf{r})V(\mathbf{r}-\mathbf{r}_n)$$
$$= \frac{1}{\Omega}\sum_n \int d^3r e^{i\mathbf{qr}}V(\mathbf{r}-\mathbf{r}_n) = \frac{1}{\Omega}V_{\mathbf{q}}\sum_n e^{i\mathbf{qr}_n}, \tag{3}$$

where Ω is the volume,

$$\mathbf{q} = (\mathbf{p}-\mathbf{p}')/\hbar, \quad V_{\mathbf{q}} = \int V(\mathbf{r})e^{i\mathbf{qr}}d^3r. \tag{4}$$

The transition probability is proportional to

$$|\langle \mathbf{p}'|\mathscr{V}||\mathbf{p}\rangle|^2 = \frac{1}{\Omega^2}|V_{\mathbf{q}}|^2\sum_{n,n'} e^{i\mathbf{q}(\mathbf{r}_n-\mathbf{r}_{n'})}$$
$$= \frac{1}{\Omega^2}|V_{\mathbf{q}}|^2\left[\mathscr{N}+2\sum_{n\neq n'}\cos\mathbf{q}(\mathbf{r}_n-\mathbf{r}_{n'})\right]. \tag{5}$$

The first term in the square brackets is a result of summation over $n=n'$. It gives the total number of scatterers $\mathscr{N}$. The second term is a sum of $\mathscr{N}(\mathscr{N}-1)$ random items that can have either sign. For a fixed value of $\mathbf{q}$ it is of the same order as the first term. This means that Eq. (5) cannot be used directly for derivation of the Boltzmann equation with a configuration averaged collision term. (There is an interesting generalization of a transport equation where the positions of scattering centres in the collision term are fixed [3]. However, it cannot be used directly for calculation of an entropy production).

Now we will assume that along with the impurity scattering there is a phase relaxation with characteristic length L_φ (see papers [4–7]). The phase destruction of electron wave function can be brought about for instance by electron–phonon or electron–electron interaction. Then instead of the product of four wave functions one should introduce a two-particle density matrix

$$\rho_{\mathbf{pp}'}(\mathbf{r},\mathbf{r}') = \overline{\psi^*_{\mathbf{p}}(\mathbf{r})\psi^*_{\mathbf{p}'}(\mathbf{r}')\psi_{\mathbf{p}}(\mathbf{r}')\psi_{\mathbf{p}'}(\mathbf{r})} \tag{6}$$

and instead of Eq. (5) one gets

$$|\langle \mathbf{p}'|\mathscr{V}||\mathbf{p}\rangle|^2 = \sum_{n,n'} \int d^3r \int d^3r' \overline{\psi^*_{\mathbf{p}}(\mathbf{r})\psi^*_{\mathbf{p}'}(\mathbf{r}')\psi_{\mathbf{p}}(\mathbf{r}')\psi_{\mathbf{p}'}(\mathbf{r})} \times V(\mathbf{r}-\mathbf{r}_n)V(\mathbf{r}'-\mathbf{r}_{n'}). \quad (7)$$

As the correlation described by the density matrix relaxes over the length L_φ one can write

$$\overline{\psi^*_{\mathbf{p}}(\mathbf{r})\psi^*_{\mathbf{p}'}(\mathbf{r}')\psi_{\mathbf{p}}(\mathbf{r}')\psi_{\mathbf{p}'}(\mathbf{r})} = \frac{1}{\Omega} e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')} e^{-|\mathbf{r}-\mathbf{r}'|/L_\varphi}. \quad (8)$$

The electron de Broglie wavelength is usually much smaller than L_φ, so that one has for characteristic values of q

$$q \gg L_\varphi^{-1}. \quad (9)$$

Now we will discuss the situation where the dimensions of the specimen are bigger than L_φ. As a result, we get instead of Eq. (5)

$$|\langle \mathbf{p}'|\mathscr{V}||\mathbf{p}\rangle|^2 = \frac{\mathscr{N}}{\Omega^2}\left[1 + \mathscr{O}(L_\varphi^3/\Omega)\right], \quad (10)$$

where the second term in the square brackets is of the order of

$$L_\varphi^3/\Omega \ll 1, \quad (11)$$

i. e. negligibly small. This inequality is sufficient to get a standard (configuration averaged) electron–impurity collision term of the Boltzmann equation.

As $\mathscr{N}$ is the total number of impurities, $n_i = \mathscr{N}/\Omega$ is their concentration that appears in the collision term

$$\left[\frac{\partial F_{\mathbf{p}}}{\partial t}\right]_{\text{coll}} = n_i \int \frac{d^3p'}{(2\pi\hbar)^3} w(\mathbf{p}', \mathbf{p})(F_{\mathbf{p}'} - F_{\mathbf{p}}). \quad (12)$$

$w(\mathbf{p}, \mathbf{p}')$ is the specific probability of electron–impurity scattering from state $\mathbf{p}'$ into state $\mathbf{p}$; in the Born approximation it is symmetric in regard to $\mathbf{p} \leftrightarrow \mathbf{p}'$ and equal to

$$w(\mathbf{p}', \mathbf{p}) = \frac{2\pi}{\hbar} |V_{\mathbf{q}}|^2 \delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'}), \quad (13)$$

where $\epsilon_{\mathbf{p}}$ is the energy of the state $\mathbf{p}$.

We will present the electron distribution function in the form

$$F_{\mathbf{p}} = F^{(0)}(\epsilon_{\mathbf{p}}) + \Delta F_{\mathbf{p}}, \quad (14)$$

where

$$F^{(0)} = \frac{1}{\exp[(\epsilon_{\mathbf{p}} - \mu)/T] + 1} \quad (15)$$

is the equilibrium Fermi function that is symmetric in regard of $\mathbf{p} \to -\mathbf{p}$ while the second term is antisymmetric. The linearized Boltzmann equation (for an arbitrary anisotropy of the electron spectrum and interaction with impurities) is

$$I\Delta F = -\frac{\partial F^{(0)}(\epsilon_{\mathbf{p}})}{\partial \epsilon_{\mathbf{p}}} e\mathbf{E}\mathbf{v}, \quad (16)$$

where $\mathbf{E}$ is the electric field, $\mathbf{v} = \partial\epsilon_{\mathbf{p}}/\partial\mathbf{p}$, and I is the linearized collision operator with the impurities; we assume it to be of the order of $1/\tau_e$, τ_e being the characteristic time of elastic collisions. The integral

$$\int d\xi_{\mathbf{p}} I\Delta F$$

vanishes as the electron–impurity collisions conserve the number of electrons. Here $d\xi_{\mathbf{p}} \equiv d^3p/(2\pi\hbar)^3$, and the factor 2 due to the spin summation is implied where necessary. The integral over $d\xi_{\mathbf{p}}$ of the function on the right-hand side of Eq. (16) also vanishes as $\mathbf{v}$ is an odd function of $\mathbf{p}$ while the other functions are even. This indicates that Eq. (16) has a solution. Now, operator I is defined within the class of functions whose average over any surface of constant energy vanishes. The function on the right-hand side of Eq. (16) belongs to such a class. This means that one can introduce the inverse operator and write the solution of Eq. (16) in the following symbolic form

$$\Delta F = -\frac{\partial F^{(0)}(\epsilon_{\mathbf{p}})}{\partial \epsilon_{\mathbf{p}}} e\mathbf{E} I^{-1}\mathbf{v} = \frac{1}{T} F^{(0)}\left(1 - F^{(0)}\right) e\mathbf{E} I^{-1}\mathbf{v}. \quad (17)$$

Here I^{-1} is the inverse operator acting on the electron velocity $\mathbf{v}$.

One can write for the entropy production due to the electron–impurity collisions (see for instance Ref. [1])

$$S = -[F_{\mathbf{p}} \ln F_{\mathbf{p}} + (1 - F_{\mathbf{p}}) \ln(1 - F_{\mathbf{p}})], \quad (18)$$

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}} = \int d\xi_{\mathbf{p}} \ln \frac{1 - F_{\mathbf{p}}}{F_{\mathbf{p}}} \left[\frac{\partial F}{\partial t}\right]_{\text{coll}}. \quad (19)$$

One gets for the heat release per unit volume

$$\frac{dQ}{dt} = T\left[\frac{\partial S}{\partial t}\right]_{\text{coll}} = Tn_i \int d\xi_{\mathbf{p}} \int d\xi_{\mathbf{p}'} w(\mathbf{p}', \mathbf{p})(F_{\mathbf{p}} - F_{\mathbf{p}'}) \ln \frac{(1 - F_{\mathbf{p}'})F_{\mathbf{p}}}{(1 - F_{\mathbf{p}})F_{\mathbf{p}'}}, \quad (20)$$

where $Q = \mathscr{E}/\Omega$. One can see that expression (20) is nonnegative. It vanishes if $F_{\mathbf{p}}$ is an arbitrary function of electron energy, $\epsilon_{\mathbf{p}}$. Physically this means that collisions of electrons with impurities relax the electron distribution function within a constant energy surface.

Taking into account comparatively rare inelastic collisions one can see that $F^{(0)}$ is a Fermi function of an electron temperature $T_e = T + \Delta T$. Here ΔT is determined by a small parameter proportional to $E^2\tau_e\tau_i$ where τ_i ($\tau_i \gg \tau_e$) is the characteristic time of inelastic collisions. Its exact value is immaterial for, as we will see, in the case of Fermi degeneracy it does not enter the final result for the heat

generation. Making use of Eq. (17) we get

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}} = -\int d\xi_{\mathbf{p}} \frac{\Delta F_{\mathbf{p}}}{F_{\mathbf{p}}^{(0)}\left(1-F_{\mathbf{p}}^{(0)}\right)} I\Delta F_{\mathbf{p}}, \qquad (21)$$

or

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}} = -\frac{1}{T_e{}^2} E_i E_k \int d\xi_{\mathbf{p}} F_{\mathbf{p}}^{(0)}\left(1-F_{\mathbf{p}}^{(0)}\right) v_i I^{-1} v_k. \quad (22)$$

Integration over $d\xi_{\mathbf{p}}$ can be split into two independent integrations in the following way

$$\int d\xi_{\mathbf{p}} \cdots = \int d\epsilon \int d\nu_\epsilon \ldots \qquad (23)$$

where the first integration is over the energy while the second one is over the surface of constant energy $\epsilon_{\mathbf{p}} = \epsilon$ (and includes the factor $2(2\pi\hbar)^{-3}$). The first integration is easily carried out provided the electrons are degenerate. As a result, we get

$$\frac{d\mathscr{E}}{dt} = T_e \left[\frac{\partial \hat{\mathcal{S}}}{\partial t}\right]_{\text{coll}} = \Omega\sigma_{ik} E_i E_k, \qquad (24)$$

where

$$\sigma_{ik} = -e^2 \int d\xi_{\mathbf{p}} \delta(\epsilon_{\mathbf{p}} - \epsilon) v_i I^{-1} v_k. \qquad (25)$$

It is instructive to consider this problem for nanostructures, such as quantum wells. Then one has to take into consideration electron scattering by the impurities that are within or outside the quantum well. The spectrum of electrons in a quantum well consists of a number of minibands of spatial quantization. We assume that all the occupied states and the scattering processes are within the lowest miniband, so that the band index can be omitted. The Boltzmann equation describing the impurity scattering has the form

$$\left[\frac{\partial F_{\mathbf{p}}}{\partial t}\right]_{\text{coll}} = \int dz \int \frac{d^2 p}{(2\pi\hbar)^2} n_i(z)\, w(\mathbf{p}', \mathbf{p}; z)(F_{\mathbf{p}'} - F_{\mathbf{p}}). \qquad (26)$$

Here $\mathbf{p}$ is a two-component electron quasimomentum parallel to the plane of quantum well, z indicates the z-coordinate of impurity; the z-axis is perpendicular to the plane of quantum well. The scattering probability depends on z as a parameter. This means that for a quantum well one should in general deal with several sorts of scatterers. Further derivation goes along the same lines as above, so it is needless to repeat it. The result is Eq. (24) for the heat generation where σ_{ik} is a 2D conductivity and volume Ω should be replaced by the area of the quantum well.

In summary, we have come to the conclusion that the amount of generated heat can be determined by elastic collisions. This has a clear physical meaning. The amount of order in the electron distribution resulting in electric current can bring about mechanical work. For instance, one can let the current flow through a coil and a magnetic rod can be drawn into the coil. In such a way the electrons transferring the current can execute a work on the rod. As a result of scattering the amount of order in the electron distribution diminishes and this means dissipation of mechanical energy of the electron system into heat.

In the example considered in the present paper inelastic collisions *do not determine the generated heat.* If the electron contribution to the specific heat is predominant over the lattice (Debye) contribution the energy will remain within the electron system even for the case there is some inelastic electron–phonon scattering. For the opposite specific heat ratio, it may eventually go to the lattice. But even in such a case, if the electron–impurity collisions are predominant (i. e. are more efficient than the electron–phonon ones) it is they that determine the heat generation. Of course, *the inelastic processes are necessary for the electron system to reach full equilibrium as well as for the dephasing.* However, under our assumptions they do not manifest essential explicit influence on the resistance and heat generation.

In future it would be very useful to investigate in more detail the conditions of applicability of the Boltzmann equation with electron–impurity collision term (12). I believe that the condition (11) for applicability of this equation can be relaxed. It would be interesting to find out the particulars of such a relaxation.

It it a great honor for me to present a paper for V.I. Perel' memorial issue of this journal. V.I. Perel' was an outstanding scientist whose profound understanding of physics, readiness to lend an ear for discussions with his colleagues, his human kindness and willingness to give his advice and help will be remembered for long.

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