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Heat generation by electric current in nanostructures

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Heat generation for collisionless Ohmic electric conductance in quantum semiconductor microstructures joining two classical reservoirs is investigated. Spatial distribution of the heat generated by current through a semiconductor microstructure is calculated. The heat is spread over the length of electron mean free path in the reservoirs. We find that the amount of heat generated per second in both reservoirs that are joined by the nanostructure is the same. [S0163-1829(97)06007-4]

I. INTRODUCTION

During recent years various properties of quantum point contacts were investigated theoretically and on experiment. Among them one can name a steplike variation of conductance (Ohmic and non-Ohmic), shot noise, thermoelectric properties, and a number of other transport effects. The total amount of heat generated by a quantum contact can be determined by simple energy conservation considerations provided that the contact conductance G is known. However, such considerations tell nothing about the spatial distribution of the heat which can be expressed via the rate of entropy production. Meanwhile the heat distribution is an important characteristic of a contact. It can be measured on experiment. Moreover, calculation of the heat provides an alternative method of computation of a contact conductance which under certain circumstances may be more efficient than the existing methods. The purpose of the present paper is to investigate the heat generation in current-carrying semiconductor quantum nanostructures.[1]

The resistance of a classical ballistic point contact between two metals was considered by Sharvin.[2] The characteristic dimensions of the contact were assumed to be much larger than the de Broglie wavelength. Kulik, Shekhter, and Omelyanchouk[3] pointed out that the processes leading to electric resistance and heat generation are spatially separated in a classical point contact. The spatial distribution of Joule heat generated by current across such a ballistic point contact was treated in the diffusive limit by Rokni and Levinson.[4]

As a further development of the Landauer-Büttiker-Imry[5,6] approach we consider the heat generation in the case of ballistic Ohmic conduction in semiconductor quantum nanostructures (microcontacts). We assume that the microcontact has a transverse dimension of the order of electron de Broglie wavelength λ. It is joining two reservoirs, each being in independent equilibrium. We will show that to measure a quantum conductance the reservoirs *should be assumed to be classical*. It will be indicated that this fact is in accordance with the general quantum theory of measurements.

We wish to emphasize that we do not make any assumptions concerning the potential distribution along the structure assuming only that it is smooth on the scale of the electron's de Broglie wavelength. We consider this a point of some importance as there is a difference between the problem of electrostatic potential distribution in metallic microcontacts and the distribution in semiconductor nanowires. In metals the potential profile is determined by the spatial distribution of the current and strong screening of the charges (see Refs. 7–9). In semiconductor nanostructures the electron concentrations are usually rather low and the screening may be not of so much importance. The potential distribution is mainly determined by the arrangement and the potentials of the gate electrodes. Usually there is zero current between the nanostructure and these electrodes. Then the surfaces of gate electrodes are at constant potentials. By manipulating these potentials one can, in principle, create various potential profiles. We consider inelastic electron scattering in the contacts (which, as we have mentioned, are assumed to be classical) and find that for any potential distribution in the nanostructure the heat generation in both contacts is the same.

We also find that practically all the heat is generated in the classical reservoirs rather than in the quantum contact. Our theory permits us to resolve the following seemingly paradoxical situation. On the one hand, the rate of Joule heat generation is determined by the relaxation mechanism(s) for the physical system in consideration, or, in other words, by relaxation rates. On the other hand, quite often in nanostructures there is the so-called collisionless transport where the conductance G is independent of any relaxation rate. This means, in other words, that the resistance and therefore the overall heat production does not depend on any mechanism of electrons' relaxation. We will show by consideration of heat generation in classical reservoirs how these two facts can be reconciled.

In conclusion we briefly discuss the non-Ohmic conduction on a qualitative level. We discuss also the situation where the electrons of the nanowire are weakly scattered by the phonons so that the heat may be partly released in the vicinity of the nanowire.

It will be convenient to consider an isolated system. Therefore we will have in mind the following physical situation. There is a capacitor which is discharged through the conductor of interest. The product RC of the whole system, R and C being the resistance and capacitance, respectively, is much bigger than any relaxation time characterizing the electron or phonon system of the conductor. This means that for all the practical purposes the conduction process can be looked upon as a stationary one. The total energy of the system, $\mathcal{U}$, is conserved while its total entropy, $\hat{\mathcal{S}}$, is growing. The rate of heat generation is expressed through $T\partial\hat{\mathcal{S}}/\partial t$ where T is the temperature. So our main purpose will be to calculate the rate of the entropy production.

II. MECHANICAL ENERGY AND HEAT

An isolated macroscopic system possesses a *mechanical energy*, $\mathcal{E}$ (see Landau and Lifshitz[10]). This means that owing to internal processes, without a resulting variation of its volume, the system can execute work on external systems. In general, the amount of work depends on how the internal state of the system under consideration is changed. Mechanical energy is the maximal amount of work that can be produced if the system finally reaches the state of thermodynamic equilibrium.

It is well known (see Ref. 10) that

$$\mathcal{E}=\mathcal{U}-\mathcal{U}_0(\hat{\mathcal{S}}), \tag{1}$$

where $\mathcal{U}_0(\hat{\mathcal{S}})$ is the total energy of the system in thermodynamic equilibrium expressed as a function of its entropy $\hat{\mathcal{S}}$ given by the relations of equilibrium thermodynamics. Calculating its time derivative one can write

$$\frac{d\mathcal{E}}{dt}=\frac{d\mathcal{U}}{dt}-\frac{d\mathcal{U}_0}{d\hat{\mathcal{S}}}\frac{d\hat{\mathcal{S}}}{dt}=\frac{d\mathcal{U}}{dt}-T_0\frac{d\hat{\mathcal{S}}}{dt}, \tag{2}$$

$T_0(\hat{\mathcal{S}})$ being the temperature of the equilibrium system whose entropy is equal to $\hat{\mathcal{S}}$. As the first term on the right-hand side vanishes because of the conservation of energy of an isolated system, one gets

$$-\frac{d\mathcal{E}}{dt}=T_0\frac{d\hat{\mathcal{S}}}{dt}. \tag{3}$$

This means that the mechanical energy of an isolated system, unlike its total energy, is not conserved. While the relaxation processes tending to bring the system into equilibrium take place its mechanical energy dissipates into heat. Equation (3) describes the rate of dissipation in the nonequilibrium system in consideration or, in other words, the rate of Joule heat generation.

III. TRANSPORT IN QUANTUM NANOSTRUCTURE

Let us consider a nanostructure where there is a direction (x axis) along which the electron motion is infinite and a current flows. Along the perpendicular direction(s), $\mathbf{r}_\perp$ the electron motion is quantized. To be definite we will discuss a 3D case although one can turn to a 2D case by a simple change of notation. We will consider the so-called adiabatic transport (see Glazman *et al.*[11]) where the potential profile varies smoothly along x axis on the scale of λ (where λ is the electron de Broglie wavelength). We assume that the electron mean free path is much bigger than the characteristic dimensions of the microstructure. Then there is a system of one-dimensional (1D) electron bands (*channels*) describing the electrons' motion in the x direction both in the microstructure and in the adjoining parts of the contacts. This motion will be considered (quasi-)classically. The transverse motion is quantized. In the spirit of an approach by Glazman *et al.*[11] we assume that the variables x and $\mathbf{r}_\perp$ are separable in the adiabatic approximation. This means that for each value of x the $\mathbf{r}_\perp$ dependence of the potential determines the wave function of transverse quantization $\eta_n(\mathbf{r}_\perp;x)$ that depends on x as a parameter. Here n is the quantum number of transverse quantization. The electron spectrum depends on x and this dependence has the following form:

$$\epsilon_n(p;x)=p^2/2m+\epsilon_n(0;x), \tag{4}$$

where m is the electron effective mass and $\epsilon(0,x)$ is the position of the band's bottom that depends on x as a parameter. $\epsilon_n(0;x)$ is the solution of the eigenvalue problem for the Hamiltonian

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+e\phi(\mathbf{r}_\perp;x). \tag{5}$$

The electron wave functions can be presented in the following form:

$$\psi(\mathbf{r})=\text{const}\frac{1}{\sqrt{p(x)}}\exp\left[i\int p(x')dx'/\hbar\right]\eta_n(\mathbf{r}_\perp;x). \tag{6}$$

Here the wave functions of the transverse quantization η_n depend on x as a parameter, n is the corresponding quantum number.

The energy conservation relation for such a system can be written in the following integral form:

$$\frac{d\mathcal{U}}{\partial t}=JV, \tag{7}$$

where

$$\mathcal{U}=\sum_n\int dx\int d\xi_p\epsilon_{np}F_{np}. \tag{8}$$

J is the total current across the nanostructure which is given by

$$J=\sum_n\int d\xi_p v_{np}F_{np}. \tag{9}$$

Here $d\xi_p=dp/2\pi\hbar$ (summation over the spin variable is implied; we assume that the electron energy is spin independent), $v_{np}=\partial\epsilon_{np}/\partial p=p/m$ is the electron group velocity (which does not depend explicitly on n), $F_{np}(x)$ is the electron distribution function that depends on the quantum number n as a parameter while p (the x component of the electron quasimomentum) and x are classical variables. $F_{np}(x)$ satisfies the Boltzmann equation

$$v\frac{\partial F_{np}(x)}{\partial x}-\frac{\partial F_{np}(x)}{\partial p}\frac{\partial\epsilon_{np}(x)}{\partial x}=\left[\frac{\partial F_{np}}{\partial t}\right]_{\text{coll}}. \tag{10}$$

IV. CALCULATION OF ENTROPY PRODUCTION FOR A NANOSTRUCTURE

The general expression for the rate of heat generation by a nanostructure is given by Eq. (3). To calculate the entropy production for the electron system in consideration interacting with phonons one should treat simultaneously the electron-phonon and phonon-electron collisions. The entropy production is given by (we will set $k_B=1$ throughout the paper)

$$\frac{d\hat{\mathcal{S}}}{dt}=\int dx\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}, \tag{11}$$

$$\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}=\sum_n \int d\xi_p \ln\frac{1-F_{np}}{F_{np}}\left[\frac{\partial F_{np}}{\partial t}\right]_{\mathrm{coll}} + \int d\eta_{\mathbf{q}} \ln\frac{1+N_{\mathbf{q}}}{N_{\mathbf{q}}}\left[\frac{\partial N_{\mathbf{q}}}{\partial t}\right]_{\mathrm{coll}}, \tag{12}$$

where S is the 1D entropy density. Now,

$$\begin{aligned}\left[\frac{\partial F}{\partial t}\right]_{\mathrm{coll}}=\sum_{n'} \int d\xi_{p'}\int d\eta_{\mathbf{q}}\{&w_{nn'}(p,p';\mathbf{q})\\ &\times[F'(1-F)(N_{\mathbf{q}}+1)-F(1-F')N_{\mathbf{q}}]\\ &+w_{n'n}(p',p;\mathbf{q})[F'(1-F)N_{\mathbf{q}}\\ &-F(1-F')(N_{\mathbf{q}}+1)]\},\end{aligned} \tag{13}$$

where $F=F_{np}$, $F'=F_{n'p'}$, $d\eta_{\mathbf{q}}=d^3q/(2\pi)^3$; the summation over the phonon branches is implied while

$$w_{nn'}(p,p';\mathbf{q})\propto\delta_{p',p+\hbar q_x}\delta(\epsilon_{n'p'}-\epsilon_{np}-\hbar\Omega_{\mathbf{q}}). \tag{14}$$

$w_{nn'}(p,p';\mathbf{q})$ is proportional to the probability of an electron to make a transition from the state specified by the quantum numbers n',p' to the state n,p accompanied by emission of a phonon with wave vector $\mathbf{q}$. In such a general form this equation is valid for any phonon states. If one considers interaction of the electrons of a nanowire with bulk phonons then perturbation theory gives (cf. with Refs. 12,13)

$$\begin{aligned}w_{nn'}(p,p',\mathbf{q})=\frac{2\pi}{\hbar}&|c_{\mathbf{q}}|^2|\langle n|\exp(i\mathbf{q}_\perp\mathbf{r}_\perp)|n'\rangle|^2\\ &\times\delta[\epsilon_n(p)-\epsilon_{n'}(p')+\hbar\Omega_{\mathbf{q}}]\delta_{p',p+\hbar q_x}.\end{aligned} \tag{15}$$

Here $c_{\mathbf{q}}$ is the matrix element of the interaction of electrons with bulk phonons; $\mathbf{r}_\perp$ denotes y,z; while $\mathbf{q}_\perp$ denotes q_y,q_z.

Now,

$$\begin{aligned}\left[\frac{\partial N_{\mathbf{q}}}{\partial t}\right]_{\mathrm{coll}}=\frac{1}{\mathcal{A}}\sum_{nn'}\int d\xi_p\int d\xi_{p'}&w_{nn'}(p,p';\mathbf{q})\\ &\times[F'(1-F)(N_{\mathbf{q}}+1)-F(1-F')N_{\mathbf{q}}],\end{aligned} \tag{16}$$

where $\mathcal{A}$ is the area of a cross section of the wire. Employing Eq. (12) we finally get

$$\begin{aligned}\left[\frac{\partial\hat{\mathcal{S}}}{\partial t}\right]_{\mathrm{coll}}=\int dx\sum_{nn'}\int d\xi_p\int d\xi_{p'}\int d\eta_{\mathbf{q}}&w_{nn'}(p,p';\mathbf{q})\\ &\times\ln\frac{F_{n'p'}(1-F_{np})(N_{\mathbf{q}}+1)}{F_{np}(1-F_{n'p'})N_{\mathbf{q}}}\\ &\times[F_{n'p'}(1-F_{np})(N_{\mathbf{q}}+1)-F_{np}(1-F_{n'p'})N_{\mathbf{q}}].\end{aligned} \tag{17}$$

This equation can be compared with the entropy production in a bulk sample which we will need below when we will treat the region outside the nanostructure, within the reservoir region. The result is (see Ref. 14)

$$\begin{aligned}\left[\frac{\partial\hat{\mathcal{S}}}{\partial t}\right]_{\mathrm{coll}}&=\int d^3r\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}\\ &=\int d^3r\int d\xi_{\mathbf{p}}\int d\xi_{\mathbf{p}'}\int d\eta_{\mathbf{q}}w(\mathbf{p},\mathbf{p}';\mathbf{q})\\ &\quad\times\ln\frac{(1-F_{\mathbf{p}})F_{\mathbf{p}'}(N_{\mathbf{q}}+1)}{(1-F_{\mathbf{p}'})F_{\mathbf{p}}N_{\mathbf{q}}}\\ &\quad\times[F_{\mathbf{p}'}(1-F_{\mathbf{p}})(N_{\mathbf{q}}+1)-F_{\mathbf{p}}(1-F_{\mathbf{p}'})N_{\mathbf{q}}],\end{aligned} \tag{18}$$

where $d\xi_{\mathbf{p}}=d^3p/(2\pi\hbar)^3$ (the summation over the spin variable is implied) and we use the same notation S for the 1D entropy density and 3D entropy density. Here $w(\mathbf{p},\mathbf{p}';\mathbf{q})$ is the specific probability of an electron-phonon collision. It is proportional to $\delta(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'}+\hbar\Omega_{\mathbf{q}})$. For phonon emission the second argument corresponds to the initial electron state. As for the quasimomenta of electrons and phonon, they satisfy the conservation law

$$\mathbf{p}-\mathbf{p}'+\hbar\mathbf{q}=\hbar\mathbf{b}, \tag{19}$$

where $\mathbf{b}$ is a vector of the reciprocal lattice. For normal processes $\mathbf{b}=\mathbf{0}$ and we have

$$\mathbf{p}-\mathbf{p}'+\hbar\mathbf{q}=0. \tag{20}$$

In the general case of Umklapp processes Eq. (19) with $\mathbf{b}\neq\mathbf{0}$ is valid.

We do not give here the corresponding rate for the interaction of electrons with impurities within the nanowire. The point is that the item of our main interest will be nanowires where the impurity scattering is of no importance. Where it is of importance it may be difficult to describe it because the widely used procedure of averaging over the impurity positions is not applicable within a nanostructure. However, such a procedure is usually applicable outside the nanostructure, within the reservoir region where it gives (see Refs. 15,14)

$$\begin{aligned}\left[\frac{\partial\hat{\mathcal{S}}}{\partial t}\right]_{\mathrm{coll}}=\int d^3r\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}=n_i\int d^3r\int d\xi_{\mathbf{p}}\int d\xi_{\mathbf{p}'}&w(\mathbf{p}',\mathbf{p})\\ &\times\ln\frac{(1-F_{\mathbf{p}'})F_{\mathbf{p}}}{(1-F_{\mathbf{p}})F_{\mathbf{p}'}}(F_{\mathbf{p}}-F_{\mathbf{p}'}).\end{aligned} \tag{21}$$

Here n_i is the impurity concentration, $w(\mathbf{p}',\mathbf{p})=w(\mathbf{p},\mathbf{p}')$ is the specific probability of electron-impurity scattering from state $\mathbf{p}$ into state $\mathbf{p}'$. $w(\mathbf{p}',\mathbf{p})$ is proportional to $\delta(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'})$ because of the energy conservation. For simplicity, we have written this formula for a case where a crystal and an impurity have a center of symmetry.

The contribution of the electron-electron interaction to entropy production within a nanowire can be described, in principle, by a straightforward generalization of Eq. (22) (see below). However, the possibility of electron-electron collisions is severely restricted for this case (see Ref. 16). Indeed, one can easily check that because of 1D electron dynamics the conditions for the energy and quasimomentum conservation in the course of electron-electron collisions cannot usually be satisfied. (We can also remark that for sufficiently small values of the relative velocity of two interacting electrons these collisions cannot be treated by a perturbation theory.) This is why we are not giving here the corresponding expression.

Outside the nanowire, within a contact region one can use the following equation for the electron-electron collisions (cf. with Ref. 17). Again we will assume that the crystal has a center of symmetry. Then

$$\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}=\frac{1}{4}\int d\xi_{\mathbf{p}}\int d\xi_{\mathbf{p}'}\int d\xi_{\mathbf{p}_1}\int d\xi_{\mathbf{p}_1'}w(\mathbf{p}_1,\mathbf{p}_1';\mathbf{p},\mathbf{p}')$$
$$\times\ln\frac{(1-F_{\mathbf{p}'})(1-F_{\mathbf{p}})F_{\mathbf{p}_1}F_{\mathbf{p}_1'}}{(1-F_{\mathbf{p}_1})(1-F_{\mathbf{p}_1'})F_{\mathbf{p}}F_{\mathbf{p}'}}$$
$$\times[(1-F_{\mathbf{p}'})(1-F_{\mathbf{p}})F_{\mathbf{p}_1}F_{\mathbf{p}_1'}$$
$$-(1-F_{\mathbf{p}_1})(1-F_{\mathbf{p}_1'})F_{\mathbf{p}}F_{\mathbf{p}'}]. \tag{22}$$

Here $w(\mathbf{p}_1,\mathbf{p}_1';\mathbf{p},\mathbf{p}')=w(\mathbf{p},\mathbf{p}';\mathbf{p}_1,\mathbf{p}_1')$ is the specific probability of electron-electron collisions where $\mathbf{p},\mathbf{p}'$ refer to the initial electron states while $\mathbf{p}_1,\mathbf{p}_1'$ refer to the final states. It is proportional to $\delta(\epsilon_{\mathbf{p}}+\epsilon_{\mathbf{p}'}-\epsilon_{\mathbf{p}_1}-\epsilon_{\mathbf{p}_1'})$. The entropy change in Eq. (22) vanishes provided that $F_{\mathbf{p}}$ is a Fermi function $F^{(0)}$ depending on an arbitrary chemical potential and temperature. If the electron quasimomentum $\mathbf{p}$ is conserved during the electron-electron collisions $[dS/dt]_{\mathrm{coll}}$ vanishes also when $F_{\mathbf{p}}$ is a function of the form

$$F^{(0)}(\epsilon_{\mathbf{p}}-\mathbf{pV}-\mu) \tag{23}$$

where $\mathbf{V}$ is an arbitrary vector having the physical meaning of electron drift velocity. This quasimomentum conservation usually takes place in semiconductors.

A few words about the phonon-phonon collisions will follow. We will discuss only the bulk phonons. We will consider three-phonon processes due to the cubic anharmonic terms in the interaction Hamiltonian. We have (see Ref. 18)

$$\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}=\frac{1}{2}\int d\eta_{\mathbf{q}}\int d\eta_{\mathbf{q}'}w(\mathbf{q},\mathbf{q}',-\mathbf{q}'')$$
$$\times[(N_{\mathbf{q}}+1)(N_{\mathbf{q}'}+1)N_{\mathbf{q}''}-N_{\mathbf{q}}N_{\mathbf{q}'}(N_{\mathbf{q}''}+1)]$$
$$\times\ln\frac{(N_{\mathbf{q}}+1)(N_{\mathbf{q}'}+1)N_{\mathbf{q}''}}{N_{\mathbf{q}}N_{\mathbf{q}'}(N_{\mathbf{q}''+1})}, \tag{24}$$

where $w(\mathbf{q},\mathbf{q}',-\mathbf{q}'')$ is the specific probability of the corresponding three-phonon process[apart from the factors $N_{\mathbf{q}}$ and $(N_{\mathbf{q}}+1)$]. For the case where a phonon is absorbed and two phonons are emitted, the two first arguments correspond to the emitted phonons. $w(\mathbf{q},\mathbf{q}',-\mathbf{q}'')$ is proportional to $\delta(\Omega_{\mathbf{q}}+\Omega_{\mathbf{q}'}-\Omega_{\mathbf{q}''})$. Here

$$\mathbf{q}''=\mathbf{q}+\mathbf{q}'+\mathbf{b}, \tag{25}$$

where $\mathbf{b}$ is either 0 (normal processes) or a vector of reciprocal lattice (Umklapp processes). If the Umklapp processes are of importance then Eq. (24) vanishes provided that $N_{\mathbf{q}}$ is the Bose function with an arbitrary temperature.

For collisions of phonons with the lattice defects the explicit expression for $[dS/dt]_{\mathrm{coll}}$ does not differ very much from Eq. (21) (see Ref. 18), and we will not give it here. It vanishes for $N_{\mathbf{q}}$ being an arbitrary function of the phonon energy, $\hbar\Omega_{\mathbf{q}}$.

V. OHM'S LAW FOR A NANOSTRUCTURE

In the present section we discuss an important case where there is a linear relation between the voltage and the current so that the deviation of the distribution functions from the equilibrium is small

$$F_{np}=F^{(0)}(\epsilon_{np})+\Delta F_{np}, \quad N_{\mathbf{q}}=N^{(0)}(\Omega_{\mathbf{q}})+\Delta N_{\mathbf{q}}, \tag{26}$$

where ΔF_{np} and $\Delta N_{\mathbf{q}}$ satisfy the *linearized* Boltzmann equations. ΔF_{np} and $\Delta N_{\mathbf{q}}$ should be proportional to the external potential difference which we assume to be the sole source of the deviation of the functions from equilibrium. As the collision terms vanish for the equilibrium parts of the distribution functions, one can express the heat production through the linearized collision operators, I, acting on ΔF_{np} and $\Delta N_{\mathbf{q}}$. The linear terms in ΔF_{np} and $\Delta N_{\mathbf{q}}$ vanish in the equation for the entropy production. This can be either easily checked directly or established using the following physical considerations. A linear term in ΔF_{np} or $\Delta N_{\mathbf{q}}$ can be of either sign whereas the rate of heat generation should be non-negative.

To give the leading terms of expansion in Eq. (17), in the most concise form it will be convenient to introduce the functions $\chi_{\mathbf{p}}$ and $\nu_{\mathbf{q}}$ defined as follows:

$$\Delta F_{np}=\chi_{np}F^{(0)}(\epsilon_{np})[1-F^{(0)}(\epsilon_{np})],$$
$$\Delta N_{\mathbf{q}}=\nu_{\mathbf{q}}N^{(0)}(\Omega_{\mathbf{q}})[N^{(0)}(\Omega_{\mathbf{q}})+1]. \tag{27}$$

We have for the electron-phonon and phonon-phonon collisions, respectively,

$$\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}=\sum_{nn'}\int d\xi_{p}\int d\xi_{p'}\int d\eta_{\mathbf{q}}F^{(0)}_{np}(1-F^{(0)}_{n'p'})$$
$$\times N^{(0)}_{\mathbf{q}}w_{nn'}(p,p';\mathbf{q})(\chi_{np}-\chi_{n'p'}+\nu_{\mathbf{q}})^2, \tag{28}$$

$$\left[\frac{\partial S}{\partial t}\right]_{\mathrm{coll}}=\frac{1}{2}\int d\eta_{\mathbf{q}}\int d\eta_{\mathbf{q}'}\int d\eta_{\mathbf{q}''}N^{(0)}_{\mathbf{q}}(N^{(0)}_{\mathbf{q}}+1)$$
$$\times w(\mathbf{q},\mathbf{q}',-\mathbf{q}'')(\nu_{\mathbf{q}}+\nu_{\mathbf{q}'}-\nu_{\mathbf{q}''})^2. \tag{29}$$

To get the total rate of heat production one should integrate these equations over the whole length of the conductor and multiply the result by temperature T.

As we have already mentioned Eqs. (28) and (29) are quadratic in the deviations of the distribution functions form the equilibrium values. This means that *to calculate the Joule heat it is sufficient to solve the Boltzmann equation up to the first order in the potential difference*.

In view of further applications it is worthwhile to indicate that these equations can be presented in a different form. As an example we consider Eq. (28). Then one can write

$$\left[\frac{\partial(F^{(0)}+\Delta F)}{\partial t}\right]_{\text{coll}}=I\Delta F. \tag{30}$$

In the same way one can write

$$\left[\frac{\partial(N^{(0)}+\Delta N)}{\partial t}\right]_{\text{coll}}=I\Delta N, \tag{31}$$

where we use the same notation I for the linearized collision operators acting upon ΔF and ΔN. Now,

$$\ln\frac{1-F^{(0)}}{F^{(0)}}=\frac{\epsilon_{\mathbf{p}}-\mu}{T},\quad \ln\frac{1+N^{(0)}}{N^{(0)}}=\frac{\hbar\Omega_{\mathbf{q}}}{T}$$

and one can see that due to energy conservation and electron number conservation in the course of electron-phonon collisions, the terms linear in ΔF and ΔN vanish. This is as it should be because the linear terms can be of either sign whereas the entropy production should be nonnegative. The quadratic term can be written in the following form:

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}}=-\sum_n\int d\xi_p\frac{\Delta F_{np}}{F_{np}^{(0)}(1-F_{np}^{(0)})}I\Delta F_{np}-\int d\eta_{\mathbf{q}}\frac{\Delta N_{\mathbf{q}}}{N_{\mathbf{q}}^{(0)}(1+N_{\mathbf{q}}^{(0)})}I\Delta N_{\mathbf{q}}. \tag{32}$$

Equation (29) can be also transformed to a similar form.

Now, if the relaxation processes within the phonon system are rapid, one can neglect the second term in Eq. (32) and we are left with

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}}=-\sum_n\int d\xi_p\frac{\Delta F_{np}}{F_{np}^{(0)}(1-F_{np}^{(0)})}I\Delta F_{np}. \tag{33}$$

I is a linear integral operator acting on ΔF_{np}. Its explicit expression for the electron-phonon collisions is

$$\begin{aligned}\left[\frac{\partial F_{np}}{\partial t}\right]_{\text{coll}}=&\sum_{n'}\int d\xi_{p'}\int d\eta_{\mathbf{q}}\Delta F_{n'p'}\{w_{nn'}(p,p';\mathbf{q})\\&\times[(1-F_{np}^{(0)})N_{\mathbf{q}}+F_{np}^{(0)}(N_{\mathbf{q}}+1)]+w_{n'n}(p',p;\mathbf{q})\\&\times[(1-F_{np}^{(0)})(N_{\mathbf{q}}+1)+F_{np}^{(0)}N_{\mathbf{q}}]\}\\&-\Delta F_{np}\sum_{n'}\int d\xi_{p'}\int d\eta_{\mathbf{q}}\{w_{nn'}(p,p';\mathbf{q})\\&\times[F_{n'p'}^{(0)}(N_{\mathbf{q}}^{(0)}+1)+(1-F_{n'p'}^{(0)})N_{\mathbf{q}}^{(0)}]\\&+w_{n'n}(p',p;\mathbf{q})\\&\times[F_{p'}^{(0)}N_{\mathbf{q}}^{(0)}+(1-F_{p'}^{(0)})(N_{\mathbf{q}}^{(0)}+1)]\}.\end{aligned} \tag{34}$$

It is an algebraic sum of two terms. One of them is an integral term where $\Delta F_{n'p'}$ is in the integrand. The other one is a time-of-relaxation term which has the form

$$\left[\frac{\partial F_{np}}{\partial t}\right]_{\text{coll}}^{(\tau)}=-\frac{\Delta F_{np}}{\tau_{np}}, \tag{35}$$

where the relaxation time τ_{np} is given by

$$\begin{aligned}\frac{1}{\tau_{np}}=&\sum_{n'}\int d\xi_{p'}\int d\eta_{\mathbf{q}}\{w_{nn'}(p,p';\mathbf{q})[F_{n'p'}^{(0)}(N_{\mathbf{q}}^{(0)}+1)\\&+(1-F_{n'p'}^{(0)})N_{\mathbf{q}}^{(0)}]+w_{n'n}(p',p;\mathbf{q})\\&\times[F_{n'p'}^{(0)}N_{\mathbf{q}}^{(0)}+(1-F_{n'p'}^{(0)})(N_{\mathbf{q}}^{(0)}+1)]\}.\end{aligned} \tag{36}$$

In the relaxation time approximation, where for some physical reasons the integral term can be discarded, we have

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}}=\sum_n\int d\xi_p\frac{(\Delta F_{np})^2}{\tau_{np}F_{np}^{(0)}(1-F_{np}^{(0)})}. \tag{37}$$

Again for a bulk sample (for instance, within the reservoirs) one can write instead of Eq. (37)

$$\left[\frac{\partial S}{\partial t}\right]_{\text{coll}}=\int d\xi_{\mathbf{p}}\frac{(\Delta F_{\mathbf{p}})^2}{\tau_{\mathbf{p}}F_{\mathbf{p}}^{(0)}(1-F_{\mathbf{p}}^{(0)})}. \tag{38}$$

One can use this expression if $\Delta F_{\mathbf{p}}$ has a sharp maximum for some value(s) of $\mathbf{p}$ and the integral in Eq. (37) is dominated by the values of $\Delta F_{\mathbf{p}}$ near the maximum (see, for instance, Abrikosov,[19] Sec. 7.3). Such a situation will be considered below, in Sec. VI.

VI. JOULE HEAT GENERATED BY BALLISTIC CURRENT THROUGH NANOSTRUCTURE

In the spirit of the Landauer-Büttiker-Imry[5,6] approach we assume the quantum microstructure to be connected with the reservoirs which we call ''left'' (+) and ''right'' (−), each of these being in independent equilibrium. We assume that the electrons enter the contacts adiabatically (see Ref. 11). As, however, the width of the classical contacts is much larger than the width of the microstructure the number of the channels within the contacts is also much larger. Most of these channels are not current carrying as the electrons belonging to them are reflected from the wire backward into the corresponding contact. So we start with consideration of the current-carrying channels within the nanostructure.

As is shown in Ref. 11 unless the bottom of an electron 1D band almost touches the Fermi level (the situation we do not consider in the present paper) the electron transport through a nanostructure is practically reflectionless, which will be assumed here. Let us, for example, consider the case $p>0$. Then we will be interested in the region $x>0$ where the relaxation and therefore heat production takes place. The states in the current-carrying channels entering the contact region, i.e., at $x=0$, will have the distribution function $F^{(0)}(\epsilon_{pn}-\mu^{(+)})$. For $x<0$ this distribution function is the same as for all other states at $x<0$. This means that the current-carrying states with $p>0$ are at equilibrium with all other states in the region $x<0$. Indeed, at $x<0$ all the states with $p>0$ as well as with $p<0$ have the distribution function of the same form $F^{(0)}(\epsilon_{pn}-\mu^{(+)})$. To the contrary, for $x>0$ the distribution of electrons in the current-carrying channels will be out of equilibrium relative to the rest of electrons [whose distribution is $F^{(0)}(\epsilon_{pn}-\mu^{(-)})$]. This means that in this region the relaxation processes should tend to bring the current-carrying states into equilibrium. It is these processes that we are going to investigate to calculate the overall heat production and its spatial distribution.

We consider the ballistic transport of electrons within the nanostructure which means that the scattering of electrons there is negligibly weak. For the sake of definiteness let us assume that the electrons relax in the contacts due to collisions with phonons and the phonon relaxation due to anharmonicity and scattering by lattice defects (as well as to the escape of the nonequilibrium phonons from the microcontact region) is rapid so that Eq. (33) is valid, the phonon system being in equilibrium. The electrons to be scattered should penetrate rather deeply into the contact region. Physically this means that the number of channels in the contact region is large as compared with the number in the microstructure. As the number of electrons in the contacts is large they can be treated as a 3D electron gas so that the usual Bloch wave representation can be used instead of the channel representation when this is more convenient. For adiabatic transport the number of nodes of a function of transverse quantization $\eta_n(\mathbf{r}_\perp ;x)$ for a current-carrying channel is invariant in x and is small. Far from the microstructure the bottoms of the channels, $\epsilon(0,x)$ are approaching each other. This means that a few electron states that are out of equilibrium have transverse parts of their quasimomenta small as compared to the longitudinal part. In other words, their quasimomenta have practically the same value $\mathbf{p}$, i.e., only a few electron states of all the states belonging to the contact region are out of equilibrium. This means that the nonequilibrium part of the electron distribution function is a sharp function of the quasimomentum $\mathbf{p}$ and we are dealing with the situation discussed after Eq. (37). The integral part of the collision operator should be negligibly small as compared to the relaxation time term, Eq. (37), so one can use the relaxation time approximation.[20]

Within this approximation the nonequilibrium part of the distribution function, ΔF_{np}, satisfies the following equation:

$$v_{np}\frac{\partial \Delta F_{np}}{\partial x}+\frac{\Delta F_{np}}{\tau}=0. \tag{39}$$

Strictly speaking, the boundary condition for this equation should be formulated somewhere near the border of the contact region. However, by our assumption the electrons do not experience collisions within the nanostructure, or, in other words, the electron mean free path is much bigger than the longitudinal dimension of the nanostructure. Therefore we practically would introduce no mistake by formulating the boundary conditions at $x=0$,

$$\Delta F_{np}|_{x=0}=\frac{\partial F_{np}}{\partial \mu}\Delta\mu, \tag{40}$$

where $\Delta\mu=\mu^{(+)}-\mu^{(-)}=eV$. We assume here that $eV\ll T$.

The solution of Eq. (39) with the boundary condition given by Eq. (40) is

$$\Delta F_{np}=\frac{\partial F^{(0)}_{np}}{\partial \mu}\Delta\mu \exp\left(-\frac{x}{v\tau_{\mathbf{p}}}\right). \tag{41}$$

Here we have neglected the difference between the channel velocity v_{np} and the 3D velocity $v_{\mathbf{p}}$. Inserting Eq. (41) into Eq. (37) we get for the spatial distribution of the rate of heat production

$$T\left[\frac{\partial S}{\partial t}\right]_{\text{coll}}=2(eV)^2\sum_n \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\,\frac{1}{\tau_{\mathbf{p}}}\,\frac{\partial F^{(0)}_{np}}{\partial \mu}\exp\left(-\frac{2x}{v\tau_{\mathbf{p}}}\right). \tag{42}$$

Taking into account Eqs. (3) and (11) we get for the overall heat production within the reservoir

$$-\frac{d\mathcal{E}}{dt}=\frac{(eV)^2}{\tau_{\mathbf{p}}}2\mathcal{N}\int_0^{\infty}\frac{dp}{2\pi\hbar}\int_0^{\infty}dx\ \exp\left(-\frac{2x}{v\tau_{\mathbf{p}}}\right)\frac{\partial F^{(0)}_{np}}{\partial \mu}. \tag{43}$$

After the integration we get for the contact region

$$-\frac{d\mathcal{E}}{dt}=\frac{(eV)^2}{2\pi\hbar}\mathcal{N}, \tag{44}$$

where $\mathcal{N}$ is the number of active channels, i.e., the channels whose bottoms are below the Fermi level. Calculating the contribution of the region $x<0$ we find that for the considered case the full rate of heat generation *is the same in both contacts* (even though the values of the relaxation times $\tau_{\mathbf{p}}$ may be different). This is true irrespective to the actual form of the potential profile. Equation (43) gives the spatial distribution of the generated heat. The heat is spread over regions of length equal to the mean free path $v\tau_{\mathbf{p}}$, i.e., well outside the nanostructure.

One can present the total rate of heat generation for the entire system in the form

$$-\frac{d\mathcal{E}}{dt}=GV^2, \tag{45}$$

where for G one has the well-known expression,[21]

$$G = \frac{e^2}{\pi\hbar}\mathcal{N}. \tag{46}$$

Thus the calculation of the heat production provides an alternative method to calculate the conductance of nanostructure. We can also remark that the fact that the relaxation time $\tau_{\mathbf{p}}$ was due to the electron-phonon collisions was not crucial for the derivation of Eq. (43). We would have come to the same relation if, for instance, $\tau_{\mathbf{p}}$ had been due to another scattering mechanism within the classical contact (for example, the electron-electron collisions).

A crucial point for our derivation was the fact that we have neglected the difference between the channel velocity v_{np} and the 3D velocity $v_{\mathbf{p}}$. In other words, this means that *we treat the reservoir regions classically*. This fact agrees with the general concept of quantum theory of measurements. To perform a quantum measurement (of a conductance in the present case) one needs a classical measuring device (i.e., classical reservoirs for the present case).

One can obtain the same result using classical equation (37) for the entropy production. We are going to outline here briefly such a calculation. We have

$$\left[\frac{\partial \hat{\mathcal{S}}}{\partial t}\right]_{\text{coll}} = \int_0^\infty dx \int d^2\mathbf{r}_\perp \int d\xi_{\mathbf{p}} \frac{(\Delta F_{\mathbf{p}})^2}{\tau_{\mathbf{p}} F_{\mathbf{p}}^{(0)}(1-F_{\mathbf{p}}^{(0)})}. \tag{47}$$

For ΔF one can use Eq. (41) where (as is stated above) one can disregard the dependence on the small transverse components of quasimomentum $\mathbf{p}_\perp$, or, in other words, on the channel number n. Now, the integration over $d^2\mathbf{r}_\perp d^2\mathbf{p}_\perp$ can be replaced by summation over discrete values of $\mathbf{p}_\perp$. As indicated above, the number of terms in such a sum should be equal to the number of open channels, and we again end up with Eq. (44) irrespective to the actual scattering mechanism that is responsible for the relaxation time τ. The only dependence of this result on the actual form of the potential profile within the nanostructure is in the number of active channels $\mathcal{N}$.

VII. CONCLUSION

The methods developed here can also be applicable for other problems. One example is heat release in the contacts in the course of tunneling of electrons.

In the present paper we discuss mostly the Ohmic conduction. The simplest example of non-Ohmic conduction is a ballistic resistance for $eV \gg T$.[22,12,23] Again the heat generation takes place well outside the nanostructure, within the contacts. Its calculation should go along the line developed in Sec. VI.

More complicated are various aspects of the so-called phonon-assisted ballistic resistance, both Ohmic and non-Ohmic.[12,13,24] In the classical regime, nonlinear phenomena in the current-voltage characteristics of point contacts between normal metals were observed and discussed in a pioneering work by Yanson.[25] Here we mean a quantum situation where the conduction electrons experience some scattering within the nanostructure. As indicated in Ref. 26, the situation here is quite unlike the usual collisionless transport where the electron-phonon (as well as the electron-electron and electron-impurity) interactions are restricted to the contacts and hence all the heat is released in the contacts only. In the mentioned case some energy is transferred to phonons and may be released as a heat by the phonon system outside both the wire and the contacts.

In summary, we have calculated the Joule heat release in the course of collisionless Ohmic transport of electric current through a quantum nanostructure. We come to the conclusion that to calculate the Joule heat for this case (as well as for any case of Ohmic conduction) it is sufficient to solve the Boltzmann equation up to the first order in the voltage drop across the nanostructure (or in electric field **E**). We find that the heat is spread over the length of the electron mean free path in the reservoirs. Even if the electron mean free paths in both reservoirs are different the total rate of heat generation in each reservoir is the same. We indicate that a calculation of the heat generation may provide an alternative method of computation of collisionless conductance.

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[1] Some aspects of this work are briefly discussed in V. L. Gurevich, Pis'ma Zh. Éksp. Teor. Fiz. **63**, 61 (1996) [Sov. Phys. JETP Lett. **63**, 70 (1996)].

[2] Yu. V. Sharvin, Zh. Éksp. Teor. Fiz. **48**, 984 (1965) [Sov. Phys. JETP **21**, 655 (1965)].

[3] I. O. Kulik, R. I. Shekhter, and A. N. Omelyanchouk, Solid State Commun. **23**, 301 (1977).

[4] M. Rokni and Y. Levinson, Phys. Rev. B **52**, 1882 (1995).

[5] R. Landauer, IBM J. Res. Dev. **1**, 233 (1957); **32**, 306 (1989).

[6] Y. Imry, in *Directions in Condensed Matter Physics*, edited by G. Grinstein and G. Mazenko (World Scientific, Singapore, 1986), p. 101; M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).

[7] I. O. Kulik, R. I. Shekhter, and A. G. Shkorbatov, Zh. Éksp. Teor. Fiz. **81**, 2126 (1981) [Sov. Phys. JETP **54**, 1130 (1981)].

[8] I. F. Itskovich, I. O. Kulik, and R. I. Shekhter, Solid State Commun. **50**, 421 (1984).

[9] Y. B. Levinson, Zh. Éksp. Teor. Fiz. **95**, 2175 (1989) [Sov. Phys. JETP **68**, 1257 (1989)].

[10] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, 3rd ed. (Pergamon Press, Oxford, 1993), Part 1.

[11] L. I. Glazman, G. B. Lesovik, D. E. Khmel'nitskii, and R. I. Shekhter, Pis'ma Zh. Éksp. Teor. Fiz. **48**, 218 (1988) [Sov. Phys. JETP Lett. **48**, 238 (1988)].

[12] V. L. Gurevich, V. B. Pevzner, and K. Hess, Phys. Rev. B **51**, 5219 (1995).

[13] V. L. Gurevich, V. B. Pevzner, and K. Hess, J. Phys. Condens. Matter **6**, 8363 (1994).

[14] A. G. Aronov, Yu. M. Galperin, V. L. Gurevich, and V. I. Kozub, Adv. Phys. **30**, 539 (1981). The results for normal metals can be obtained from the equation for superconductors given in this paper by going to the limit $\Delta \rightarrow 0$ where Δ is the superconducting gap.

[15] J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, 1960).

[16] J. P. Leburton, Phys. Rev. B **45**, 11 022 (1995).

[17] E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics* (Pergamon Press, Oxford, 1981).

[18] V. L. Gurevich, *Transport in Phonon Systems* (North-Holland, Amsterdam, 1986).

[19] A. A. Abrikosov, *Fundamentals of the Theory of Metals* (North-Holland, Amsterdam, 1988).

[20] One can see that the relaxation time approximation is actually unnecessary for calculation of the overall heat release within the contact region(s). It is, however, essential for calculation of the spatial distribution of the heat.

[21] See, for instance, C. W. J. Beenakker and H. van Houten, in *Solid State Physics: Advances in Research and Applications*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1991), Vol. 44.

[22] V. L. Gurevich and V. B. Pevzner (unpublished).

[23] V. L. Gurevich, V. B. Pevzner, and G. J. Iafrate, Phys. Rev. Lett. **75**, 1352 (1995).

[24] V. L. Gurevich, V. B. Pevzner, and E. W. Fenton, Phys. Rev. B **51**, 9465 (1995).

[25] I. K. Yanson, Sov. Phys. JETP **39**, 506 (1974).

[26] V. L. Gurevich, V. B. Pevzner, and G. J. Iafrate, J. Phys. Condens. Matter **7**, L445 (1995).