Reduced differential current: A conserved quantity in short-scale transport

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An electronic transport invariant, the reduced differential current (RDC), is introduced. The RDC is approximately conserved over short distances typical for modern semiconductor devices. In a steady-state transport, the divergence of the RDC vanishes if the only source of inelastic collisions is due to the interaction with monochromatic optical phonons. Rates of the violation of the RDC invariance due to the inelastic acoustic-phonon scattering and to the dispersion of optical phonons are calculated for exemplary nonequilibrium electron distributions.

I. INTRODUCTION

In this paper we discuss a quantity $\mathbf{G}(\mathbf{r},E)$ that is approximately conserved in a short-scale electronic transport. It is a vector field and a function of the electron energy, defined by the following expression:

$$\mathbf{G}(\mathbf{r},E)=\sum_{\{\nu(\mathbf{r})\}}\frac{\partial\mathbf{J}(\mathbf{r},E+\nu\hbar\omega_0)}{\partial E}\ ,$$

$$E-U(\mathbf{r})+\nu\hbar\omega_0>0\ , \quad (1)$$

where $\mathbf{J}(\mathbf{r},E)$ is the contribution to the total current density $\mathbf{J}(\mathbf{r})$ from electrons traveling at the point $\mathbf{r}$ with a total energy $E=E_{\rm kin}+U(\mathbf{r})$, where $E_{\rm kin}$ is the kinetic and $U(\mathbf{r})$ the potential electron energy. The summation in Eq. (1) is carried over all integer values of $\nu=0,\pm1,\pm2,\ldots$ consistent with the condition of positive kinetic energy $E_{\rm kin}=E-U+\nu\hbar\omega_0>0$, where $\hbar\omega_0$ is the optical-phonon energy. We shall call $\mathbf{G}(\mathbf{r},E)$ the reduced differential current, or RDC. The argument E in Eq. (1) is an independent variable, not a function of $\mathbf{r}$; on the other hand, the range of the summation over ν depends on $\mathbf{r}$ through the condition $E_{\rm kin}>0$.

It is clear from the definition (1) that $\mathbf{G}$ is a periodic function of E. The total current density can be expressed in terms of the RDC as follows:

$$\mathbf{J}(\mathbf{r})=\int_0^{\infty}\frac{\partial\mathbf{J}[\mathbf{r},U(\mathbf{r})+E_{\rm kin}]}{\partial E_{\rm kin}}dE_{\rm kin}$$

$$=\int_0^{\hbar\omega_0}\mathbf{G}[\mathbf{r},U(\mathbf{r})+E_{\rm kin}]dE_{\rm kin}\ . \quad (2)$$

The useful property of the RDC concept is that it is invariant in a steady-state transport, $\mathrm{div}\mathbf{G}(\mathbf{r},E)=0$, for any scattering model in which inelastic collisions result only from dispersionless optical phonons. This property reflects the fact that the combined action of an electric field and scattering by monochromatic phonons conserves the total number of particles that extend over a ladder of total-energy levels separated by $\hbar\omega_0$. The spatial density of particles per unit energy interval in a given ladder,

$$N_{\rm ext}(\mathbf{r},E)=\sum_{\{\nu(\mathbf{r})\}}\frac{\partial n(\mathbf{r},E+\nu\hbar\omega_0)}{\partial E}\ ,$$

$$E-U(\mathbf{r})+\nu\hbar\omega_0>0\ , \quad (3)$$

where $n(\mathbf{r},E)$ is the density of electrons of energy E, must, therefore, satisfy a continuity equation of the form

$$\frac{e\partial N_{\rm ext}(\mathbf{r},E)}{\partial t}+\mathrm{div}\mathbf{G}(\mathbf{r},E)=0\ . \quad (4)$$

It is not hard to see that the generalized current $\mathbf{G}$ in (4) coincides with the RDC. In what follows this fact will be formally proven from the Boltzmann equation. This approach will also enable us to assess the rate at which the continuity equation (4) is violated by inelastic acoustic-phonon scattering and by a non-negligible optical-phonon dispersion.

II. DERIVATION OF THE RDC CONTINUITY EQUATION

Let $f_{\mathbf{k}}(\mathbf{r})$ be the electron distribution function, satisfying the kinetic equation in its general form:

$$\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial t}=-\frac{1}{\hbar}\frac{\partial E_{\mathbf{k}}}{\partial\mathbf{k}}\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial\mathbf{r}}+\frac{1}{\hbar}\frac{\partial U}{\partial\mathbf{r}}\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial\mathbf{k}}$$

$$+[\hat{S}_{\mathbf{k}}^{(+)}f_{\mathbf{k}}(\mathbf{r})-\hat{S}_{\mathbf{k}}^{(-)}f_{\mathbf{k}}(\mathbf{r})]\ , \quad (5)$$

where $\hat{S}_{\mathbf{k}}^{(+)}$ and $\hat{S}_{\mathbf{k}}^{(-)}$ are the collision operators describing, respectively, the scattering into and from a point $\mathbf{k}$ of the momentum space. The differential current density due to particles whose total energy equals E is given by

$$\frac{\partial\mathbf{J}}{\partial E}=\frac{2e}{\hbar(2\pi)^3}\int\frac{\partial E_{\mathbf{k}}}{\partial\mathbf{k}}f_{\mathbf{k}}(\mathbf{r})\delta[E-E_{\mathbf{k}}-U(\mathbf{r})]d^3\mathbf{k}\ . \quad (6)$$

Taking the divergence of (6), we find

$$\operatorname{div}\left[\frac{\partial \mathbf{J}(\mathbf{r},E)}{\partial E}\right]=\frac{2e}{\hbar(2\pi)^3}\int\frac{\partial E_{\mathbf{k}}}{\partial \mathbf{k}}\cdot\left[\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial \mathbf{r}}+\frac{\partial U}{\partial \mathbf{r}}f_{\mathbf{k}}(\mathbf{r})\frac{\partial}{\partial E_{\mathbf{k}}}\right]\delta(E-E_{\mathbf{k}}-U)d^3\mathbf{k}$$

$$=\frac{2e}{\hbar(2\pi)^3}\int\left[\frac{\partial E_{\mathbf{k}}}{\partial \mathbf{k}}\cdot\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial \mathbf{r}}+\frac{\partial U}{\partial \mathbf{r}}f_{\mathbf{k}}(\mathbf{r})\frac{\partial}{\partial \mathbf{k}}\right]\delta(E-E_{\mathbf{k}}-U)d^3\mathbf{k}$$

$$=\frac{2e}{\hbar(2\pi)^3}\int\left[\frac{\partial E_{\mathbf{k}}}{\partial \mathbf{k}}\cdot\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial \mathbf{r}}-\frac{\partial U}{\partial \mathbf{r}}\cdot\frac{\partial f_{\mathbf{k}}(\mathbf{r})}{\partial \mathbf{k}}\right]\delta(E-E_{\mathbf{k}}-U)d^3\mathbf{k}\ . \tag{7}$$

Multiplying Eq. (5) by $2(2\pi)^{-3}\delta(E-E_{\mathbf{k}}-U)$, integrating over $d^3\mathbf{k}$, and using relation (7), we obtain

$$\frac{\partial}{\partial t}N(\mathbf{r},E)+\frac{1}{e}\operatorname{div}\left[\frac{\partial \mathbf{J}(\mathbf{r},E)}{\partial E}\right]$$

$$=\int[\hat{S}_{\mathbf{k}}^{(+)}f_{\mathbf{k}}(\mathbf{r})-\hat{S}_{\mathbf{k}}^{(-)}f_{\mathbf{k}}(\mathbf{r})]\delta(E-E_{\mathbf{k}}-U)\frac{2d^3\mathbf{k}}{(2\pi)^3}\ , \tag{8}$$

where $N(\mathbf{r},E)$ is the differential electron concentration defined by

$$N(\mathbf{r},E)\equiv\frac{\partial n(\mathbf{r},E)}{\partial E}=\frac{2}{(2\pi)^3}\int f_{\mathbf{k}}(\mathbf{r})\delta(E-E_{\mathbf{k}}-U)d^3\mathbf{k}\ . \tag{9}$$

Had we integrated Eq. (8) over all energies E we would have obtained the usual continuity equation. In the right-hand side terms containing $\hat{S}_{\mathbf{k}}^{(+)}$ and $\hat{S}_{\mathbf{k}}^{(-)}$ cancel after the integration: each of these terms describes the total number of collision-induced transitions in the system. This cancellation, of course, does not depend on the nature of collisions. Clearly, for *elastic* collisions only—whatever their nature—terms containing $\hat{S}_{\mathbf{k}}^{(+)}$ and $\hat{S}_{\mathbf{k}}^{(-)}$ cancel without an integration over E and the right-hand side of (8) vanishes.

To prove Eq. (4), we sum Eq. (8) over all energies $E^{(\nu)}>0$ in the extended set:

$$E^{(\nu)}(E)=E+\nu\hbar\omega_0-U(\mathbf{r})\ . \tag{10}$$

The right-hand side $R(E)$ of the resultant equation

$$\frac{\partial N_{\text{ext}}(\mathbf{r},E)}{\partial t}+\frac{\operatorname{div}\mathbf{G}(\mathbf{r},E)}{e}=R(E) \tag{11}$$

must be evaluated for concrete inelastic-scattering processes. In this work we restrict our consideration to phonon scattering, leaving out the contribution to $R(E)$ from electron-electron collisions. This means that our treatment should be valid in the limit of low carrier concentration.

III. PHONON SCATTERING

For electrons interacting with phonons of a branch j, the expression for $R(E)$ can be brought into the form

$$R^{(j)}(E)=\sum_{\nu}^{\{E^{(\nu)}>0\}}\int\frac{d^3\mathbf{q}}{(2\pi)^3}\frac{2d^3\mathbf{k}}{(2\pi)^3}|W_{\mathbf{q}}^{(j)}|^2[(N_{\mathbf{q}}^{(j)}+1)f_{\mathbf{k}+\mathbf{q}}(1-f_{\mathbf{k}})-N_{\mathbf{q}}^{(j)}f_{\mathbf{k}}(1-f_{\mathbf{k}+\mathbf{q}})]$$

$$\times\delta(E_{\mathbf{k}+\mathbf{q}}-E_{\mathbf{k}}-\hbar\omega_{\mathbf{q}}^{(j)})[\delta(E^{(\nu)}-E_{\mathbf{k}})-\delta(E^{(\nu)}-E_{\mathbf{k}+\mathbf{q}})]\ , \tag{12}$$

where $N_{\mathbf{q}}^{(j)}\equiv[\exp(\hbar\omega_{\mathbf{q}}^{(j)}/T)-1]^{-1}$ is the Planck function and $W_{\mathbf{q}}^{(j)}$ is a coefficient proportional to the electron-phonon interaction matrix element. For the interaction with acoustic phonons the $W_{\mathbf{q}}^{(j)}$ is given by $|W_{\mathbf{q}}^{\text{ac}}|^2=(\pi E_{\text{ac}}^2/\rho s)|\mathbf{q}|$, where E_{ac} is the deformation-potential constant, ρ the material density, and s the sound velocity.

In the case of monochromatic optical phonons, $\hbar\omega_{\mathbf{q}}^{(j)}=\hbar\omega_0$, each of the two δ-function terms in (12) contributes the same amount, since they are different only by the order of their appearance in the sum. Consequently, $R^{(j)}(E)$ vanishes for this interaction. For other inelastic interactions, in general, $R^{(j)}(E)\neq 0$; in particular, $R^{\text{ac}}\neq 0$ for the acoustic-phonon scattering.

In evaluating the right-hand side of (11), we shall neglect the nonsymmetric part of the nonequilibrium distribution function. Moreover, in the example below we shall assume that the symmetric part is a Maxwellian function characterized by an effective temperature T_e,

$$f(E_{\mathbf{k}})=\frac{n_0}{2}\left[\frac{2\pi\hbar^2}{mT_e}\right]^{3/2}e^{-E_{\mathbf{k}}/T_e}\ , \tag{13}$$

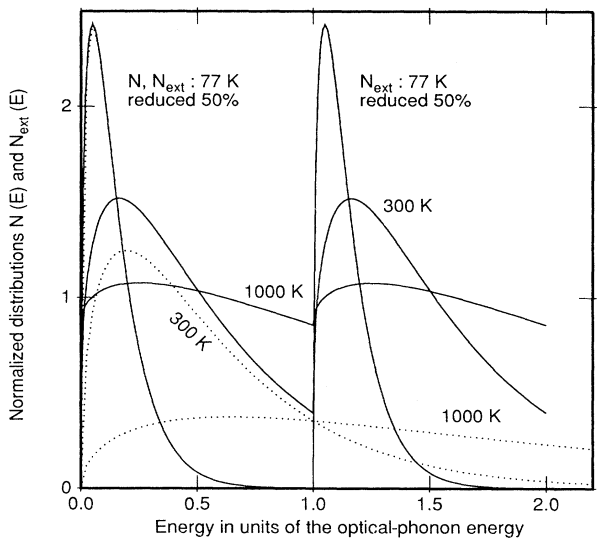

FIG. 1. Normalized distributions $N_{\text{ext}}(E)$, defined by Eq. (3), and $N(E)\propto\sqrt{E}f(E)$. Solid lines show N_{ext}, calculated from Eq. (14); dotted lines correspond to N.

and that the electron distribution is nondegenerate, $f(E_{\mathbf{k}}) \ll 1$.

It is clear that functions defined by the summation over ν, such as those in Eqs. (1), (3), and (12), are periodic in energy. We shall characterize the degradation of RDC by calculating the ratio $R^{(j)}(E)/N_{\rm ext}(E)$ as a function of the energy in the interval $0 \le E \le \hbar\omega_0$. This ratio determines the rate of change of $N_{\rm ext}(E)$ by collisions and is a functional of the distribution function $f(E)$.

With the distribution function (13), the differential number of particles $N_{\rm ext}(E)$ in the extended set (3) is given by

$$N_{\rm ext}(E) = \frac{m^{3/2}(2\hbar\omega_0)^{1/2}}{\pi^2\hbar^3} f(E) \times \sum_{\nu=0}^{\infty} (E/\hbar\omega_0 + \nu)^{1/2} e^{-\nu\hbar\omega_0/T_e} . \quad (14)$$

Figure 1 plots Eq. (14) for several values of T_e and the $\hbar\omega_0$ of GaAs. For a semiconductor with a different optical phonon energy $\hbar\omega_0'$, these plots describe the $N_{\rm ext}$ at a different set of temperatures ($T_e' = T_e\hbar\omega_0'/\hbar\omega_0$).

For inelastic interactions with acoustic phonons at an equilibrium temperature T, and an electronic ensemble distributed according to Eq. (13), it is possible to derive from (12) an analytic expression for $R^{\rm ac}(E)$ in a closed form:

$$R^{\rm ac}(E) = \frac{m^4 E_{\rm ac}^2 \beta(T_e - T) f(E)}{\pi^3 \rho \hbar^7} \frac{2(\Phi - 1 + N_\beta) - \beta[(\Phi - 1 + N_\beta)^2 + N_\beta(N_\beta - 1)]}{1 - \exp(-\beta)} , \quad (15)$$

where $0 \le \Phi \equiv E/\hbar\omega_0 \le 1$, $\beta \equiv \hbar\omega_0/T_e$, and $N_\beta = [1 - \exp(-\beta)]^{-1}$. Derivation of Eq. (15) relies on the smallness of the acoustic-phonon energy relative to the electron energy[1] and is valid only provided $T, T_e \gtrsim 10$ K. The calculated energy dependences of the ratio $R^{\rm ac}/N_{\rm ext}$ are plotted in Fig. 2 for two values of T_e in Si and in GaAs. The lattice temperature is assumed low ($T = 77$ K) to emphasize the behavior away from equilibrium. However, for $T_e = 1000$ K, the curves at $T = 300$ K are practically indistinguishable from those at $T = 77$ K. The ratio of 3×10^{-2} between the curves corresponding to GaAs and Si is mainly owing to the difference in the effective electron mass. If all other parameters were equal (including $\hbar\omega_0$), then the ratio $R^{\rm ac}/N_{\rm ext}$ would scale in proportion to $m^{5/2}$ (the relevant value for silicon being[2] $m_l^2 m_t^{1/2}$).

The energy dependence of $R^{\rm ac}/N_{\rm ext}$ is of qualitatively expected shape. Because of the small phonon energy, the gain and/or loss of energy is determined by derivatives of the distribution function. For $T_e > T$, the number of particles decreases in the range $E > T_e$, which corresponds to the direction toward equilibrium. The decrease of $R^{\rm ac}$ in the range $E < T_e$ is due to the depletion of the distribution at energies $E + \hbar\omega_0$, $E + 2\hbar\omega_0$, etc., which overwhelms the enhancement at E. In the intermediate range of energies $R^{\rm ac}$ is positive, corresponding to an increasing RDC. It is clear that $R^{\rm ac}$ must change sign in different energy ranges, since the integral over E vanishes exactly in light of the current continuity.

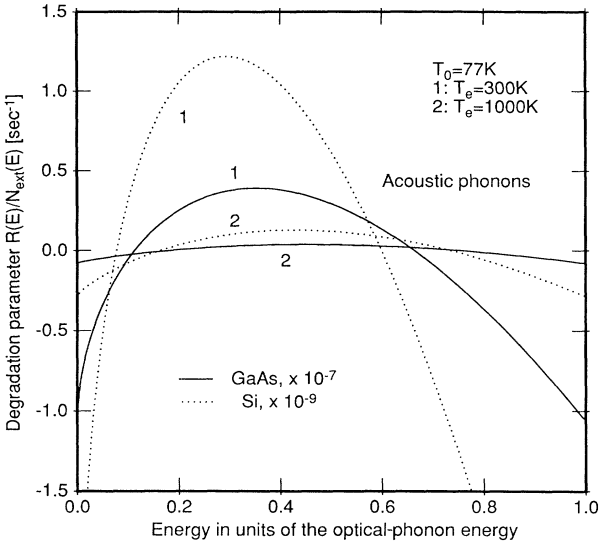

FIG. 2. Degradation parameter $R^{\rm ac}(E)/N_{\rm ext}(E)$ calculated according to Eqs. (14) and (15) for the nonequilibrium electron distribution described by Eq. (12) with $T_e = 300$ and 1000 K and the lattice temperature $T = 77$ K.

As seen from Fig. 2, the degradation of RDC is a rather slow process. The spatial scale of the variation of **G** due to the acoustic-phonon scattering is of the order $N_{\rm ext} R^{-1} v_{\rm sat} \approx 0.1$ cm for GaAs and ≈ 30 μm for Si (here $v_{\rm sat} \sim 10^7$ cm/s is the scattering-limited electron velocity).

Another possible mechanism for the degradation of the RDC is associated with the fact that optical phonons are not exactly monochromatic. The dispersion of optical phonons can be described[3] by an expression of the form $\hbar\omega_{\mathbf{q}}^{(\rm op)} - \hbar\omega_0 - \gamma q^2 = \hbar\omega_0 - \tilde{\gamma} E_q$, where $E_q \equiv \hbar^2 q^2/2m$. The dimensionless parameter $\tilde{\gamma}$ approximately equals 10^{-4} in GaAs and 6×10^{-4} in Si.[4] We have carried out estimates based on Eq.(12), taking

$$|W_{\mathbf{q}}^{{\rm op}(P)}|^2 = \frac{4\pi^2 e^2 \omega_0}{|\mathbf{q}|^2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) ,$$

$$|W_{\mathbf{q}}^{{\rm op}(N)}|^2 = \frac{\pi E_{\rm op}^2 \omega_0}{\rho s^2} ,$$

for polar (GaAs) and nonpolar (Si) optical phonons, respectively, where ϵ_0 and ϵ_∞ are the static and the optical-frequency dielectric permittivities of the semiconductor. Typically, the estimated rate $R^{\rm op}$ of the RDC degradation due to the optical-phonon dispersion turns out to be *higher* than $R^{\rm ac}$ given by Eq. (15). Indeed, the width of the optical-phonon band is only an order of magnitude smaller than the characteristic energy of

acoustic phonons that interact with electrons while the optical-phonon scattering rate is much higher. It should be noted, however, that optical phonons can appreciably degrade the RDC only after *multiple* emission and/or absorption processes, upon the accumulation of small differences in energy. In order that an electron belonging to the ladder $E+\nu\hbar\omega_0$ could end up in the ladder $E'+\nu\hbar\omega_0$, one needs at least $2(E-E')/\gamma E_q$ emission and absorption processes. For a scatter in energy $(E-E')$ in typical electron distributions of interest, this number is very large. Therefore the inclusion of optical phonons can be of importance in the degradation of RDC only for an unusually narrow electron distribution peaked at a high energy. Another situation, when the optical-phonon dispersion may be important, corresponds to sufficiently high temperatures and multiple emission and reabsorption of $\hbar\omega_{\mathbf{q}}$. This situation is more relevant for GaAs, where the optical-phonon energy is relatively low. However, in this case the degradation of RDC is further suppressed by the $\mathbf{q}$ dependence of $W_{\mathbf{q}}^{\mathrm{op}(P)}$ that favors small momentum transfers.

IV. CONCLUSION

We have introduced the concept of RDC, which should be useful in the studies of transport in short-scale semiconductor devices. So long as the RDC is conserved, the Boltzmann transport equation can be split into independent equations for electrons belonging to different energy ladders, $E+\nu\hbar\omega_0$. Another situation where the RDC can be extremely helpful corresponds to a coexistence of a region of high electric field, where electronic transport is fast, with a low-field region, where both the RDC and N_{ext} rapidly collapse into the usual differential current density $\partial J/\partial E$ and the differential concentration $\partial N/\partial E \sim \sqrt{E} f(E)$. The power of this approach was recently demonstrated[5] by applying it to the problem of current oscillations in $GaAs/Al_xGa_{1-x}As$ heterostructure-tunneling diodes. It was found that the RDC was responsible for transporting the tunnel-injected structure in the electron energy distribution over micrometer-length distances; this allowed us to obtain a satisfactory explanation of a long-standing puzzle.

The conservation of RDC has been rigorously demonstrated in the limit of low carrier concentration, which is the case where the theory[5] was applied. In this limit, the electronic system can be expected to exhibit unusual transport and thermodynamic properties. Such a situation can arise both in a nonuniform system with a steady-state electron flow,[5] and in a spatially uniform nonstationary system on a short temporary scale.[6] Equation (11) describes the general case. It should be noted, however, that electron-electron collisions make an important contribution to the right-hand side of (11). Preliminary Monte Carlo estimates[7] show that in bulk GaAs this contribution becomes dominant already for electron concentrations of order 10^{16} cm^{-3}. Analysis of the degradation of RDC by interelectronic scattering will be presented in a separate publication.

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