Parallel channel to the Boltzmann band conduction: Scattering by charged screened impurities in semiconductors

V. Čápek
Institute of Physics of Charles University, Ke Karlovu 5, CS-121 16 Prague 2, Czechoslovakia
(Received 1 February 1988; revised manuscript received 19 April 1988)

With use of generalized master equations, an additive correction to the mobility of nondegenerate single-type carriers in a parabolic band scattered by charged screened random impurities is found to the lowest order in the impurity scattering. This correction may become important at low temperatures.

I. INTRODUCTION

Standard Boltzmann theory of the band conduction gets problematic for scattering by charged impurities once the concentration n of carriers providing screening becomes sufficiently low. The cutoff procedure by Conwell and Weisskopf[1] (though successful in several respects) remains just an artificial procedure and the Brooks[2] and Herring method of including screening becomes inoperative (due to too strong scattering on almost unscreened Coulomb centers) when $n \to 0$. Here, we report on a new method of calculating the mobility, starting from the generalized master equations (GME).[3,4] The Ohmic current in the dc (and similarly ac) field results as a sum of a Boltzmann-like term and a new non-Boltzmann contribution. Corresponding additive correction to the Boltzmann dc mobility can be made explicit for a parabolic band and single-type nondegenerate carriers (electrons henceforth) screening charged random impurities in an exponential manner to[2] the lowest (second) order in the impurity potential provided that the impurities are the only relevant scattering mechanism.

II. GENERALIZED MASTER EQUATIONS

Let us designate d, $\mathcal{E}(t)$ and $\delta\rho(t)$ the electronic dipole moment, acting electric field, and linear (in $\mathcal{E}$) change of the electron density matrix $\rho(t)$. Assuming that $\mathcal{E}(t) \to 0$ for $t \to -\infty$, i.e., that $\rho(t) \to \rho_{\rm eq}$, $t \to -\infty$ ($\rho_{\rm eq}$ being canonical), the linearized GME reads

$$\frac{\partial}{\partial t}[D\,\delta\rho(t)] = -iDLD\,\delta\rho(t) + \frac{i}{\hbar}D\mathcal{E}(t)[d,\rho_{\rm eq}] + \int_{-\infty}^{t} DLe^{-i(1-D)L(t-\tau)}(1-D) \times \left[-LD\,\delta\rho(\tau) + \frac{1}{\hbar}\mathcal{E}(\tau)[d,\rho_{\rm eq}]\right] d\tau \,. \tag{1}$$

Here $L(\cdots) = \hbar^{-1}[H,(\cdots)]$ is the Liouville superoperator,[4] H is the electron Hamiltonian, and D is the standard Zwanzig[3] projector

$$[D\rho(t)]_{\{k\}\{k'\}} = [\rho(t)]_{\{k\}\{k\}}\delta_{\{k\}\{k'\}} \,, \tag{2a}$$

$$|\{k\}\rangle = \prod_{gs\in\{k\}} a_{gs}^{\dagger}|{\rm vac}\rangle \tag{2b}$$

($a_{gs}^{\dagger}$ being the creation operator of an electron with momentum g and spin s). For every linear idempotent D ($=D^2$) [(2a)–(2b)], the solution to (1) reads[5]

$$D\,\delta\rho(t) = \int \frac{d\omega}{2\pi} e^{-i(\omega+i\delta)t} D\,\delta\rho^{\omega+i\delta} \,,$$
$$D\,\delta\rho^{\omega+i\delta} = -D\frac{1}{\hbar}\frac{1}{\omega+i\delta-L}\mathcal{E}^{\omega+i\delta}[d,\rho_{\rm eq}] \,. \tag{3}$$

For the current density operator having no off-diagonal elements in representation (2b), we have from (3)

$$\langle j_\alpha\rangle(t) = \sum_{\gamma=1}^{3}\int \frac{d\omega}{2\pi} e^{-i(\omega+i\delta)t}\sigma_{\alpha\gamma}(\omega+i\delta)\mathcal{E}_{\gamma}^{\omega+i\delta} \,, \tag{4a}$$

$$\sigma_{\alpha\gamma}(z) = -\frac{1}{\hbar}{\rm Tr}\left[j_\alpha D\frac{1}{z-L}D[d_\gamma,\rho_{\rm eq}]\right] - \frac{1}{\hbar}{\rm Tr}\left[j_\alpha D\frac{1}{z-L}(1-D)[d_\gamma,\rho_{\rm eq}]\right] \equiv \sigma_{B,\alpha\gamma}(z) + \sigma_{{\rm NB},\alpha\gamma}(z), \quad \alpha,\gamma = 1,2,3, \quad z = \omega+i\delta \,. \tag{4b}$$

Now, let us specify our Hamiltonian as

$$H = \sum_{\mathbf{g}} \varepsilon_{\mathbf{g}} a_{\mathbf{g}s}^{\dagger} a_{\mathbf{g}s} + \sum_{\mathbf{g}_1\neq\mathbf{g}_2}\sum_{s}\langle \mathbf{g}_1|\sum_{j} v(\mathbf{r}-\mathbf{r}_j)|\mathbf{g}_2\rangle a_{\mathbf{g}_1 s}^{\dagger} a_{\mathbf{g}_2 s} \equiv H_0 + \mathcal{H} \,. \tag{5}$$

It describes band electrons (H_0) scattered by impurities ($\mathcal{H}$). Here $\sum_j$ means summation over random impurities. Using (2a), we have

$$DL_0 = L_0 D = 0, \quad L_0(\cdots) = \frac{1}{\hbar}[H_0,(\cdots)], \quad DLD = 0 \,, \tag{6}$$

so that $\sigma_B(z)$ may be rewritten as

$$\sigma_{B,\alpha\gamma}(z)=-\frac{1}{\hbar}\,\mathrm{Tr}\left[j_\alpha\frac{D}{z-\mathcal{L}\left[\frac{1-D}{z-L}\right]\mathcal{L}}[d_\gamma,\rho_{eg}]\right],\qquad z=\omega+i\gamma\ , \tag{7a}$$

$$\mathcal{L}=(\cdots)\frac{1}{\hbar}[\mathcal{H},(\cdots)]\ . \tag{7b}$$

Owing to a typical ω dependence, σ_B may be easily identified with the Boltzmann-like contribution to the conductivity σ. Approximating

$$\mathcal{L}\frac{1-D}{z-L}\mathcal{L}\approx\mathcal{L}\frac{1-D}{z-L_0}\mathcal{L}\ , \tag{8a}$$

$$[d_\gamma,\rho_{eq}]\approx[d_\gamma,e^{-\beta H_0}/\mathrm{Tr}(e^{-\beta H_0})] \tag{8b}$$

gives for σ_B the Brooks and Herring value for the dc conductivity in the limit $z\to 0$ as long as we assume

$$\langle g_1|v(r)|g_2\rangle=\left\langle g_1\left|\pm\frac{Ze^2}{\varepsilon_0 r}e^{-g_{FT}r}\right|g_2\right\rangle \approx\pm\frac{4\pi Ze^2}{\varepsilon_0\Omega[(g_1-g_2)^2+g_{FT}^2]}\ . \tag{9}$$

III. NON-BOLTZMANN CONDUCTIVITY CHANNEL

This channel is given by σ_{NB}, where NB denotes non-Boltzmann, in (4b). It is worth mentioning that once we neglect $\mathcal{H}$ in both the denominator and in ρ_{eq} in the second term (σ_{NB}) in the first equality of (4b), $\sigma_{NB}(z)$ turns to zero. (This procedure is justified by analyticity and absence of any divergency.) Direct expansion of σ_{NB} starts with positive powers of $\mathcal{H}$, i.e., for randomly distributed impurities, it is proportional to positive powers of the impurity concentration c. To the second order in $\mathcal{H}$ and in the dc limit $z\to 0$, we obtain

$$\sigma_{NB,\alpha\gamma}\equiv\sigma_{NB,\alpha\gamma}(z\to 0)=\frac{\pi e^2\beta^3\hbar}{2}c\sum_{g_1\neq g_2}\sum_s\delta(\varepsilon_{g_1}-\varepsilon_{g_2})|\langle g_1|v(r)|g_2\rangle|^2 \times[\mathbf{v}_{g_1}+\mathbf{v}_{g_2}]_\alpha[\mathbf{v}_{g_1}+\mathbf{v}_{g_2}]_\gamma\{n_F(\varepsilon_{g_1})[1-n_F(\varepsilon_{g_2})]\}^2+o(\mathcal{H}^2),\quad \lim_{x\to 0}\frac{o(x^2)}{x^2}=0 \tag{10a}$$

$$n_F(y)=\frac{1}{e^{\beta(y-\mu)}+1},\quad \beta=\frac{1}{k_BT}\ . \tag{10b}$$

Here μ is the chemical potential.

Let us now assume one parabolic band

$$\varepsilon_g=\frac{\hbar^2g^2}{2m^*}\ , \tag{11}$$

the form of the matrix element as in (9) and extend the integration in (10a) to infinity. Then

$$\sigma_{NB,\alpha\gamma}=\delta_{\alpha\gamma}\sigma_{NB}\ ,$$

$$\sigma_{NB}=\frac{4Z^2e^6\beta^3}{3\pi\varepsilon_0^2\hbar}c\int_0^{+\infty}d\varepsilon\{n_F(\varepsilon)[1-n_F(\varepsilon)]\}^2\times\left[\frac{\varepsilon}{\varepsilon_{FT}}+\frac{1}{4}\ln\frac{\varepsilon_{FT}}{4\varepsilon+\varepsilon_{FT}}\right]+o(\mathcal{H}^2)\ ,$$

$$\varepsilon_{FT}=\frac{\hbar^2g_{FT}^2}{2m^*}\ . \tag{12}$$

For nondegenerate electrons,

$$\{n_F(\varepsilon)[1-n_F(\varepsilon)]\}^2\approx e^{-2\beta(\varepsilon-\mu)}\ ,$$

$$g_{FT}^2=\frac{4\pi ne^2}{\varepsilon_0k_BT}\ . \tag{13}$$

Then (12) gives the non-Boltzmann additive correction to the mobility

$$\mu_{NB}\equiv\frac{\sigma_{NB}}{|e|n}=\frac{\pi Z^2|e|^3\hbar^3\beta^3}{3\varepsilon_0(m^*)^2}c\times[1+\tfrac{1}{2}\beta\varepsilon_{FT}\exp(\tfrac{1}{2}\beta\varepsilon_{FT})Ei(-\tfrac{1}{2}\beta\varepsilon_{FT})]+o(\mathcal{H}^2) \tag{14}$$

where $Ei(z)=\int_{-\infty}^{z}dt\,e^t/t$ is the exponential integral. For $Z=1$ and numerically in $\mathrm{cm^2\,V^{-1}\,sec^{-1}}$,

$$\mu_{NB}=7.69\left[\frac{m}{m^*}\right]^2\left[\frac{300}{T}\right]^3\frac{10^{-18}c}{\varepsilon_0}\times[1+\tfrac{1}{2}\beta\varepsilon_{FT}\exp(\tfrac{1}{2}\beta\varepsilon_{FT})Ei(-\tfrac{1}{2}\beta\varepsilon_{FT})]+o(\mathcal{H}^2) \tag{15}$$

with T in K and c in $\mathrm{cm^{-3}}$. In typical semiconductor situations, $\frac{1}{2}\beta\varepsilon_{FT}$ is less or much less than unity. Consequently, the second term in square brackets in (15) becomes negligible. Therefore, $\mu_{NB}\sim c/T^3$ so that this non-Boltzmann additive correction to the total mobility

$$\mu_{tot}=\mu_B+\mu_{NB} \tag{16}$$

(μ_B being the Boltzmann mobility) might become important at low T and high enough c. This fully corresponds to general criteria of validity of the Boltzmann theory which certainly ceases to apply under these conditions due to very strong scattering at the least. In this context,

one should mention that the standard Boltzmann theory of the conduction in solids[6,7,8] is the lowest-order theory summing up higher orders in scattering strength (in the final conductivity formula) only partially. The origin of the additive correction (15) to $\mu_{\rm tot}$ in (16) should therefore be sought in higher-order corrections to the Boltzmann conduction.[9,10]

Physically, for, e.g, $m^*/m \approx 0.3, n = 10^{16}$ cm^{-3}, $c = 10^{17}$ cm^{-3}, and $T = 100$ K; $\mu_{\rm NB}/\mu_B$ attains values $\gtrsim 10^2$, due to too low values of μ_B resulting from the Boltzmann treatment. This shows the significance of our treatment. It is expected that (15) and (16) might apply for slightly compensated samples when the conduction is still inside the bands of extended states. For, e.g., extremely low n (very low T) when conduction is mainly in tails of the bands (or inside impurity bands), neither the Boltzmann treatment nor that presented here are sufficiently accurate.

[1]E. M. Conwell and V. F. Weisskopf, Phys. Rev. **77**, 388 (1950).
[2]H. Brooks, Phys. Rev. **83**, 879 (1951).
[3]R. W. Zwanzig, in *Lectures in Theoretical Physics,* edited by W. E. Brittin, B. W. Downs, and J. Downs (Interscience, New York, 1961), Vol. 3, p. 106.
[4]E. Fick and G. Sauermann, *Quantenstatistik Dynamischer Prozesse* (Geest and Portig, Leipzig, 1985), Vol. II a, p. 22.
[5]V. Čápek, Phys. Rev. B **36**, 7442 (1987).
[6]W. Kohn and J. Luttinger, Phys. Rev. **108**, 590 (1957).
[7]J. M. Luttinger and W. Kohn, Phys. Rev. **109**, 1892 (1958).
[8]W. Jones and N. H. March, *Theoretical Solid State Physics* (Wiley-Interscience, London, 1973), Vol. 2, p. 736.
[9]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962), p. 102.
[10]J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986).