Letter to the Editor

EQUATIONS FOR THE STEADY STATE DENSITY MATRIX IN A HIGH ELECTRIC FIELD

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УРАВНЕНИЯ ДЛЯ МАТРИЦЫ ПЛОТНОСТИ СТАЦИОНАРНОГО СОСТОЯНИЯ В СИЛЬНОМ ЭЛЕКТРИЧЕСКОМ ПОЛЕ

When a strong electric field is applied to a crystal, electrons are localized on certain planes perpendicular to the direction of the field. The stronger the field is, the sharper is the localization of electrons. If this localization is sharp enough, the electric charge is transfered only by means of hopping between the localized states. The interaction of electrons with the scattering system, namely with phonons, is responsible for such transitions. The stronger this interaction is, the more probable are the transitions and the more intensive is the electric current. In these cases a direct expression for the current density can be found [1—3] as a consequence of the fact that only the lowest order terms must be determined when solving the density matrix equation. But as long as the applied field is not strong enough the localization of the electron states is smeared and the transfer of the electric charge is not so simple. However, the situation differs from the standard case of conductivity in which an electron is between two succeeding collisions accelerated by the electric field and the gained energy is delivered to the scattering system in the event of collision. In this case the electric current drops with increasing electron-phonon interaction. Sawaki [4] in his recent paper approached this problem in a way utilizing an infinite subseries of a perturbation expansion of the density matrix equation for the weak electron-phonon coupling. Since the processes neglected in this work play a role in the charge transport this method is not so general as one would expect. We shall therefore suggest a simpler approach based on a solution of the density matrix equation with a different initial condition.

In order that we may find the direct expression for the current density in a new situation, we should count an infinite number of terms in the expansion of the density matrix in the powers of the electron--phonon interaction. The standard transport theory applicable to systems exposed to a weak electric field was in a similar situation. A solution of this problem appeared to be in the kinetic equation for the electron distribution function and not in finding the direct expression for current density. We shall follow a similar pattern but since we are interested in the region of strong electric fields we shall use the Wannier--Kane representation. However, the knowledge of the distribution function is not enough because the velocity operator (in the expression for the current density) has nondiagonal matrix elements. That is why we must look for equations for the elements of the density matrix. In our investigation we shall assume that phonons remain in thermal equilibrium in spite of their interaction with electrons. Even in case of the electric field which is not strong enough to ensure a good definition of

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the Wannier--Stark levels we may use the Wannier--Kane representation since it is a natural representation for an electron exposed to a periodic potential and an electric field. Instead of the adiabatic application of the interaction with the scattering system we may assume a weak interaction of the system with its environment [5]. Then the density matrix equation takes the form

$$\frac{\partial \varrho}{\partial t} = \frac{1}{\hbar}[\varrho, H_0 + H_F + H_i] - \frac{\varrho - \varrho_s}{\tau} \tag{1}$$

in which the second term in the right-hand side represents for $\tau \to \infty$ the weak interaction of the system with the environment tending to preserve the steady state (experiments are always arranged in such a way). Here H_0 is the Hamiltonian of free electrons and phonons, H_i represents their interaction, H_F the interaction of an electron with the electric field and ϱ_s is the density matrix of the steady state. Knowing the density matrix at a certain time we can express it at a later time with the aid of the density matrix equation. As long as we are interested in a steady state we may assume that if the time evolution of our system is long enough, the density matrix does not alter any more.

If we write $\varrho(t) = \varrho(t') + \Delta\varrho(t, t')$, then for $t - t'$ large enough there must be $\varrho(t) = \varrho(t')$. Thus the condition $\Delta\varrho = 0$ represents the equation for ϱ. To preserve the technique of our recent paper [3] we shall choose the earlier time in such a way that $t' \to -\infty$ and we shall look for the solution of the density matrix equation satisfying the initial condition $\varrho(t) \to \varrho_s$ for $t \to -\infty$. We must keep in mind that ϱ_s (contrary to ϱ_0 from the mentioned paper) does not commute with $H_0 + H_F$. Equation (1) has the following formal solution

$$\varrho(t) = \varrho_s + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} \exp\frac{t'-t}{\tau} \exp\left\{-\frac{\mathrm{i}}{\hbar}(t'-t)(H_0+H_F)\right\}\{[\varrho(t'), H_i] + [\varrho_s, H_0 + H_F]\} \exp\left\{\frac{\mathrm{i}}{\hbar}(t'-t)(H_0+H_F)\right\} \mathrm{d}t' . \tag{2}$$

Now we shall express the solution in the above mentioned representation. The wave functions are the the product of the Wannier-Kane functions χ_{nk}, and the phonon functions and we shall denote them just by capital letters. Since the velocity operator is nondiagonal in the Wannier--Kane representation and has zero diagonal elements (see, e.g., [1]) we shall be interested in nondiagonal matrix elements of ϱ. Thus we can write

$$\langle A|\varrho(t)|B\rangle = \langle A|\varrho_s|B\rangle + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} \exp\frac{t'-t}{\tau} \exp\left\{\frac{\mathrm{i}}{\hbar}(t-t')(\varepsilon_A - \varepsilon_B)\right\} \times \left\{\langle A|\varrho_s|B\rangle(\varepsilon_B - \varepsilon_A) + \sum_c [\langle A|\varrho(t')|c\rangle \langle c|H_i|B\rangle - \langle A|H_i|c\rangle \langle c|\varrho(t')|B\rangle]\right\} \mathrm{d}t' . \tag{3}$$

This is an integral equation for ϱ which can be solved by an iterative process starting from $\varrho(t') = \varrho_s$. Up to the first non vanishing term we obtain

$$\langle A|\varrho(t)|B\rangle = \langle A|\varrho_s|B\rangle + \frac{1}{\hbar^2}\int_{-\infty}^{t} \exp\frac{t'-t}{\tau} \exp\left\{\frac{\mathrm{i}}{\hbar}(\varepsilon_A - \varepsilon_B)(t-t')\right\} \times \int_{-\infty}^{t'} \exp\left\{\frac{t''-t'}{\tau}\right\} \sum_{C,D} \left\{\exp\left\{\frac{\mathrm{i}}{\hbar}(t'-t'')(\varepsilon_A - \varepsilon_C)\right\}[\langle A|H_i|D\rangle \langle D|\varrho_s|C\rangle - \langle A|\varrho_s|D\rangle \langle D|H_i|C\rangle]\langle C|H_i|B\rangle - \exp\left\{\frac{\mathrm{i}}{\hbar}(t'-t'')(\varepsilon_C - \varepsilon_B)\right\}\langle A|H_i|C\rangle \langle C|H_i|D\rangle \langle D|\varrho_s|B\rangle - \langle C|\varrho_s|D\rangle \langle D|H_i|B\rangle\right\} \mathrm{d}t'' \mathrm{d}t' . \tag{4}$$

If we now perform time integration and set $\langle A|\Delta\varrho|B\rangle = 0$, we have

$$\frac{1}{\varepsilon_A - \varepsilon_B + \frac{i\hbar}{\tau}} \sum_{C,D} \left\{ \frac{[\langle A|H_i|D\rangle\langle D|\varrho|C\rangle - \langle A|\varrho|D\rangle\langle D|H_i|C\rangle]\langle C|_i|B\rangle}{\varepsilon_A - \varepsilon_C + \frac{i\hbar}{\tau}} - \frac{\langle A|H_i|C\rangle[\langle C|H_i|D\rangle\langle D|\varrho|B\rangle - \langle C|\varrho|D\rangle\langle D|H_i|B\rangle]}{\varepsilon_C - \varepsilon_B + \frac{i\hbar}{\tau}} \right\} = 0 . \tag{5}$$

Instead of ϱ_s here is simply written ϱ. For $\tau \to \infty$ we can use the relation

$$\frac{-1}{\varepsilon_A - \varepsilon_C + \frac{i\hbar}{\tau}} = \frac{i\pi}{\hbar}\delta\left(\frac{\varepsilon_C - \varepsilon_A}{\hbar}\right) + \frac{1}{\hbar} P\left(\frac{\hbar}{\varepsilon_C - \varepsilon_A}\right)$$

in which $P(1/x)$ is the principal value of $(1/x)$ and $\delta(x)$ is the Dirac delta function. Then after some rearrangement we obtain

$$\begin{aligned}
\langle A|\varrho|B\rangle = \Big\{ & \sum_C \langle B|H_i|C\rangle\langle C|H_i|B\rangle \left[i\pi\delta\left(\frac{\varepsilon_C - \varepsilon_A}{\hbar}\right) + P\left(\frac{\hbar}{\varepsilon_C - \varepsilon_A}\right)\right] + \sum_C \langle A|H_i|C\rangle\langle C|H_i|A\rangle \left[i\pi\delta\left(\frac{\varepsilon_B - \varepsilon_C}{\hbar}\right) + \right. \\
& \left. + P\left(\frac{\hbar}{\varepsilon_B - \varepsilon_C}\right)\right] \Big\}^{-1} \Big\{ \sum_{C,D} \langle A|H_i|D\rangle\langle D|\varrho|C|H_i|B\rangle \left[i\pi\delta\left(\frac{\varepsilon_C - \varepsilon_A}{\hbar}\right) + \right. \\
& \left. + i\pi\delta\left(\frac{\varepsilon_B - \varepsilon_D}{\hbar}\right) + P\left(\frac{\hbar}{\varepsilon_C - \varepsilon_A}\right) + P\left(\frac{\hbar}{\varepsilon_B - \varepsilon_D}\right)\right] - \sum_{\substack{C,D \\ D \neq A}} \langle A|H_i|C\rangle \\
& \langle C|H_i|D\rangle\langle D|\varrho|B\rangle \left[i\pi\delta\left(\frac{\varepsilon_B - \varepsilon_C}{\hbar}\right) + P\left(\frac{\hbar}{\varepsilon_B - \varepsilon_C}\right)\right] - \\
& - \sum_{\substack{C,D \\ D \neq B}} \langle A|\varrho|D\rangle\langle D|H_i|C\rangle\langle C|H_i|B\rangle \left[i\pi\delta\left(\frac{\varepsilon_C - \varepsilon_A}{\hbar}\right) + P\left(\frac{\hbar}{\varepsilon_C - \varepsilon_A}\right)\right] \Big\} .
\end{aligned} \tag{6}$$

These are the equations for the matrix elements of the steady density matrix which can be solved in a selfconsistent manner starting with the simplest form of ϱ corresponding to the absence of interaction with phonons. The starting function ϱ^0 of [3] may be convenient for this purpose. These equations can be used for intermediate cases when both standard charge transport and phonon assisted hopping between the Wannier-Stark levels fail.

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