Frequency dependence of the hopping magnetoconductivity in disordered systems

H. Böttger
Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, PF 4120, 39016 Magdeburg, Germany

V. V. Bryksin
A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia

F. Schulz
Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, PF 4120, 39016 Magdeburg, Germany

(Received 5 July 1995)

We examine the frequency dependence of the hopping conductivity and magnetoconductivity (MC) in the framework of the effective-medium method. The calculation of the MC requires the inclusion of at least three-site hopping probabilities, which makes the studies considerably more difficult than those for $H = 0$. As a result, we find a simple relation between the ratio of the MC for $\omega \neq 0$ to the static MC and the conductivity for $H = 0$. The ratio between the MC for $\omega \neq 0$ and $\omega = 0$ is independent of the magnetic field at low and medium frequencies, where the critical hopping length does not considerably deviate from its static value. Numerical calculations are performed, which confirm the analytical results.

The frequency dependence of the hopping conductivity is directly related to the presence of disorder in the considered medium (see, e.g., Ref. 1). Studies of the frequency dependence of the conductivity $\sigma(\omega)$ have been performed in the framework of the two-site model,[2] which is appropriate in the region of very high frequencies, where the conductivity $\sigma(\omega)$ of real materials is affected by interaction with phonons. The effective-medium method has been found to be the most effective tool for theoretical examinations of the conductivity $\sigma(\omega)$ in the region of low frequencies—from the static limit, where the electron moves through an infinite cluster, up to the region of multiple hopping, where the electron moves through a finite cluster of large extent.[3–5]

One should expect that the frequency dependence of the hopping magnetoconductivity (MC) is as characteristic of disordered systems as the frequency dependence of the conductivity $\sigma(\omega)$. Theoretical studies of transport phenomena in the presence of a magnetic field H are much more difficult than those for $H = 0$, because at least three-site hopping processes have to be taken into account.[6] The fact that the measurement of the Hall effect in materials with low mobility is very difficult due to its smallness stimulated the study of alternating current (ac) transport phenomena. For the Hall and Faraday effects, examinations have been carried out in the framework of the three-site model,[6–9] which is appropriate only in the high-frequency region like the two-site model for studying $\sigma(\omega)$.

The present paper is devoted to the theoretical examination of the frequency dependence of the hopping MC on the basis of an effective-medium method, i.e., in the region of low and medium values of the frequency. The static MC has been calculated in Ref. 10 using the effective-medium method. Below, we will use results of that paper.

The basic equation for our calculations in the framework of the effective-medium method is the self-consistency equation

$$\langle (G_{mm'} - G)/(G_{mm'} + \chi G) \rangle = 0 \tag{1}$$

for the effective conductance G between the sites m and m'. Here $G_{mm'}$ is the random conductance between sites m and m' and $\langle\ \rangle$ denotes the averaging over all possible configurations. The function $\chi = \chi(\omega/W)$ is defined in Ref. 3, where W is the effective hopping probability, related to G by $G = \frac{e^2}{kT} W$. In the static limit $\omega = 0$ we have $\chi(0) = d-1$, where d denotes the spatial dimension.

In the presence of a magnetic field, the random conductance between the sites consists of a two-site and a three-site contribution $G_{mm'} = G^{(2)}_{mm'} + G^{(3)}_{mm'}$. Accordingly, we define the effective conductance G and probability W as $G = G^{(2)} + G^{(3)}$ and $W = W^{(2)} + W^{(3)}$, respectively, where $G^{(i)} = \frac{e^2}{kT} W^{(i)}$. The two-site conductance $G^{(2)}$ determines the frequency dependence of the conductivity in the absence of the magnetic field. It can be obtained from the self-consistency equation

$$\langle (G^{(2)}_{mm'} - G^{(2)})/(G^{(2)}_{mm'} + \chi_0 G^{(2)}) \rangle = 0 \ , \tag{2}$$

where χ_0 is given by $\chi_0 = \chi\left(\omega/W^{(2)}\right)$. $\sigma(\omega)$ has been studied in Ref. 3 on the basis of (2) in the R hopping regime. The R-ε hopping regime is considered below.

Our examination of the frequency dependence of the conductivity $\sigma(\omega, H)$ is based on the linearized self-consistency equation (1). In order to linearize (1), we take into account that $|G^{(3)}_{mm'}| \ll G^{(2)}_{mm'}$ and, consequently, $|G^{(3)}| \ll G^{(2)}$ and $|W^{(3)}| \ll W^{(2)}$. We obtain

$$G^{(3)} = G^{(2)} \frac{g_3 \chi_0}{g_2 \left(\chi_0 - \frac{e^2}{kT}\frac{\omega}{G^{(2)}}\chi_0'\right) + \frac{e^2}{kT}\frac{\omega \chi_0'}{(1+\chi_0)^2 G^{(2)\,2}}} \ , \tag{3}$$

where

$$g_{2,3} = \langle G^{(2,3)}_{mm'} / (G^{(2)}_{mm'} + \chi_0 G^{(2)})^2 \rangle \tag{4}$$

and $\chi_0' = d\chi_0(x)/dx$ with $x = \omega/W^{(2)}$. Calculating (3) we used that χ can be represented as

$$\chi = \chi_0 - \chi_0'(e^2/kT)\omega(G^{(3)}/G^{(2)\,2}) \tag{5}$$

to lowest order in $G^{(3)}$. In the static limit we find[10] that

$$G^{(3)} = G^{(2)} g_3/g_2 \ , \tag{6}$$

where χ_0 has to be replaced by $d-1$ in the definition of g_i, simultaneously.

The electric conductivity $\sigma(\omega, H)$ is related to the effective conductance between the sites by[3,10]

$$\sigma(\omega, H) = L^2(\omega, H)kTG(\omega, H)d\nu/d\varepsilon_F \ , \tag{7}$$

where ν denotes the concentration of electrons, which depends on the Fermi energy ε_F. L is the characteristic hopping length, depending, in general, on frequency and on the magnetic field. However, the hopping length is basically determined by the large two-site hopping probabilities. Therefore, we neglect the dependence of L on the magnetic field in the following. As function of frequency, the hopping length decreases with increasing frequency from R_c (length of the critical hop in the infinite cluster for $\omega = 0$) down to a value of order α^{-1} (localization length in the high frequency region of the two-site model). We are interested in the region of low and medium frequencies. In this region we can set $L \cong R_c$ (up to logarithmic corrections), neglecting the dependence of L on frequency as well as on the magnetic field.[1,3]

Using now (7), we can represent the relative MC as

$$\frac{\sigma(\omega, H) - \sigma(\omega)}{\sigma(\omega)} \equiv \frac{\Delta\sigma(\omega, H)}{\sigma(\omega)} = \frac{G^{(3)}(\omega, H)}{G^{(2)}(\omega)} \ .$$

Taking into account (3), we get

$$\Delta\sigma(\omega, H)/\sigma(\omega) = \{[g_3(\omega, H) - g_3(\omega, 0)]/g_2(\omega)\}F(\omega) \ , \tag{8}$$

where

$$F(\omega) = \left\{1 + \frac{\chi_0'}{\chi_0}\frac{e^2}{kT}\frac{\omega}{G^{(2)}}\left[\frac{1}{g_2 G^{(2)}\,(1+\chi_0)^2} - 1\right]\right\}^{-1} . \tag{9}$$

The expression (9) for $F(\omega)$ can be simplified by representing (2) as

$$\langle G^{(2)}_{mm'}/(G^{(2)} + \chi_0 G^{(2)})\rangle = 1/(1+\chi_0) \tag{10}$$

and differentiating it with respect to ω. This procedure results in

$$g_2(\omega) = \frac{1}{G^{(2)}\,(1+\chi_0)^2}\,\frac{1 - \frac{\omega}{G^{(2)}}\frac{dG^{(2)}}{d\omega}}{1 + \frac{dG^{(2)}}{d\omega}\left(\frac{kT}{e^2}\frac{\chi_0}{\chi_0'} - \frac{\omega}{G^{(2)}}\right)} \ .$$

On the basis of the above expression we find for $F(\omega)$ the relation

$$F(\omega) = 1 - \frac{\omega}{G^{(2)}}\frac{dG^{(2)}}{d\omega} = 1 - \omega\frac{d\ln\sigma(\omega)}{d\omega} \ , \tag{11}$$

which obviously depends only on the frequency dispersion $\sigma(\omega)$ in the absence of the magnetic field.

Now, we consider the term $[g_3(\omega, H) - g_3(\omega, 0)]/g_2(\omega)$, occurring in (8). This quantity has been examined in Ref. 10 in the static limit $\omega = 0$ [i.e., for the case where χ_0 in (4) is replaced by $d-1$]. g_3 is determined by averaging over the three-site configurations of the conductance $G^{(3)}_{mm'}$. This averaging has been performed in Ref. 10 in two steps. The first step consists of averaging over the third site with respect to a given random configuration of the pair of sites m, m'. We label the resulting quantity by $\langle G^{(3)}_{mm'}\rangle_2$. The averaging over the third site is independent of χ_0. Therefore, calculating $\langle G^{(3)}_{mm'}\rangle_2$, we can immediately use the results obtained in Ref. 10. In accordance with (41) of that paper, we have

$$\langle G^{(3)}_{mm'}\rangle_2 = AG^{(2)}_{mm'}K_d(|\mathbf{R}_{mm'}|) \ , \tag{12}$$

where A is a coefficient, which does not depend on the random variables, and $K_d(|\mathbf{R}_{mm'}|)$ is a function of the distance $|\mathbf{R}_{mm'}|$ between the selected pair of sites.

The second step of the calculation of $g_3(\omega, H)$ consists of averaging over the random two-site configuration. This means for R hopping averaging over the distance $|\mathbf{R}_{mm'}|$ and for R-ε hopping, additionally, averaging over the random site energies ε_m and $\varepsilon_{m'}$. Performing this averaging in the static limit, the random distance $|\mathbf{R}_{mm'}|$ in the function $K_d(|\mathbf{R}_{mm'}|)$ in (12) is replaced by the critical hopping length R_c. For R hopping $R_c = \eta_d N^{-1/d}$, where N denotes the concentration of sites and η_d is a numerical coefficient. By direct calculation using (4) we get $\eta_d = [d/\pi(d-1)]^{1/d}$. The values $\eta_2 \approx 0.93$ and $\eta_3 \approx 0.86$ have been obtained by means of numerical studies.[1] In Ref. 10 the relation $2\alpha R_c = (T_{0d}/T)^{2/(d+2)}$ has been found for the critical hopping length in the R-ε hopping regime. The expression for the characteristic temperature T_{0d} is given as Eq. (30) in the above cited paper. It should be noted that the self-consistency equation (1) leads to the temperature dependence

$$\sigma(0) = \sigma_0 \exp\{-(T_{0d}/T)^{\frac{2}{d+2}}\} \tag{13}$$

of the static conductivity in the R-ε hopping regime. This result differs from the Mott law. Some discussion concerning this point can be found in Ref. 10.

Averaging over the two-site configurations for $\omega \neq 0$, the random distance $|\mathbf{R}_{mm'}|$ in the function $K_d\,(|\mathbf{R}_{mm'}|)$ changes to the critical hopping length of the finite cluster $L(\omega)$, which decreases logarithmically with increasing frequency (see above and in Refs. 1 and 3). The quantity $L(\omega)$ can be obtained from

$$L(\omega) = R_c - (1/2\alpha)\ln\sigma(\omega)/\sigma(0) \ . \tag{14}$$

In the region of not too high frequencies, in which we are interested, the length $L(\omega)$ deviates only weakly from R_c, i.e., $[R_c - L(\omega)]/R_c \ll 1$. Therefore, we can set in (12) $K_d\,(|\mathbf{R}_{mm'}|) \to K_d\,(R_c)$ in the frequency range from $\omega = 0$ up to the regime of multiple hopping. This has analogously been done in Ref. 10 for calculating the static MC. Afterward, we find that $[g_3(\omega, H) - g_3(\omega, H)]/g_2(\omega) \cong \Delta\sigma(0, H)/\sigma(0)$. Consequently, we obtain from (8) and (11)

$$S_H(\omega) = F(\omega)S(\omega) = -\omega^2\{(d/d\omega)[S(\omega)/\omega]\} \ . \tag{15}$$

Here we have introduced the relative quantities

$$S_H(\omega) = \Delta\sigma(\omega, H)/\Delta\sigma(0, H), \ \ S(\omega) = \sigma(\omega)/\sigma(0) \ . \tag{16}$$

Equation (15) is the central result of the present paper. It determines the relation between the frequency dependence of the MC $S_H(\omega)$ and the frequency dependence of the conductivity $S(\omega)$ in the absence of the magnetic field. It is important to note that $S_H(\omega)$, obtained using the above mentioned approximations, is independent of the magnetic field. This feature is valid only for not too high frequencies if the electron moves through a large cluster and the critical hopping length does not much deviate from its static value R_c.

We now turn to the problem of calculating the frequency dependence of the electric conductivity $S(\omega)$ in the absence of the magnetic field, which is determined by the self-consistency equation (10) in the framework of the effective-medium theory. The two-site averaging, which has to be performed, was done in Ref. 10 for $\omega = 0$. For $\omega \neq 0$ it can be performed analogously and leads to the replacement of $d-1$ by χ_0 in Eq. (29) of Ref. 10

$$G^{(2)} = (G_0/\chi_0)\exp\{-2\alpha R_c[d/(1+\chi_0)]^{1/\gamma}\} . \tag{17}$$

Here $\gamma = d$ for R hopping and $\gamma = d+2$ for R-ε hopping. The critical hopping lengths R_c for both types of hopping transport are given above. The pre-exponential factor G_0 has been calculated in Ref. 10 for the cases of weak as well as strong coupling with phonons.

For not too high frequencies the function $\chi_0\left(\omega/W^{(2)}\right)$ may be expanded in a series with respect to ω (see Ref. 3)

$$\chi_0 \cong d - 1 + i\xi_d d\omega/W^{(2)} , \tag{18}$$

where ξ_d is a numerical coefficient ($\xi_3 = 0.253$) and the self-consistency equation (17) takes the form[3,11,12]

$$S(\omega) = \exp\{i\Omega/S(\omega)\} . \tag{19}$$

Here we introduced the dimensionless frequency $\Omega = \omega/\omega_0$ with $\omega_0 = \frac{W_c}{2\alpha R_c}\frac{\gamma}{\xi_d}$. The probability of the critical hop W_c is given by $W_c = W_0\exp(-2\alpha R_c)$ and $G_0 = \frac{e^2}{kT}W_0$.

Equation (19) for the frequency dependence of the conductivity is confirmed by both computer calculations and numerous experimental results.[12] However, note that a regular series expansion of χ_0 with respect to the frequency does not exist for two-dimensional systems, where singular (logarithmic) corrections occur. This leads to a more difficult expression for the frequency dependence of the conductivity than (19) in two dimensions (see below). Using (19), the relation between the frequency dependences of the MC and the conductivity in the absence of the magnetic field (15) can be represented as

$$S_H(\omega) = S^2(\omega)/[S(\omega) + i\Omega] . \tag{20}$$

To check the relation (15), we performed numerical calculations of the frequency dependence of the MC in the R hopping regime for two-dimensional systems of 5000 sites. To this end, we generate square model systems of randomly distributed sites. We put electrodes at the boundaries of the systems in the direction of the electric field $\mathbf{E} = \mathbf{E_0}e^{i\omega t}$ and set the voltages at the electrodes equal to zero and one, respectively. The current through the systems can be calculated on the basis of the linearized set of rate equations for the electrochemical potentials $U_m = -\mathbf{E}\cdot\mathbf{R}_m + \mu_m/e$ at the sites derived in Ref. 13, which is under R hopping conditions given by

$$i\tilde{\Omega}(U_m + \mathbf{E}\cdot\mathbf{R}_m) = \sum_{m'}\tilde{G}_{m'm}(U_{m'} - U_m) . \tag{21}$$

Here we introduced the dimensionless conductance $\tilde{G} = G/G_0$. The dimensionless frequency $\tilde{\Omega}$ is related to Ω by $\tilde{\Omega} = B_0 f(1-f)e^{-2\alpha R_c}\Omega$, $f = \{\exp[-\varepsilon_F/(kT)]+1\}^{-1}$ and $B_0 \approx 3.7094$ (an analytical expression for B_0 can be found in Ref. 5). Using the solutions U_m of the above set of equations, the current (in units of G_0) can be calculated by the formula

$$j_x(\tilde{\Omega}, H) = \frac{1}{L}\sum_m (U_{\rm el} - U_m)\tilde{G}^{(2)}_{{\rm el}\,m} - \frac{i\tilde{\Omega}}{L^2}\sum_m x_m(U_m + E_0 x_m) , \tag{22}$$

where L denotes the length of the systems. The x axis has been directed along the electric field and x_m is the x component of the radius vector to site m. The subscript el denotes the electrode at $x = L$. Numerical calculations have been performed for different values of the magnetic field H. The quantity S_H is obtained from the numerical results using Eq. (16).

The results of our numerical calculations of ReS and ImS are represented by solid lines in Figs. 1(a) and 1(b), respectively. In this figure we have drawn results from the effective-medium theory too (dashed lines). However,

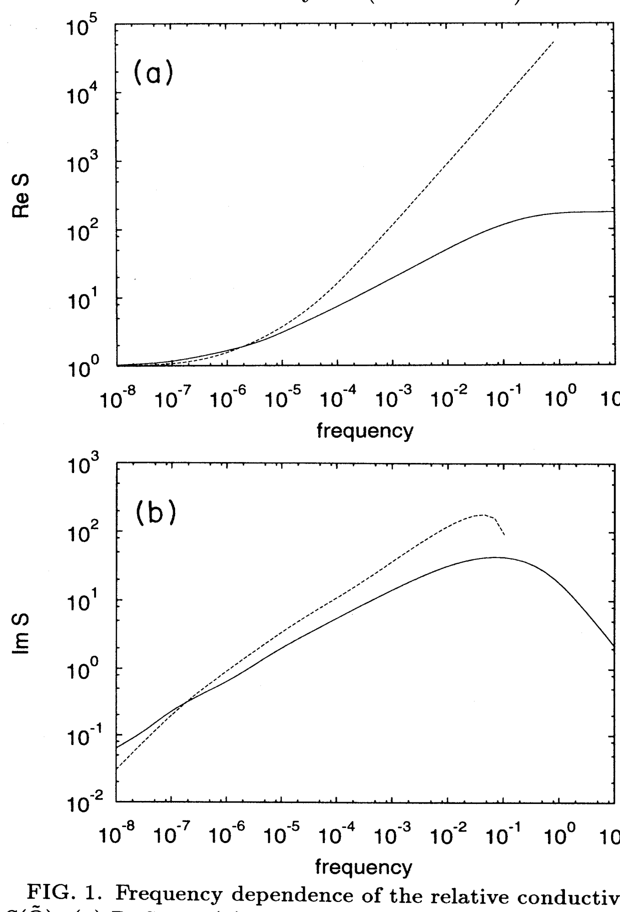

FIG. 1. Frequency dependence of the relative conductivity $S(\tilde{\Omega})$: (a) ReS and (b) ImS.

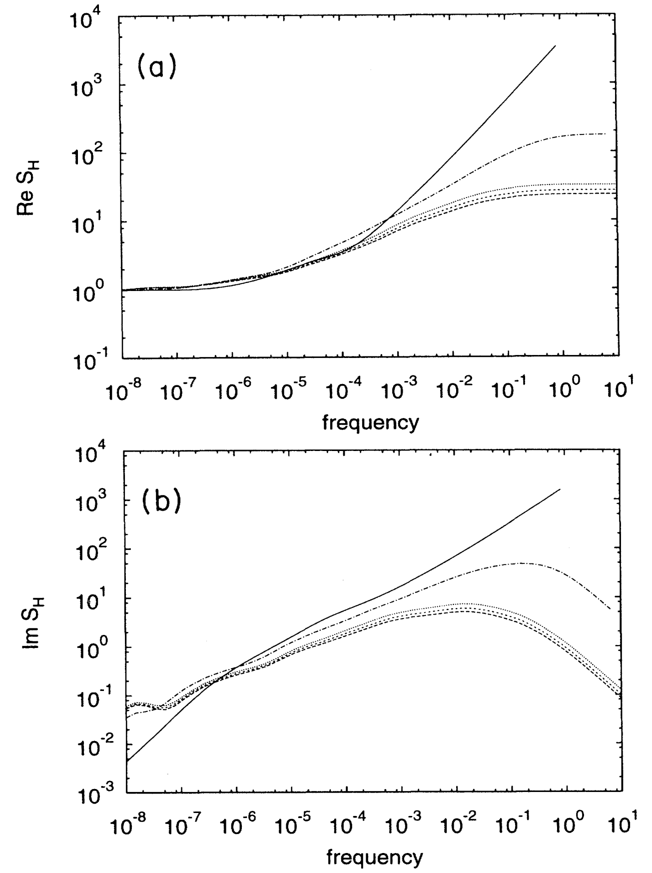

FIG. 2. Frequency dependence of $S_H(\tilde{\Omega})$: (a) ReS_H and (b) ImS_H.

because we treat two-dimensional systems we cannot use Eq. (19). Instead, we calculated the theoretical curves by means of another relation.[5,14] In two-dimensional systems, the equation for $S(\omega)$ takes the form

$$S(\omega) = \exp\{-\kappa[i\Omega/S(\omega)]\ln[i\Omega/S(\omega)]\} , \qquad (23)$$

where the quantity $\kappa = 4\alpha R_c/B_0$ has been introduced.[5] Comparing the numerically and analytically obtained curves in Fig. 1, we find that they coincide well in the region of not too high frequencies. The occurrence of a high-frequency plateau of the numerically obtained ReS and simultaneously the occurrence of the dependence Im$S \propto 1/\omega$ are characteristic of the two-site model and are not described by (19) or (23).[1,3]

In Figs. 2(a) and 2(b) we give the numerical results for the calculation of the frequency dependence of the MC ReS_H and ImS_H. Additionally, we show analytical curves, which are calculated by two different methods. The dash-dotted curves are obtained applying (15) to the numerical results for S presented in Figs. 1(a) and 1(b). The solid lines are calculated using (15) and (23), which lead in two dimensions to the expression

$$S_H(\omega) = \frac{S(\omega)}{1-\kappa\frac{i\Omega}{S(\omega)}\left[1+\ln\left(\frac{i\Omega}{S(\omega)}\right)\right]} . \qquad (24)$$

The dotted lines in Figs. 2(a) and 2(b) are numerical results for the values 0.2, 0.4, and 0.6 of the magnetic-field parameter $\Phi = eHR_c^2/(2\hbar c)$ (see, e.g., Ref. 13), which are chosen to be in the interval where the static MC has its strongest slope.[10]

The analytically and numerically obtained results for the frequency dependence of the MC coincide well for low and medium frequencies, i.e., in that frequency region where (15) and (23) may be applied, due to the approximations made in deriving them. The numerically obtained MC has a plateau at high frequencies [as it is characteristic of the conductivity $\sigma(\omega)$ (Refs. 1 and 3)]. This shape is characteristic of the two- and three-site models. Therefore, the analytical dependence, obtained using (15) and (23), does not exhibit a plateau at high frequencies.

The frequency dependence of the MC is a characteristic feature of disordered systems as is the frequency dependence of the electric conductivity in the absence of a magnetic field. The dependence of the MC on frequency is weaker than that of the conductivity (preserving all other conditions). A characteristic feature is the independence of the relative quantity S_H on the magnetic field in a wide range of the field for not too high frequencies. The analytical and numerical calculations performed in this paper show that the frequency dependence of the MC is related to the frequency dependence of the electric conductivity by the parameterless relation (15). To our knowledge, up to now there have been no experimental studies of the ac MC. Therefore, the verification of our results is a challenge to experimentalists.

[1] H. Böttger and V. V. Bryksin, *Hopping Conduction in Solids* (Akademie-Verlag, Berlin, 1985).
[2] M. Pollak and T. M. Geballe, Phys. Rev. **122**, 1742 (1961).
[3] V. V. Bryksin, Fiz. Tverd. Tela (Leningrad) **22**, 2441 (1980) [Sov. Phys. Solid State **22**, 1421 (1980)].
[4] B. Movaghar, B. Pohlmann, and G. W. Sauer, Phys. Status Solidi B **97**, 533 (1980).
[5] V. V. Bryksin, Fiz. Tverd. Tela (Leningrad) **26**, 1362 (1984).
[6] T. Holstein, Phys. Rev. **124**, 1329 (1961).
[7] M. Amitay and M. Pollak, J. Phys. Soc. Jpn. Suppl. **21**, 549 (1966).
[8] I. I. Fishchuk and V. N. Rudko, J. Phys. C **13**, 2703 (1980).
[9] R. S. Klein, Phys. Rev. B **31**, 2014 (1985).
[10] O. Bleibaum, H. Böttger, V. V. Bryksin, and F. Schulz, Phys. Rev. B **51**, 14020 (1995).
[11] J. C. Dyre, Phys. Rev. B **48**, 12 511 (1993).
[12] J. R. Macdonald, Phys. Rev. B **49**, 9428 (1994).
[13] H. Böttger, V. V. Bryksin, and F. Schulz, Phys. Rev. B **49**, 2447 (1994).
[14] V. V. Bryksin and P. Kleinert, Fiz. Tverd. Tela (Leningrad) (to be published) [Phys. Solid State (to be published)].