Frequency dependence of the hopping conductivity in a quasi-1D system with a pronounced disorder

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The kinetics of carriers in 1D and quasi-1D systems with a pronounced disorder is analyzed. It is assumed that as the carriers interact inelastically with, say, phonons they can hop between deeply localized states. The resulting conductivity is analyzed over the entire frequency range on the basis of exact equations derived by the Berezinskiĭ method [Sov. Phys. JETP **38**, 620 (1974)]. An exact asymptotic expansion is derived for σ in the limit of small ω. Resummation of this expansion gives rise to a paired (two-site) approximation. The results are compared with the various approximations. Possible applications of the model to real systems are pointed out.

1. INTRODUCTION

It was shown previously[1] in a calculation of the state density that the technique developed by Berezinskiĭ[2] can be used to sum all the perturbation-theory diagrams in a disordered 1D system. It thus becomes possible to analyze the effects of disorder in the fluctuation region. Classical diffusion in a random chain is another case in which no finite set of diagrams is sufficient. Here again it is necessary to sum the entire perturbation-theory series, since this problem has nothing analogous to a quantum-mechanical parameter such as $p_F l \gg 1$.

Classical diffusion in a 1D system can be described by the equation

$$\frac{dP_{nn_0}}{dt}=\sum_{g=\pm 1}(W_{n\,n+g}P_{n+g\,n_0}-W_{n+g\,n}P_{nn_0}), \tag{1.1}$$

where W_{nm} is the probability for an electron to hop from the m-th site to the n-th site or for a transition from a localized state centered at the point r_m, say, to a state centered at the point r_n. The probability W_{nm} depends on the distance $r=|r_n-r_m|$ between sites and also on the positions of the local energy levels of these sites. This probability can be found by the "golden rule" of quantum mechanics. The quantity $P_{nn_0}(t)$ in (1.1) is a conditional probability; i.e., $P_{nn_0}(t)$ is the probability that an electron will be at site n at the time t if at the time $t=0$ it was at the site n_0 [$P_{nn_0}(0)=\delta_{nn_0}$].

In the absence of collective effects, the hopping transport described by Eq. (1.1) is the only conductivity mechanism which can operate in a 1D system, since an electron in a 1D system is localized regardless of the degree of disorder.[2] In the case of a slight disorder (Mott localization due to above-barrier reflection) it can be assumed that an electron is localized wherever it originally happens to be. In this case Eq. (1.1) can be solved immediately, as was demonstrated by Gogolin *et al.*,[3] who also derived Eq. (1.1) from microscopic theory.

Hopping transport becomes more complicated if the disorder is pronounced and a localized electron is concentrated primarily at a strong fluctuation of the random potential (deep Anderson or classical localization, $p_F l \lesssim 1$). The hopping probability W_{nm} is a random function in this case since it depends on the random distance between sites n and m. Since the localization is exponential we can set

$$w=W_{nm}=\nu(T)e^{-2\beta r}, \quad r=|r_n-r_m|, \tag{1.2}$$

where β^{-1} is the localization radius, and the parameter $\nu(T)$ is determined by the particular mechanism which causes the hops. We will not need the explicit function $\nu(T)$ below, although it has already been calculated for certain models.[4–7] We will also ignore a possible energy disorder, assuming that kT is much larger than the width of the local levels. We will therefore assume that ν in (1.2) is an average over the energy position at the n-th and m-th sites. It may be assumed in general that in the case of a pronounced disorder the fluctuational properties are statistically independent, so that the random variable r in (1.2) obeys a Poisson distribution; i.e.,

$$\Pi(r)\,dr=\exp(-r/l)\,dr/l, \tag{1.3}$$

where l is the average distance between sites (or between states).

The phenomenological model introduced here [Eqs. (1.1)–(1.3)] may thus be valid for describing the kinetics in systems with a pronounced nondiagonal disorder. The problem of impurity-band conductivity could be taken as a classical example of the application of this model.[7] In this case $l=1/c$, where c is the impurity concentration, β^{-1} is the first Bohr radius of the wave function, and the parameter ν is approximately equal to the phonon frequency. It is assumed that kT is greater than the width of the impurity band.

One result of this study is that the low-frequency conductivity of the system is ultimately determined exclusively by the w distribution. In other words, it can be assumed that the sites or states are arranged in a regular manner spatially, while the hopping probabilities w remain random independent variables which obey some specified distribution $\rho(w)$. This circumstance raises the hope that the model may apply to a broader class of disordered systems. To calculate the corresponding distribution function $\rho(w)$ from a microscopic model is a separate problem. One particular approach is described by Berezinskiĭ and Gor'kov.[4]

The model of this paper may be pertinent to research on

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the transport properties of systems with a short mean free path ($p_F l \lesssim 1$), e.g., the salt Qn(TCNQ)$_2$ with radiation defects,[8,9] ion conductivity,[10,11] and polyacetylene (see Ref. 12, where it is assumed[6] that the electrons hop between soliton states whose spatial positions are random).

Equations of the type in (1.1)–(1.3) also arise in many physical problems (see the review by Bernasconi *et al.*[11]), in particular, in a study of a random ferromagnetic chain in the random-phase approximation.[11,13] In this case the role of $R_{nn_0}(t)$ is played by a Green's function

$$P_{nn_0}(t)=\langle\langle S_n^+(t);\ S_{n_0}^-(0)\rangle\rangle, \tag{1.4}$$

and that of W_{nm} in (1.1) is played by exchange integrals. It was shown in Refs. 4 and 5 that a similar model can describe the thermodynamics of a weakly interacting Fermi gas with a slight disorder at low temperatures. The corresponding parameters in this case are

$$l=\frac{3l_0}{g_{\text{eff}}},\quad \beta=\frac{1}{8l_0},\quad \nu=2\pi\frac{g_{\text{eff}}}{\tau}, \tag{1.5}$$

where l_0 and τ are the mean free time and mean free path of the electron, and g_{eff} is a dimensionless interaction constant.

Hopping conductivity has already been analyzed in this model by a variety of methods, including the binary and cluster approximations, the effective-medium approximation, a similarity hypothesis, etc., (again, see the review by Bernasconi *et al.*[11]). All such methods, however, are based to some extent or other on unverifiable approximations or hypotheses. The 1*D* case requires a special approach, since there is no small parameter which can be used as the basis for an approximation. We would thus like to derive an exact solution for this model and compare the results with those of the approximate approaches.

2. BASIC EQUATIONS

The dynamics of the electrons in this model can be described completely by the Green's function

$$G(q,s)=\int_0^\infty dt e^{-st}\left\langle \sum_n \exp[-iq(r_n-r_m)]P_{nm}(t)\right\rangle, \tag{2.1}$$

where $P_{nm}(t)$ is the solution of Eq. (1.1), and the angle brackets denote a configurational average. In particular, the conductivity can be expressed in terms of $G(q,s)$ as follows:

$$\sigma(\omega)=\frac{e^2n}{2kT}\int_0^\infty e^{-st}dt\left\langle\left(\frac{dr}{dt}\right)^2\right\rangle=\frac{e^2n}{2kT}s^2\sum_n\langle r_n^2P_{nm}(s)\rangle$$
$$=\frac{e^2n}{kT}\left(-\frac{s^2}{2}\right)\frac{d^2G}{dq^2}\Big|_{q=0,s=i\omega}, \tag{2.2}$$

where $n=n_0e^{-\mu/kT}$ is the carrier density.

Exact equations for the average Green's function $G(q,s)$ can be derived by the Berezinskiĭ method,[2] as was shown in Ref. 14 (see also Ref. 1). The equations found as a result may be written in the form

$$G(q,s)=\frac{1}{s}\int_{-i\infty}^{i\infty}\frac{dx}{2\pi i}\frac{x}{(x-1)^2}[F(x,q)$$
$$+F(x,-q)]\left[\Phi\left(\frac{x}{1-x}\right)-\frac{x-1}{x}\right]-G_{00}, \tag{2.3}$$

$$G_{00}(s)=-\frac{1}{s}\int_{-i\infty}^{i\infty}\frac{dx}{2\pi i}\left[\Phi(x)-\frac{1}{x}\right]\left[\Phi\left(\frac{x}{1-x}\right)-\frac{x-1}{x}\right], \tag{2.4}$$

where $G_{00}(s)=\langle P_{00}(s)\rangle$ is an autocorrelation function, and the functions Φ and F satisfy the equations

$$(1-x)[1+(1-x)\Phi(x)]=\hat{p}\Phi(x/(1-x)-s/w), \tag{2.5}$$
$$(1-x)[F(x)+x\Phi(x)-1]=\hat{p}e^{-iqr}F(x/(1-x)-s/w). \tag{2.6}$$

Here the operator $\hat{p}$ averages over r with distribution function (1.3). We recall that w depends on r, according to (1.2). Equations (2.5) and (2.6) are supplemented with the normalization condition

$$\int_{-i\infty}^{i\infty}\frac{dx}{2\pi i}\left[\Phi(x)-\frac{1}{x+0}\right]=-1. \tag{2.7}$$

We seek the frequency dependence of the conductivity. Using the expansion

$$F(x,q)=-\Phi(x)+iqA+{}^1/_2(iq)^2B+\ldots,$$

we find directly the following expression for $\sigma(\omega)$:

$$\sigma=\frac{e^2n}{kT}s\int_{-i\infty}^{i\infty}\frac{dx}{2\pi i}\frac{x}{(x-1)^2}B(x)\left[\Phi\left(\frac{x}{x-1}\right)-\frac{x-1}{x}\right], \tag{2.8}$$

where the functions A and B are to be found from the equations

$$(1-x)A(x)=\hat{p}r\Phi\left(\frac{x}{1-x}-\frac{s}{w}\right)+\hat{p}A\left(\frac{x}{1-x}-\frac{s}{w}\right),$$
$$(1-x)B(x)=-\hat{p}r^2\Phi\left(\frac{x}{1-x}-\frac{s}{w}\right) \tag{2.9}$$
$$-2\hat{p}rA\left(\frac{x}{1-x}-\frac{s}{w}\right)+\hat{p}B\left(\frac{x}{1-x}-\frac{s}{w}\right).$$

We begin the solution of Eqs. (2.5)–(2.9) by noting that in the absence of disorder the solution of (2.5) is

$$\Phi(x)=\frac{1}{x-x_0},\quad x_0=-\frac{s}{2w_0}+\left[\left(\frac{s}{2w_0}\right)^2+\frac{s}{w_0}\right]^{1/2}, \tag{2.10}$$

with a similar result for (2.9). It is thus natural to adopt the following form for the solution in the case of a disordered system:

$$\Phi(x)=\int_0^\infty\frac{f(y)}{x-y}dy,\quad A(x)=\int_0^\infty\frac{a(y)}{x-y}dy,\quad B(x)=\int_0^\infty\frac{b(y)}{x-y}dy. \tag{2.11}$$

We then find the following equations for the distribution functions of the poles from (2.5) and (2.9):

$$\int_0^\infty dyf(y)\left[\frac{1-y}{x-y}-\int_0^\infty\frac{w\rho(w)\,dw}{w(x-y(1-x))-s(1-x)}\right]=0, \tag{2.12}$$

$$\int_0^\infty dya(y)\left[\frac{1}{x-y}-\int_0^\infty\frac{wdw\rho(w)}{w(x-y(1-x))-s(1-x)}\right]$$
$$=\int_0^\infty f(y)dy\int_0^\infty\rho(w)\frac{rwdw}{w(x-y(1-x))-s(1-x)}, \tag{2.13}$$

$$\int_0^\infty dy b(y)\left[\frac{1}{x-y}-\int_0^\infty \rho(w)\frac{wdw}{w(x-y(1-x))-s(1-x)}\right]$$

$$=\int_0^\infty dy\int_0^\infty dw w\rho(w)\frac{r^2f(y)-2ra(y)}{w(x-y(1-x))-s(1-x)}, \quad (2.14)$$

$$\int_0^\infty dyf(y)=1, \quad (2.15)$$

where $\rho(w)$, the probability density of w, is found from (1.2) and (1.3) to be

$$\rho(w)=\begin{cases}(1-\alpha)/w^\alpha, & w<1\\ 0, & w>1\end{cases}; \quad r=l\ln\frac{1}{w}, \quad \alpha=1-\frac{1}{2\beta l}. \quad (2.16)$$

Here and below, w and s are expressed in units of ν.

A high-frequency solution of (2.12)–(2.14) can be derived directly through an expansion in inverse powers of s. To find the low-frequency solution we perform the scale transformation

$$x\to\Delta x, \quad y\to\Delta y, \quad f(y)=\frac{1}{\Delta}h\left(\frac{y}{\Delta}\right),$$
$$a(y)=\frac{l}{\Delta^2}g\left(\frac{y}{\Delta}\right), \quad b(y)=-\frac{2l^2}{\Delta^3}\varphi\left(\frac{y}{\Delta}\right). \quad (2.17)$$

Equation (2.12) can then be rewritten as

$$\int_0^\infty dy\, h(y)\frac{y^2(1-\Delta x)}{(x-y)[x-y(1-\Delta x)]}$$

$$=\int_0^\infty dyh(y)\frac{s}{\Delta^2}\frac{1-\Delta x}{x-y(1-\Delta x)}$$

$$\times\int_0^\infty dw\frac{\rho(w)}{w(x-y(1-\Delta x))-s(1-\Delta x)/\Delta}. \quad (2.18)$$

Equations (2.13) and (2.14) are rewritten analogously. Now choosing $\Delta(s)$ such that in the limit $s\to 0$ we have $\Delta(s)\to 0$ and $s/\Delta(s)\to 0$, we can attempt to solve Eq. (2.18) by successive approximations.

3. ASYMPTOTIC SOLUTION OF THE EQUATIONS IN THE LIMIT $\omega\to 0$

The averaging over w in (2.18) and (2.13), (2.14) reduces to evaluating integrals of the type

$$J_1=(1-\alpha)u\int_0^1\frac{dw}{w+u}\frac{1}{w^\alpha},$$

$$J_2=(1-\alpha)^2\int_0^1\frac{dw}{w+u}w^{1-\alpha}\ln\frac{1}{w},$$

$$J_3=\frac{(1-\alpha)^3}{2}\int_0^1\frac{dw}{w+u}w^{1-\alpha}\ln^2\frac{1}{w},$$

for which we have the following expansion in the regions $u\ll 1$ and $u\gg 1$:

$$J_1=\varkappa u^{1-\alpha}-\psi(u,1,\alpha)=u\psi(1/u,1,1-\alpha), \quad (3.1)$$

$$J_2=1+\varkappa u^{1-\alpha}(1-\alpha)\ln u+\varkappa^2u^{1-\alpha}\cos\pi\alpha$$
$$-\psi(u,2,\alpha)=\psi(1/u,2,2-\alpha), \quad (3.2)$$

$$J_3=1-{}^1/_2\varkappa u^{1-\alpha}(1-\alpha)^2\ln^2u$$
$$+\varkappa^2u^{1-\alpha}(1-\alpha)(\ln u)\cos\pi\alpha-\varkappa^3u^{1-\alpha}(1-{}^1/_2\sin^2\pi\alpha)$$
$$+\psi(u,3,\alpha)=\psi(1/u,3,2-\alpha), \quad (3.3)$$

where

$$\varkappa=\frac{\pi(1-\alpha)}{\sin\pi\alpha}, \quad \psi(z,k,v)=(1-\alpha)^kz\sum_{n=0}^\infty\frac{(-z)^n}{(n+v)^k}. \quad (3.4)$$

We see thus that in the limit $s\to 0$ the quantity $\Delta(s)$ in (2.18) should be set equal to

$$\Delta(s)=s^{(1-\alpha)/(2-\alpha)}. \quad (3.5)$$

For $h(y,s)$ we then find

$$h(y,s)=h(y)+O(s^\mu), \quad \mu=\min\left(\frac{\alpha}{2-\alpha};\frac{1-\alpha}{2-\alpha}\right), \quad (3.6)$$

where $h(y)$ satisfies the equation

$$\int_0^\infty dyh(y)\left[\frac{y^2}{(y-x)^2}-\Gamma(\alpha)\Gamma(2-\alpha)\frac{1}{(y-x)^{2-\alpha}}\right]=0. \quad (3.7)$$

Here $\Gamma(\alpha)$ is the gamma function. Multiplying the last equation by $\exp(-\eta x)$, and integrating over x along the imaginary axis, we find

$$\frac{d^2\phi}{d\eta^2}=\frac{\Gamma(\alpha)}{\eta^\alpha}\phi, \quad \phi(0)=1, \quad (3.8)$$

where $\phi(\eta)$ is the Laplace transform of $h(x)$. Analogously, in the limit $s\to 0$, we find the following equations for the Laplace transforms of $g(x)$ and $\varphi(x)$ [$u(\eta)$ and $v(\eta)$, respectively] from Eqs. (2.13), (2.14), and (2.17):

$$\frac{d}{d\eta}\eta\frac{du}{d\eta}=\Gamma(\alpha)\eta^{1-\alpha}u-\phi, \quad (3.9)$$

$$\frac{d}{d\eta}\eta\frac{dv}{d\eta}=\Gamma(\alpha)\eta^{1-\alpha}v-u. \quad (3.10)$$

The change of variables

$$\eta=\left(\frac{z}{\lambda}\right)^{2\beta}, \quad \beta=\frac{1}{2-\alpha}, \quad \lambda=2\beta(\Gamma(\alpha))^{1/2} \quad (3.11)$$

reduces Eqs. (3.8)–(3.10) to Bessel's equations. The solution of (3.8)–(3.10) can thus be written:

$$\phi=Nz^\beta K_\beta(z), \quad N=2^{1-\beta}/\Gamma(\beta), \quad (3.12)$$

$$u=-\frac{N}{\Gamma(\alpha)}\lambda^{2(1-\beta)}\left\{I_0(z)\int_z^\infty d\zeta\zeta^{3\beta-1}K_0(\zeta)K_\beta(\zeta)\right.$$
$$\left.+K_0(z)\int_0^z d\zeta\zeta^{3\beta-1}I_0(\zeta)K_\beta(\zeta)\right\}, \quad (3.13)$$

$$v=\frac{\lambda^{2(1-\beta)}}{\Gamma(\alpha)}\left\{I_0(z)\int_z^\infty d\zeta\zeta^{2\beta-1}K_0(\zeta)u(\zeta)\right.$$
$$\left.+K_0(z)\int_0^z d\zeta\zeta^{2\beta-1}I_0(\zeta)u(\zeta)\right\}. \quad (3.14)$$

Substituting the solution into (2.8), we finally find the following expression for the conductivity $\sigma(\omega)$:

$$\frac{\sigma(\omega)}{\sigma_0}=\left(\frac{i\omega}{\nu}\right)^\gamma\left[C_0(\alpha)+C_1(\alpha)\left(\frac{i\omega}{\nu}\right)^\mu+\ldots\right], \quad (3.15)$$

where

$$\sigma_0=\frac{e^2n}{kT}l^2\nu,\quad \gamma=\frac{\alpha}{2-\alpha}.$$

The coefficient $C_0(\alpha)$ in (3.15) is

$$C_0(\alpha)=2\int_0^\infty dz v(z)\frac{d\phi}{dz}. \tag{3.16}$$

To evaluate it we make use of the following property of Bessel functions:

$$\frac{2}{\pi^2}\int_0^\infty \frac{\operatorname{sh}\pi\xi}{\xi}K_{i\xi}(\zeta)K_{i\xi}(z)\,d\xi = \begin{cases} I_0(z)K_0(\zeta) & (0<z<\zeta)\\ I_0(\zeta)K_0(z) & (0<\zeta<z)\end{cases}.$$

As a result we find

$$C_0(\alpha)=\left(\frac{\beta}{\pi\Gamma(\beta)}\right)^3\frac{4}{[\beta^2\Gamma(\alpha)]^{2\beta}\Gamma(2\beta)\Gamma(3\beta)} \times\int_0^\infty dv\operatorname{ch}\pi v\int_0^\infty\frac{d\mu}{\mu}\operatorname{sh}2\pi\mu|\Gamma(\beta+i\mu)\Gamma(2\beta+i\mu) \times\Gamma(\beta+i(\nu+\mu))\Gamma(\beta+i(\nu-\mu))\Gamma(\beta+i\nu)|^2. \tag{3.17}$$

The integral in (3.17) is a so-called Mellin-Barnes double integral. To evaluate it, we use the Slater theorem[15] and the Dixon theorem[16] in succession. We find

$$C_0(\alpha)=4\pi\left(\frac{\beta}{\Gamma(\beta)}\right)^3\times\frac{1}{[\beta^2\Gamma(\alpha)]^{2\beta}}\frac{\Gamma(\beta)}{\Gamma^3(3\beta)}N_\beta, \tag{3.18}$$

$$N_\beta=\frac{1}{2\pi}\int_0^\infty\frac{d\mu}{\mu}\operatorname{sh}2\pi\mu|\Gamma(\beta+i\mu)\Gamma(2\beta+i\mu)|^4. \tag{3.19}$$

Here N_β, the Meijer function[16] with unity argument, exists in series form. For certain particular values of the parameter β we can find N_β explicitly:

$$N_{1/2}=\pi/8,\quad N_1=1/2\pi, \qquad N_{2/3}=2\cdot9^{-2}(2\pi+9-\psi(^2/_3))\approx0.3039, \tag{3.20}$$

etc., where ψ is the trigamma function. In the interval $1/2<\beta<1$ the function N_β can be approximated by

$$N_\beta=0{,}796-0{,}756\beta+0{,}198\beta^2. \tag{3.21}$$

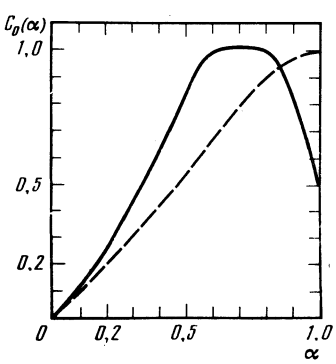

FIG. 1. Coefficient of the first term in the asymptotic expansion of the conductivity. Solid curve—Exact result; dashed curve—prediction of the effective-medium approximation.

Figure 1 shows the function $C_0(\alpha)$ calculated from (3.18)–(3.21).

We also find an expression for autocorrelation function (2.4) in the limit $s\to0$:

$$G_{00}(s)=s^{-1/(2-\alpha)}[\beta^2\Gamma(\alpha)]^\beta\Gamma(2-\beta)/\Gamma(1+\beta). \tag{3.22}$$

The s dependence of G_{00} is of course the same as that derived by Kirkpatrick[17] by Dyson's approach. An expression for the coefficient in (3.22) was not found in Ref. 17.

4. INTERMEDIATE AND HIGH FREQUENCIES

It can be seen from (3.15) that our expansion for $\sigma(\omega)$ holds if

$$\left|\frac{\omega}{\nu}\right|^\mu\ll1,\quad \mu=\frac{1}{2}\frac{1-|1-2\alpha|}{2-\alpha}. \tag{4.1}$$

In the case of pronounced disorder, $(1-\alpha)\ll1$, condition (4.1) corresponds to extremely low frequencies, so there is a rather broad frequency range in which the subsequent terms of the expansion in (3.15) must be taken into account. The corresponding coefficients can be found by the method described above. If $(1-\alpha)\ln(\nu/\omega)\ll1$, i.e., if $1-\alpha\ll1$ and $\omega\ll\nu$, the asymptotic expansion in (3.15) should be revised. In this frequency interval we have, according to (3.1)–(3.3),

$$J_1=1+\zeta,\quad J_2=\zeta^2/2,\quad J_3=\zeta^3/6,\quad \zeta=(1-\alpha)\ln(1/u). \tag{4.2}$$

Using (4.2) and proceeding by analogy with the approach above, we find from (2.12) and (2.13)

$$f(y)=\delta(y-1),\quad \xi=(1-\alpha)\ln(\nu/\omega),$$
$$b(y)=^1/_6l^2\xi^3\delta(y-^1/_2),\quad a(y)=^1/_4l\xi^2\delta(y-^1/_2).$$

Again substituting the solution into (2.8), we find the following expression for the conductivity in this frequency range:

$$\frac{\sigma}{\sigma_0}=\frac{(1-\alpha)^3}{2}\frac{\omega}{\nu}\left[\frac{\pi}{2}+\frac{i}{3}\ln\frac{\nu}{\omega}\right]\ln^2\frac{\omega}{\nu}. \tag{4.3}$$

This result corresponds to the so-called binary approximation.[18]

In the case of a slight disorder ($\alpha\ll1$) the first term in (3.15) is the dominant term if

$$^1/_2\alpha\ln(\nu/\omega)\gg1,\quad \omega\ll\nu. \tag{4.4}$$

If $\frac{1}{2}\alpha\ln(\nu/\omega)\ll1$, we have an expansion in the following form for the right side of (2.18) and Eqs. (2.13) and (2.14), according to (3.1)–(3.3):

$$J_1=u\ln(1/u),\quad J_2=J_3=1. \tag{4.5}$$

We then find the following asymptotic solution of Eqs. (2.12)–(2.14):

$$\Delta^2(s)=^1/_2s\ln(2/s),\quad h=g=\varphi=\delta(y-1). \tag{4.6}$$

In turn, the conductivity turns out to be

$$\frac{\sigma}{\sigma_0}=2/\ln\frac{\nu}{\omega}+i\pi/2\ln^2\frac{\nu}{\omega}. \tag{4.7}$$

A high-frequency expression for the conductivity can be derived by expanding in inverse powers of s. Retaining only the first few terms of the expansion, we find

$$\frac{\sigma}{\sigma_0}=2\left(\frac{1-\alpha}{2-\alpha}\right)^3+\frac{2i\nu}{\omega}\left(\frac{1-\alpha}{3-\alpha}\right)^3. \tag{4.8}$$

5. QUALITATIVE SOLUTION AND COMPARISON WITH OTHER METHODS

We can derive a simple qualitative solution of the original equations. We write the unknown solution in the form

$$\Phi=\frac{1}{x-x_c} \quad A=\frac{a}{x-x_c}, \quad B=\frac{b}{x-x_c}, \tag{5.1}$$

where the effective parameters x_c, a, and b are found by substituting (5.1) into (2.12)–(2.14) and then setting $x=0$. As a result we find the following general expression for $\sigma(\omega)$:

$$\sigma=\frac{e^2n}{kT}\frac{s}{2-x_c}\left[\left\langle\frac{r^2w}{x_cw+s}\right\rangle+2\left\langle\frac{rw}{x_cw+s}\right\rangle\right], \tag{5.2}$$

where x_c satisfies the equation

$$x_c=\langle s/(x_cw+s)\rangle. \tag{5.3}$$

These equations differ from the corresponding effective-medium equations only in details.[11,17,19] For distribution (1.2), (1.3), Eqs. (5.2) and (5.3) can be rewritten as

$$\frac{\sigma}{\sigma_0}=\frac{2}{2-s/u}\left[uJ_3+\frac{1}{s}(uJ_2)^2\right], \tag{5.4}$$

$$s=uJ_1, \quad s=i\omega/\nu, \tag{5.5}$$

where J_i are the same integrals as those in the exact equations [see (3.1)–(3.3)]. A point worth noting is that it is the nature of the expansion of these integrals J_i which ultimately determines the nature of the expansion of the conductivity in ω. The qualitative solution thus yields the correct asymptotic dependence of σ on ω. According to (5.5), in the limit $s\to 0$ we have

$$u=\left(\frac{s}{\varkappa}\right)^{1/(2-\alpha)}, \quad \varkappa=\frac{\pi(1-\alpha)}{\sin\pi\alpha}, \tag{5.6}$$

and for the conductivity we then find expansion (3.15) with the coefficient

$$C_{\text{eff}}(\alpha)=\varkappa^{-2/(2-\alpha)}. \tag{5.7}$$

Figure 1 shows the value of $C_{\text{eff}}(\alpha)$ for comparison with the exact result. The coefficient C_{eff} also differs from the exact coefficient by a factor of 2 in the case of expansion (4.3) at intermediate frequencies.

The effective-medium approximation [Eqs. (5.2)–(5.5)] thus reproduces the correct asymptotic frequency dependence of σ. A disadvantage of this approximation can be seen by comparing (5.1) and (2.11). According to the exact solution, the functions $f(y)$, $a(y)$, and $b(y)$ are definitely not δ-functions, even in the limit $s\to 0$. Consequently, the Green's function found in the effective-medium approximation ($s\to 0$, $q\to 0$),

$$G^{-1}(q,\ s)=s+w_{\text{eff}}(s)q^2, \tag{5.8}$$

may not correspond to reality. Working from the exact solution, we might instead expect $G(q, s)$ to be represented in the form

$$G(q,s)=\int\frac{dxR(x)}{s+s(xq)^2}, \tag{5.9}$$

where again $R(x)$ is not a δ-function. If we assume that in the limit $s\to 0$ we have

$$R(x)=\frac{1}{\Delta}r\left(\frac{x}{\Delta}\right),$$

we would have a situation corresponding to the similarity hypothesis of Bernasconi *et al.*[20]

As might be expected, the cluster approximation[11,21] gives the correct dependence $\sigma(\omega)$ in the limit of pronounced disorder, $1-\alpha\ll 1$, where we have

$$\sigma/\sigma_0=(i\omega/\nu)^{1-1/\beta l};$$

here $\beta l\gg 1$.

6. DISCUSSION OF RESULTS

The static conductivity of a $1D$ system with pronounced disorder thus remains equal to zero at a nonzero temperature. The physical reason is the large fluctuations of the random potential, which come close to amounting to breaks in the chain. By virtue of the one-dimensional nature of the motion, a carrier cannot circumvent these parts of the path, and it is forced to spend most of its time overcoming them. Nevertheless, the carriers do not become localized, as can be seen from (3.22). It is correct to say that the carrier mobility μ eventually approaches zero. The derivation of $\sigma(\omega)$ carried out above is in fact a calculation of μ as a function of the time.

Comparison with the results of the approximate methods shows that the effective-medium approximation correctly reproduces the asymptotic behavior of σ at low frequencies ω. This fact is itself particularly interesting, since in terms of diagrams this approximation would correspond to the summation of only those diagrams which lack intersections (it would correspond to simply a gathering of beams in the "cross technique"). This result may mean that, if the nucleating Green's function is chosen appropriately for this approximation, (5.8), then the usually dangerous interference diagrams will make the same contribution to the conductivity as do the diagrams without intersections. As a result, only the coefficients in the asymptotic expansion will be determined by the sum of all the diagrams. It is actually a rather complicated mathematical problem to evaluate the coefficient of the first term in (3.15), and the result cannot be expressed in terms of elementary functions, in contrast with $C_{\text{eff}}(\alpha)$.

When these results are applied to real systems it is necessary to consider the possibility that electrons will hop between chains. Such a hopping would lead to new terms of the type

$$\sum_j w_\perp^{i\,i+j}\left[P_{nn_0}^{i+j\,i_0}-P_{nn_0}^{ii_0}\right] \tag{6.1}$$

on the right side of Eq. (1.1). Here the superscripts i, i_0, and $i+j$ specify the chain, and $w_\perp^{i\,i+j}$ is assumed to be nonzero, equal to $w_\perp$, only for nearest chains, packed in a $2D$ lattice, say. Allowance for the departure term in (6.1) after the transformation to the Laplace time representation reduces to the substitution $s\to s+4w_\perp$ on the left side of (1.1). The arrival term in (6.1) can be studied in the ladder approximation, whose validity depends on the number of nearest neighbors. As a result, we find the following expression for the Green's function:

$$G_{3d}^{-1}(q,s)=G_{1d}^{-1}(s+4w_\perp,q_z)-2w_\perp(\cos q_x d+\cos q_y d). \quad (6.2)$$

For the conductivity we thus find

$$\sigma_{3d}=\sigma_{1d}(s+4w_\perp)=C_0(\alpha)\sigma_0\left(\frac{4w_\perp+i\omega}{\nu}\right)^\gamma. \quad (6.3)$$

The effective probability for hops between chains can be estimated from

$$w_\perp=\nu\exp\{-2((d\beta_\perp)^2+l^2\beta^2)^{1/2}\}, \quad (6.4)$$

where d is the distance between chains, and $\beta_\perp$ is the localization radius of the wave function in the direction transverse to the chains. The quasi-1D situation, which is the situation to which Eqs. (6.1)–(6.4) apply, strictly speaking, corresponds to the case $d\beta_\perp \gg l\beta$, i.e., to the case of rare hops between chains. In this case we may ignore the fluctuations of $w_\perp$.

According to (6.3), the static conductivity of a quasi-1D system depends strongly on $w_\perp$:

$$\frac{\sigma_{dc}}{\sigma_0}=C_0(\alpha)\left(\frac{w_\perp}{\nu}\right)^\gamma, \quad (6.5)$$

$$\left(\frac{\sigma_\perp}{\sigma_\parallel}\right)_{dc}=\frac{1}{C_0(\alpha)}\left(\frac{d}{l}\right)^2\left(\frac{w_\perp}{\nu}\right)^{1-\gamma}. \quad (6.6)$$

In the region $\omega \gtrsim w_\perp$, there is again a strong frequency dependence, which can be seen most easily in the relaxation of the current upon the sudden application of an electric field E:

$$j(t)=\int_{-i\infty}^{i\infty}\frac{ds}{2\pi i}e^{st}\frac{\sigma(s)}{s}E.$$

Substituting in (6.3), we find

$$j(t)-j_c=j_0 e^{-w_\perp t}/(t\nu)^\gamma, \quad (6.7)$$

where $j_c=\sigma_{dc}E$ and $j_0=\sigma_0 E$. The steady state is thus reached in a basically power-law fashion, since $w_\perp$ may be extremely small, according to (6.4). It has been pointed out previously[14] that the asymptotic behavior $j(t)$ found on the basis of the linear conductivity is valid at the times $t \ll t_c$, where

$$t_c=\frac{1}{\nu}\left(\frac{2kT}{elE}\right)^{2\beta l+1}.$$

At $t \gg t_c$, the nonlinear effects become important.[14,22]

The model of this paper might be applied, in the form outlined above, to a physical system such as polyacetylene.[6,12] The kinetics of polyacetylene is presently interpreted on the basis of a 3D model of hopping conductivity.[6] The anisotropy of the conductivity of polyacetylene, however, has not been measured directly. Data on spin diffusion[24] imply[1)] that the anisotropy could be extremely great (10^6), so that our model might apply. Measurements of $\sigma(\omega)$ in polyacetylene have been carried out over the frequency range from 10 to $10^6\,s^{-1}$ (Ref. 12). The results reveal no variance at room temperature, while they reveal a strong dependence $\sigma_{AC}\propto\omega^\gamma$ ($\gamma\approx 0.6$) at temperatures on the order of 100 K. Hopping transport could have a power-law dependence $\sigma_{AC}(\omega)$ in a quasi-1D system, as was shown above, while this dependence would not hold in the 3D case[6] (see also Ref. 12).

According to (6.3) and (4.1), the power-law dependence $\sigma_{AC}(\omega)$ in a quasi-1D system is restricted to the frequency range $4w_\perp(T) \ll \omega \ll \exp[-1/(1-\alpha)]\nu(T)$. Estimates in Ref. 6 and experimental data[12] on $\sigma_{dc}(T)$ [see (6.5)] reveal $\nu(T)=10^{17}(300\ K/T)^\varkappa\ s^{-1}$, where $\varkappa=14.7$. According to (6.4), the T dependence of $w_\perp$ is of the same nature, $w_\perp(T)=w_\perp^0(300\ K/T)^\varkappa$, and $w_\perp^0$ can be estimated from data on spin diffusion,[24] $w_\perp^0=4.5\cdot10^7\ s^{-1}$. With these parameters, Eq. (6.3) gives a qualitatively correct description of the experimental dependence $\sigma(\omega)$ in polyacetylene.[12] According to (6.6), the values of the parameters ν, $w_\perp$, and γ also correspond to a pronounced anisotropy. The value of the exponent γ, however, corresponds to too high a soliton concentration, if we use Eq. (3.15). Noting that[6] $\beta^{-1}=7a$, where a is the lattice constant, we conclude that the value $\gamma=0.6$–0.8 corresponds to a degree of doping $C=7$–3%. It may be that the hops not only occur betwen soliton formations but also involve other defects, since a similar dependence, $\sigma_{AC}\propto\omega^{0.8}$, has been observed in an isomer of polyacetylene[12] in which there are no soliton states. A final conclusion will require an experimental study of $\sigma(\omega)$ over a broader frequency range and at various degrees of doping. The model discussed above might apply at any rate to polyacetylene with a high degree of doping.[6]

Another system in which the power-law dependence studied here might be seen is $Qn(TCNQ)_2$. According to Refs. 4, 5, and 25, the low-temperature ($T \lesssim 10$ K) phase of $Qn(TCNQ)_2$ can be described by a model of spins with a random exchange interaction. Using (1.4) and the model of this paper, we find the spin-wave component of the heat capacity[11]:

$$C\propto T^{(1-\alpha)/(2-\alpha)}. \quad (6.8)$$

This result becomes the same as that found by the cluster approach[5] if we set $\alpha\approx 1$. The NMR relaxation time depends on the magnetic field in accordance with

$$T_1(H)\sim G_{00}\propto\left(\frac{\nu}{\omega_l+w_\perp}\right)^{1/(1-\alpha)}, \quad \omega_l=\mu_B H, \quad (6.9)$$

where the parameters α and ν were determined in (1.5). Measurements[25] reveal a value of 0.73 for the parameter α ($g_{eff}=1/5$), while the parameter τ in (1.5) can be estimated from[25] $1/\tau=0.7\cdot10^{14}\ s^{-1}$, so that we would have $\nu=10^{14}\ s^{-1}$. An estimate of $w_\perp$ can be found from data[9] on spin diffusion at $T=30$ K: $w_\perp=3.4\cdot10^7\ s^{-1}$ (10^{-4} K). This value of $w_\perp$ is also in agreement with data on the anisotropy ($\sigma_\parallel/\sigma_\perp=2500$) if we use (6.6). According to (4.1), the upper frequency limit on the region with a power-law dependence is $\omega_c=\exp[-1/(1-\alpha)]\nu=2.5\cdot10^{12}\ s^{-1}$ (18 K). Consequently, the behavior in (6.8) and (6.9) corresponds to a quasi-1D situation.

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[1)]The inference could be justified on the basis that potential impurities would trap charged and neutral solitons in an identical way.[23] The charge and spin transport mechanisms might therefore be the same.

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