

Kinetics of one-dimensional disordered systems with localized carriers

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The Berezinskii method is used to study nonstationary phenomena that occur in a one-dimensional chain with random probabilities of intersite hopping when an electric field is turned on. The asymptotic behavior of the current $j(t)$ as $t \rightarrow \infty$ depends substantially on the field strength. In the case of weak field, the asymptotic behavior is governed by carrier relaxation near the cluster boundaries, and in strong fields the main contribution is made by hops over large-size clusters. The results are generalized to include the quasi-one-dimensional case.

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It is known that in a one-dimensional system an electron is localized independently of the degree of disorder, so that its motion along such a system consists of hops at finite temperatures.¹ In the case of deep Anderson localization, the probabilities of hopping between neighboring localized states are in turn random quantities.

Hopping conduction in the presence of disorder is the subject of an extensive literature (see, e.g. the reviews^{2–5} and their cited references). Various methods were used to analyze this problem: the cluster approximation, the effective-medium method, the percolation method, and others, but all are based on various *a priori* unproven assumptions. Comparison with the results of the present paper will show that the use of such assumptions is not always valid.

It should be noted that in a chain in which the probabilities of the intersite hops has a large scatter the dc conductivity is zero, so that actual interest attaches to the study of nonstationary conduction in such systems. We consider in fact the time dependence of the current $j(t)$ produced by an instantaneous application of a dc electric field E . Concrete results are obtained for two disorder models: a chain of sites with randomly distributed breaks, and a chain of sites with random coordinates.

An effective method of investigating one-dimensional disordered systems is the use of the Berezinskii diagram technique,¹ a variant of which as applied to the problem of hopping conduction was recently proposed by one of us.⁶ This method yields exact equations for the Green's functions of the disordered chain. These equations will be investigated in the present paper for the case of the aforementioned two types of disorder.

1. THE MODEL. BASIC EQUATIONS

We consider an electron whose motion along a one-dimensional chain is by hopping from site to site. The probability of finding the electron on site number n at the instant of time t , $P_n(t)$, satisfies the balance equation

$$dP_n/dt = w_+(n-1)P_{n-1} + w_-(n)P_{n+1} - [w_+(n) + w_-(n-1)]P_n, \quad (1.1)$$

where $w_{\pm}(n)$ denotes the random quantities—probabilities of hops respectively between the sites n and $n+1$: from left to right and from right to left. It is assumed that the system is

an electric field E , so that

$$w_{\pm}(n) = w(n) \exp \left[\pm \frac{eE}{2kT} (r_{n+1} - r_n) \right], \quad (1.2)$$

where coordinate r_n of the n th site is also generally speaking a random quantity.

The distribution $w(n)$ of random quantities is determined by the character of the disorder in the system. We shall consider two types of disorder, and in both cases $w(n)$ are independent random quantities for different n .

1. *The broken chain model.* Here $w(n)$ takes on values 0 to w with respective probabilities c and $1-c$. The distance between all neighboring sites are equal, $r_{n+1} - r_n = a$.

2. *Model of randomly distributed sites.* Here $w(n)$ is a function of the distance between sites, $w(n) = w(r_{n+1} - r_n)$,

$$w(r) = \nu \exp(-2\beta r/\bar{r}); \quad (1.3)$$

where r is assumed to have a Poisson distribution:

$$P(r) = \bar{r}^{-1} \exp(-r/\bar{r}). \quad (1.4)$$

In these formulas \bar{r} is the average distance between neighboring sites, \bar{r}/β is the electron-localization radius, and ν is a quantity of the order of the phonon frequency.

It is convenient to express the physical quantities in terms of averaged Green's functions (GF). We define the GF in the site approximation in the following manner:

$$D_{nn'}(t) = \langle \tilde{D}_{nn'}(t) \rangle, \quad (1.5)$$

where $\tilde{D}_{nn'}$ is the solution of Eq. (1.1) with initial condition $\tilde{D}_{nn'}(0) = \delta_{nn'}$, and the angle brackets denote averaging over the realizations of the random quantities. We shall need also the GF in the coordinate representation, whose Fourier transform is given by

$$G(q, t) = \left\langle \sum_n \exp[-iq(r_n - r_{n'})] \tilde{D}_{nn'}(t) \right\rangle. \quad (1.6)$$

After changing over into the Laplace representation with respect to time, the current $j(s)$ in the system, where s is the Laplace variable, is expressed in terms of $G(q, s)$ as follows:

$$j(s) = enis \frac{dG(q, s)}{dq} \Big|_{q=0}, \quad (1.7)$$

where n is the electron density.

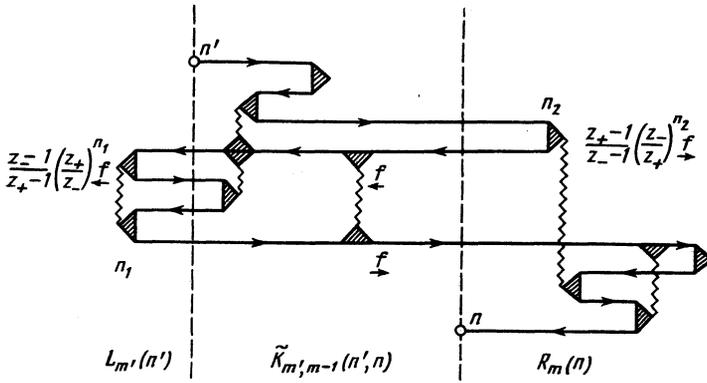


FIG. 1. Example of diagram for the Green's function $D_{nn'}$. The vertex types are shown with the corresponding multipliers. The dashed sections break up the diagram into blocks corresponding to $R_m(n)$, $L_m'(n')$, and $K_{m',m-1}^{~}(n',n)$; in this example $m' = 2 = m$.

For a regular lattice, the GF has the standard form

$$D_{nn'}^0(s) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{e^{ik(n-n')}}{s + w_+(1 - e^{-ik}) + w_-(1 - e^{ik})}.$$

It can be easily seen that in the site representation $D_{nn'}$ can be represented as a product of two factors pertaining to the sites n and n' . The Berezinskii method¹ can therefore be used to analyze this problem. The details of the method itself can be found in Berezinskii's original paper and in Gogolin's review.²

A characteristic feature of the method is the use of diagrams ordered along the chain. The diagram for the GF $D_{nn'}$ is a line going from n' to n , on which, as is done in the cross technique, a definite number of vertices localized on the bonds is placed; the vertices localized on one bond are joined into a bundle (Fig. 1). Each such diagram can be broken up into three factors that contain respectively vertices lying to the right of sites n and n' , to their left, and between them. For the sum of the diagrams of the right, left, and central parts, at a definite number of pairs of incoming and outgoing lines, we can obtain the following equations (for details see Ref. 6):

$$R_m(n) = \hat{p} \sum_{m'} W_{mm'}^r(n+1) R_{m'}(n+1), \quad (1.8)$$

$$L_m(n) = \hat{p} \sum_{m'} W_{mm'}^l(n) L_{m'}(n-1), \quad (1.9)$$

$$\tilde{K}_{m'm}(n', n) = \hat{p} \sum_{m''} V_{mm''}^r(n) \tilde{K}_{m''m'}(n', n-1) \quad \text{at } n > n'; \quad (1.10)$$

$$\tilde{K}_{m'm}(n', n) = \hat{p} \sum_{m''} V_{mm''}^l(n) \tilde{K}_{m''m'}(n', n+1) \quad \text{at } n < n'. \quad (1.11)$$

Here $R_m(n)$ [$L_m(n)$] is the sum of all the diagrams in which the vertices lie to the right (left) of the site $n+1$ and have m pairs of lines in the section passing through this site. In the diagrams for $\tilde{K}_{m'm}(n', n)$ the vertices lie between the sites $n'+1$ and $n+1$, the numbers of line pairs in the corresponding sections are m' and m , and furthermore they contain each one more line directed from the site $n'+1$ to the site $n+1$. The symbol \hat{p} denotes averaging over the realizations of all the random quantities located on its right.

The expressions for the transition matrices $W_{mm'}^r(n)$ and $V_{mm'}^r(n)$ are⁶

$$W_{mm'}^r(n) = \left(\frac{1-z_-}{z_+-1} \right)^{m'-m} \left(\frac{z_+}{z_-} \right)^{n(m'-m)} W_{mm'}^r, \quad (1.12)$$

$$W_{mm'}^r = \sum_k C_m^k C_{m'-1}^{k+m'-m} (1+f_{\rightarrow})^{m-k} (1+f_{\leftarrow})^{m-k} (-f_{\rightarrow})^k (-f_{\leftarrow})^{k+m'-m}, \quad (1.13)$$

$$V_{mm'}^r(n) = \left(\frac{z_+-1}{1-z_-} \right)^{m'-m} \left(\frac{z_-}{z_+} \right)^{n(m'-m)} V_{mm'}^r, \quad (1.14)$$

$$V_{mm'}^r = \sum_k C_m^k C_{m'}^{k+m'-m} (1+f_{\rightarrow})^{m-k+1} (1+f_{\leftarrow})^{m-k} (-f_{\rightarrow})^{k+m'-m} (-f_{\leftarrow})^k, \quad (1.15)$$

the transition matrices with index l are obtained by making the substitutions $z_+ \leftrightarrow z_-$ and $f_{\rightarrow} \leftrightarrow f_{\leftarrow}$. The quantities z_+ , z_- and f_{\rightarrow} , f_{\leftarrow} are connected respectively with the parameters of the chosen zeroth approximation (ordered chain with hopping probabilities \bar{w}_+ and \bar{w}_- to the right and to the left, respectively) and with the fluctuations about this approximation, $u_{\pm}(n) = w_{\pm}(n) - \bar{w}_{\pm}$, in the following manner:

$$z_{\pm} = \frac{1}{2\bar{w}_{\pm}} \{s + \bar{w}_+ + \bar{w}_- \pm [(s + \bar{w}_+ + \bar{w}_-)^2 - 4\bar{w}_+\bar{w}_-]^{1/2}\}, \quad (1.16)$$

$$f_{\rightarrow} = \frac{(1-z_-)(z_-^{-1}u_+ - u_-)}{\bar{w}_-(z_+ - z_-) + u_+(1 - z_+^{-1}) + u_-(1 - z_-)}; \quad (1.17)$$

f_{\leftarrow} differs from f_{\rightarrow} by the substitutions $z_+ \leftrightarrow z_-^{-1}$ and $u_+ \leftrightarrow u_-$. Going from R_m , L_m , and $\tilde{K}_{m'm}$ to their generating functions:

$$R(z) = \sum_{m=0}^{\infty} R_m z^m, \quad R_m = \left(\frac{z_+-1}{1-z_-} \right)^m \left(\frac{z_-}{z_+} \right)^{mn} R_m(n); \quad (1.18)$$

$$L(z) = \sum_{m=0}^{\infty} L_m z^m, \quad L_m = \left(\frac{z_+-1}{1-z_-} \right)^m \left(\frac{z_-}{z_+} \right)^{m(n+1)} L_m(n); \quad (1.19)$$

$$K(z', z; n', n) = \sum_{m', m} K_{m'm}(n', n) z'^{m'} z^m, \quad K_{m'm}(n', n) = \left(\frac{z_+-1}{1-z_-} \right)^{m-m'} \left(\frac{z_-}{z_+} \right)^{mn-m'(n'+1)} \times \begin{cases} z_-^{-n'} & \text{if } n > n' \\ z_+^{n'-n} & \text{if } n < n' \end{cases} \tilde{K}_{m'm}(n', n) \quad (1.20)$$

and transforming the latter as follows:

$$R(z') = \frac{1}{1-z'} + \frac{2z'}{(1-z')^2} \frac{z_+ - z_-}{2} \times \Phi_r \left[z_+ z_- \frac{x'}{1-x'} - (z_+ - 1)(1 - z_-) \right], \quad (1.21)$$

$$L(z) = \frac{1}{1-z} + \frac{2z}{(1-z)^2} \frac{z_+ - z_-}{2z_+ z_-} \times \Phi_l \left[\frac{1}{z_+ z_-} \frac{x}{1-x} - \frac{(z_+ - 1)(1 - z_-)}{z_+ z_-} \right], \quad (1.22)$$

$$K(z', z; n', n) = \frac{1}{1-z'} \frac{1}{1-z} \frac{z_+ - z_-}{z_-} \times F \left(z_+ z_- \frac{x'}{1-x'} - (z_+ - 1)(1 - z_-), \frac{1}{z_+ z_-} \frac{x}{1-x} - \frac{(z_+ - 1)(1 - z_-)}{z_+ z_-}; n', n \right), \quad (1.23)$$

and introducing new variables x' and x :

$$x' = \frac{z'(1-z_-) + z_- - z_-/z_+}{z' - z_-/z_+}, \quad (1.24)$$

where x is connected with z in similar fashion with the substitution $z_+ \leftrightarrow z_-^{-1}$, we arrive at the following equations for $\Phi_{r,l}$ and K :

$$(1-x) [1 + (1-x)\Phi_{r,l}(x)] = \hat{p} \frac{w_{\pm}}{w_{\mp}} \Phi_{r,l} \left(\frac{w_{\pm}}{w_{\mp}} \frac{x}{1-x} - \frac{s}{w_{\mp}} \right), \quad (1.25)$$

$$(1-x)F(x', x; n', n) = \hat{p}F \left(x', \frac{w_-}{w_+} \frac{x}{1-x} - \frac{s}{w_+}; n', n-1 \right) \quad \text{at } n > n', \quad (1.26)$$

$$(1-x)F(x', x; n', n) = \hat{p}F \left(x', \frac{w_+}{w_-} \frac{x}{1-x} - \frac{s}{w_-}; n', n+1 \right) \quad \text{at } n < n'.$$

These equations should be supplemented by conditions that follow from the obvious requirements $R_0 = L_0 = 1$ and $K_{m'm}(n, n) = \delta_{m'm}$:

$$\int_{-i\infty}^{+i\infty} \frac{dx}{2\pi i} \left[\Phi_{r,l}(x) - \frac{1}{x+0} \right] = 1, \quad (1.27)$$

$$F(x', x; n', n) = \frac{1}{(x'-1)(x-1)-1}. \quad (1.28)$$

It is convenient to combine the function F with Φ_l at $n > n'$ and with Φ_r at $n < n'$, by introducing the functions $Q_{r,l}$:

$$Q_{r,l}(x; n', n) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} \frac{x' dx'}{(x'-1)^2} \left[\Phi_{r,l} \left(\frac{x'}{x'-1} \right) - \frac{x'-1}{x'} \right] F(x', x; n', n), \quad (1.29)$$

the equations for which will be similar to (1.26), and the initial condition (1.28) must be replaced by

$$Q_{r,l}(x; n, n) = \Phi_{r,l}(x). \quad (1.30)$$

After changing to the Fourier representation with respect to the site numbers

$$D(k) = \sum_n e^{-ik(n-n')} D_{nn'}, \quad (1.31)$$

the Green's functions $D(k)$ will be expressed in terms of the functions introduced above in the following manner:

$$D(k) = D_+(k) + D_-(-k) - D_{00}, \quad (1.32)$$

$$D_{00} = \frac{1}{2\pi i s} \int_{-i\infty}^{+i\infty} \frac{x dx}{(x-1)^2} \left[\Phi_l(x) - \frac{1}{x} \right] \left[\Phi_r \left(\frac{x}{x-1} \right) - \frac{x-1}{x} \right], \quad (1.33)$$

$$D_{\pm}(k) = \sum_{n=0}^{\infty} D_{\pm n, 0} e^{ikn} = \frac{1}{2\pi i s} \int_{-i\infty}^{+i\infty} \frac{x dx}{(x-1)^2} \left[\Phi_{l,r} \left(\frac{x}{x-1} \right) - \frac{x-1}{x} \right] Q_{r,l}(x, k). \quad (1.34)$$

The equations for the functions $Q_{r,l}(x, k)$ are of the form

$$(1-x) [Q_{r,l}(x, k) + x\Phi_{r,l}(x) - 1] = e^{-ik} \hat{p} Q_{r,l} \left(\frac{w_{\pm}}{w_{\mp}} \frac{x}{1-x} - \frac{s}{w_{\mp}}, k \right) \quad (1.35)$$

Similarly, the GF $G(q)$ can be represented in the form

$$G(q) = G_+(q) + G_-(-q) - D_{00}, \quad (1.36)$$

$$G_{\pm}(q) = \frac{1}{2\pi i s} \int_{-i\infty}^{+i\infty} \frac{x dx}{(x-1)^2} \left[\Phi_{l,r} \left(\frac{x}{x-1} \right) - \frac{x-1}{x} \right] \Gamma_{r,l}(x, q), \quad (1.37)$$

where the generating functions $Q_{r,l}(x, q)$ of the central part satisfy the following equations:

$$(1-x) [\Gamma_{r,l}(x, q) + x\Phi_{r,l}(x) - 1] = \hat{p} e^{-iq} \Gamma_{r,l} \left(\frac{w_{\pm}}{w_{\mp}} \frac{x}{1-x} - \frac{s}{w_{\mp}}, q \right). \quad (1.38)$$

Expanding expressions (1.36)–(1.38) in powers of q and substituting in Eq. (1.7) for the current, we obtain

$$j(s) = \frac{en}{2\pi i} \int_{-i\infty}^{+i\infty} \frac{x dx}{(x-1)^2} \times \left\{ B_l(x) \left[\Phi_r \left(\frac{x}{x-1} \right) - \frac{x-1}{x} \right] + B_r(x) \left[\Phi_l \left(\frac{x}{x-1} \right) - \frac{x-1}{x} \right] \right\}, \quad (1.39)$$

where the functions $B_{l,r}(x)$ are defined as follows:

$$\Gamma_{r,l}(x, q) = A_{r,l}(x) - iqB_{r,l}(x) + \dots, \quad (1.40)$$

and must be sought by solving the system of equations

$$(1-x)A_{r,l}(x) - \hat{p}A_{r,l} \left(\frac{w_{\pm}}{w_{\mp}} \frac{x}{1-x} - \frac{s}{w_{\mp}} \right) = (1-x) [1 - x\Phi_{r,l}(x)], \quad (1.41)$$

$$(1-x)B_{r,l}(x) - \hat{p}B_{r,l} \left(\frac{w_{\pm}}{w_{\mp}} \frac{x}{1-x} - \frac{s}{w_{\mp}} \right) = \hat{p}rA_{r,l} \left(\frac{w_{\pm}}{w_{\mp}} \frac{x}{1-x} - \frac{s}{w_{\mp}} \right). \quad (1.42)$$

2. CHAIN WITH BROKEN BONDS

In this model, the broken bonds make a zero contribution to the right-hand sides of Eqs. (1.25), (1.41), and (1.42),

so that these equations take the form

$$(1-x)[1+(1-x)\Phi_i(x)]=(1-c)e^{-2\theta}\Phi_i\left(e^{-2\theta}\frac{x}{1-x}-\frac{s}{w}e^{-\theta}\right), \quad (2.1)$$

$$(1-x)[A_i(x)+x\Phi_i(x)-1]=(1-c)A_i\left(e^{-2\theta}\frac{x}{1-x}-\frac{s}{w}e^{-\theta}\right), \quad (2.2)$$

$$(1-x)B_i(x)=(1-c)A_i\left(e^{-2\theta}\frac{x}{1-x}-\frac{s}{w}e^{-\theta}\right) + (1-c)B_i\left(e^{-2\theta}\frac{x}{1-x}-\frac{s}{w}e^{-\theta}\right), \quad (2.3)$$

where $\theta = eEa/2kT$. The corresponding equations for the functions with index r are obtained by substituting $\theta \rightarrow -\theta$. Making the following substitutions:

$$x = \frac{\lambda z + \mu}{z + 1}, \quad z = \frac{\mu - x}{x - \lambda}, \quad (2.4)$$

$$\Phi_i(x) = (1+z)^2 \left[\frac{\tilde{\Phi}_i(z)}{(1-\mu)^2} - \frac{1}{\lambda-\mu} \frac{1}{1+z} \right], \quad (2.5)$$

$$A_i(x) = \frac{\tilde{A}_i(z)}{(1-\mu)^2} (1+z) + \frac{\lambda(1-\mu)}{(\lambda-\mu)(c-\mu)} (1+z), \quad (2.6)$$

$$B_i(x) = \frac{\tilde{B}_i(z)}{(1-\mu)^2} (1+z) + \frac{\lambda(1-\mu)c}{(\lambda-\mu)(c-\mu)^2} (1+z), \quad (2.7)$$

where we have introduced the parameters

$$\lambda = 1 - e^{-\theta}/u, \quad \mu = 1 - e^{-\theta}u, \quad (2.8)$$

$$u = r + (r^2 - 1)^{1/2}, \quad r = \text{ch } \theta + s/2w,$$

we can reduce (2.1)–(2.3) to the form

$$\tilde{\Phi}_i(z) = b(1-c)\tilde{\Phi}_i(bz) + c \frac{(1-\lambda)(1-\mu)}{\lambda-\mu} \frac{1}{1+bz}, \quad (2.9)$$

$$\tilde{A}_i(z) + (\lambda z + \mu)\tilde{\Phi}_i(z) = \frac{1-c}{1-\mu} \tilde{A}_i(bz), \quad (2.10)$$

$$\tilde{B}_i(z) = \frac{1-c}{1-\mu} \tilde{A}_i(bz) + \frac{1-c}{1-\mu} \tilde{B}_i(bz), \quad (2.11)$$

where $b = (1-\lambda)/(1-\mu)$. Equations (2.9)–(2.11) can be solved by applying to both sides the Mellin transformation

$$f^M(\eta) = \int_0^\infty z^{\eta-1} f(z) dz,$$

as a result of which we obtain for the Mellin transforms of the corresponding functions

$$\tilde{\Phi}_i^M(\eta) = \frac{\pi}{\sin \pi \eta} c \frac{(1-\mu)(1-\lambda)}{\lambda-\mu} \frac{b^{-\eta}}{1-(1-c)b^{1-\eta}}, \quad (2.12)$$

$$\tilde{A}_i^M(\eta) = \frac{\lambda \tilde{\Phi}_i^M(\eta+1) + \mu \Phi_i^M(\eta)}{1-(1-c)b^{-\eta}/(1-\mu)}, \quad (2.13)$$

$$\tilde{B}_i^M(\eta) = \frac{(1-c)b^{-\eta}/(1-\mu)}{[1-(1-c)b^{-\eta}/(1-\mu)]^2} [\lambda \tilde{\Phi}_i^M(\eta+1) + \mu \tilde{\Phi}_i^M(\eta)]. \quad (2.14)$$

After taking the inverse Mellin transforms, the expressions (2.12)–(2.14) go over into

$$\tilde{\Phi}_i(z) = c \frac{(1-\mu)(1-\lambda)}{\lambda-\mu} \sum_{n=0}^{\infty} \frac{(1-c)^n b^n}{1+zb^{n+1}}, \quad (2.15)$$

$$\tilde{B}_i(z) = -\frac{(1-c)}{(c-\mu)^2} \lambda \frac{(1-\mu)^2}{\lambda-\mu} + c(1-c) \frac{1-\lambda}{\lambda-\mu} \sum_p \frac{((1-c)/(1-\mu))^p}{1+zb^{p+2}} t_p, \quad (2.16)$$

$$t_p = \frac{\lambda}{b\mu^2} [(1-\mu)^{p+2} + (2+p)\mu - 1] - \frac{\mu}{\lambda^2} [(1-\lambda)^{p+2} + (2+p)\lambda - 1]. \quad (2.17)$$

Substituting (2.15)–(2.17) in (1.39) we get after lengthy but straightforward calculations an expression for the Laplace transform of the current

$$j(s) = j_0 \frac{f(u)}{w}, \quad (2.18)$$

$$f(u) = c^2(1-c)(u-u^{-1})$$

$$\sum_{n=0}^{\infty} \left\{ \frac{u^{-2n}}{[1-(1-c)u^{-2n}][1-(1-c)u^{-2n-2}]} \right\}^2 \times \frac{1-(1-c)^2 u^{-4n-2}}{[e^{-\theta}u - (1-c)u^{-2n}][e^{\theta}u - (1-c)u^{-2n}]}, \quad (2.19)$$

where $j_0 = 2ena \sinh \theta$ is the current in the unbroken chain.

Taking the inverse Laplace transform we obtain

$$j(t) = j_0 e^{-2wt \text{ch } \theta} \oint_{|u| > \text{ch } \theta} \frac{du}{2\pi i} e^{wt(u+u^{-1})} f(u). \quad (2.20)$$

It can be seen from (2.19) that the set of singularities of the function $f(u)$ is a family of poles that condense on approaching the unit circle. At $(1-c)e^{\theta} < 1$ all the poles are inside the unit circle so that the asymptotic form of $j(t)$ as $t \rightarrow \infty$ is

$$j(t) \sim j_0 \exp[-2wt(\text{ch } \theta - 1)]. \quad (2.21)$$

At $(1-c)e^{\theta} > 1$ one of the families of the poles of $f(u)$ goes inside the unit circle and then, taking into account only the poles farthest to the right, we obtain for the asymptotic form of $j(t)$

$$j(t) \sim \frac{j_0}{1-c} \left[\frac{(1-c)^2 e^{2\theta} - 1}{(1-c)e^{2\theta} - 1} \right]^2 \exp\left\{-wt \left[ce^{\theta} + \frac{c}{1-c} e^{-\theta} \right]\right\}. \quad (2.22)$$

Equations (2.21) and (2.22) offer evidence that the asymptotic form of $j(t)$ as $t \rightarrow \infty$ depends substantially on the field strength. The behavior of $j(t)$ determined by the function $\sigma(\omega)$ takes place only in the region of not too large t . For a more detailed consideration of this question we turn to the case of low density of broken pairs, $c \ll 1$. Under this assumption Eqs. (2.18)–(2.20) takes the form

$$j(s) = j_0 \varphi(u^2) / wc^2, \quad (2.23)$$

$$\varphi(\eta) = \frac{1}{\eta - v^2} \left\{ 1 + \frac{2\eta^{1/2}}{\eta - v^2} + \frac{1}{\eta - v^2} \left[2\psi\left(\frac{1}{2\eta^{1/2}}\right) - \psi\left(\frac{1}{2} + \frac{1+v}{2\eta^{1/2}}\right) - \psi\left(\frac{1}{2} + \frac{1-v}{2\eta^{1/2}}\right) \right] \right\}, \quad (2.24)$$

$$j(t) = j_0 e^{-v^2 t} \int_{-\infty}^{+\infty} \frac{d\eta}{2\pi i} e^{\eta t} \varphi(\eta). \quad (2.25)$$

Here $v = \theta/c$, $u^2 = v^2 + s/wc^2$, and $\tau = wc^2t$, and ψ is the digamma function. The function $\varphi(\eta)$ has the following singularities: a cut going from 0 to $-\infty$ and poles due to the digamma functions. If $v < 1$ the poles are located on the second sheet. Closing the integration contour on the right, we have only the contribution from the cut

$$j(t) = 2j_0 e^{-v^2\tau} \int_0^\infty \frac{x dx}{(1+v^2x^2)^2} e^{-x^2\tau} \operatorname{cth} \frac{\pi x}{2} \frac{1 + \operatorname{ch} \pi v x}{\operatorname{ch} \pi x + \operatorname{ch} \pi v x}. \quad (2.26)$$

This integral is calculated at $\tau \gg 1$ by the saddle-point method, after which we obtain

$$j(t) = \frac{2j\pi^{1/2}x}{(1+x_c^2v^2)(2\tau)^{1/2}} \exp \left[-v^2\tau - 3 \left(\frac{\pi(1-v)}{2} \right)^{2/3} \tau^{1/3} \right], \quad (2.27)$$

where $x_c = [2\tau/\pi(1-v)]^{1/3}$. It can be noted that as $v \rightarrow 0$ the asymptotic form of $j(t)$ has an unusual behavior:

$$j(t) \sim j_0 \exp \left\{ - \left[\frac{\pi(c-\theta)}{2} \right]^{2/3} (wt)^{1/3} \right\}.$$

The reason is that as $\omega \rightarrow 0$ the function $\sigma(\omega)$ has an essential singularity, $\sigma(\omega) \propto \exp(-1/\omega^{1/2})$.

At $v > 1$ the pole singularities $\varphi(\eta)$ go over to the first sheet, and as $t \rightarrow \infty$ we have

$$j(t) \sim j_0 \frac{4(v-1)^2}{(2v-1)^2} \exp[-(2v-1)\tau], \quad (2.28)$$

which corresponds to the behavior described by Eq. (2.22).

3. MODEL WITH RANDOM SITE DISTRIBUTION

The exact solution of Eqs. (1.25) and (1.26) in the case of the distribution (1.3), (1.4) is a complicated mathematical problem even in a zero field.⁶ Allowance for the field aggravates the difficulties, and we therefore restrict ourselves to calculation of the exponent of the first power of the asymptote of $j(s)$ as $s \rightarrow 0$. We determine the corresponding coefficient only in the case of a weak field.

Recognizing that for a regular chain the solution of Eqs. (1.25) and (1.26) is in the form of a pole, we seek the solution of (1.25) in the form

$$\Phi_l(x) = \int_0^\infty \frac{f_l(y) dy}{x-y/(1+y)}. \quad (3.1)$$

Substituting (3.1) in (1.25) and taking into account the normalization condition (1.27), which now takes the form

$$\int_0^\infty f_l(y) dy = 1,$$

we obtain for the pole distribution density $f_l(y)$ the equation

$$\int_0^\infty dy f_l(y) \hat{p} \left[\frac{y}{x+y} \frac{y-(e^{2\theta}-1)}{x(1+y)+ye^{2\theta}} - s \left(\frac{1+y}{x(1+y)+ye^{2\theta}} \right)^2 \left\{ w_- + s \frac{1+y}{x(1+y)+ye^{2\theta}} \right\}^{-1} \right] = 0, \quad (3.2)$$

where $\theta = eEr/2kT$. In the derivation of (3.2) we have made the substitution $x \rightarrow -x/(1-x)$. We note that at $s = 0$ this equation has a nonzero solution, so that the asymptotic expansion of $f_l(y)$ as $s \rightarrow 0$ begins with the zeroth order in s . The corresponding term of the expansion can be calculated for an arbitrary field. We indicate here only that in the weak-field limit the solution of Eq. (3.2) takes at $s = 0$ the form

$$f_l(y) = \delta(y-2\mu), \quad \mu = eEr/2kT. \quad (3.3)$$

We turn now to the equations for the central part with the index l . Substituting A_l in the form

$$A_l(x) = \int_0^\infty \frac{a_l(y) dy}{x-y/(1+y)} \quad (3.4)$$

in (1.41), we obtain for $a_l(y)$ the equation

$$\int_0^\infty dy a_l(y) \hat{p} \left[\frac{x(1+y)}{x+y} \frac{y-(e^{2\theta}-1)}{x(1+y)+ye^{2\theta}} + s \frac{e^{2\theta}(1+y)^2}{[x(1+y)+ye^{2\theta}]^2} \left\{ w_- + s \frac{1+y}{x(1+y)+ye^{2\theta}} \right\}^{-1} \right] = - \int_0^\infty dy f_l(y) \frac{y}{x+y}. \quad (3.5)$$

Multiplying the latter by $x^{\eta-1}$ and integrating with respect to x from 0 to ∞ we have

$$\begin{aligned} & \tilde{a}_M(\eta) - (1-2\mu\eta) [a_M(\eta+1) + a_M(\eta)] \\ & = s^{1-\lambda} \Gamma(\lambda) \frac{\Gamma(2-\lambda-\eta)}{\Gamma(1-\eta)} \tilde{a}(\eta-1+\lambda) + \sum_{k=0}^{\infty} \frac{1-\lambda}{k+\lambda} (-s)^{k+1} \frac{\Gamma(2-k-\eta)}{\Gamma(2+k)\Gamma(1-\eta)} \tilde{a}(\eta-1-k) + f_M(\eta+1), \end{aligned} \quad (3.6)$$

where $a_M(\eta)$ is the Mellin transform of $a(y)$, and by $\tilde{a}(\eta)$ is denoted the following integral transformation of $a(y)$:

$$\tilde{a}(\eta) = \int_0^\infty dy a(y) \left(\frac{y}{1+y} \right)^{\eta-1}. \quad (3.7)$$

The functions $a_M(y)$ and $\tilde{a}(y)$ are connected by the relations

$$\begin{aligned} a_M(\eta) &= \sum_{k=0}^{\infty} (-1)^k \frac{\Gamma(2-\eta)}{\Gamma(k+1)\Gamma(2-\eta-k)} \tilde{a}(\eta+k), \\ \tilde{a}(\eta) &= \sum_{k=0}^{\infty} \frac{\Gamma(2-\eta)}{\Gamma(k+1)\Gamma(2-\eta-k)} a_M(\eta+k). \end{aligned}$$

We put $\eta = 0$ in (3.6); the left-hand side of the equation is then identically zero. Recognizing that $f_M(1) = 1$, we can conclude that the expansion of $a(y)$ as $s \rightarrow 0$ begins with a term of the form

$$a(y, s) = a(y) s^{-1/(2\beta-\mu)}. \quad (3.8)$$

We note that the derivation of (3.8) above is based actually on the condition of integrability, at infinity, of the second iteration of (3.5).

Similar arguments for $b_l(y, s)$ lead to the conclusion that its asymptotic form as $s \rightarrow 0$ is

$$b_l(y, s) = b_l(y) s^{-2/(2\beta-\mu)}. \quad (3.9)$$

In the weak-field limit $b_l(y)$ is equal to

$$b_l(y) = \bar{r} \delta(y-2\mu).$$

We turn now to the equation for the function $\Phi_r(x)$. The corresponding equation for the distribution function of the poles of $f_r(y)$ differs from (3.2) in that $\theta \rightarrow -\theta$. After this substitution, however, Eq. (3.2) has at $s=0$ only a zero solution. This means that the second term in (3.2) must be taken into account on a par with the first. To this end it is necessary to carry out the scale transformation $y \rightarrow sy$. In other words, the asymptotic form of $\Phi_r(x)$ as $s \rightarrow 0$ is

$$\Phi_r(x) = \int_0^\infty \frac{h(y) dy}{x-sy}, \quad (3.10)$$

where $h(y)$ satisfy in the limit as $s \rightarrow 0$ the equation

$$\int_0^\infty dy h(y) \bar{p} \left[\frac{y}{x+y} \frac{e^{2\theta}-1}{y+xe^{2\theta}} - \frac{e^{2\theta}}{(y+xe^{2\theta})^2} \left\{ we^{-\theta} + \frac{1}{1+e^{2\theta}x} \right\}^{-1} \right] = 0. \quad (3.11)$$

In the Mellin representation, the last equation takes the form

$$2\mu\Gamma(2-\eta) h_M(\eta) - \Gamma(\rho)\Gamma(2-\rho-\eta) h_M(\eta-1+\rho) + \sum_{k=0}^{\infty} \frac{1-\rho}{k+\rho} \frac{\Gamma(k+2-\eta)}{\Gamma(k+2)} h_M(\eta-k-1) = 0, \quad (3.12)$$

$$\rho = 1 - \frac{1+2\mu(\eta-1)}{2\beta+\mu}.$$

It follows from (3.12) that $h_M(\eta)$ has only pole singularities located on the real axis, and the singularity farthest to the left is located at $\eta = \eta_c$, where $\eta_c = 1 + 1/(2\beta - \mu)$. Consequently, the function $h(y)$ decreases exponentially [like $\exp(-1/y)$] at zero and in power fashion at infinity:

$$h(y) \sim y^{-\eta_c} \frac{2\beta+\mu}{2\beta-\mu}. \quad (3.13)$$

The explicit form of $h(y)$ in the case of weak field is given in the Appendix.

It is possible to establish in similar form the asymptotic behavior of A_r and B_r . It can be noted, however, that the most diverging among the functions with index l are B_l , therefore the main contribution to the asymptotic form of $j(s)$ is made by the first term in (1.39). Substituting (3.9) and (3.10) in (1.39), we have

$$j(s) = -ena \int_0^\infty dx b_l(x) \int_0^{1/s} dy h_r(y) \frac{sy(1+x)}{x+sy} = -enab_l^M(1) \times \int_0^{1/s} dy y h(y). \quad (3.14)$$

The last integral in (3.14) diverges as $s \rightarrow 0$. Taking (3.13) into account, we obtain ultimately

$$j(s) = j_0(\mu) s^{-1/(2\beta-1)}, \quad (3.15)$$

where $j_0(\mu)$ is calculated in the Appendix for the case of a weak field and is equal to

$$j_0(\mu) = en\bar{r} \frac{2\beta}{2\beta-1} \mu^{2\beta}. \quad (3.16)$$

From (3.15) we conclude that the current falls off with time in power-law fashion

$$j(t) = j_0(\mu) t^{-(1-1/(2\beta-\mu))}. \quad (3.17)$$

We note that the presence of an electric-field threshold follows from (3.15).

4. CONCLUSION

We have obtained the general expressions (1.25), (1.39), (1.41), and (1.42), which make it possible to determine the kinetic characteristics of a large class of disordered systems whose behavior is described by an equation of the type (1.1). The method itself can be generalized also for a larger class of one-dimensional systems with disorder.

The results obtained in Secs. 2 and 3 indicate that the hopping conductivity of one-dimensional system is nonlinear. The behavior of $j(t)$ conforms to the relation $\sigma(\omega)$ only at small t ; thus, in the broken-bond model, at $t \ll t_c = \pi(c-\theta)/\theta^3$ (at $\theta \ll 1$ and $c \ll 1$) [see (2.7)]. The asymptotic form of $j(t)$ as $t \rightarrow \infty$, as can be seen from (2.21), (2.22), and (3.17), is not connected with the character of the $\sigma(\omega)$ dependence even in the weakest fields. In this sense any field is strong in the systems considered.

We present now a physical interpretation of the results. When an electric field is turned on the carrier distribution, which is equally probable over all the sites of a given cluster, begins to go over into a new Boltzmann distribution. In the course of this redistribution, a carrier current sets in and relaxes with a characteristic time $t \sim (w_+ + w_- - w)^{-1}$. This can be easily verified using as an example the problem with two sites, into which our problem is changed as $c \rightarrow 1$. The carriers located initially at the start of the cluster should then move through the cluster.

Depending on the strength of the field, two regimes can be distinguished in the behavior of $j(t)$ as $t \rightarrow \infty$. In the weak-field regime the main contribution to the current stems precisely from the processes that spread over the carriers, and the $j(t)$ dependence is described by Eq. (2.21). It is clear that in this case calculation of $j(s)$ from the formula $j(s) = \sigma(s)E/s$ is incorrect at small s , since this formula does not take the spreading into account.

In the strong field regime, the main contribution to the current comes from the carrier drift over the clusters along the field. In this case a contribution to $j(t)$ at the instant t will be made only by clusters having a dimension l much larger than w_+t . The statistical weight of such clusters is

$$W = c \int_l^\infty dx e^{-cx} = e^{-lc}.$$

Consequently the current decreases like $\exp(-w_+tc)$, in agreement with (2.22).

In the model with randomly distributed sites the carrier will continue to move over the field at a certain finite t , and only at $t \rightarrow \infty$ will it reach a bond where $w_+ \rightarrow 0$. Therefore $j(t)$ is here not an exponential but a power-law function, with the exponent depending on the field strength.

Using the results of Ref. 6, we can indicate times \bar{t} starting with which the power-law behavior mentioned above sets in. In the case of weak fields, $2\beta - \mu \gg 1$ (it assumed that $\beta \gg 1$) we have $\bar{t} \approx \nu^{-1} \exp(2\beta - \mu)$. At times shorter than \bar{t} , $j(t)$ will fall off more slowly than $1/t$, according to Ref. 6, by a logarithmic factor. Near the threshold field value ($2\beta - \mu - 1 \ll 1$)

$$\bar{t} \approx \exp \left[2 \frac{2\beta - \mu}{2\beta - \mu - 1} \right].$$

At $t \ll \bar{t}$ one can expect in this case $j(t)$ to fall off like $1/\ln^2 t$. Recognizing that $\nu \sim 10^{13} \text{ sec}^{-1}$ and $\beta \gtrsim 10$, \bar{t} can become quite appreciable.

As seen from (3.15), in fields in which a finite dc conductivity appears above a certain threshold, the threshold field is

$$E_c = \frac{2kT}{e\bar{r}}(2\beta - 1). \quad (4.1)$$

Fields below the threshold correspond to a finite value $\langle 1/w_+ \rangle$. In real systems such a situation can be realized only in fields on the order of intra-atomic.

One can attempt to generalize the results to include the case of quasi-one-dimensional systems. Allowance for hopping from a string to a string leads, in the effective-medium approximation, to the substitution $s \rightarrow s + w_1$ in the formulas obtained for the one-dimensional chain. Here w_1 is the probability of hopping from string to string:

$$w_1 = \nu \exp(-2\beta_1 r_1) \ll w_2. \quad (4.2)$$

In this case $j(t)$ has a finite limit as $t \rightarrow \infty$, corresponding in weak fields to $\sigma(\infty)$. For the broken-bonds model

$$\sigma_{sd} = \frac{e^2 a^2 n}{kT} \frac{w_1}{c^2}, \quad c \ll 1; \quad (4.3)$$

for the model of randomly distributed sites

$$\sigma_{sd} = \frac{e^2 \bar{r}^2 n}{kT} \nu \left(\frac{w_1}{\nu} \right)^{(2\beta-1)/(2\beta+1)} C(\alpha). \quad (4.4)$$

The results can be used to interpret the experimental data on quasi-one-dimensional compounds such as $\text{QN}(\text{TCNQ})_2$ (Ref. 7), and also on charge transport along linear dislocations,⁸ where the considered type of hopping conduction is possibly realized.

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APPENDIX

In the case of a weak field we put

$$h_{\mathbf{x}}(\eta) = (2\mu)^{(1-\eta)/(1-\alpha)} \chi(\eta). \quad (A.1)$$

According to (3.12), in the limit $\mu \rightarrow 0$ we have for $\chi(\eta)$

$$\nu \chi(\eta+1) + \chi(\eta) - \Gamma(\alpha) \frac{\Gamma(2-\alpha-\eta)}{\Gamma(2-\eta)} \chi(\eta-1+\alpha) = 0, \quad (A.2)$$

where $\alpha = 1 - 1/2\beta$. In (A.2) we took into account also the first term of the expansion in s , $\nu = s/(2\mu)^{(2-\alpha)/(1-\alpha)}$.

We write next $\chi(\eta)$ in the form

$$\chi(\eta) = \frac{1}{\Gamma(\eta-1)} \int_0^\infty t^{-\eta} g(t) dt, \quad (A.3)$$

and from (A.2) we obtain the following equation for $g(t)$:

$$\left[\nu \frac{d^2}{dt^2} - \frac{d}{dt} - \frac{\Gamma(\alpha)}{t^\alpha} \right] g(t) = 0, \quad g(0) = 1. \quad (A.4)$$

We note that $g(t)$ and $h(y)$ are connected by a Laplace transformation.

An asymptotic solution of (A.4) can be obtained by using boundary-layer theory.⁹ At sufficiently large t the solution is obtained by direct interaction of Eq. (A.4) with respect to ν :

$$g(t) = C_0 \exp \left[-\frac{\Gamma(\alpha)}{1-\alpha} t^{1-\alpha} \right] \left[1 + \frac{\nu \Gamma(\alpha)}{t^\alpha} \left(1 + \frac{\Gamma(\alpha)}{1-2\alpha} t^{1-\alpha} \right) \right] + O(\nu^2). \quad (A.5)$$

This expression is applicable at $t \gg \nu^{1/\alpha}$.

To obtain the solutions in the region of small t we make the change of variable $t = \nu p$, after which (A.4) takes the form

$$\left[\frac{d^2}{dp^2} - \frac{d}{dp} - \nu^{1-\alpha} \frac{\Gamma(\alpha)}{p^\alpha} \right] g(p) = 0. \quad (A.6)$$

Integrating (A.6) with respect to the small parameter $\nu^{1-\alpha}$ we obtain

$$g(p) = 1 - \nu^{1-\alpha} \Gamma(\alpha) \left\{ \frac{p^{1-\alpha}}{1-\alpha} + \int_0^\infty dk e^{-k} [(k+p)^{-\alpha} - k^{-\alpha}] \right\}. \quad (A.7)$$

The region of validity of (A.7) is bounded by the condition $p \gg 1$ or $t \gg \nu$. Matching together (A.5) and (A.7) we can write an asymptotic equation that is suitable everywhere

$$g(t) = \exp \left[-\frac{\Gamma(\alpha)}{1-\alpha} t^{1-\alpha} \right] - \Gamma(\alpha) \int_0^\infty dq e^{-q/\nu} [(q+t)^{-\alpha} - q^{-\alpha}]. \quad (A.8)$$

This result leads to two conclusions. The first is that the function $h(y, \mu)$ as $\mu \rightarrow 0$ can asymptotically be represented in the form

$$h(y, \mu) = \frac{1}{\mu} \frac{1}{1-\alpha} \bar{h} \left(\frac{y}{\mu^{1/(1-\alpha)}} \right).$$

The second is that the asymptotic form (3.13) is valid at $y \ll s^{-\alpha}$. Consequently the integral in (3.14) can be calculated using the asymptotic relation (3.13), and its value as $s \rightarrow 0$ is

$$\int_0^{s^{-\alpha}} y h(y) dy = \frac{1}{\alpha} \mu^{1/(1-\alpha)} s^{-\alpha}. \quad (A.9)$$

¹V. L. Berezinskiĭ, Zh. Eksp. Teor. Fiz. 65, 1251 (1973) [Sov. Phys. JETP 38, 620 (1974)].

²A. A. Gogolin, Preprint University of Helsinki, 1981.

³H. Böttger and V. V. Bryksin, Phys. Stat. Sol. (b) 78, 9, 415 (1976).

⁴S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, Rev. Mod. Phys. 53, 175 (1981).

⁵B. I. Shklovskii and A. A. Éfros, Usp. Fiz. Nauk 117, 401 (1975) [Sov. Phys. Usp. 18, 845 (1975)].

⁶V. N. Prigodin, J. Phys. C, 16, 12 (1983).

⁷G. Grüner, Bull. Am. Phys. Soc. 25, 255 (1980).

⁸Yu. A. Osip'yants, V. I. Tal'yanskii, and S. A. Shevchenko, Zh. Eksp. Teor. Fiz. 72, 1543 (1977) [Sov. Phys. JETP 45, 810 (1977)].

⁹J. D. Cole, Perturbation Methods in Applied Mathematics, Xerox College, 1968.

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