

## SOURCE-SOURCE DISTRIBUTION FUNCTIONS AND THE ELECTRON TRANSPORT IN DISORDERED SOLIDS

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The correlation and distribution functions for the local sources of the current are used in a new formulation of the conductivity problem of solids. Some general properties of the source-source distribution functions are derived. The theory is applied to the Anderson model of the disordered solid. The Brownian diffusion and the transport in the vicinity of mobility edges are discussed.

### *1. Introduction*

This paper is concerned with the electron mobility in low mobility solids. A new approach to the conductivity problem based on the source-source correlation and distribution functions is presented. In order to explain the basic ideas we start with the Anderson model<sup>1)</sup> of the solid with the cellular disorder. The corresponding single-particle Hamiltonian is defined on a reduced Hilbert space in which there is a single  $s$ -level associated with each site on a primitive lattice. This model Hamiltonian may be written as

$$H = \sum_i \varepsilon_i |i\rangle \langle i| + \sum_{ij} V_{ij} |i\rangle \langle j|, \quad (1.1)$$

where  $|i\rangle$  represents the Wannier state at the site  $i$  of a Bravais lattice,  $\varepsilon_i$  is the corresponding energy, and  $V_{ij} = V_{ji}$  is the intercell transfer matrix element. The energies on different sites are taken to be random, statistically independent, and to share a common distribution.

Studies of the conductivity are usually reduced to calculations of the current-current correlation functions. We consider here a symmetric correlation function

$$F_{\mu\nu}(t) = \frac{1}{4} \langle [j_\mu(t), j_\nu(0)]_+ + [j_\nu(t), j_\mu(0)]_+ \rangle, \quad (1.2)$$

where  $j_\mu$  is the  $\mu$ -th component of the current density operator,  $[\ ]_+$  denotes the anticommutator, and  $\langle \ \rangle$  represents both the thermal and the ensemble average. In terms of  $F_{\mu\nu}(t)$  the static conductivity tensor  $\sigma_{\mu\nu}$  is given by

$$\sigma_{\mu\nu} = \beta V \int_0^\infty F_{\mu\nu}(t) dt, \quad (1.3)$$

where  $\beta = 1/kT$  and  $V$  is the volume (Kubo<sup>2</sup>).

We first introduce the operator  $I_{ij}$  for the current flowing in the bond  $(i, j)$  from the site  $i$  to the site  $j$ :

$$I_{ij} = -ieV_{ij}(c_j^\dagger c_i - c_i^\dagger c_j); \quad \hbar = 1, \quad (1.4)$$

$e$  being the particle charge. Here,  $c_i^\dagger$  and  $c_i$  are respectively the creation and annihilation operators for a fermion particle in the state  $|i\rangle$ . Now, we may express  $j_\mu$  as

$$j_\mu = \frac{1}{V} \sum_{i>j} I_{ij} (X_{j\mu} - X_{i\mu}), \quad (1.5)$$

where  $X_{i\mu}$  is the  $\mu$ -th component of the lattice vector  $\vec{X}_i$  of the site  $i$ . By exploiting the property  $I_{ij} = -I_{ji}$ , we may also write

$$j_\mu = -\frac{1}{V} \sum_i X_{i\mu} S_i, \quad (1.6)$$

where  $S_i$  is the operator for the source of the current at the site  $i$  and is defined by

$$S_i = \sum_j I_{ij}. \quad (1.7)$$

$S_i$  represents the sum of all currents which flow from the site  $i$ . Note the important property

$$\sum_i S_i = 0, \quad (1.8)$$

which is a consequence of the charge conservation.

In view of (1.6) and (1.8) the current-current correlation function may be written as

$$F_{\mu\nu}(t) = -\frac{1}{V^2} \sum_{i>j} (X_{i\mu} - X_{j\mu})(X_{i\nu} - X_{j\nu}) G_{ij}(t), \quad (1.9)$$

where  $G_{ij}(t)$  is the source-source correlation function

$$G_{ij}(t) = \frac{1}{4} \langle \{[S_i(t), S_j(0)]_+ + [S_j(t), S_i(0)]_+\rangle. \quad (1.10)$$

Further,

$$\sigma_{\mu\nu} = -\frac{\beta}{V} \sum_{i>j} (X_{i\mu} - X_{j\mu})(X_{i\nu} - X_{j\nu}) K_{ij}, \quad (1.11)$$

$K_{ij}$  being the source-source distribution function, defined by

$$K_{ij} = \int_0^{\infty} G_{ij}(t) dt. \quad (1.12)$$

Charge fluctuations in the solid give rise to local sources and sinks of the current. The time and position correlations of the source and sink intensities are described by the functions  $G_{ij}(t)$  and  $K_{ij}$ .

The validity of the expression (1.11) for the conductivity tensor is not restricted only to the case of the Hamiltonian (1.1). The formula (1.11) is with the self-evident modifications applicable to any system. To prove this we consider a continuous distribution of the charge density  $\rho(\vec{x}, t)$ . The corresponding current density  $j_\mu(t)$  is given by

$$j_\mu(t) = -\frac{1}{V} \int d^3x x_\mu S(\vec{x}, t), \quad (1.13)$$

where

$$S(\vec{x}, t) = -\frac{\partial \rho(\vec{x}, t)}{\partial t} \quad (1.14)$$

is the current source density at the position  $\vec{x}$  and the time  $t$ . Substituting this expression for the current density in (1.2) and (1.3) we find

$$\sigma_{\mu\nu} = -\frac{\beta}{2V} \int d^3x_1 \int d^3x_2 (x_{1\mu} - x_{2\mu})(x_{1\nu} - x_{2\nu}) K(\vec{x}_1, \vec{x}_2), \quad (1.15)$$

where the source-source distribution function

$$K(\vec{x}_1, \vec{x}_2) = \int_0^\infty dt G(\vec{x}_1, \vec{x}_2; t) \tag{1.16}$$

is derived from the source-source correlation function

$$G(\vec{x}_1, \vec{x}_2; t) = \frac{1}{4} \langle [S(\vec{x}_1, t), S(\vec{x}_2, 0)]_+ + [S(\vec{x}_2, t), S(\vec{x}_1, 0)]_+ \rangle. \tag{1.17}$$

The expression (1.15) can be obtained directly from Eq. (1.11) by replacing the sums over the lattice sites with the space integrations.

The purpose of this paper is to study the properties of the source-source distribution functions, particularly in the regime of low mobilities. In Section 2 some general properties of  $K(\vec{x}_1, \vec{x}_2)$  are derived. The Brownian diffusion and the transport in the vicinity of mobility edges are discussed in Section 3. The advantages of the new approach to the conductivity problem are examined in Section 4.

## 2. Source-source distribution function

The following properties of the source-source distribution function can be easily proved:

1.  $K(\vec{x}_1, \vec{x}_2)$  is real and

$$\int d^3x_1 K(\vec{x}_1, \vec{x}_2) = \int d^3x_2 K(\vec{x}_1, \vec{x}_2) = 0. \tag{2.1}$$

This follows directly from (1.17) and (1.8).

2.  $K(\vec{x}_1, \vec{x}_2)$  is invariant with respect to the exchange of the coordinates. This follows from the symmetry of  $G(\vec{x}_1, \vec{x}_2; t)$ .

3. For translationally invariant systems  $K(\vec{x}_1, \vec{x}_2)$  is an even function of  $\vec{x}_1 - \vec{x}_2$ . In disordered systems the translational symmetry may result only after the ensemble averaging.

4. Considering a single system of non-interacting fermion particles we find by utilizing the representation of one-particle energy states  $|\alpha\rangle$  the following expression for the corresponding source-source distribution function

$$K(\vec{x}_1, \vec{x}_2) = \frac{\pi}{\beta} \sum_{\alpha\beta} \left[ -\frac{df(E)}{dE} \right]_{E=\varepsilon_\alpha} \langle \alpha | S(\vec{x}_1) | \beta \rangle \langle \beta | S(\vec{x}_2) | \alpha \rangle \delta(\varepsilon_\alpha - \varepsilon_\beta), \tag{2.2}$$

where  $f(E)$  is the Fermi-Dirac function,  $\varepsilon_\alpha$  the energy of the state  $|\alpha\rangle$ , and  $S(\vec{x})$  operates in the one-particle space.

In case of translationally invariant systems it is convenient to consider the Fourier transform  $K(\vec{q})$ ,

$$K(\vec{x}_1 - \vec{x}_2) = \frac{1}{V} \sum_{\vec{q}} K(\vec{q}) \exp [i\vec{q} \cdot (\vec{x}_1 - \vec{x}_2)]. \quad (2.3)$$

Note that

$$K(\vec{q}) = \int_0^\infty dt G(\vec{q}, t), \quad (2.4)$$

where  $G(\vec{q}, t)$  is the Fourier transform of the source-source correlation function (1.17). Introducing also the Fourier transform  $S(\vec{q}, t)$  of the current source density we find

$$G(\vec{q}, t) = \frac{1}{4V} \langle \{ [S(\vec{q}, t), S(-\vec{q}, 0)]_+ + [S(-\vec{q}, t), S(\vec{q}, 0)]_+ \} \rangle. \quad (2.5)$$

For particles of the charge  $e$  and mass  $m$  in the plane wave representation

$$S(\vec{q}) = -\frac{ie}{m} \sum_{\vec{k}} (\vec{k} \cdot \vec{q}) c_{\vec{k}-\vec{q}/2}^\dagger c_{\vec{k}+\vec{q}/2}. \quad (2.6)$$

An instructive example represents a degenerate Fermi gas with a slow exponential decay of electron-hole excitations. If we assume, that all excitations decay with the same relaxation time  $\tau = 1/\Gamma$  and further that  $\Gamma \ll \varepsilon_f$ , where  $\varepsilon_f$  is the Fermi energy, then approximately

$$K(\vec{q}) = \frac{e^2}{V m^2} \sum_{\vec{k}} (\vec{k} \cdot \vec{q})^2 f(\varepsilon_{\vec{k}-\vec{q}/2}) [1 - f(\varepsilon_{\vec{k}+\vec{q}/2})] \frac{\Gamma}{\left(\frac{\vec{k} \cdot \vec{q}}{m}\right)^2 + \Gamma^2}. \quad (2.7)$$

Here,  $\varepsilon_{\vec{k}} = k^2/2m$ .

In the long-wavelength limit  $q \ll k_f$ , where  $k_f$  is the Fermi surface wave number, and for  $kT \ll \varepsilon_f$  we find

$$K(\vec{q}) = \frac{e^2 N(\varepsilon_f) \Gamma}{\beta} \left[ 1 - \frac{m \Gamma}{k_f q} \operatorname{arctg} \left( \frac{k_f q}{m \Gamma} \right) \right], \quad (2.8)$$

where  $N(\varepsilon_f)$  is the density of states per unit volume on the Fermi surface.  $K(\vec{x})$ , which corresponds to (2.8), has a positive delta function peak at  $\vec{x} = 0$  and for  $\vec{x} \neq 0$  is negative and decays exponentially according to

$$K(\vec{x}) = - \frac{e^2 N(\varepsilon_f) \Gamma}{4\pi \beta} \left( \frac{m\Gamma}{k_f} \right) \frac{1}{x^2} \exp \left[ - \left( \frac{m\Gamma}{k_f} \right) x \right]. \quad (2.9)$$

Note that  $k_f/m\Gamma$  represents the particle free path. The substitution of (2.9) for  $K(\vec{x})$  in (1.15) gives the Drude formula

$$\sigma = \frac{n e^2}{m \Gamma}, \quad (2.10)$$

where  $n$  is the concentration of particles.

### 3. The Brownian diffusion and the transport in the vicinity of mobility edges

The purpose of this section is to study the conductivity in the low mobility regime. Systems which can be described by the model Hamiltonian (1.1) are considered. Further, we assume that the ensemble averaged conductivity is a scalar. In view of (1.11) and (2.2) we may write

$$\sigma = \frac{e}{\beta} \int dE \langle N(E) \rangle \left[ - \frac{df(E)}{dE} \right] \mu(E), \quad (3.1)$$

where  $N(E)$  is the density of states per unit volume and  $\mu(E)$  is the energy dependent mobility, given by

$$\begin{aligned} \mu(E) = - \frac{\pi\beta}{eV \langle N(E) \rangle} \sum_{i>j} (X_{ix} - X_{jx})^2 \langle \sum_{\alpha\beta} \langle \alpha | S_i | \beta \rangle \langle \beta | S_j | \alpha \rangle \times \\ \times \delta(E - \varepsilon_\alpha) \delta(E - \varepsilon_\beta) \rangle. \end{aligned} \quad (3.2)$$

According to (1.4) and (1.7)

$$\langle \alpha | S_i | \beta \rangle = ie \sum_l V_{il} (\langle \alpha | i \rangle \langle l | \beta \rangle - \langle \alpha | l \rangle \langle i | \beta \rangle). \quad (3.3)$$

Introducing the spectral density functions

$$A_{ij}(E) = \sum_{\alpha} \langle i | \alpha \rangle \langle \alpha | j \rangle \delta(E - \varepsilon_\alpha) \quad (3.4)$$

we can rewrite (3.2) in the following way

$$\mu(E) = \frac{\pi \beta e}{V \langle N(E) \rangle} \sum_{ij} (X_{ix} - X_{jx})^2 \sum_{lk} V_{il} V_{jk} \langle \text{Re} [A_{kl}(E) A_{lj}(E) - A_{jl}(E) A_{ik}(E)] \rangle. \quad (3.5)$$

In the original paper Anderson took that the distribution of site energies  $\varepsilon_i$  is uniform in the energy interval  $-\frac{1}{2}W$  and  $\frac{1}{2}W$ . This represents an unimportant simplification. Further, it is reasonable to assume that the transfer of particles takes place mostly between neighbouring sites. The structure of the energy eigenfunctions  $\langle i|\alpha\rangle$  in the energy region of extended states is very sensitive to the ratio of  $W$  and the energy band width  $B$  for the corresponding perfect crystal, i.e. if  $\varepsilon_i = 0$ . For small values of  $W/B$  the amplitude of the wavefunction does not change much by going from one to another site. In the approximation of a constant amplitude

$$|\alpha\rangle = \frac{1}{\sqrt{N}} \sum_i \exp(i\alpha_i) |i\rangle, \quad (3.6)$$

where  $N$  is the number of sites and  $\alpha_i$  the phase of the wavefunction at the site  $i$ . As far as the particle mean free path  $l$  is larger than the characteristic wavelength corresponding to the energy  $\varepsilon_\alpha$  in a perfect crystal a well defined correlation exists between the phases for sites which are separated by less than  $l$ . If  $W$  is of the order of  $B$  the phase coherence is lost already at distances of the order of the lattice spacing. This is the stage of the minimum metallic conductivity<sup>3)</sup> or the Brownian diffusion. In this regime the phases of the particle wavefunction at two neighbouring sites are random and therefore

$$\langle A_{lj}(E) A_{kl}(E) \rangle = \langle A_{il}^2(E) \rangle \delta_{lj} \delta_{kl}. \quad (3.7)$$

Hence,

$$\mu(E) = \frac{N \pi \beta e}{V \langle N(E) \rangle} \langle A_{il}^2(E) \rangle \sum_j (X_{jx} - X_{ix})^2 V_{ij}^2. \quad (3.8)$$

Note that the density of states per unit volume is

$$N(E) = \frac{1}{V} \sum A_{il}(E). \quad (3.9)$$

The particle motion consists here of successive uncorrelated jumps. The expression (3.8) has a simple meaning. Each term in it may be derived from the golden rule formula for the probability that the particle jumps from the site  $i$  to the site  $j$ .

The Brownian limit (3.8) does not represent the smallest possible mobility in the region of extended states. In fact, for larger ratios  $W/B$  the mobility may be considerably lower than (3.8) in particular if the energy  $E$  is close to mobility

edges. This happens because now the assumption of the constant amplitude  $|\langle i|a\rangle|$  and the random phase approximation are no more justifiable. In order to get a better insight into the structure of the particle wavefunction we use an approach which is based on the qualitative theory of localization proposed by Thouless<sup>4)</sup>. We shall consider the case when the ratio  $W/B$  is considerably greater than unity. Let the energy  $E$  be well within the range of the site energies  $\varepsilon$ . Then the wavefunction has largest amplitude on those sites whose energy lies within the energy interval  $E \pm xB$ , where  $x$  is a constant of the order  $1/2z$ ,  $z$  being the co-ordination number of the lattice. For small values of  $W/B$  the sites with the largest amplitude of the wavefunction may form an infinite cluster. In this case the band or the Brownian diffusion type motion of the particle is still possible along the percolation paths. In addition to infinite clusters we may have also finite clusters. In the quantum theory of disordered systems finite clusters are usually strongly coupled to infinite ones. For larger values of  $W/B$  only finite clusters survive. In order to construct an approximate wavefunction for this case we imagine finite clusters to grow in size until they touch one another. The lattice site  $i$  can be either inside of one of the clusters or on the surface which separates one cluster from another. The surface, where clusters mutually touch, is here considered to be formed by lattice sites. We shall denote the clusters by capital letters. First, we introduce the concept of the cluster Hamiltonian. The cluster Hamiltonian  $H_A$  for the cluster  $A$  is defined by

$$H_A = \sum_{i \in A} \varepsilon_i |i\rangle \langle i| + \sum_{i \in A, j \in A} V_{ij} |i\rangle \langle j|, \quad (3.10)$$

where the summations run over all sites in the cluster or on its surface. Note that the Hamiltonian (1.1) is not equal to the sum of all cluster Hamiltonians because the terms  $\varepsilon_i |i\rangle \langle i|$  for the surface sites appear in the sum at least twice. The Hamiltonian  $H_A$  has so many eigenstates as there are sites within and on the surface of the cluster. If the cut of the lattice into clusters has been done in an appropriate way we may expect that one of these states has the energy very close to  $E$ . These particular states, one for each cluster  $A$  and denoted by  $|A\rangle$ , we now use in the tight-binding construction of approximate eigenstates of (1.1):

$$|a\rangle = \frac{1}{\sqrt{N_c}} \sum_A \exp(i\alpha_A) |A\rangle, \quad (3.11)$$

where  $N_c$  is the number of clusters and  $\alpha_A$  is the phase of the state  $|A\rangle$ . By making a suitable choice of phases  $\alpha_A$  we hope that (3.11) represents a good approximation for the eigenstates of  $H$  on the energy shell  $E$ . It is obvious that one can construct  $N_c$  different states of this kind which are mutually orthogonal. The normalization of  $|a\rangle$  to  $\langle a|a\rangle = 1$  is only approximate because of the small overlap contributions  $\langle A|B\rangle$ .

It is important to note that the assumption of the same amplitude of the wavefunction  $\langle A|a\rangle$  on different clusters  $A$  can be justified only for states in the region of extended states. If clusters are large the possibility for the existence of extended states is small. Namely, the energy band of all possible states of the type (3.11) is much narrower than  $B$  because  $|\langle A|H|C\rangle| \ll B$  also for the neighbouring

clusters  $A$  and  $C$ . Therefore, already small fluctuations of the cluster energies  $\langle A | H | A \rangle$  may produce the localization.

In order to see the efficiency of the approximation (3.11) we consider first the case of the one-dimensional crystal with two sites, 1 and 2, in the primitive cell. The site energies in the cell are  $\varepsilon$  and  $-\varepsilon$ , respectively. Further, the particle transfer takes place only between neighbouring sites. Therefore,

$$H = \sum_n \varepsilon (|n, 1\rangle \langle 1, n| - |n, 2\rangle \langle 2, n|) + \sum_n w (|n, 1\rangle \langle 2, n| + |n, 2\rangle \langle 1, n| + |n, 2\rangle \langle 1, n+1| + |n+1, 1\rangle \langle 2, n|), \quad (3.12)$$

where  $|n, i\rangle$  represents the Wannier state at the site  $i = 1, 2$  of the  $n$ -th cell and  $w$  is the transfer matrix element. The eigenenergies of (3.12) are

$$E(\alpha) = \pm \left( \varepsilon^2 + 4w^2 \cos^2 \frac{\alpha}{2} \right)^{1/2}; \quad -\pi < \alpha < \pi. \quad (3.13)$$

The energy spectrum is split in two bands. In case  $E(\alpha) > 0$ , the corresponding eigenstates  $|\alpha\rangle$  are

$$|\alpha\rangle = \frac{1}{\sqrt{N}} \cos \varphi \sum_n [ |n, 1\rangle + \frac{w}{E(\alpha) + \varepsilon} (|n, 2\rangle + |n-1, 2\rangle) ] \exp(in\alpha), \quad (3.14)$$

where  $N$  is the number of primitive cells and

$$\operatorname{tg} \varphi = \frac{2w}{E(\alpha) + \varepsilon} \cos \frac{\alpha}{2}. \quad (3.15)$$

If energy bands are narrow and well separated,  $\varphi \approx 0$  and  $E(\alpha) \approx \varepsilon$ . Then, the expression in the curly brackets of (3.14) does not depend on  $\alpha$  and represents an approximate eigenstate of the three-site cluster Hamiltonian

$$H_n = \varepsilon (|n, 1\rangle \langle 1, n| - |n-1, 2\rangle \langle 2, n-1| - |n, 2\rangle \langle 2, n|) + w (|n-1, 2\rangle \langle 1, n| + |n, 1\rangle \langle 2, n-1| + |n, 2\rangle \langle 1, n| + |n, 1\rangle \langle 2, n|). \quad (3.16)$$

In case  $E(\alpha) < 0$  the  $n$ -th cluster is formed by sites  $(n, 1)$ ,  $(n, 2)$ , and  $(n+1, 1)$ .

Next we consider again the one-dimensional crystal but now with 4 sites, 1–4, in the primitive cell. The site energies are  $\varepsilon$ , 0,  $-\varepsilon$ , and 0, respectively. Between neighbouring sites a slow particle transfer,  $w$  is much smaller than  $\varepsilon$ , takes place. The energy spectrum

$$E(\alpha) = \pm \left\{ \frac{1}{2} (\varepsilon^2 + 4w^2) \pm \frac{1}{2} \left[ (\varepsilon^2 + 4w^2)^2 - 16w^4 \sin^2 \frac{\alpha}{2} \right]^{1/2} \right\}^{1/2}; \quad -\pi < \alpha < \pi, \quad (3.17)$$

is here split into three bands.

The energies in the upper and lower band are given approximately by

$$E(\alpha) \approx \pm \left( \varepsilon + \frac{2w^2}{\varepsilon} - \frac{2w^4}{\varepsilon^3} \sin^2 \frac{\alpha}{2} \right). \quad (3.18)$$

The corresponding band width is  $2w^4/\varepsilon^3$ . In the upper band the  $n$ -th cluster is formed by sites  $(n-1, 3)$ ,  $(n-1, 4)$ ,  $(n, 1)$ ,  $(n, 2)$ , and  $(n, 3)$  so that a good approximation for the eigenstate  $|\alpha\rangle$  is

$$|\alpha\rangle \approx \frac{1}{\sqrt{N}} \sum_n \left[ |n, 1\rangle + \frac{w}{\varepsilon} (|n, 2\rangle + |n-1, 4\rangle) + \frac{w^2}{2\varepsilon^2} (|n, 3\rangle + |n-1, 3\rangle) \right] \exp(in\alpha). \quad (3.19)$$

One can verify this by comparing with exact solutions. The expression in the square brackets represents a cluster state and can be derived easily by using the perturbation expansion.

In the middle band

$$E(\alpha) \approx \pm \frac{2w^2}{\varepsilon} \sin \frac{\alpha}{2} \quad (3.20)$$

and the band width is  $4w^2/\varepsilon$ . Here, we have twice as much of clusters as there are primitive cells. One type of clusters are formed by sites  $(n, 1)$ ,  $(n, 2)$ ,  $(n, 3)$  and the other by sites  $(n, 3)$ ,  $(n, 4)$ ,  $(n+1, 1)$ . Here, we find

$$|\alpha\rangle \approx \frac{1}{\sqrt{2N}} \sum_n \left[ \left[ |n, 2\rangle + \frac{w}{\varepsilon} (|n, 3\rangle - |n, 1\rangle) \right] \exp(in\alpha) \mp \left[ |n, 4\rangle + \frac{w}{\varepsilon} (|n, 3\rangle - |n+1, 1\rangle) \right] \exp \left[ i \left( n + \frac{1}{2} \right) \alpha \right] \right]. \quad (3.21)$$

Note that the upper and lower band are much narrower than the middle one. The narrowness of the band is related to the size of clusters. The band shrinks when clusters grow in size.

In periodic structures the phase  $\alpha_A$  in (3.11) is well defined. On the contrary, in disordered systems the phase  $\alpha_A$  can be considered usually as a random variable, In the random phase approximation

$$\langle \alpha | S_i | \beta \rangle \langle \beta | S_j | \alpha \rangle = \frac{1}{N_c^2} \sum_{AB} \langle A | S_i | B \rangle \langle B | S_j | A \rangle. \quad (3.22)$$

In this approximation the value of  $\langle \alpha | S_i | \beta \rangle \langle \beta | S_j | \alpha \rangle$  does not depend on the particular choice of the pair of states  $|\alpha\rangle, |\beta\rangle$ . Therefore, the expression (3.2) for the mobility assumes the following form

$$\mu(E) = \frac{\pi \beta}{e \langle N(E) \rangle} \langle N^2(E) R(E) \rangle, \quad (3.23)$$

where

$$R(E) = -\frac{V}{N_c^2} \sum_{i>j} (X_{ix} - X_{jx})^2 \sum_{AB} \langle A | S_i | B \rangle \langle B | S_j | A \rangle. \quad (8.24)$$

The structure of clusters  $A$  depends on the choice of the energy  $E$ . This is the cause of the energy dependence of  $R(E)$ .

The coefficients in the expansion of cluster states  $|A\rangle$  in terms of Wannier states  $|i\rangle$  are real and therefore, according to (3.3),  $\langle A | S_j | A \rangle = 0$ . Further,  $\langle A | S_i | B \neq A \rangle$  is different from zero only on very restricted conditions. Consider the sites  $l$  in the neighbourhood of the site  $i$  for which  $V_{il} \neq 0$ . Then  $\langle A | S_i | B \rangle$  is different from zero only if either  $i$  is in the cluster  $A$  and at least one of  $l$  in the cluster  $B$  or viceversa. The sites  $i, l$  may be also the sites on the cluster surface. In case of large cluster the site  $i$  must be close or on the surface of the cluster  $A$  or  $B$ . It is evident that the above considerations restrict  $A$  and  $B$  to the nearest neighbours.

For the illustration we again consider the one-dimensional crystal with two sites in the primitive cell as described by the Hamiltonian (3.12). If  $w/\varepsilon \ll 1$ , we deal with three-site clusters and narrow energy bands. Hence,

$$R(E) = \frac{2a^2 e^2 w^4}{\varepsilon^2}, \quad (3.26)$$

where  $a$  is a distance between the neighbouring sites. It is instructive to compare this result with

$$R(E) = a^3 e^2 w^2 \quad (3.26)$$

in the case  $\varepsilon = 0$ , where each site represents a cluster.

Next, we consider the one-dimensional crystal with 4 sites in the primitive cell and the energy spectrum (3.18). In the upper and lower band each cluster occupies 5 sites and

$$R(E) = \frac{4a^3 e^2 w^8}{\varepsilon^6}. \quad (3.27)$$

In the middle band clusters are formed by 3 sites and

$$R(E) = \frac{8a^3 e^2 w^2}{\varepsilon^2}. \quad (3.28)$$

#### 4. Discussion

Source-source distribution functions represent a convenient tool for the study of low mobility transport problems. These functions have a simple physical meaning. In the energy region of extended states a local charge density fluctuates in

time. Charge fluctuations are accompanied with random sources and sinks of the current. The spatial correlation between the sources and sinks is described by the source-source distribution function. The particle mobility is proportional to the average of the square of the distance between the source and the sink of the current. In low mobility materials this length is small and the source-source distribution function decays very fast with the increasing distance  $|\vec{x}_1 - \vec{x}_2|$ .

If the conductivity tensor is expressed in terms of the current-current correlation functions the following expression results for the particle mobility (Gosar and Prelovšek<sup>5)</sup>):

$$\mu(E) = -\frac{\pi \beta e}{V \langle N(E) \rangle} \sum_{ijkl} (X_{ix} - X_{jx})(X_{kx} - X_{lx}) V_{ij} V_{kl} \langle A_{li}(E) A_{jk}(E) \rangle. \quad (4.1)$$

This should be compared with the equivalent Eq. (3.5) which is derived from the source-source distribution function. Eq. (3.5) is more concise and transparent. Nevertheless, the real advantage of the new approach is not in the use of the Eq. (3.5) but of the expression (3.2). Unfortunately, so far no simple prescription is known for the direct calculation of the source-source distribution functions.

The new approach to the conductivity problem, as proposed in the present paper, is not applicable only to systems with a cellular disorder. It can be used also in case of a time dependent or a dynamic disorder which results from the coupling of the charge particle to lattice vibrations.

#### References

- 1) P. W. Anderson, Phys. Rev. **109** (1959) 1492;
- 2) R. Kubo, J. Phys. Soc. Jap. **12** (1957) 570;
- 3) N. F. Mott and E. A. Davis, *Electronic Processes in Non-Crystalline Materials*, Clarendon Press, Oxford 1979;
- 4) D. J. Thouless, Phys. Rep. **13** (1974) 93;
- 5) P. Gosar and P. Prelovšek, Z. Phys. **266** (1974) 299.

### DISTRIBUCIJSKE FUNKCIJE IZVIR-IZVIR IN ELEKTRONSKI TRANSPORT V NEUREJENIH TRDNIH SNOVEH

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Originalno znanstveno delo

Predstavljena je nova formulacija problema prevodnosti v trdnih snoveh, ki sloni na korelacijskih in distribucijskih funkcijah lokalnih izvirov toka. Izpeljane so nekatere splošne lastnosti distribucijskih funkcij izvir-izvir. Teorija je uporabljena pri Andersonovem modelu neurejene snovi. Obravnavana sta Brownova difuzija in transport v bližni gibljivostnih robov.