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Effective medium theory of hopping transport

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An effective medium theory for the calculation of the conductivity in the presence of inelastic scattering has been developed. Our approach turns out to be quite universal and applicable to arbitrary types of disorder. In contrast to other effective medium theories, our method does not rely on the introduction of an ordered lattice but focuses on the diffusion processes in the disordered media. We obtain a quantum diffusion equation in the presence of inelastic scattering which takes into account the Fermi correlation. The form of this equation shows the inapplicability of the concept of a spectral density for the conductivity used in earlier effective medium treatments. Furthermore, we apply our formalism to the calculation of the conductivity in the variable range hopping regime. For the dc conductivity we obtain Mott's law. In addition, we derive a simple formula for the frequency dependence of the ac conductivity. [S0163-1829(96)00132-4]

I. INTRODUCTION

So far, numerous papers have been devoted to the study of hopping transport in disordered media (see Refs. 1 and 2 and references therein). One of the most intricate problems in this field is the calculation of the impurity-averaged conductivity. To tackle this problem several methods have been applied. Among them, the percolative approach and the effective medium theory have proved to be particularly useful. Both methods rely on an interpretation of the system of transport equations as a random resistor network. While the percolative approach takes advantage of the fact that the admittances of the network vary by many orders of magnitude and therefore the current mainly follows the path of least resistance, the standard effective medium theory[3] focuses on a typical admittance of the network. This admittance is considered to be placed in a network with equal admittances forming an ordered lattice. The ordered network is chosen to imitate the average surroundings as well as possible, which is done by requiring that the electric field around the typical admittance is equal to the homogeneous field of the effective medium.

For nearest neighbor hopping (NNH), where the spread of the energy levels is neglected, both methods lead to similar results, which fully agree with the experimental situation. In the case of variable range hopping (VRH), where the transitions are inelastic, the situation is more intricate. In this case the application of percolation theory to the calculation of the conductivity leads to Mott's law.

In Ref. 4 Mott's law was found by means of a modified effective medium theory, which is based on the Kubo-Greenwood formula. However, the weakness of this approach is that the conductivity is expressed through the spectral density, which ignores the inelastic character of the transitions. Accordingly, only an averaging over the difference of the site energies was performed.

On the other hand, a deviation from Mott's law was detected in Ref. 5, where the standard effective medium theory was used. In this approach the conductances were considered to be random quantities in a $(d+1)$-dimensional space, where d is its spatial dimension. Accordingly, an independent averaging over the initial and the final sites was performed.

The reasons for the deviation of the effective medium result from the percolative one were discussed in Ref. 6 and Ref. 7. To achieve correspondence, the authors of Ref. 6 suggest restriction of the averaging procedure to sites having energies of order $kT\ln\sigma/\sigma_0$ near the Fermi level, where σ is the conductivity and σ_0 a normalization factor. In consequence of this restriction the site density becomes temperature dependent and the conductivity obeys Mott's law. However, it is not clear how to incorporate this restriction into the standard effective medium theory.

The aim of the present paper is the development of an effective medium theory which copes with the above-mentioned difficulties. Moreover, the theory should also be applicable to the study of the influence of a magnetic field on the transport properties in the hopping regime. To do so, we generalize an effective medium treatment which was suggested in Ref. 8 for the calculation of the conductivity in the NNH regime to the case of inelastic scattering. The advantage of this method lies in the fact that it does not rely on the introduction of an ordered lattice, which implies the definition of nearest neighbors, but focuses on the diffusion processes in disordered media. In particular, in the case of VRH, where the transitions do not occur between nearest neighbors in the d-dimensional configuration space, but between nearest neighbors in a $(d+1)$-dimensional space, this fact is certainly advantageous.

Below we represent an effective medium approach that is based on a transition from discrete to continuous coordinates in a $(d+1)$-dimensional space. The method turns out to be quite universal and applicable to arbitrary types of disorder.

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In our approach the diffusion in a $(d+1)$-dimensional space turns out to be most important. The diffusion process, which also implies the diffusion of energy between environments with different energies, leads to integral equations with respect to the energy. Owing to the Fermi correlation the kernel of these integral equations not only depends on difference coordinates but also on sum variables. The character of these integral equations shows clearly the inapplicability of notions like the spectral density for the conductivity in the VRH regime. Moreover, we obtain the quantum diffusion equation in the presence of inelastic scattering, which fully takes into account the Fermi correlation reproducing the characteristics of VRH.

Furthermore, we demonstrate the applicability of our method to the investigation of the frequency dependence of the conductivity in the VRH regime. Here, the advantages of our method show up in the emergence of a natural restriction of the electronic transport processes to a small region near the Fermi surface, as suggested in Ref. 6.

II. THE CONDITIONAL PROBABILITY FUNCTION

In order to establish a theory for the conductivity we start with an expression for the current. In the linear approximation with respect to the external electric field E, the current can be written in the form[5]

$$\mathbf{j}=\frac{e^2\beta s}{\Omega}\sum_m \mathbf{R}_m C_m(U_m+\mathbf{E}\cdot\mathbf{R}_m). \tag{1}$$

Here $C_m=f_m(1-f_m)$, where $f_m=f(\epsilon_m)$ is the Fermi distribution function with site energy ϵ_m, $\mathbf{R}_m$ is the position vector of site m, Ω is the volume, β the inverse temperature, e the unit charge, and $s=-i\omega$, where ω is the frequency of the applied external electric field. The quantity U_m has the interpretation of the electrochemical potential at site m. It is related to the chemical potential μ_m through $U_m=-\mathbf{E}\cdot\mathbf{R}_m+\mu_m/e$. To obtain the dc current the limit $s\rightarrow 0$ has to be taken in Eq. (1).

In order to calculate the quantity U_m we use the rate equations linearized with respect to the external electric field.[1] They are given by

$$sC_m(U_m+\mathbf{E}\cdot\mathbf{R}_m)=\sum_m \Gamma_{m'm}(U_{m'}-U_m). \tag{2}$$

The quantities $\Gamma_{m'm}$, which are related to the two site transition probabilities entering the rate equations in the absence of the field, can be represented in the form

$$\Gamma_{m'm}=\gamma_{m'm}\sqrt{C_mC_{m'}}, \tag{3}$$

where $\gamma_{m'm}$ is defined by

$$\gamma_{m'm}=\frac{J^2_{m'm}}{\hbar^2}e^{-2S_T}\int_{-\infty}^{\infty}dt\left\{\exp\left[\frac{i}{\hbar}(\epsilon_{m'}-\epsilon_m)t+\sum_{\mathbf{q}}\frac{\gamma_q^2[1-\cos(\mathbf{q}\cdot\mathbf{R}_{m'm})]}{N\sinh(\hbar\omega_{\mathbf{q}}/2kT)}\cos(\omega_{\mathbf{q}}t)\right]-1\right\}. \tag{4}$$

Here $\omega_{\mathbf{q}}$ is the frequency of a phonon with wave vector $\mathbf{q}$, $\gamma_{\mathbf{q}}$ the electron-phonon coupling constant, $\mathbf{R}_{m'm}=\mathbf{R}_{m'}-\mathbf{R}_m$, N is the number of sites of the sytem under consideration, and

$$S_T=\frac{1}{2N}\sum_{\mathbf{q}}\gamma_{\mathbf{q}}^2[1-\cos(\mathbf{q}\cdot\mathbf{R}_{m'm})]\coth\left(\frac{\hbar\omega_{\mathbf{q}}}{2kT}\right). \tag{5}$$

The resonance integrals $J_{m'm}$ are supposed to have the form

$$J_{m'm}=J_0\exp(-2\alpha|R_{m'm}|), \tag{6}$$

where α^{-1} is the localization length. Expression (4) is valid for arbitrary electron-phonon coupling strength. Owing to their definition the quantities $\gamma_{m'm}$ are symmetric with respect to their indices. Furthermore, they depend only on difference coordinates, i.e., they have the form

$$\gamma_{m'm}=\gamma(|\mathbf{R}_{m'm}|,|\epsilon_{m'm}|). \tag{7}$$

To solve Eq. (2) we use the Green's function method. In reminiscence of the NNH problem we require the Green's function P to satisfy an equation of the type

$$sP_{m'm}=\delta_{m'm}+\sum_{m''}(P_{m'm''}V_{m''m}-P_{m'm}V_{mm''}). \tag{8}$$

To achieve correspondence we choose the coefficients α_m and the potentials $V_{m'm}$ in accordance with the rate equations (2). Doing so, we obtain the following equation for the Green's function P:

$$sP_{m'm}=\delta_{m'm}+\sum_{m''}\gamma_{m''m}\left(\sqrt{\frac{C_m}{C_{m''}}}P_{m'm''}-\sqrt{\frac{C_{m''}}{C_m}}P_{m'm}\right). \tag{9}$$

Using the solution of Eq. (9) the electrochemical potentials are determined according to

$$C_mU_m=-\sum_{m'}sC_{m'}(\mathbf{E}\cdot\mathbf{R}_{m'})P_{m'm}. \tag{10}$$

Owing to the principle of detailed balance and the law of probability conservation, the Green's function P satisfies the sum rules

$$\sum_{m'}sC_{m'}P_{m'm}=C_m, \tag{11}$$

$$\sum_m sP_{m'm}=1. \tag{12}$$

Both properties can be easily derived from Eq. (9). Using the sum rules the current can be represented in the form

$$\mathbf{j}=\frac{e^2\beta s^2}{2\Omega}\sum_{m'm}\mathbf{R}_{m'm}C_{m'}P_{m'm}(\mathbf{E}\cdot\mathbf{R}_{m'm}). \tag{13}$$

The introduction of the Green's function P reminds one of the diffusion function in a four-dimensional space with coordinates $\rho_m=\{\mathbf{R}_m,\epsilon_m\}$. However, as the transition probabilities between the sites, i.e., the quantities $\gamma_{m'm}\sqrt{C_m/C_{m'}}$, are nonsymmetric and moreover do not only depend on difference coordinates but also on sum variables, the nature of this diffusion process is rather strange. This fact is obviously related to the Fermi correlation acting differently for NNH and for VRH. In the latter case the transitions are inelastic. Therefore, one is not only concerned with diffusion in space but also with diffusion of energy.

III. THE CONTINUOUS REPRESENTATION

In order to proceed further it is expedient to convert to continous coordinates. This can be achieved by defining the new Green's function

$$P(\rho',\rho)=\sum_{m'm}\delta(\rho'-\rho_{m'})P_{m'm}\delta(\rho-\rho_m), \tag{14}$$

where $\rho=(\mathbf{R},\epsilon)$. Using the definition (14) the equation of motion for the Green's function (9) can be written in the form

$$sP(\rho',\rho)=\eta(\rho')\delta(\rho'-\rho)+\int d\rho_1 P(\rho',\rho_1)V(\rho_1,\rho), \tag{15}$$

where $\eta(\rho)=\Sigma_m\delta(\rho-\rho_m)$. In three dimensions the function $\eta(\mathbf{R})$ represents the well known structural factor describing the atomic structure of materials. The potential V, which is linear in the function η containing the disorder, is given by

$$V(\rho',\rho)=\int d\rho_1 w_{\rho_1}(\rho',\rho)\eta(\rho_1), \tag{16}$$

where

$$w_{\rho_1}(\rho',\rho)=w(\rho',\rho_1)[\delta(\rho_1-\rho)-\delta(\rho'-\rho)], \tag{17}$$

$$w(\rho',\rho)=\gamma(\rho',\rho)\sqrt{\frac{C(\epsilon)}{C(\epsilon')}}. \tag{18}$$

Here $\gamma(\rho',\rho)=\gamma_{m'm}|_{\rho_{m'}=\rho',\rho_m=\rho}$. Owing to their structure, the quantities (17) have the properties

$$w_{\rho'}(\rho',\rho)=0\ , \tag{19}$$

$$\int d\rho w_{\rho_1}(\rho',\rho)=0\ . \tag{20}$$

In addition, the transition probabilities (18) satisfy the relation

$$C(\epsilon')w(\rho',\rho)=C(\epsilon)w(\rho,\rho'). \tag{21}$$

Equations (20) and (21) represent the law of probability conservation and the principle of detailed balance on the level of transition probabilities. Due to property (19) double occupacy of points in the configuration space is prevented.

Equation (15) has the advantage that all random quantities are comprised in the Green's function P and in the function η. Furthermore, the expression for the Green's function P is quite close to the Green's function equation usually considered in the theory of impurity scattering. Reiterating Eq. (15), we obtain the following equation for the Green's function P:

$$P=\frac{1}{s}\sum_{n=0}^{\infty}\eta\left(\frac{1}{s}V\right)^n. \tag{22}$$

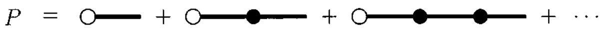

FIG. 1. Diagrams contributing to the Green's function P. All points are numbered consecutively. The empty point denotes the single structural factor η. A solid line starting at the point i and ending at j represents a factor $\delta(\rho_i-\rho_j)/s$. Every full dot is associated with a potential $V(\rho_i,\rho_j)$.

The series expansion (22) can be represented diagrammatically in the customary way depicted in Fig. 1. As the lowest-order term in (22) contains the function η, the diagrammatic representation differs slightly from those considered in the theory of impurity scattering.

In this representation the requirements of the principle of detailed balance and the law of probability conservation read

$$\int d\rho sP(\rho',\rho)=\eta(\rho'), \tag{23}$$

$$\int d\rho' sC(\epsilon')P(\rho',\rho)=C(\epsilon)\eta(\rho). \tag{24}$$

Using the new Green's function P the conductivity can be represented as

$$\sigma_{\alpha\beta}=\frac{e^2\beta s^2}{2\Omega}\int d\rho' d\rho(R'-R)_\alpha(R'-R)_\beta C(\epsilon')P(\rho',\rho). \tag{25}$$

IV. A DIAGRAMMATIC THEORY FOR THE CONFIGURATIONAL AVERAGED GREEN'S FUNCTION

In order to calculate the configurational averaged Green's function we apply the methods of standard perturbation theory. To do so, we first define a proper averaging procedure. In order to calculate the configurational average we assume the sites to be statistically independently and uniformly distributed in space. Furthermore, we suppose the probability distribution of site energies to be given by some function $p(\{\epsilon_m\})$. Therefore, the configurational average of an arbitrary quantity A depending on the random variables $\{\mathbf{R}_m\}$ and $\{\epsilon_m\}$ is calculated according to

$$\langle A\rangle=\int\prod_m\frac{d\mathbf{R}_m}{\Omega}d\epsilon_m p(\{\epsilon_m\})A(\{\mathbf{R}_m,\epsilon_m\}). \tag{26}$$

In particular, the application of the averaging procedure to the function η serves as definition for the density of states $N(\epsilon)$ of the configurational averaged system, i.e., $\langle\eta(\rho)\rangle=N(\epsilon)$.

In order to calculate the configurational averaged Green's function we average the series (22) term by term. Furthermore, we represent the resulting expansion in the customary way depicted in Fig. 2.

It can be seen from Fig. 2 that the set of all diagrams can be decomposed into two subsets, the set S containing all diagrams connected with the empty point and the class F

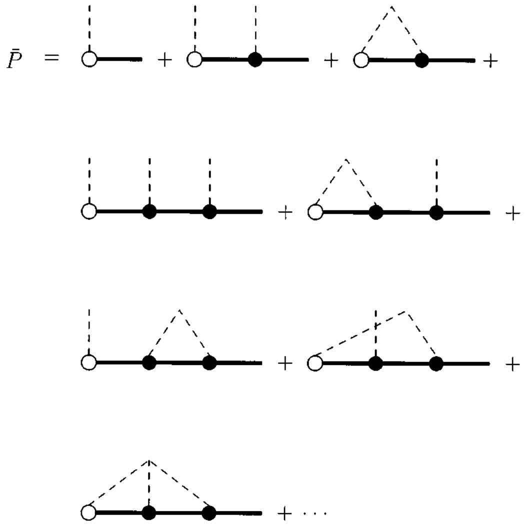

FIG. 2. Diagrams contributing to the configurational averaged Green's function. The performance of the averaging procedure is symbolized by dashed lines. Correlated averaging is denoted by joint lines.

containing all other diagrams. Owing to this decomposition the configurational averaged Green's function can be written as

$$\overline{P(\rho',\rho)}=\int d\rho_1 S(\rho',\rho_1)F(\rho_1,\rho). \tag{27}$$

Furthermore, the class F can be divided into the class of irreducible diagrams Π and the class of reducible diagrams. Owing to this procedure the function F can be shown to satisfy the Dyson equation

$$sF(\rho',\rho)=\delta(\rho',\rho)+\int d\rho_1 \Pi(\rho',\rho_1)F(\rho_1,\rho). \tag{28}$$

To obtain the functional dependence of the function Π with respect to F we have to perform a summation of diagrams contributing to Π. However, as the consideration of all diagrams is impossible we are forced to use an approximation. To perform a partial summation we neglect all interference diagrams. In consequence of this neglect the functions Π and S can be represented by the diagrams depicted in Fig. 3 and Fig. 4.

The set of diagrams depicted in Fig. 3 can be generated by means of the propagator $\Pi_{\widetilde{\rho}}$, being a solution of the equation

$$\Pi_{\widetilde{\rho}}=w_{\widetilde{\rho}}+w_{\widetilde{\rho}}F\Pi_{\widetilde{\rho}}. \tag{29}$$

Here we have used a matrix notation for brevity. Owing to the relations (19) and (20) the propagator $\Pi_{\widetilde{\rho}}$ satisfies

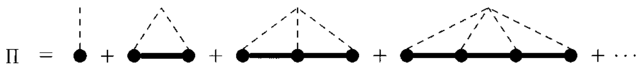

FIG. 3. Diagrams contributing to the function S. Here every solid line connecting the points i and j is associated with a function $F(\rho_i,\rho_j)$.

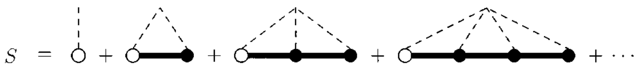

FIG. 4. Diagrams contributing to the irreducible part Π. Every solid line is associated with a function $F(\rho_i,\rho_j)$.

$$\Pi_{\rho'}(\rho',\rho)=0, \tag{30}$$

$$\int d\rho \Pi_{\widetilde{\rho}}(\rho',\rho)=0. \tag{31}$$

By means of $\Pi_{\widetilde{\rho}}$ the irrducible part Π is obtained from the equation

$$\Pi(\rho',\rho)=\int d\widetilde{\rho}N(\widetilde{\epsilon})\Pi_{\widetilde{\rho}}(\rho',\rho). \tag{32}$$

Furthermore, the diagrammatic expansion for the function S depicted in Fig. 4 can be cast into the form

$$S(\rho',\rho)=N(\epsilon')\left(\delta(\rho'-\rho)+\int d\rho_1 F(\rho',\rho_1)\Pi_{\rho'}(\rho_1,\rho)\right). \tag{33}$$

The relations (23) and (24) result in additional requirements on the functions S and F. Using the sum rules they can be shown to satisfy the relations

$$s\int d\rho F(\rho',\rho)=1, \tag{34}$$

$$\int d\rho' C(\epsilon')S(\rho',\rho)=C(\epsilon)N(\epsilon). \tag{35}$$

In order to obtain an expression for the conductivity we insert $\overline{P}$ in Eq. (25). Furthermore, we take into account the translational invariance and isotropy of the impurity averaged system. Doing so, we obtain

$$\sigma=\frac{e^2\beta}{2d}\int dr d\epsilon' d\epsilon r^2 C(\epsilon')N(\epsilon')\left\{\Pi(r|\epsilon',\epsilon)\right.$$
$$\left.+S^2\int d\rho_1 \delta S(r-r_1|\epsilon',\epsilon_1)F(r_1|\epsilon_1,\epsilon)\right\}, \tag{36}$$

where

$$\delta S(r|\epsilon',\epsilon)=\int d\rho_1 F(r-r_1|\epsilon',\epsilon_1)\Pi_{r,\epsilon'}(r_1,\epsilon_1|\mathbf{0},\epsilon). \tag{37}$$

V. THE EFFECTIVE MEDIUM

Despite the neglect of interference diagrams the system of equations (28), (29), and (32) is still complicated and nonlinear. To solve it approximately we generalize the effective medium theory suggested in Ref. 8 to the case of VRH.

To introduce the effective medium we decompose F into two parts, one part containing the effective medium and a part $\widetilde{F}$ describing the deviations from the effective medium solution, according to

$$F(\rho',\rho)=\widetilde{F}(\rho',\rho)+\sigma(\rho')\,\delta(\rho'-\rho). \tag{38}$$

In order to investigate the consequences of this decomposition we insert Eq. (38) into (29). Doing so, the effect is a partial summation of diagrams. Owing to this partial summation the unrenormalized transition probabilities (18) are replaced by renormalized ones according to

$$\widetilde{w}(\rho',\rho)=\frac{w(\rho',\rho)}{1+\sigma(\rho')w(\rho',\rho)}. \tag{39}$$

Furthermore, the series for the propagator $\Pi_{\tilde{\rho}}$ can be represented in the form

$$\Pi_{\tilde{\rho}}=\widetilde{w}_{\tilde{\rho}}+\widetilde{w}_{\tilde{\rho}}\widetilde{F}\Pi_{\tilde{\rho}}, \tag{40}$$

where the quantity $\widetilde{w}_{\tilde{\rho}}$ is the transition probability (17) with $w(\rho',\rho_1)$ replaced by $\widetilde{w}(\rho',\rho_1)$.

Let us now elaborate the structure of the function $\sigma(\rho)$ further. Due to the fact that the function P, like the functions F and S, has to meet the requirements of detailed balance and of probability conservation, the choice of the function $\sigma(\rho)$ is not arbitrary. As on the level of transition probabilities the fulfillment of these requirements is guaranteed by the relations (20) and (21), we demand that the renormalized transition probabilities satisfy these relations too. This requirement can be incorporated if the function $\sigma(\rho)$ is chosen according to

$$\sigma(\rho)=fC(\epsilon), \tag{41}$$

where f is a parameter depending neither on position nor on energy.

To fix f we investigate the formula (36) for the conductivity further. After the insertion of Eq. (40) into Eq. (36) the conductivity can be represented as $\sigma=\sigma_1+\sigma_2$. The contributions σ_1 and σ_2 are given by

$$\sigma_1=\frac{e^2\beta}{2d}\int dr\,d\epsilon'\,d\epsilon\,r^2N(\epsilon')N(\epsilon)W(r|\epsilon',\epsilon), \tag{42}$$

$$\begin{aligned}\sigma_2=\frac{e^2\beta}{2d}\int & d\rho\,d\rho_1\,d\epsilon'\,r^2C(\epsilon')N(\epsilon')\\ &\times\{N(\epsilon_1)\,\delta\Pi_{\rho_1}(r,\epsilon'|\mathbf{0},\epsilon)\\ &+s^2\delta S(r-r_1|\epsilon',\epsilon_1)F(r_1|\epsilon_1,\epsilon)\},\end{aligned} \tag{43}$$

where

$$\delta\Pi_{\tilde{\rho}}(\rho',\rho)=\int d\rho_1d\rho_2\widetilde{w}_{\tilde{\rho}}(\rho',\rho_1)\widetilde{F}(\rho_1,\rho_2)\Pi_{\tilde{\rho}}(\rho_2,\rho), \tag{44}$$

$$W(r|\epsilon',\epsilon)=C(\epsilon')\widetilde{w}(r|\epsilon',\epsilon). \tag{45}$$

Owing to the relation (21) the quantity $W(r|\epsilon',\epsilon)$ is symmetric with respect to its arguments.

Equation (42) has just the well known structure that one would expect to encounter in an effective medium theory. Its contribution to the conductivity is proportional to the square of the hopping length multiplied by an effective transition probability. Furthermore, the characteristics of the inelastic transitions result in integrations over the initial and the final energy. The occurrence of two integrations prevents the introduction of a spectral density for the conductivity or the usage of the Kubo-Greenwood formula, suggested in Ref. 4.

The contribution of σ_2 to the conductivity is proportional to the fluctuations $\widetilde{F}$, i.e., it vanishes for vanishing fluctuations. In order to fix f we require that

$$\sigma_2=0\,. \tag{46}$$

Doing so, we obtain a self-consistency equation for the effective medium f. Furthermore, the frequency dependence of the part σ_2 results in a frequency dependence of the effective medium.

As Eq. (46) is a complicated implicit equation for the effective medium f, the determination of f by means of (46) seems to be hopeless. Therefore, a further approximation is needed. Assuming the fluctuations to be small, we linearize the self-consistency equation (46) with respect to the fluctuations. This procedure is analoguous to the calculation of the effective medium on the basis of the vanishing of the t matrix in the standard perturbation theory. Retaining only the first order contribution of Eq. (46) with respect to the fluctuations, we obtain

$$\begin{aligned}0=\int & dr\,d\epsilon'\,d\epsilon\,C(\epsilon')N(\epsilon')r^2\\ &\times\left\{\int d\rho_1N(\epsilon_1)\,\delta\Pi^{(1)}_{\rho_1}(r,\epsilon'|\mathbf{0},\epsilon)+s\,\delta S^{(1)}(r|\epsilon',\epsilon)\right\},\end{aligned} \tag{47}$$

where

$$\begin{aligned}\delta\Pi^{(1)}_{\tilde{\rho}}(r,\epsilon'|\mathbf{0},\epsilon)=\int & d\rho_1d\rho_2\widetilde{w}_{\tilde{\rho}}(r,\epsilon'|\rho_1)\widetilde{F}(\rho_1,\rho_2)\\ &\times(\widetilde{w}_{\tilde{\rho}}(\rho_2|\mathbf{0},\epsilon),\end{aligned} \tag{48}$$

$$\delta S^{(1)}(r|\epsilon',\epsilon)=\int d\rho_1\widetilde{F}(r-r_1|\epsilon',\epsilon_1)\widetilde{w}_{r,\epsilon'}(\rho_1|\mathbf{0},\epsilon). \tag{49}$$

To eliminate the fluctuations $\widetilde{F}$ we replace $\widetilde{F}$ by F according to Eq. (38). However, as the full function F is calculated from the Dyson equation (28) this procedure results again in an infinite series in the fluctuations. As we have already neglected higher-order terms in the fluctuations retaining these contributions is not justified. Therefore, we have to use the the lowest order approximation of the function F with respect to the fluctuations. Doing so, the self-consistency equation takes the form

$$2\int d\mathbf{k}\,d\epsilon'\,d\epsilon\,d\tilde{\epsilon}\,N(\tilde{\epsilon})N(\epsilon')\nabla W(\mathbf{k}|\tilde{\epsilon},\epsilon')\Phi(\mathbf{k}|\epsilon',\epsilon)\nabla W(\mathbf{k}|\epsilon,\tilde{\epsilon})=f\int d\mathbf{k}\,d\epsilon'\,d\epsilon\,N(\epsilon')N(\epsilon)[\nabla W(\mathbf{k}|\epsilon',\epsilon)]^2, \tag{50}$$

where $W(\mathbf{k}|\epsilon',\epsilon)$ is the Fourier transform of the quantity (45). The function Φ, defined by

$$\Phi(\mathbf{k}|\epsilon',\epsilon)=F(\mathbf{k}|\epsilon',\epsilon)C^{-1}(\epsilon), \tag{51}$$

contains the function F only to lowest order with respect to the fluctuations. Accordingly, it satisfies the equation

$$\begin{aligned} sC(\epsilon')\Phi(\mathbf{k}|\epsilon',\epsilon)=\delta(\epsilon'-\epsilon)+\int d\epsilon_1 N(\epsilon_1) \\ \times\{W(\mathbf{k}|\epsilon',\epsilon_1)\Phi(\mathbf{k}|\epsilon_1,\epsilon) \\ -W(\mathbf{0}|\epsilon',\epsilon_1)\Phi(\mathbf{k}|\epsilon',\epsilon)\}. \end{aligned} \tag{52}$$

To complete the approximation scheme we elaborate the transition probabilities further. Using Eq. (45) the effective transition probabilities take the form

$$W(\rho',\rho)=\frac{\Gamma(\rho',\rho)}{1+f\Gamma(\rho',\rho)}, \tag{53}$$

where

$$\begin{aligned} \Gamma(\rho',\rho)=\nu\exp\biggl(-2\alpha|\mathbf{R}-\mathbf{R}'| \\ -\frac{|\epsilon'-\epsilon_f|+|\epsilon-\epsilon_F|+h|\epsilon'-\epsilon|}{2kT}\biggr). \end{aligned} \tag{54}$$

The function $\Gamma(\rho',\rho)$ is the continuous analog of the quantity $\Gamma_{m'm}$ defined by Eq. (3). The parameter h entering Eq. (54) is equal to 1 for weak and 0 for strong coupling with phonons. Whereas in the first case the factor ν is only weakly temperature dependent, it is of activation type in the latter case. Using Eqs. (53) and (54) we obtain

$$W(\mathbf{k}|\epsilon',\epsilon)=\nu\exp(-\rho_c)\int d\mathbf{R}\frac{e^{i\mathbf{k}\cdot r}}{1+\exp[-\rho_c+2\alpha R+(|\epsilon'-\epsilon_F|+|\epsilon-\epsilon_F|+h|\epsilon'-\epsilon|)/2kT]}, \tag{55}$$

where $\rho_c=\ln f\nu$ is a dimensionless parameter, which measures the critical length of a hop. As we are interested in the region of large ρ_c we approximate the integrand in Eq. (55) by a step function, which is zero for $\rho_c>2\alpha R+[|\epsilon'-\epsilon_F|+|\epsilon-\epsilon_F|+h|\epsilon'-\epsilon|]/2kT$. Doing so, we obtain

$$W(\mathbf{k}|\epsilon',\epsilon)=\nu\exp(-\rho_c)\left(\frac{2\pi\mu}{q}\right)^{d/2}\left(\frac{\rho_c}{2\alpha}\right)^{d}J_{d/2}(q\mu)\Theta(\mu), \tag{56}$$

where $J_n(x)$ is the Bessel function, $\Theta(x)$ the step function, $q=\rho_c k/(2\alpha)$, and $y=\epsilon/(2kT\rho_c)$. The quantity μ entering Eq. (56) is defined by

$$\mu=1-|y'-y_F|-|y-y_F|-h|y'-y|. \tag{57}$$

Approximation (56), which relies on the properties of Fermi integrals, is strongly related to the ideas of percolation theory.[1] This description corresponds to a transition to the picture of a hypersphere in a $(d+2)$-dimensional space with coordinates $\mathbf{R}$, ϵ', and ϵ. The parameter ρ_c has the interpretation of the critical diameter at which hopping conduction occurs. However, rather often only jumps across the Fermi surface are taken into account, which permits the consideration of the percolation problem in a $(d+1)$-dimensional space with coordinates $\mathbf{R}$ and $\epsilon'-\epsilon$.[9]

VI. TEMPERATURE AND FREQUENCY DEPENDENCE OF THE CONDUCTIVITY IN THE VRH REGIME

In order to calculate the conductivity we insert the effective transition probability (56) into Eq. (42). Owing to the step function the range of integration is restricted to a small region of width kT/ρ_c near the Fermi level. If the density of states within this range has no peculiarities we can replace the density of states by the density of states at the Fermi level. Doing so, we obtain

$$\begin{aligned} \sigma(\omega)=\frac{a\pi^{d/2}}{(d+3)(d+4)\Gamma(2+d/2)}\frac{\nu e^2N_F^2 2kT\rho_c^{d+4}}{(2\alpha)^{d+2}} \\ \times\exp(-\rho_c), \end{aligned} \tag{58}$$

where $\Gamma(x)$ is the Gamma function and a is a numerical coefficient, which is equal to 4 for strong coupling and 3/2 for weak coupling with phonons. The frequency dependence of the conductivity is entirely contained in the frequency dependence of the effective medium.

To elaborate the dependence of the conductivity on the frequency and on the temperature further we have to solve the self-consistency equation (50). However, as mentioned above, the calculation of the effective medium f relies on the solution of the integral equation (52). Only in the case of NNH, where $N(\epsilon)=n\delta(\epsilon)$, does the integral equation (52) reduce to an algebraic equation which can be solved easily. In this case, Eq. (52) describes diffusion in an effective homogeneous coordinate space. As for NNH our results agree fully with those obtained in Ref. 8, we do not pursue this problem further.

In the case of VRH Eq. (52) takes into account the inelastic character of the transitions and describes diffusion in a four-dimensional space with coordinates $\mathbf{R}$ and ϵ. In particular, for homogenuous particle distributions $(q\to 0)$ it describes the diffusion of energy without mass transport.

Owing to the difficult structure of the integral equation (52) further progress seems to be impossible. However, it turns out that for low frequencies a lot of physical information can be extracted from the structure of the function Φ. Using the dimensionless coordinates introduced above, the integral equation (52) can be rewritten in the form

$$s\frac{(2\alpha)^d\exp(\rho_c)C(2\rho_c y' kT)\phi(q|y',y)}{\nu N_F kT\rho_c^{d+1}} = \delta(y'-y)+\int dy_1[v(q|y',y_1)\phi(q|y_1,y) - v(0|y',y_1)\phi(q|y',y)], \tag{59}$$

where

$$\phi(q|y',y)=\frac{\nu N_F(kT)^2\rho_c^{d+2}}{(2\alpha)^d\exp(\rho_c)}\Phi(\mathbf{k}|\epsilon',\epsilon), \tag{60}$$

$$v(q|y',y)=\left(\frac{2\pi\mu}{q}\right)^{d/2}J_{d/2}(q\mu)\Theta(\mu). \tag{61}$$

Furthermore, the self-consistency equation (50) takes the form

$$\frac{2(2\alpha)^d}{N_F kT\rho_c^{d+1}}\int dy' dy dy_1 dq q^{d-1}\frac{dv(q|y_1,y')}{dq}\phi(q|y',y)\frac{dv(q|y,y_1)}{dq} = \int dy' dy dq q^{d-1}\left(\frac{dv(q|y',y)}{dq}\right)^2. \tag{62}$$

In the dc case the left hand side of Eq. (59) vanishes. Therefore the function $\phi^{(0)}=\phi|_{s=0}$ is determined from the equation

$$\int dy_1\{v(0|y',y_1)\phi^{(0)}(q|y',y)-v(q|y',y_1)\phi^{(0)}(q|y_1,y)\}=\delta(y'-y). \tag{63}$$

As the function $\phi^{(0)}$ depends only on the coordinates $q,\ y'$, and y its further calculation leads only to a determination of a numerical coefficient entering the self-consistency equation (62). Comprising this contribution into a parameter A, we obtain

$$\rho_c=\left(\frac{T_0}{T}\right)^{1/(d+1)}, \tag{64}$$

where $T_0=2A(2\alpha)^d/N_F k$. The coefficient A is determined from the equation

$$A=\frac{\int dy' dy dy_1 dq q^{d-1}[dv(q|y_1,y')/dq]\phi^{(0)}(q|y',y)dv(q|y,y_1)/dq}{\int dy' dy dq q^{d-1}[dv(q|y',y)/dq]^2}. \tag{65}$$

Inserting the expression (64) into Eq. (58) we obtain

$$\sigma(0)=\frac{aA\pi^{d/2}}{(d+3)(d+4)\Gamma(2+d/2)}\frac{e^2N_F\nu}{\alpha^2}\left(\frac{T_0}{T}\right)^{3/(d+1)} \times\exp\left[-\left(\frac{T_0}{T}\right)^{1/d+1}\right]. \tag{66}$$

The exponential factor occurring in Eq. (66) obeys Mott's law. The preexponential factor is proportional to $T^{-3/d+1}$. It is to be mentioned that the preexponential factor has been investigated by a numbers of authors.[1] However, as all those investigations are based on the notion of the correlation length of a critical cluster and therefore rely on the critical index, the results differ from our result.

Let us now investigate the frequency dependence of the conductivity. This dependence is entirely contained in the frequency dependence of the parameter ρ_c. In the framework of percolation theory it corresponds to a decrease of the critical cluster size with increasing ω.[10] Below we restrict the calculation to a range of small frequencies, which is determined as $[\rho_c(0)-\rho_c(\omega)]/\rho_c(0)\ll 1$.

To calculate the frequency dependence of the effective medium we expand the function ϕ up to the first order with respect to the parameter s. Doing so, we obtain

$$\phi^{(1)}=\frac{sT_0\exp(\rho_c)}{2A\nu T\rho_c^{d+1}}\int dy_1\phi^{(0)}(q|y',y_1)C(2\rho_c kTy_1) \times\phi^{(0)}(q|y_1,y). \tag{67}$$

For large ρ_c the quantity $C(2\rho_c kTy_1)$, which is given by $C(2\rho_c kTy_1)=[2\cosh(\rho_c y_1)]^{-2}$, is a strongly peaked function centered at $y_1=0$. As the function $\phi^{(0)}$ is slowly varying as compared to $C(2\rho_c kTy_1)$, the integration in Eq. (67) can be approximately performed and yields

$$\phi^{(1)}=\frac{sT_0\exp(\rho_c)}{4A\nu T\rho_c^{d+1}}\phi^{(0)}(q|y',0)\phi^{(0)}(q|0,y). \tag{68}$$

Taking into account the first order contribution (68) the self-consistency equation (62) reads

$$\rho_c^{d+1}=\frac{T_0}{T}\left(1+\frac{sBT_0}{2\nu A^2T\rho_c^{d+2}}\exp(\rho_c)\right). \tag{69}$$

The numerical coefficient B is given by

$$B=\frac{\int dy'dydy_1dqq^{d-1}[dv(q|y_1,y')/dq]\phi^{(0)}(q|y',0)\phi^{(0)}(q|0,y)dv(q|y,y_1)/dq}{\int dy'dydqq^{d-1}[dv(q|y',y)/dq]^2}. \tag{70}$$

To obtain the frequency dependence we replace s by $-i\omega$. Furthermore, we use Eq. (58) for the conductivity to cast Eq. (69) into the form

$$\frac{\sigma(\omega)}{\sigma(0)}\ln\frac{\sigma(\omega)}{\sigma(0)}=i\frac{\omega}{\omega_0}, \tag{71}$$

where ω_0 is given by

$$\omega_0=\frac{2A^2(d+1)}{B}\nu\exp\left[-\left(\frac{T_0}{T}\right)^{1/d+1}\right]$$
$$\sim\sigma(0)\frac{\alpha^2}{e^2N_F}\left(\frac{T}{T_0}\right)^3\bigg/(d+1). \tag{72}$$

To obtain Eq. (71) we have neglected the frequency dependence of the preexponential of the conductivity.

The equations (71) and (72) for the frequency dependence of the conductivity and the characteristic frequency ω_0 represent the main concrete result of our work.

VII. RESULTS

In the present article we have developed an effective medium theory which takes into account the effect of inelastic scattering. In contrast to other effective medium theories our approach does not focus on a particular admittance of a certain random resistor network but on the diffusion processes in a disordered medium. Within our theory the characteristics of inelastic scattering are reflected by integral equations with respect to the energy. The structure of these equations shows clearly the inapplicability of notions like a spectral density for the conductivity used in earlier effective medium treatments. Only for NNH, where the transitions occur on a surface with fixed energy, do the integral equations reduce to algebraic ones and the introduction of a spectral density for the conductivity becomes admissible. In the presence of inelastic scattering the diffusion process is described by the quantum diffusion equation (52), which takes into account the Fermi correlation reproducing the characteristics of VRH. For NNH or for hopping motion of small polarons in crystals this equation reduces to the standard diffusion equation in configuration space. In that case the features of the disorder show up in a strong dependence of the diffusion coefficient on the frequency for small frequencies. In the time dependent representation this dependence corresponds to a non-Markovian behavior of the diffusion process, a fact which is strongly related to the theory of dispersive transport.[11] The fact that in the presence of inelastic scattering the diffusion equation is an integral equation should be reproduced by the theory of dispersive transport. However, this problem has not been tackled in the literature so far.

One of the main advantages of the method is the fact that it does not rely on the introduction of the nearest neighbor conception but leads to an automatic determination of the critical hopping length. Thus it leads to a temperature dependent hopping length for VRH and to transitions between nearest neighbors in the configuration space for NNH. Moreover, the applicability of the method is not restricted to either of these limiting cases but covers the whole range of crossover between them. Furthermore, it is applicable to arbitrary types of disorder. To do so, it is only nessecary to modify the averaging procedure and its application to the structural factor η. If one performed these modifications the method would permit the study of systems with short range order too. To do so, the dependence of the structural factor η on the wave vector could be taken from neutron scattering experiments (e.g., on amourphous materials or liquids) which reproduce the characteristics of the short range order.

Furthermore, we have employed our formalism to calculate the conductivity in the VRH regime. In that case a natural restriction of the transport processes to a region near the Fermi surface appears. For vanishing frequencies of the driving field we obtain Mott's law. However, the preexponential factor obtained by means of our method differs from those obtained by other methods. In addition, we have derived a simple formula for the frequency dependence of the conductivity for low frequencies. Although Eq. (71) has not been derived so far on the basis of a microscopic foundation for VRH, but only for NNH,[8] it has been frequently used for the discussion of the experimental data.[12,13]

It is to be mentioned that the derivation of Eq. (71) presumes the convergence of the integrals in Eq. (70). In the NNH regime the nominator of Eq. (70) diverges logorithmically for small k. In this case the corrections to Eq. (69) can be shown to be proportional to $\ln(\omega/\omega_0)$. For three-dimensional systems the integrals in Eq. (70) converge. In that case a further consideration of the corrections to Eq. (69) reveals that they are of order $\omega^{3/2}$. In the VRH regime the situation is obscured by the absence of an explicit solution of Eq. (52). However, owing to Eq. (34) and Eq. (52) it is to be expected that the same statement holds also in the VRH regime.

However, the investigation of the temperature dependence of the conductivity in the range of crossover obviously requires further numerical calculations or the usage of additional approximations. Such an approximation could be the usage of the concept of quasielastic scattering, which permits the diffusion equation (52) to be written as a differential equation. Owing to the universal charcter of the method presented above we hope that it proves to be useful in studying the influence of a magnetic field on hopping conduction. As the latter problem requires at least the consideration of three site probabilities, further modifications have to be performed. Further work in this direction is in progress.

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