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2003 J. Phys.: Condens. Matter 15 1719

(http://iopscience.iop.org/0953-8984/15/10/319)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) 1719–1731 PII: S0953-8984(03)57074-6

Random-resistor network description for hopping transport in the presence of Hubbard interaction

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Received 3 December 2002
Published 3 March 2003
Online at stacks.iop.org/JPhysCM/15/1719

Abstract

On the basis of the linearized rate equations for hopping electrons in the presence of Hubbard interaction we derive a random resistor network analogue of the transport equations. In contrast to the ordinary Miller–Abraham network our network has two nodes per site. The occurrence of the second node is related to the capability of the system to propagate excitations, and thus is characteristic for the interacting situation. Our random resistor network can be used for the investigation of the transport properties in alternating electric fields and for the investigation of properties of excitations. The network analogue is applied to the calculation of the dynamical conductivity in the nearest-neighbour hopping regime for all Hubbard-interaction strength.

1. Introduction

In recent years there has been increasing interest in the investigation of interaction effects on conductivity in the hopping regime. As well as the long-range Coulomb interaction, the impact of the Hubbard interaction has also received a lot of attention. The effects of Hubbard interaction have recently been detected in magneto-resistance measurements in different materials [1–7]. In the absence of spin–orbit scattering the consideration of the Hubbard interaction leads to a positive magneto-resistance due to the Kamimura–Kurobe effect [8–11]. Spin–orbit scattering is expected to change this picture, and to result in an enhancement of the conductivity due to an increase in the effective density of states [12]. The ϵ_2-conduction, which appears in a very narrow range of impurity concentration and compensation, is also assumed to be caused by the impact of the Hubbard interaction [13].

From the theoretical point of view the physical picture in the presence of Hubbard interaction is much more involved than for non-interacting electrons. The strong electron

correlation between electrons on the same site leads naturally to the introduction of four types of transition probabilities, since the charge carriers can jump from single or double occupied sites to empty or single occupied sites [8, 15, 16]. This raises the question whether or not the traditional methods for the calculation of the conductivity in the hopping regime, that is either the percolation theory or effective medium methods, can also be used in the interacting situation.

Since the percolation theory for the hopping conductivity is based on the notion that the transport equations can be cast into the form of an equivalent random resistor network, the answer to this question depends on the introduction of a suitable random resistor network. While most authors agree that in the interacting situation percolation theory can also be applied to the investigation of the hopping conductivity, there is no general answer to the question of what the equivalent random resistor network looks like. While some authors use networks with one node per site (see, e.g., [17]) other authors use networks with two nodes per site (see, e.g., [9, 15, 18]). It is unclear, however, whether or not these two approaches are equivalent to each other. For finite frequencies no generalized random resistor networks have been published in the literature so far.

For the effective medium theories the consideration of the Hubbard interaction also represents a new challenge. Since in the interacting situation the state of each site has to be characterized at least by two variables the transport equations become matrix equations, which are more difficult to handle. Thus it is not surprising that only one effective medium theory for such systems has been published so far [19]. In this theory the impact of the Hubbard interaction reflects itself in four types of effective differential conductivity, which have to be considered. On the other hand the number of fluctuating quantities in the presence of the Hubbard interaction is the same as in the non-interacting situation, if fluctuations of the Hubbard-interaction strength are ignored. This is especially apparent in the activated transport regime. In this transport regime only the positions of the sites are considered as disordered quantities. The spread of the site energies of the band of first occupied states is ignored. If we assume that the system is strongly localized then the transitions mainly occur between nearest neighbours. In this case there is only one fluctuating quantity, the distance between the sites. The transport is characterized by a fixed percolation path, which does not shift with temperature [20]. Thus, at least for the nearest-neighbour-hopping (NNH) regime, which occurs in strongly localized systems, it should be possible to derive an effective medium theory, which has only one effective parameter, the characteristic hopping length. If the system is not very strongly localized, but the wavefunctions are widely spread, the transitions do not necessarily happen between nearest neighbours only. In such systems with widely spread wavefunctions, often an activated behaviour is also observed, although these systems are not NNH like in the sense used above. However such systems, although interesting in their own right, are not within the scope of the present paper. We would like to note that in the variable-range-hopping (VRH) regime the situation is in principle similar.

The aim of the present paper is to find answers to the questions raised above. Starting with the transport equations for hopping electrons in the presence of Hubbard interaction we derive a random resistor network with two nodes per site, which can also be used for the investigation of hopping transport problems in alternating electric fields. By doing so, we restrict the consideration to the NNH regime and focus on the strongly localized regime. To answer the question under which conditions the nodes of the network can be joint, that is under which conditions the random resistor network with two nodes per site is equivalent to a random resistor network with one node per site, we generalize the standard effective medium theory in such a way that it can also be used for the investigation of such systems, and apply it to the investigation of the dynamical conductivity in the whole range of frequencies.

2. The model

We consider localized electrons interacting via Hubbard repulsion and with the phonon system. The Hamilton operator of the electron system is given by

$$H_e = \sum_{m,\sigma}(\epsilon_m + e\boldsymbol{E}(t)\boldsymbol{R}_m)a^+_{m\sigma}a_{m\sigma} + \sum_{mm'\sigma} J_{mm'}\Phi_{mm'}(t)a^+_{m\sigma}a_{m'\sigma} + \frac{U}{2}\sum_{m\sigma} a^+_{m\sigma}a_{m\sigma}a^+_{m-\sigma}a_{m-\sigma}. \tag{1}$$

The operators $a^+_{m\sigma}$ ($a_{m\sigma}$) are electron creation (annihilation) operators. They create localized electrons with spin σ at site m with position vector $\boldsymbol{R}_m$, site energy ϵ_m, and localization radius α^{-1}. Both the positions of the sites and their site energies are random quantities. The coupling between the electron and phonon system is provided by the resonance integral

$$J_{mm'} = J_0 \exp(-\alpha|\boldsymbol{R}_{mm'}|) \tag{2}$$

and the multi-phonon operator $\Phi_{mm'}(t)$ [14]. The impact of the electron system on the phonon system is neglected. Accordingly, the evolution of the multi-phonon operator is governed by the Hamilton operator

$$H_{ph} = \sum_{\boldsymbol{q}} \hbar\omega_q (b^+_q b_q + \tfrac{1}{2}) \tag{3}$$

only, where b^+_q (b_q) are creation (annihilation) operators for acoustic phonons with momentum q, and $\hbar\omega_q$ is the energy for a phonon with wavevector q.

3. The transport equations

In order to investigate transport we have to derive transport equations for such systems in the strongly localized regime. To this end it is sufficient to focus on the expected values of the one-particle density matrix in the non-interacting situation, since products of particle number operators can safely be Hartree–Fock decoupled in this case. In the presence of the Hubbard interaction, however, Hartree–Fock decoupling cannot be applied to products of particle number operators at the same site, but only to products of particle number operators at different sites, since the latter are only coupled by the resonance integral and the electron–phonon interaction, and tunnelling can be ignored in the hopping regime. Consequently, in deriving the transport equations we have to take into account that every site can be either empty, double occupied, or single occupied with an electron in a certain spin direction. To take into account this fact it is convenient to introduce the expection values of the Hubbard operators

$$f^{(0)}_m = \langle(1 - n_{m\uparrow})(1 - n_{m\downarrow})\rangle, \tag{4}$$
$$f^{(2)}_m = \langle n_{m\uparrow} n_{m\downarrow}\rangle, \tag{5}$$
$$f_{m\downarrow} = \langle n_{m\downarrow}(1 - n_{m\uparrow})\rangle, \tag{6}$$
$$f_{m\uparrow} = \langle n_{m\uparrow}(1 - n_{m\downarrow})\rangle, \tag{7}$$

where $n_{m\sigma}$ is the particle number operator for particles on site m with spin σ, and to derive transport equations for these quantities [15]. For weak electron–phonon interaction such equations were first derived in [15], and the equations derived there are used in this paper. They have the form

$$\frac{\mathrm{d}f^{(2)}_m}{\mathrm{d}t} = \sum_{n\sigma}[f_{n\sigma}f_{m-\sigma}W^{(SS)}_{nm} + f^{(2)}_n f_{m-\sigma}W_{nm} - f^{(2)}_m f^{(0)}_n W^{(DU)}_{mn} - f^{(2)}_m f_{n\sigma}W_{mn}], \tag{8}$$

$$\frac{\mathrm{d}f_m^{(0)}}{\mathrm{d}t} = \sum_{n\sigma}[f_{m\sigma}f_n^{(0)}W_{mn} + f_{m\sigma}f_{n-\sigma}W_{mn}^{(SS)} - f_{n\sigma}f_m^{(0)}W_{nm} - f_n^{(2)}f_m^{(0)}W_{nm}^{(DU)}], \tag{9}$$

$$\frac{\mathrm{d}f_{m\sigma}}{\mathrm{d}t} = \sum_{n\sigma}[f_{n\sigma}f_m^{(0)}W_{nm} + f_n^{(2)}f_m^{(0)}W_{nm}^{(DU)} + f_m^{(2)}f_n^{(0)}W_{mn}^{(DU)} + f_m^{(2)}f_{n\sigma}W_{mn} - f_{m\sigma}f_n^{(0)}W_{mn} - f_{m\sigma}f_{n-\sigma}W_{mn}^{(SS)} - f_{n-\sigma}f_{m\sigma}W_{nm}^{(SS)} - f_n^{(2)}f_{m\sigma}W_{nm}]. \tag{10}$$

Here the quantities W_{nm}, $W_{nm}^{(DU)}$ and $W_{nm}^{(SS)}$ are the transition probabilities for a hop from a single occupied site to an unoccupied site, for a hop from a double occupied to an unoccupied site, and for a hop from a single occupied site to a single occupied site, respectively. Owing to the principle of detailed balance these quantities satisfy the relationships

$$\frac{W_{mn}}{W_{nm}} = \exp(-\beta V_{nm}), \tag{11}$$

and

$$\frac{W_{mn}^{(DU)}}{W_{nm}^{(SS)}} = \exp(-\beta(V_{nm} - U)), \tag{12}$$

where $V_{nm} = \epsilon_n - \epsilon_m + e\boldsymbol{E}\boldsymbol{R}_{nm}$. Since the Hubbard-interaction strength is independent of the site index, the transition probabilities for jumps between single occupied and unoccupied sites are the same as those for jumps between double occupied and single occupied sites. In order to calculate the ohmic conductivity we linearize the set of equations (8)–(10) with respect to small deviations from equilibrium due to the electric field. To do so, we first note that the expection values of the Hubbard operators are not independent of each other but satisfy the relationship

$$f_m^{(0)} + f_m^{(2)} + f_{m\uparrow} + f_{m\downarrow} = 1, \tag{13}$$

since every site is either empty, single occupied or double occupied. Moreover, if the initial conditions are chosen in such a way that the initial particle distribution is independent of the spin direction, the probability of finding a single occupied site is also independent of the spin direction. Accordingly, only two of the quantities $f_m^{(0)}$, $f_m^{(2)}$, and $f_{m\sigma}$ are independent of each other. Consequently, small deviations from equilibrium can be characterized by two generalized electrochemical potentials $U_m^{(1)}$ and $U_m^{(2)}$, which can be introduced according to the relationships

$$f_m^{(0)}(t) = f^{(0)}(1 + \beta\delta_m^{(0)}(t)), \tag{14}$$

$$f_m^{(2)}(t) = f^{(2)}(1 + \beta\delta_m^{(2)}(t)), \tag{15}$$

and

$$f_\uparrow(t) = f(1 + \beta\delta_{m\uparrow}(t)), \tag{16}$$

where

$$\delta_m^{(0)}(t) = -(1 - f^{(0)})(U_m^{(1)}(t) + e\boldsymbol{E}(t)\boldsymbol{R}_m) - f^{(2)}(U_m^{(2)}(t) + e\boldsymbol{E}(t)\boldsymbol{R}_m), \tag{17}$$

$$\delta_m^{(2)}(t) = f^{(0)}(U_m^{(1)}(t) + e\boldsymbol{E}(t)\boldsymbol{R}_m) + (1 - f^{(2)})(U_m^{(2)}(t) + e\boldsymbol{E}(t)\boldsymbol{R}_m), \tag{18}$$

and

$$\delta_{m\uparrow}(t) = f^{(0)}(U_m^{(1)}(t) + e\boldsymbol{E}(t)\boldsymbol{R}_m) - f^{(2)}(U_m^{(2)}(t) + e\boldsymbol{E}(t)\boldsymbol{R}_m). \tag{19}$$

Here

$$f^{(2)} = \frac{\mathrm{e}^{-\beta(U-2\mu)}}{1 + 2\mathrm{e}^{\beta\mu} + \mathrm{e}^{-\beta(U-2\mu)}}, \tag{20}$$

$$f^{(0)} = \frac{1}{1 + 2\mathrm{e}^{\beta\mu} + \mathrm{e}^{-\beta(U-2\mu)}} \tag{21}$$

and

$$f = \frac{\mathrm{e}^{\beta\mu}}{1 + 2\mathrm{e}^{\beta\mu} + \mathrm{e}^{-\beta(U-2\mu)}}, \tag{22}$$

are the expection values of the Hubbard operators in equilibrium. In writing down the expressions (20)–(22) we have taken into account that we are only interested in investigating the NNH regime, where the random distribution of the sites in space is the only source of disorder, since the spread of the site energies of the first occupied states can be neglected when compared to the temperature.

If we use the equations (14)–(19) to linearize the transport equations then we find that the transport equations take the form

$$\sum_{j=1}^{2} sC_{ij}(U_m^{(j)} + L_m^k) = \sum_{j=1}^{2}\sum_{n} 2\Gamma_{mn}^{ij}(U_n^{(j)} - U_m^{(i)}), \tag{23}$$

where $C_{11} = f^{(0)}(1 - f^{(0)})$, $C_{22} = f^{(2)}(1 - f^{(2)})$, $C_{12} = f^{(2)}f^{(0)}$, $L_m^k = e(\boldsymbol{ER})_m$, and $s = -\mathrm{i}\omega$ is the frequency of the external electric field. The quantities

$$\Gamma_{mm'}^{ij} = W_{ij}\,g(|\boldsymbol{R}_{mm'}|), \tag{24}$$

with

$$g(R) = \exp(-2\alpha R) \tag{25}$$

and $W_{11} = ff^{(0)}\nu$, $W_{22} = ff^{(2)}\nu$, $W_{12} = f^{(2)}f^{(0)}\nu'$ are the transition rates corresponding to the transition probabilities. The quantities ν and ν' in the transition rates are the attempt-to-escape frequencies. While in all other investigations in the literature it has been assumed that $\nu = \nu'$, in our paper we take into account that the attempt-to-escape frequencies are, in principle, different from each other. The reason for this is simply that the attempt-to-escape frequencies characterize the ability of the phonon to induce the transition. With increasing Hubbard-interaction strength, however, it becomes more and more difficult for the phonon to bridge the gap between the upper and the lower Hubbard band. Accordingly, ν' tends to zero with increasing Hubbard-interaction strength.

To calculate the current $\boldsymbol{j}(s)$ we first have to solve equation (23) and insert the solution into the equation

$$\boldsymbol{j}(s) = \frac{\beta e s}{V}\sum_{m}\boldsymbol{R}_m\sum_{k,l=1}^{2} C_{lk}(U_m^k + e(\boldsymbol{ER}_m)). \tag{26}$$

Here V is the sample volume.

4. The random resistor network analogue

A natural question that arises is the question of whether equation (23) can be translated into the language of the random-resistor network, since the application of percolation theory, one of the most powerful techniques in investigating hopping transport problems, is based on this interpretation. So far, percolation theory has been applied in most investigations on the impact of the Hubbard interaction on hopping transport. To our knowledge, most papers in the literature focus on dc properties in the VRH regime, so that the question arises of what the random resistor network looks like for finite frequencies. In addition we would like to mention that even in the dc limit there seems to be some confusion about the answer to this question: while some authors use random resistor networks with two nodes per site other authors use networks with one node per side, so that the question arises under which conditions are both approaches equivalent.

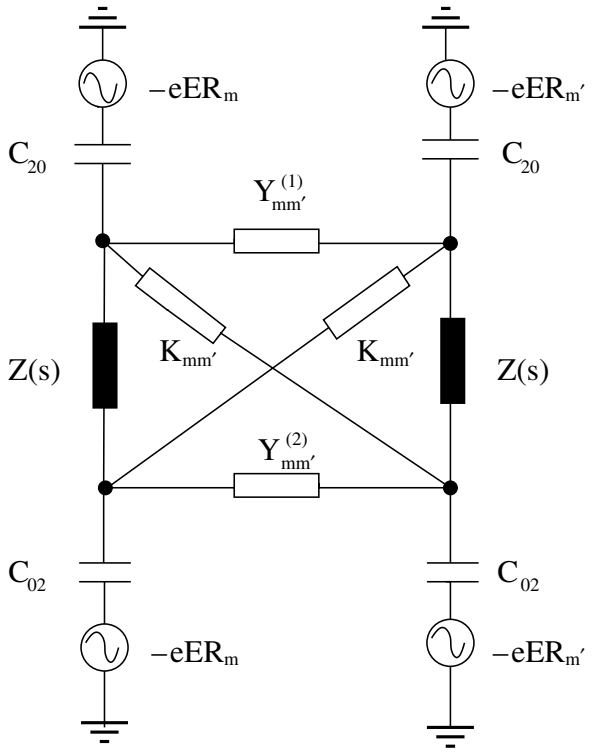

Figure 1. Random-resistor network analogue for the transport equations in the NNH regime. A typical node in the interior of the network. The capacitors are given by $C_{02} = e^2\beta f^{(0)}(1 - f^{(0)} + f^{(2)})$, $C_{20} = e^2\beta f^{(2)}(1-f^{(2)}+f^{(0)})$. The mutual electrostatic induction is $Z(s) = -se^2\beta f^{(0)} f^{(2)}$, and the resistors are $Y^{(1)}_{mm'} = (2e^2\beta\Gamma^{11}_{mm'})^{-1}$, $Y^{(2)}_{mm'} = (2e^2\beta\Gamma^{22}_{mm'})^{-1}$, and $K_{mm'} = (2e^2\beta\Gamma^{12}_{mm'})^{-1}$.

To give equation (23) a random-resistor network interpretation we write it in the form

$$sC_{02}(U^{(1)}_m + e(\boldsymbol{E}\boldsymbol{R}_m)) + Z(s)(U^{(1)}_m - U^{(2)}_m) = \sum_n 2e^2\beta\Gamma^{11}_{nm}(U^{(1)}_n - U^{(1)}_m) + 2e^2\beta\Gamma^{12}_{nm}(U^{(2)}_n - U^{(1)}_m) \tag{27}$$

$$Z(s)(U^{(2)}_m - U^{(1)}_m) + sC_{20}(U^{(2)}_m + e(\boldsymbol{E}\boldsymbol{R}_m)) = \sum_n 2e^2\beta\Gamma^{12}_{mn}(U^{(1)}_n - U^{(2)}_m) + 2e^2\beta\Gamma^{22}_{nm}(U^{(2)}_n - U^{(2)}_m). \tag{28}$$

Here $C_{02} = e^2\beta f^{(0)}(1-f^{(0)}+f^{(2)})$, $C_{20} = e^2\beta f^{(2)}(1-f^{(2)}+f^{(0)})$, and $Z(s) = -se^2\beta f^{(0)} f^{(2)}$. In this representation the quantities C_{20} and C_{02} can be interpreted as ordinary capacitors, and the quantities $(e^2\beta\Gamma^{ij}_{mn})^{-1}$ as ordinary resistors. The quantity $Z(s)$, however, is an element with a frequency dependence that agrees with that of an ordinary capacitor with negative capacity. The negative capacitor can be considered as mutual electrostatic induction. A typical node in the interior of the random resistor network, described by equations (27) and (28), is depicted in figure 1. The sites at the boundary of the random resistor network are connected to the electrodes, as depicted in figure 2. In this picture $U = -eEL$, where L is the length of the sample. In addition to the situation depicted in figure 2 there is also one electrode which is grounded. Since the sites at the boundaries are connected to the electrodes the generalized electrochemical potentials at these sites agree with each other. Therefore, their lower and upper nodes are connected.

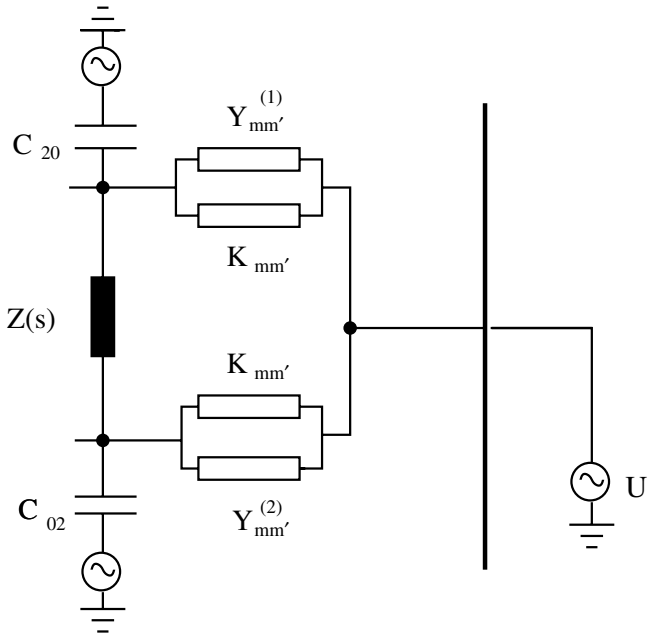

Figure 2. Node for a site connected to the electrode (right wall). All sites connected to the electrode have the same electrochemical potential, the potential of the electrode. In this picture the potential of the electrode is U.

An important question is whether the upper and lower nodes of the network can be joined. In this case the network can be treated like an ordinary Miller–Abraham network with one node per site. The answer to this question depends on the Hubbard-interaction strength, on the filling of the system, on frequency, and on the quantity of interest. If we are only interested in calculating the dc we can use the symmetry of the quantities Γ^{12}_{nm} with respect to exchange of the site indices to show that for $s = 0$ the solution with the correct boundary condition is given by $U^1_m = U^2_m = U_m$, where the quantities U_m satisfy the Miller–Abraham network equation

$$\sum_n \Gamma_{mn}(U_m - U_n) = 0, \tag{29}$$

where $\Gamma_{mn} = \Gamma^{11}_{mn} + \Gamma^{22}_{mn} + 2\Gamma^{12}_{mn}$. The solution to this equation is independent of the Hubbard-interaction strength. Accordingly, the dc conductivity σ_U in the presence of the Hubbard interaction is related to dc conductivity in the absence of the Hubbard interaction σ_0 by the simple relationship

$$\sigma_U = \frac{C_U}{C_0}\sigma_0, \tag{30}$$

where $C_U = (C_{11} + C_{22})\nu + 2C_{12}\nu'$ and $C_0 = C_{U=0}$. The factor C_U/C_0 leads to a reduction in the conductivity, which depends on the filling of the system and on the Hubbard-interaction strength (see figure 3). The largest impact of the interaction is at half-filling ($z = 1$), where

$$\left.\frac{C_U}{C_0}\right|_{z=1} = \frac{2}{1 + \exp(\beta U/2)} \tag{31}$$

if $\nu = \nu'$. If, however, $s \neq 0$ the random-resistor network can only be reduced to a Miller–Abraham network if $\nu = \nu'$. In this case equation (23) takes the well known form

$$s(U_m + e(\boldsymbol{E}\boldsymbol{R}_m)) = \sum_n \nu g(|\boldsymbol{R}_{nm}|)(U_n - U_m). \tag{32}$$

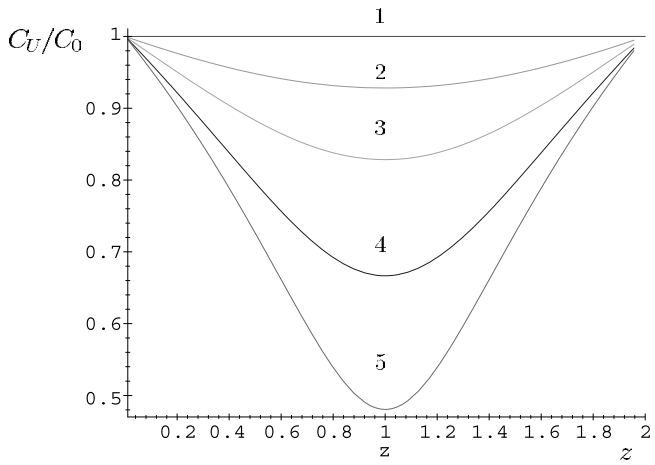

Figure 3. The ratio C_U/C_0 dependence on the filling z for different Hubbard-interaction strengths. The curves are drawn for $y = \exp(-\beta U) = 1$ (1), $y = 0.75$ (2), $y = 0.5$ (3), $y = 0.25$ (4) and $y = 0.1$ (5).

Accordingly, equation (30) also holds for all frequencies of the applied external electric field, if only $\nu = \nu'$.

If we investigate the reason for this simplification further, however, we find that this property is not of general validity. If $\nu \neq \nu'$ then the two nodes of the random resistor network cannot be joint, unless the system is half-filled. Accordingly, if we only look at the conductivity it is the difference between ν and ν' which makes the physics different from that in the non-interacting situation.

If we try to extend the random-resistor network interpretation to the VRH regime, and use instead of the quantities (24) those appropriate to VRH, then the situation becomes even more obscure. In this case we face the problem that in the VRH regime the quantities Γ^{ij}_{mn} are only symmetric with respect to simultaneous exchange of site indices (m and n) and equation indices (i and j) [15]. Therefore, they can only be interpreted as ordinary resistors in an abstract space. A point in this space is a position vector and an equation index. Due to this lack of symmetry we cannot join the upper and the lower node of the network, even if we would like to restrict the consideration to the dc conductivity, unless the Hubbard-interaction strength is either zero or large compared to the band of first occupied states. Therefore, it is *a priori* not clear whether or not those results, which have been obtained from random-resistor networks, were obtained with one node per site, or not. This question is investigated further below for the NNH regime.

5. Effective-medium approximation

The fact that at finite frequencies the nodes of the network cannot be joined to each other unless $\nu = \nu'$ raises the question of what the impact of the Hubbard interaction on the dynamical conductivity is. In order to answer this question we use the standard effective medium method of [22] in the formulation of [23]. In this method the disordered system is modelled on an ordered lattice with effective bonds. For simplicity a cubic lattice with lattice spacing $a^2 = \langle R^2 \rangle$ is used, where the brackets symbolize the configuration average. The bonds are chosen in such a way that the replacement of an arbitrary ordered bond by a disordered one

gives vanishing corrections to the current. In order to calculate the average we use the Poisson distribution

$$dp(R) = \frac{n\gamma_d}{2} R^{d-1} \exp\left(-\frac{\gamma_d n R^d}{2d}\right). \tag{33}$$

which yields for $d = 2\langle R^2\rangle = 4/(\pi n)$ and for $d = 3\langle R^2\rangle = \Gamma(5/3)(9/2\pi n)^{2/3}$.

To use the philosophy outlined above we first put the system (23) on the lattice. On the lattice it takes the form

$$\begin{aligned} sC_{11}(U_m^{(1)} + e(\boldsymbol{E}\boldsymbol{R}_m)) + sC_{12}(U_m^{(2)} + e(\boldsymbol{E}\boldsymbol{R}_m)) &= \sum_g 2\Gamma^{11}_{m+g,m}(U_{m+g}^{(1)} - U_m^{(1)}) \\ &\quad + 2\Gamma^{12}_{m+g,m}(U_{m+g}^{(2)} - U_m^{(1)}) \\ sC_{21}(U_m^{(1)} + e(\boldsymbol{E}\boldsymbol{R})_m) + sC_{22}(U_m^{(2)} + e(\boldsymbol{E}\boldsymbol{R}_m)) &= \sum_g 2\Gamma^{21}_{mm+g}(U_{m+g}^{(1)} - U_m^{(2)}) \\ &\quad + 2\Gamma^{22}_{mm+g}(U_{m+g}^{(2)} - U_m^{(2)}). \end{aligned} \tag{34}$$

Here the summation is restricted only to nearest neighbours. Due to the random distribution of the sites in the original problem the transition rates Γ^{ij}_{mm+g} are fluctuating quantities. However, since in reality the distance between the sites is the only fluctuating quantity in the problem, the distribution function for these quantities is entirely determined by the distribution function for the site separations, that is by the distribution function for the quantities $g(|\boldsymbol{R}_{mn}|)$ (see equation (25)). To incorporate this effect we replace the fluctuating quantities $g(|\boldsymbol{R}_{mn}|)$ by an effective quantity g which, in the spirit of the effective medium theory, is frequency dependent and the same for all bonds. Due this replacement the transition rates become independent of the indices m and g and therefore the current can be readily calculated. Doing so, we obtain

$$\boldsymbol{j}(s) = \beta e^2 n \boldsymbol{E}(s)\langle R^2\rangle 2C_U g(s), \tag{35}$$

where n is the concentration of sites. To calculate g, we replace one bond, the $(nn+g)$-bond, by a disordered one, that is we replace g by $g(|\boldsymbol{R}_{nn+g}|)$ for a fixed n and g. Thereafter we require that this replacement does not affect the current. This requirement leads to one self-consistency equation (see equation (A.8), appendix) for the calculation of $g(s)$, which can be solved both in the limit of high frequencies and in the limit of low frequencies.

For high frequencies, that is for frequencies s satisfying $\nu g(s)/s \ll 1$, the self-consistency equation reduces to

$$g(s) = \frac{2f^{(2)}f^{(0)}\left\langle R^2 \frac{g(R)}{s\tau_2 + g(R)}\right\rangle + f(f^{(0)} - f^{(2)})^2\left\langle R^2 \frac{g(R)}{s\tau_1 + g(R)}\right\rangle}{\langle R^2\rangle\left(\frac{2f^{(2)}f^{(0)}}{s\tau_2} + \frac{f(f^{(0)} - f^{(2)})^2}{s\tau_1}\right)}. \tag{36}$$

The remarkable fact in this expression is the occurrence of the two relaxation times

$$1/\tau_1 = 2\nu \tag{37}$$

and

$$1/\tau_2 = 2(2f\nu + (f^{(0)} + f^{(2)})\nu'). \tag{38}$$

These two relaxation times enter the current. If we simply insert equation (38) into (35) we obtain

$$\sigma_U(s) = \frac{ne^2\beta s}{d}\left[\frac{f(f^{(0)} - f^{(2)})^2}{f^{(0)} + f^{(2)}}\left\langle \frac{R^2 g(R)}{1 + s\tau_1 g(R)}\right\rangle + \frac{2f^{(2)}f^{(0)}}{f^{(0)} + f^{(2)}}\left\langle \frac{R^2 g(R)}{1 + s\tau_2 g(R)}\right\rangle\right]. \tag{39}$$

Accordingly, for very high frequencies ($s\tau_{1/2} \gg 1$) the conductivity becomes independent of frequency, as in the non-interacting situation. For $s\tau_{1/2} \ll 1$, however, two modes are present

in the current. This sets the situation apart from that of non-interacting charge carriers where only one relaxation time is present at high frequencies. In this regime we obtain

$$\sigma_U(s) = \frac{A'_d n^2 e^2 \beta}{(2\alpha)^{d+2}} \left[\frac{f(f^{(0)} - f^{(2)})^2}{f^{(0)} + f^{(2)}} \rho_{c1}^{d+2} + \frac{2 f^{(2)} f^{(0)}}{f^{(0)} + f^{(2)}} \rho_{c2}^{d+2} \right] \tag{40}$$

where $\rho_{ci} = -\ln(s\tau_i)$, and $A'_3 = 4\pi/15$, $A'_2 = \pi/4$ and $A'_1 = 1/3$.

In order to obtain the frequency dependence of the conductivity we simply have to replace s by $-\mathrm{i}\omega$. Accordingly, the real part of the conductivity satisfies the equation

$$\mathrm{Re}\,\sigma_U(\omega) = \frac{A'_d n^2 e^2 \beta}{(2\alpha)^{d+2}} \left[\frac{f(f^{(0)} - f^{(2)})^2}{f^{(0)} + f^{(2)}} \ln^{d+2}(1/\omega\tau_1) + \frac{2 f^{(2)} f^{(0)}}{f^{(0)} + f^{(2)}} \ln^{d+2}(1/\omega\tau_2) \right]. \tag{41}$$

The expression obtained in this way differs from the standard result by Pollak and Geballe [24] for non-interacting particles in the occurrence of two characteristic relaxation times. From the physical point of view the difference between these two relaxation times results from the fact that transition between sites within the same band and transitions between the band of first occupied states and the band of second occupied states occur with different attempt-to-escape frequency. If, however, we look at equation (41) in this way then we notice that obviously one of the characteristic frequencies in equation (41) is wrong, since at half-filling only transitions between the upper and the lower Hubbard band should be important. Accordingly, the result for the current should only depend on ν'. The effective medium theory becomes exact in the limit of large frequencies. Therefore, we expect that this discrepancy is produced by the Hartree–Fock decoupling, which has been used in the derivation of the rate equations in [15], and because of this only the average of the occupancy of the sites is taken into account.

For low frequencies, that is for frequencies s satisfying $s \ll \nu g$, the self-consistency equation reduces to

$$0 = \left\langle R^2 \frac{g(R) - g}{g(R) + g(d - 1 + s\tau)} \right\rangle. \tag{42}$$

In contrast to equation (36) this equation contains only one characteristic frequency. It agrees completely with the self-consistency equation for non-interacting particles [23]. Only the relaxation time τ is different. In equation (42) it is given by

$$\tau = \frac{C_U}{2\sum_{ij} W_{ij} g(0)} \sum_k \frac{1}{\phi(k)}, \tag{43}$$

where

$$\phi(k) = \sum_g (1 - \cos(\boldsymbol{k}\boldsymbol{g})). \tag{44}$$

For $s = 0$ equation (42) yields

$$g(s = 0) = \frac{\exp(-\eta_d \alpha n^{-1/d})}{d - 1}, \tag{45}$$

where $\eta_3 = 1.669$ and $\eta_2 = 1.879$. For non-zero s equation (42) can be cast into the form

$$\frac{g(s)}{g(0)} \ln \frac{g(s)}{g(0)} = \frac{s}{\omega_0}, \tag{46}$$

where the characteristic frequency

$$\omega_0 = \frac{n^{1/d} g(0)}{\alpha} \frac{d(d-1) \ln \frac{d}{d-1}}{\eta_d \xi_d} \frac{2 f (f^{(0)} + f^{(2)}) \nu + 4 f^{(2)} f^{(0)} \nu'}{2 f (f^{(0)} + f^{(2)}) + 4 f^{(2)} f^{(0)}}. \tag{47}$$

For $d = 3$ the number $\xi_3 = 0.253$. In order to obtain the frequency dependence of the conductivity we merely have to replace the Laplace frequency s by $-\mathrm{i}\omega$ in equation (47). The equation obtained in this way is the same as for non-interacting particles. Its physics is described extensively in [14].

6. Conclusions

Our investigations have shown that even for finite frequencies the transport equations in the NNH regime in the presence of the Hubbard interaction can be cast into the form of a generalized random resistor network. The random resistor network in question has two nodes per site and consists of random resistors and capacitors. In contrast to the non-interacting situation as well as capacitors with positive capacity, capacitors with negative capacity also have to be taken into account. The latter quantities can be considered as mutual electrostatic induction.

From the physical point of view the differences between the random resistor network derived in this paper and the traditional Miller–Abraham network result from the fact that in the presence of the Hubbard interaction there are more degrees of freedom which have to be taken into account than in the non-interacting situation. These additional degrees of freedom describe excitations of the system which cannot be produced in the non-interacting situation. As such there are deviations of the probability to find double occupied sites in the system from its equilibrium value. Since there is only one conserved quantity in this system, the particle number, and the number of single occupied sites is not conserved, the propagation of excitations is described by relaxation modes. In our random-resistor network this fact manifests in the occurrence of capacitors with negative capacity. These capacitors connect the upper and the lower node at the same site, and thus are important if the generalized electrochemical potentials at the same site are different from each other. Clearly, further investigation of the diffusion and decay of such excitations is very important for the development of an understanding of the impact of the Hubbard interaction on the non-equilibrium properties of strongly localized systems, since it is the ability of the interacting system to propagate excitations which sets it apart from the non-interacting one. Our random-resistor network can be used for studying some of the properties of such excitations if appropriate initial conditions are used.

While the excitations are very important for the non-equilibrium properties of the system, we cannot expect them to influence strongly the conductivity in the ohmic approximation at low frequencies of the external electric field, since excitations have first to be produced before they can be affected by an external electric field. Accordingly, excitations do not affect the dc conductivity in the dc limit. This conclusion also holds at finite frequencies if $\nu = \nu'$. If the attempt-to-escape frequencies differ from each other our random-resistor network for the calculation of the conductivity does not reduce to the ordinary Miller–Abraham network exactly, but the ordinary Miller–Abraham network describes the situation adequately in a large range of frequencies, including the range of lowest frequencies and the multiple-hopping regime. Only in the high frequency limit does the fact that the network has two nodes per site become important. In this limit the relaxation modes describing the excitations manifest themselves in a second pole of the generalized diffusion function. The second pole results from the fact that the transitions between the upper and the lower Hubbard band and the transition within a given Hubbard band occur with different attempt-to-escape frequency. However, the characteristic frequency for jumps between the lower and the upper Hubbard band, as found by direct calculation from the linearized rate equations, is obviously incorrect. Since the effective medium theory is exact in the limit of large frequencies (the two-site model yields the same result) we expect that this discrepancy is produced by the Hartree–Fock decoupling, which has been used in the derivation of the rate equations in [15]. Thus, it is doubtful that the equations derived in [15] also apply to the high frequency limit. Further investigation of the reason for this discrepancy might be useful, especially as by investigating the high frequency conductivity further information about the properties of the Hubbard gap can be obtained. The Hubbard gap in the strongly localized regime has been observed, e.g., in the experiments of [7].

Despite the fact that we have focused in our investigation on the NNH regime the random resistor network derived in this paper can also be applied to the VRH regime. Since, however, in the VRH regime the transition rates connecting sites in different Hubbard bands are not symmetric with respect to exchange of the site indices, but only symmetric with respect to simultaneous exchange of site and equation indices, the transition rates connecting the upper and the lower Hubbard band can only be considered as ordinary resistors in an abstract space. A point in this space is determined by a site index and an equation index. In ordinary space these quantities cannot be considered as ordinary resistors, but only as unipolar elements. The latter fact renders the application of the percolation theory to the VRH regime difficult.

Appendix. On the derivation of the self-consistency equation

In order to derive the self-consistency equation it is convenient to use the Green function formalism. The Green function F of equation (34) satisfies the equation

$$\sum_{k=1}^{2} sC_{ik}F^{kj}_{m'm} = \delta_{m'm}\delta_{ij} + \sum_{k=1}^{2}\sum_{n}[\Gamma^{ik}_{m'n}\Delta_{m'n}F^{kj}_{nm} - \Gamma^{ik}_{m'n}\Delta_{m'n}F^{kj}_{m'm}], \tag{A.1}$$

where $\Delta_{mn} = 1$ for $\boldsymbol{R}_m = \boldsymbol{R}_n + \boldsymbol{l}$, where $\boldsymbol{l}$ is a unit-lattice vector, and $\Delta_{mn} = 0$ otherwise. With the help of the Green function the equation for the calculation of the current can be written in the form

$$\boldsymbol{j}(s) = \frac{\beta s^2 e^2}{V}\sum_{m'm}\sum_{k,l,j,i=1}^{2}\boldsymbol{R}_{mm'}(\boldsymbol{E}(s)\boldsymbol{R}_{m'})C_{lk}F^{kj}_{m'm}C_{ji}. \tag{A.2}$$

Due to the law of probability conservation and the principle of detailed balance the Green function satisfies the sum rules

$$s\sum_{j,k=1}^{2}\sum_{m}F^{ij}_{m'm}C_{jk} = 1 \tag{A.3}$$

and

$$s\sum_{m'}\sum_{ik=1}^{2}C_{ik}F^{kj}_{m'm} = 1. \tag{A.4}$$

According to the assumptions of the effective medium theory the configuration average of the Green function F, $\bar{F}$, satisfies the equation

$$\sum_{k} sC_{ik}\bar{F}^{kj}_{m'm} = \delta_{m'm}\delta_{ij} + \sum_{k,n}[\bar{\Gamma}^{ik}_{m'n}\Delta_{m'n}\bar{F}^{kj}_{nm} - \bar{\Gamma}^{ik}_{m'n}\Delta_{m'n}\bar{F}^{kj}_{m'm}], \tag{A.5}$$

where $\bar{\Gamma}^{ik}_{mn}$ differs from Γ^{ik}_{mn} in that the quantities $g(|\boldsymbol{R}_{mn}|)$ in the latter rates are replaced by $g(s)$. To determine $g(s)$ we use the philosophy of the effective-medium approximation. We first replace one bond by a random one. This replacement amounts to the introduction of a new bond of strength $\delta\Gamma^{ik}_{m'm}\Delta_{mm'} = 2W_{ik}(g(\boldsymbol{l}) - g(s))\Delta_{mm'}$. In this approximation the equation for the Green function takes the Form

$$F = \bar{F} + \bar{F}T\bar{F}, \tag{A.6}$$

where we have used a matrix notation for brevity. The T-matrix satisfies the equation

$$T = \delta\Gamma + \delta\Gamma\bar{F}T. \tag{A.7}$$

We now require that the introduction of the additional random bond does not yields corrections to the conductivity. This is the case, if

$$0 = \sum_{ij} \sum_{mm'} \langle R^2_{mm'} T^{ij}_{mm'} \rangle. \tag{A.8}$$

Equation (A.8) is the self-consistency equation for the calculation of $g(s)$. Due to the matrix-structure equation (A.8) is difficult to handle, although further calculations are elementary. However, due to their length they are not presented here. We therefore restrict the discussion to the further approximations used.

For high frequencies, that is for $\bar{\Gamma}/s \ll 1$, the second term on the right-hand side of equation (A.5) is negligible, so that the equation for the Green function simply takes the form

$$\sum_k s C_{ik} \bar{F}^{kj}_{m'm} = \delta_{m'm} \delta_{ij}. \tag{A.9}$$

If we use this approximation then the self-consistency equation (A.8) reduces to (36).

For low frequencies, that is for $\bar{\Gamma}/s \gg 1$, the Green function can be expanded with respect to this parameter. To first order this expansion yields

$$\bar{F}(s) \approx \bar{F}(0) - s \bar{F} C \bar{F}. \tag{A.10}$$

To obtain equation (42) we use the approximation (A.10) in calculating the T-matrix according to equation (A.7). It should be mentioned that also in this case the inversion of the matrices leads, strictly speaking, to a denominator quadratic with respect to $s/(\bar{\Gamma})$, and therefore also to two modes. However, since $s/\bar{\Gamma} \ll 1$ the difference between these modes is small, and therefore only the linear terms are retained.

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