Single-particle hopping probability on a chain with interaction and disorder by the modified Lanczos algorithm

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(Received 29 April 1991)

We consider numerically a chain of ten sites (half filled) described by the Anderson-Hubbard model. The single-particle hopping probability is calculated as a function of disorder and correlation. A qualitative agreement for the logarithm of this hopping probability is found when compared with results of a calculation of the low-frequency conductivity by the Monte Carlo method.

The Hubbard model is an old problem proposed to describe electrons in narrow bands. However, nowadays it has become popular again due to its possible connection with high-T_c superconductivity.

The model reads

$$H_H=\sum_{i,j,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_i n_{i\downarrow}n_{i\uparrow}-\mu\sum_{i,\sigma} n_{i\sigma}\ . \tag{1}$$

The parameters are the effective on-site interelectronic Coulomb repulsion U and the probability of delocalization t_{ij}, which is mainly taken between nearest neighbors and isotropic μ is the chemical potential and it adjusts the number of electrons per site in the band.

Although most attempts in the context of high-T_c superconductivity are done on the Hubbard model itself, some contributions have stressed the importance of disorder as well as correlation.[1-3] Disorder is thought of in terms of the Anderson model which reads

$$H_A=\sum_{i,\sigma}\varepsilon_i n_{i\sigma}+\sum_{i,j,\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}\ . \tag{2}$$

The hopping terms t_{ij} are taken all equal and only for nearest neighbors. The energy parameters ε_i are taken from some random distribution. Here we use the box distribution, namely,

$$P(\varepsilon_i)=\begin{cases}\dfrac{1}{W} & \text{if } -\dfrac{W}{2}<\varepsilon_i<\dfrac{W}{2}\\ 0 & \text{otherwise}\ .\end{cases} \tag{3}$$

W is the parameter that characterizes the disorder and is the width of the distribution.

So, when disorder and interaction are taken into account we have to value the Anderson-Hubbard Hamiltonian, namely,

$$H_{\mathrm{AH}}=\sum_{i,\sigma}\varepsilon_i n_{i\sigma}+H_H \tag{4}$$

with ε_i random. Any attempts done on this last model are also relevant for the localization theory with interaction.

Scaling theories of the disordered interaction problem were proposed. McMillan[4] assumed a scaling theory in two parameters: the dimensionless conductance and the dimensional interaction constant. Finkelstein[5] treated the long-range Coulomb problem assuming weak disorder but retaining the interaction term to all orders. A scaling theory for interaction put with strong spin-flip scattering was considered by Castellani *et al.*[6] A renormalization-group study for weak disorder in the Hubbard Hamiltonian was performed by Bhat and Singh[7] and by Ma.[8] Recent treatment of the large-U limit was given by Zimanyi and Abrahams.[9]

Not much is known numerically about the Anderson-Hubbard model. Some preliminary results were obtained by Muramatsu and Hanke[10] using Hirsch's program.

In a previous work[11] we presented some numerical simulations on the one-dimensional Anderson-Hubbard model. It concerned localized superconducting properties of the chain through the behavior of the local pair-pair correlation function defined as

$$UD=\frac{1}{N}\sum_i\langle c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}c_{i\downarrow}c_{i\uparrow}\rangle=\frac{1}{N}\sum_i\langle n_{i\uparrow}n_{i\downarrow}\rangle\ . \tag{5}$$

The numerical procedure was based on the modified Lanczos algorithm which gives the ground-state energy eigenvalue and the corresponding eigenfunction. With this last magnitude several correlation functions can be obtained. The computational program is that used by Dagotto and co-workers.[12,13]

In Ref. 11 the test of the program was presented by comparison with calculations performed by Singh.[14] The magnetic structure factor both for $q=0$ and π was calculated:

$$S_{(q)}=\frac{1}{N}\sum_{i,j=1}^{N} e^{iq(R_i-R_j)}(n_{i\uparrow}-n_{i\downarrow})(n_{j\uparrow}-n_{j\downarrow}) \tag{6}$$

as a function of disorder W. For $q=0$ the magnetic structure factor is just the $q=0$ susceptibility.

Recently Lehr[15] and Dzierzawa and Schlüter[16] have calculated the conductivity of interacting fermions in a disordered chain using a Monte Carlo simulation. They use the Hartree-Fock approximation for the correlation and calculate the low-frequency conductivity by linear response theory.

In this paper we want to concentrate on results for the

normal-state quasiconductivity calculated by the modified Lanczos algorithm using the same program as in Ref. 11.

We calculate the following correlation function:

$$t=\frac{1}{N}\left\langle \sum_{i,\sigma} c^{\dagger}_{i+1,\sigma}c_{i\sigma}\right\rangle . \tag{7}$$

We take the mean value in the ground state as given by our program. This correlation function is the averaged probability of hopping from one site to the neighboring site of a single particle. We assume that the conductivity will follow the same trends as this hopping probability.

In Fig. 1 we show the behavior of the logarithm of the absolute value of t as a function of disorder for different values of the correlation U. We observe "quasilinear" decrease with disorder for the purely disordered sample (10 sites) ($U=0$) and for negative correlation U.

For positive, rather large correlation, nonmonotonic behavior is observed, namely, an initial increase in the hopping probability with increasing disorder is observed. Figure 1 agrees qualitatively very well with the results of Refs. 15 and 16, where an initial increase with increasing disorder is also observed for the conductivity. In Fig. 2 we show similar results for the different value of the cutoff energy.

The explanation for the increase of conductivity with disorder was given in Ref. 15. It is due to competition between interaction and disorder. For large U and small W the system occupies an ordered Mott insulating state (single-site occupation). Increasing disorder destroys the correlated state as the random potential tends to build up a pair, which leads to better conductivity. For large W the decreasing localization length leads to a decreasing conductivity again.

We estimate that the turning point for competition of

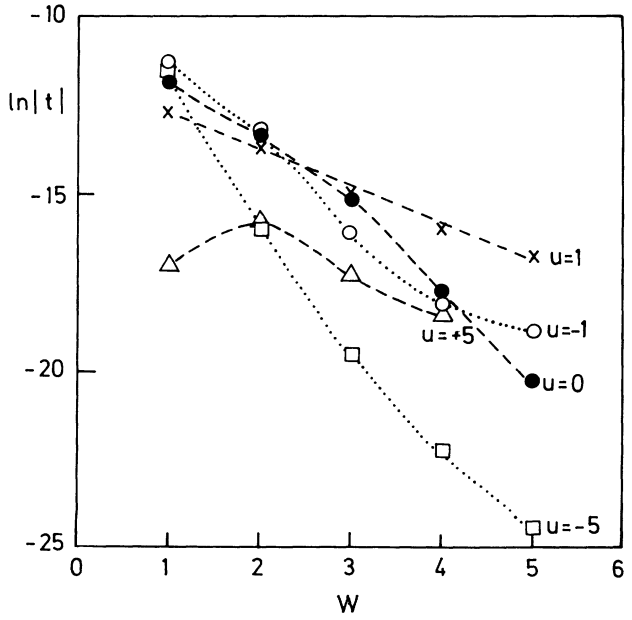

FIG. 1. Logarithm of the hopping probability t as function of disorder W for different correlations U. The cutoff energy is $E_c=6t$.

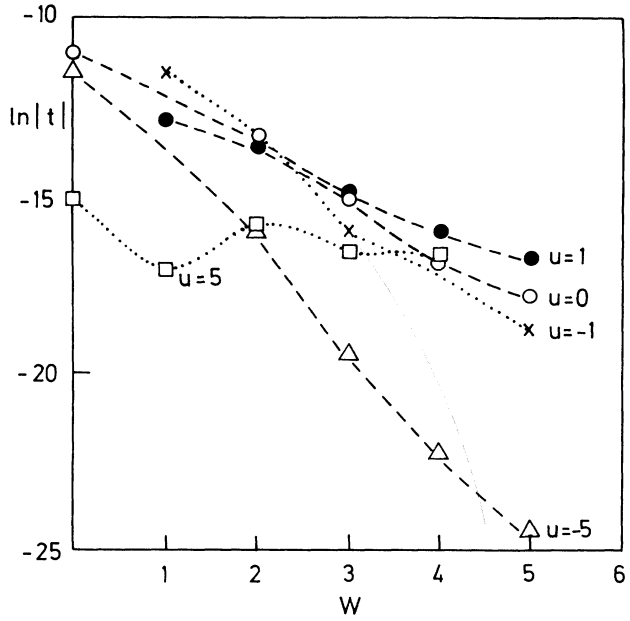

FIG. 2. As in Fig. 1 with the cutoff energy $E_c=20t$.

disorder and correlation is roughly $U=2W$. Initially, at low disorder correlation splits the density of states in two parts, each with width W. Therefore with increasing disorder, there are more states available for conduction. At the turning point, the two bands merge and further disorder localizes the states and the hopping probability decreases. The turning point is, roughly speaking, the maximum of the curve.

In Refs. 15 and 16 conductivity was calculated from linear-response theory. What we present in Fig. 1 is the logarithm of the average hopping probability for one particle jumping from one site to another.

It appears from both calculations that this is a good comparison to make. Therefore the conductivity is proportional to the logarithm of the single-particle jumping probability (at least for not too low values) of this last magnitude. This is an interesting point and we think it is the most important point of this paper. We do not have any analytic derivation of this relation.

In relation to error treatment we have not made sample averages due to the time-consuming calculation. We have used only one seed for the random-number generator, which means that we have followed only the same sample. Another factor that sets the numerical value is the precision in the determination of the ground-state energy. There also, one must compromise in order to have reasonable bounds on computational times.

Also, since with disorder the number of states needed to determine the eigenvalue grows enormously, we have decided to keep states up to a certain energy (here $E=6t$ in Fig. 1, $E=20t$ in Fig. 2).

In conclusion, we have performed the numerical calculation using the modified Lanczos algorithm of the single-particle average hopping probability for a chain of 10 sites (half-filled) with interaction and disorder. Very good qualitative agreement is obtained with the results of the Monte Carlo simulation (Refs. 15 and 16) for the

linear-response-derived conductivity if it is compared with the logarithm of our hopping probability. Both show decreasing behavior with the disordered W and an initial increase for the rather large positive U. We think that this numerical evidence for the conductivity being related to the logarithm of the hopping probability is an interesting point and it should be a subject of further research. The half-filled case is the most interesting to study as a function of disorder. As the author of Ref. 15 shows, the conductivity simply decreases with disorder out of half filling.

We wish to thank Consejo Nacional de Investigaciones Científicas y Técnicas of Argentina for financial support.

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