Modified Lanczos simulation of the localized superconductivity for a chain with interaction and disorder

C. Wiecko[1] and G. Chiappe[2]

Centro Atómico Bariloche

8400 Bariloche, Argentina

Abstract

Using the modified Lanczos algorithm we calculate numerically for a chain with ten sites and half-filled, the local pair-pair correlation function of the Anderson-Hubbard model (with the interaction both repulsive and attractive). The calculation aims to describe the phase with local superconductivity.

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[1]Fellow of Carrera del Investigador, CONICET, Argentina

[2]Fellowship holder of Comisión Nacional de Energía Atómica.

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The interest in studying the Hubbard model is greatly enhanced nowadays for its possible connexion with the high T_c problem[1]. This model is particularly useful to describe electrons in narrow bands. Thus, the simplest hamiltonian for interacting electrons reads:

$$H_H = \sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U\sum_i n_{i\downarrow} n_{i\uparrow} - u \sum_{i,\sigma} n_{i\sigma} \qquad (1)$$

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

The Hubbard model has been mapped into a 2-D Heisenberg antiferromagnet[2] for large U, where it is exact. At half-filling ($n_\uparrow + n_\downarrow = 1$, $\delta = 0$) we have a 2D AF. Doping the system, therefore with $n_\uparrow + n_\downarrow < 1$; $\delta \neq 0$; the presence of holes transforms the AF into a new type of liquid[3,4] which some people postulate as a new superconductive phase[3,5-10]. Apart from the high T_c motivation, inherent interest exists, coming from research in the one-particle Anderson localizxation theory to analyze the electron behavior when apart from disorder they interact among themselves. We have in mind the so called Anderson-Hubbard Hamiltonian which reads

$$H_{AH} = H_A + H_H = \sum_{i,\sigma} \varepsilon_i n_{i\sigma} + H_H \qquad (2)$$

with ε_i taken from some random distribution. We take here the box distribution:

$$P(\varepsilon_i) = \frac{1}{W} \text{ if } -\frac{W}{2} < \varepsilon_i < \frac{W}{2} \qquad (3)$$

$$0 \text{ otherwise}$$

W is the parameter that characterizes the disorder. Other distributions such as the gaussian or the Lorentzian are also being used.

Scaling theories of the disordered interaction problem were proposed. McMillan[11] assumed a scaling theory in two parameters: the dimensionless conductance and the dimensional interaction constant. Finkelstein[12] treated the long-range Coulomb problem assuming weak disorder but retaining the interaction term to all orders. A scaling theory for interaction but with strong spin-flip scattering was considered by Castellani et al[13]. A renormalization group study for weak disorder in the Hubbard Hamiltonian was performed by Bhat et al.[14] and by Ma[15].

Numerical simulations are being performed extensively on the Hubbard model in 1-3 dimensions at present. (For a review on simulations in the Hubbard model see Hirsch[16]). Although the size of the samples is small, different correlation functions are being calculated. However, not much is known even numerically for

the Anderson-Hubbard model. This we think is due to the fact that many people envision the Hubbard and not the Anderson-Hubbard model as the mechanism for high-T_c compounds.

The exception to this trend are the preliminary simulations using Hirsch´s program performed by Muramatsu and Hanke[17].

We are pioneering the latest point of view. Some of our previous results seem to indicate that superconducting T_c can be enhanced by disorder (at least within the approximation scheme of the mean-field type used therein)[18,19]. Being mean-field these results are mostly valid in high enough dimension. On the other hand we present here numerical simulations of the one dimensional chain of 10 sites and half filled with open boundary conditions. Our numerical procedure is based on the modified Lanczos algorithm which gives the ground-state eigenenergy and the corresponding eigenfunction. With this last magnitude, several correlation functions can be obtained. The computational program is that used previously by Dagoto et al.[20,21] and we are endebted to E. Gagliano for it.

As the program gives T = 0 magnitudes we decided that some meaningful characterization of the dependence of the superconducting state with disorder could come from the local pair-pair correlation function:

$$UD = \frac{1}{N} \sum_i \langle c^+_{i\uparrow} c^+_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \rangle = \frac{1}{N} \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle \qquad (4)$$

where the brackets mean the thermodynamic average. We think that this last magnitude is representative of the local superconductivity in the sense that it is the $t \to 0$ limit of the double-time correlation function which would give supercoductivity in the frame of the linear response theory, when describing superconductivity as:

$$H_c = - g \sum_i \Delta \, c^+_{i\uparrow} \, c^+_{i\downarrow} + c.c \qquad (5)$$

This correlation function reads:

$$C_{pair\text{-}pair} = \frac{1}{N} \sum_i \langle c_{i\uparrow}(t) \, c_{i\downarrow}(t); \, c^+_{i\downarrow}(o) \, c^+_{i\uparrow}(o) \rangle \qquad (6)$$

The same as what is usually done in critical phenomena studies of the phase can be characterized not only by the order parameter but also by the corresponding correlation function. Due to the fact that our method gives the wave function with a fixed number of particles it is not possible to calculate the traditional order parameter for local pairs directly; as:

$$\Delta = \frac{1}{N} \sum_i \langle c^+_{i\uparrow} \, c^+_{i\downarrow} \rangle \qquad (7)$$

In Fig. 1 we show the results of the simulation of UD as function of disorder for different values of the interaction U (taken both positive and negative).

The curves show the following:

1) There is a finite probability of forming the local pair with U = 0 and W = 0 due to the finite length of the system. In our ten sites calculation it is .1 (numerically it has got slighly less due to the taken precision as explained further on).

2) U>0 repulsion lowers the pairing in agreement with references 14 and 15 (Renormalization Groups treatment). It is shown clearly therefore that the repulsive interaction leads to <u>delocalization</u>.

3) U < 0 attraction (as in BCS formulated locally) enhances localization, up to a critical value (a fixed point). We get almost .4 numerically for the fixed point. Analyzing the probabilities of localization of local pairs in 10 sites we get $[1/10 + (1/9)\ (1/9)] \times \frac{45}{10}$ with 45 = 10!/(8!) (2!); slightly higher than the numerical value.

4) In all cases disorder tends to localize, therefore the value of local pairing increases with W apparently achieving saturation (at different values for different U).

Let us extrapolate some conclusions for the superconductive T_c from the behavior of the T = 0 pair-pair correlation function. We are tempted then to say that the repulsive Hubbard model gives for all disorder W, T_c smaller (or of the order with big enough W) than in the pure metal (W = 0, U = 0). On the contrary, attractive interaction, increases the value with respect to the pure metal more and more with disorder (and also with the strength of the interaction, in both cases going to fixed points). In Fig.

2 we show a plot of our correlation function as function of the interaction U, both for W = 0 and w = 5 (medium strength). These results are in good qualitative agreement with our previous work where the actual contribution to T_c from the disorder was studied within a certain approximation scheme[19]. There we have considered the effective electronic Hamiltonian obtained from having postulated the existence of two types of excitations: localized and extended both for electrons and phonons. At maximal mixing of zero and two particle levels (the most favourable situation for superconductivity) we also obtained T_c increasing with disorder and with the attractive interaction going up to a fixed point. For repulsive U a critical concentration is needed in order to obtain a phase with T_c bigger than the BCS value. This T_c is always smaller than what is got for the attractive U.

It is necessary to comment on the error treatment as, working with disordered samples, configurational averages are currently performed. Figure 1 shows the actually measured points, for a given configuration generated with different seeds for the random number generator. The lines are guides to the eye. We have not performed configurational averages but rather worked with different seeds for the different points on each curve. The sequence of values obtained in such a way allows us to think of a generic behavior.

Another factor that changes the position of the simulation points (but not the qualitative behavior) is the precision asked in the determination of the ground state energy. We show curves

both with low and with high precision for a certain U. It shows that the trend of behavior is the same.

Another point is that due to the fact that with disorder, the number of states needed in order to determine the ground state eigenvalue grows enormously we have decided to keep states up to a certain energy only (here E = 20t).

The U = 0 curve from Fig. 1 shows a very pronounced oscillation for a not too low disorder which we cannot explain. This type of behavior has not appeared for other values. It is also interesting to remark that a high enough attractive interaction leads to curves of UD practically constant with disorder which would mean good illustration of the Anderson theorem (which says that superconductivity should not be changed by static disorder).

Numerical work was done on the MicroVax, Solid State Group at Centro Atómico Bariloche.

We acknowledge E. Gagliano again for the program.

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Figure Captions

Fig. 1: The correlation function UD as function of disorder. Energy units t = 1. Precision in the ground-state energy equal to .1t unless specified otherwise.

a) U = - 20

b) U = - 10

c) U = - 5

d) U = - .2

e) U = - .2 precision in the ground state energy = 10^{-4}t.

f) U = 1 precision in the ground state energy = 10^{-4}t.

g) U = 0

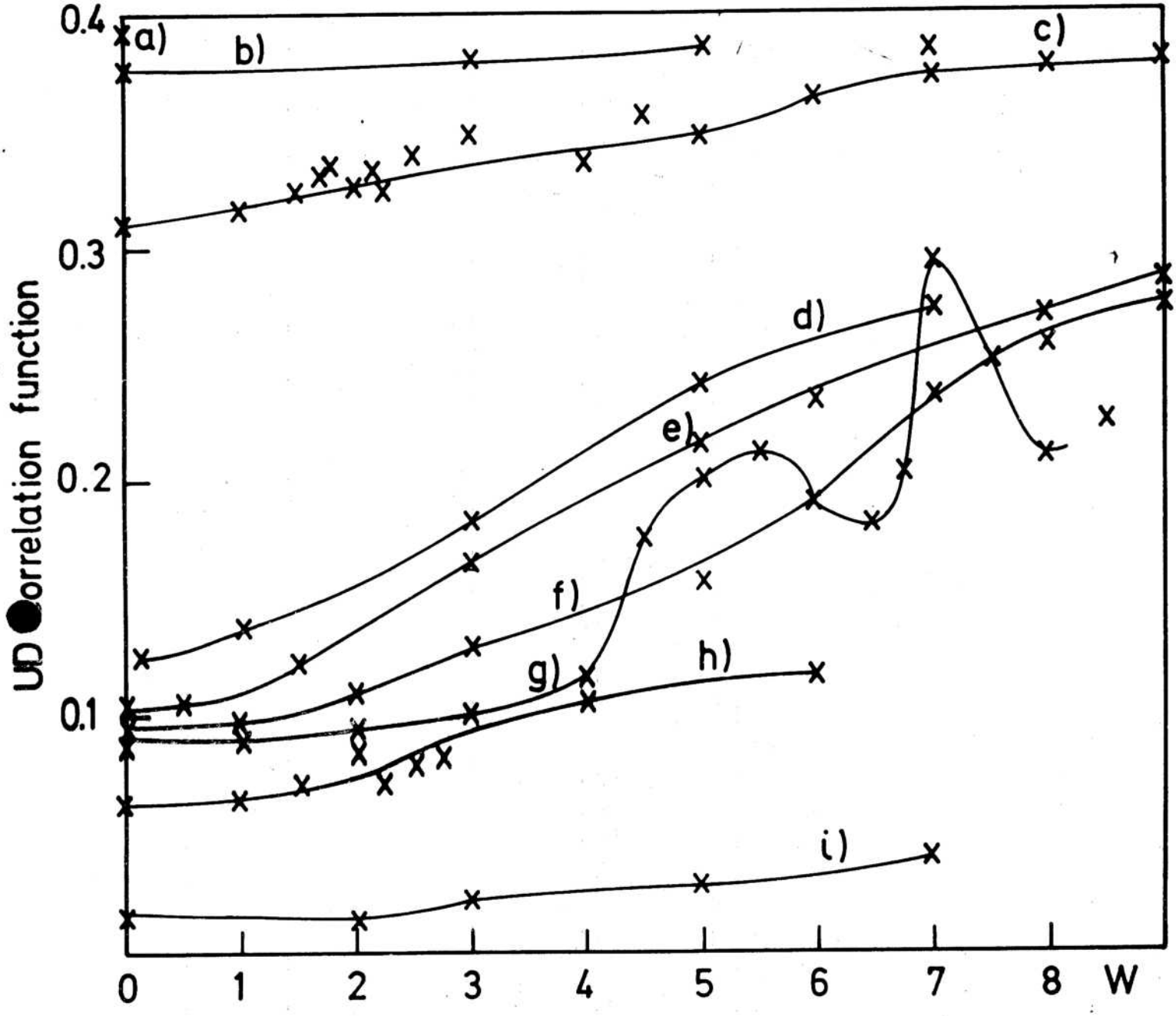
h) U = 1

i) U = 5

Fig. 2: Correlation function as a function of U for different W.

a) W = 5

b) W = 0


0.4
0.3
0.2
0.1
UD correlation function
a)
b)
c)
d)
e)
f)
g)
h)
i)
0
1
2
3
4
5
6
7
8
W

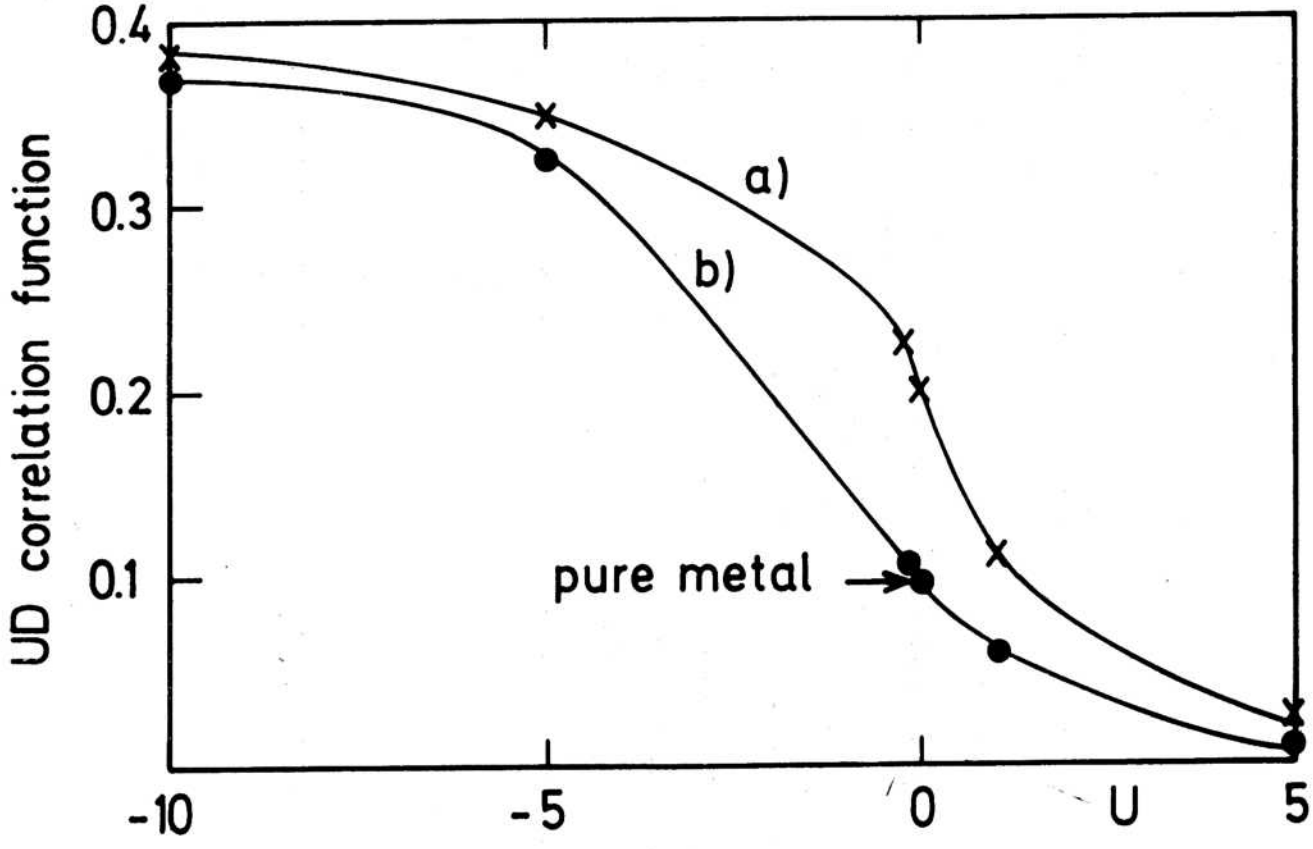


Fig 2