Random negative-U Hubbard model

G. Litak
Department of Mechanics, Technical University of Lublin, Nadbystrzycka 36, PL–20-618 Lublin, Poland

B. L. Györffy
H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

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In the case of superconductors whose electrons attract each other only if they are near certain centers, the question arises of how many such centers are needed to make the ground state superconducting? We shall examine it in the context of a random U Hubbard model. In short, we study the case where U_i is $-|U|$ and 0 with probability c and $1-c$, respectively, on a lattice whose sites are labeled i using the Gorkov decoupling and the coherent potential approximation. We argue that for this model there is a critical concentration c_0 below which the system is not a superconductor.

I. INTRODUCTION

In many attempts to construct a viable model for high-temperature superconductors the notion of negative-U centers is invoked.[1–4] In this connection there is a simple, natural question that arises: How many such centers are needed to make a superconductor. In this paper we shall argue that under certain circumstances there is a critical concentration c_0 below which there is no superconducting order. Moreover, we developed a strategy for investigating the factors which determine c_0.

In order to deal with a well posed problem we shall study a single orbital random-U Hubbard model defined by the Hamiltonian

$$H=-\sum_{ij\sigma} t_{ij}c_{i\sigma}^{+}c_{j\sigma}+\frac{1}{2}\sum_{i\sigma} U_i c_{i\sigma}^{+}c_{i\sigma}c_{i-\sigma}^{+}c_{i-\sigma} - \mu\sum_{i\sigma} c_{i\sigma}^{+}c_{i\sigma}, \tag{1}$$

where i and j label lattice sites, t_{ij} is the hopping integral connecting only nearest neighbor i and j's, μ is the electronic chemical potential, $c_{i\sigma}^{+}$, $c_{i\sigma}$ create and annihilate, respectively, electrons at the single site i with spin σ, and the coupling constant

$$U_i=\begin{cases} -|U| & \text{with probality } c, \\ 0 & \text{with probability } 1-c. \end{cases}$$

The question we shall ask is: Is there a finite concentration c_0 such that for $c<c_0$ the cofigurationally averaged, superconducting long range order parameter $\overline{\chi}$ vanishes even at zero temperature?

As is natural we define $\overline{\chi}$ by the relation

$$\overline{\chi}=\frac{1}{N}\sum_i \chi_i, \tag{2}$$

where the local pairing amplitude is given by

$$\chi_i=\langle c_{i\uparrow}c_{i\downarrow}\rangle. \tag{3}$$

Following the conventional notation $\langle\cdots\rangle$ denotes a thermodynamic average and $\overline{\Theta}$, for an arbitrary operator $\hat{\Theta}$, implies the average of $\hat{\Theta}$ over all configurations U_i, such that the fraction of negative U sites is c, with equal weight. A sample will be said to be superconducting if $\overline{\chi}\neq 0$ This implies that $\chi_i\neq 0$ on a finite fraction of all sites. Namely, if $\chi_i\neq 0$ only on a finite number of sites $\overline{\chi}$ will go to zero as $N\to\infty$ and the system will be regarded as not superconducting.

To make progress we calculate χ_i within the Hartree-Fock-Gorkov (HFG) decoupling scheme for the Green's functions and the averaging over the U configurations is accomplished with the help of the coherent potential approximation (CPA).[5] In short, at the risk of missing some important feature of the problem, such as localization of electrons, we develop a mean field theory for the phenomena described by H in Eq. (1) This approach may be justified by noting that little is known about the problem at hand systematically[1–3] and hence as a preliminary study a mean field theory is called for.

Note that the simplest approximations to the problem would be to set U_i at each site equal to its average value $\overline{U}=cU$. In some contexts this is called the virtual crystal approximation.[7,5] Since, as is well known,[3] any amount of attraction leads to superconductivity, $\overline{U}=cU$ implies superconductivity for all non zero concentrations with the transition temperature T_C decreasing albeit nonanalytically, with c. Thus before setting out the details of the above theory it is worthwhile to pause, briefly, to consider a number of fairly general arguments which suggest that the above conclusion is premature and that there is a critical concentration c_0 of negative U centers for superconductivity.

(i). Classical percolation theory for a mixture of two metals with resistivities ρ_1 and ρ_2 have been studied in the effective medium approximation.[6–8] For $\rho_1=\rho_0$ and $\rho_2=0$ (Fig. 1), namely, in the case where metal 2 is a superconductor, it yields an effective resistivity given by

FIG. 1. A mixture of normal, with resistance $\rho=\rho_0$, and super, with $\rho=0$, conductors.

$$\rho_{\text{eff}}=\begin{cases}\rho_0(1-dc) & \text{for } c<c_0=\dfrac{1}{d},\\ 0 & \text{for } c>c_0=\dfrac{1}{d},\end{cases} \tag{4}$$

where d is the number of spatial dimension in which percolation is allowed. Thus, this model predicts critical concentrations in $d=1$, 2, and 3 dimensions, More over, c_0 depends on the dimensionality d. More generally $\rho_{\text{eff}}\sim(c-c_0)^s$ near c_0 but a mean field theory cannot be expected to deal with the critical exponent s adequately.

(ii). The propagation of Cooper pairs between negative-U centers by hopping from site to site, where $U=0$ on the intermediate sites, is depicted in Fig. 2. Assuming that the distance between two negative-U centers is $c^{-1/d}$, in units of the lattice constant a on a d-dimensional lattice, we estimate the number of individual hops l necessary to reach one such center from its nearest neighbors. Assuming random walk $c^{-1/d}=l^{1/(d-1)}$ (for $d>1$). If each hop takes $\hbar/W$ seconds where W is the bandwidth for the pairs, the time to travel between two negative U centers is given by $\tau=(\hbar/W)c^{-(d-1)/d}$. Now we note that in between two centers the Cooper pair is without its binding energy U. Consequently, such travel is allowed only for such times δt that the energy uncertainty $\delta E=\hbar/\delta t>U$. Taking $\delta t=\tau$ we conclude that for $\delta E=Wc^{(d-1)/d}>U$ the pair will propagate for $\delta E=Wc^{(d-1)/d}<U$ the pair will not propagate. Thus for $c<c_0$, where

$$c_0=\left(\frac{U}{W}\right)^{d/(d-1)}, \tag{5}$$

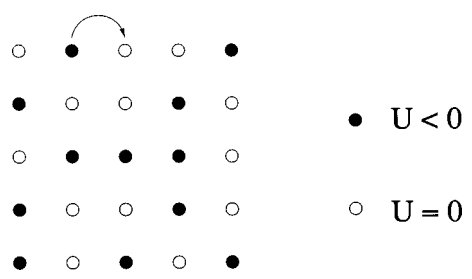

FIG. 2. The propagation of Cooper pairs between negative $U<0$ centers by hopping from site to site, where $U=0$ on the intermediate sites.

a system of negative U centers will not be superconducting. Presumably, the Cooper pairs will be localized. On the other hand for $c>c_0$ it will be a superconductor.

(iii). Localization of Cooper pairs by local charge and order-parameter-phase fluctuation is the third argument which we wish to recall briefly. It was explored in the present context by Doniach and Inui.[1] In a Ginzburg-Landau theory on a lattice the relative phases of the local order parameters $\psi_i=|\psi_i|e^{i\Theta_i}$ are determined by the quadratic term in the free energy function $F(\{\psi_i\})$. This may be written in the form of Josephson coupling energies $F(\{\Theta_i\})=\frac{1}{2}\Sigma_{ij}E_{ij}^J\cos(\Theta_i-\Theta_j)$, where the precise relationship of the coefficients to various parameters of the theory need not concern us here. To describe charge fluctuations associated with Cooper pairs arriving and leaving a site a charging energy needs to be added to F. Because, the local potential is related to the phase by Josephson voltage relation $V_i=(\hbar/2e)\dot{\Theta}_i$ this has the form of a kinetic energy term. Finally, to recover a microscopic description the local phases are treated as quantum mechanical variables by the Hamiltonian

$$H=\frac{1}{2}E_C\sum_i\left(i\frac{\partial}{\partial\Theta_i}\right)^2-\frac{1}{2}E_J\sum_{ij}\cos(\Theta_i-\Theta_j). \tag{6}$$

This is a much studied Hamiltonian in connection with granular superconductivity. In particular it was investigated by Gosset and Györffy[10] in the Hartree approximation. In short they factorized the wave function as shown below

$$\Psi(\{\Theta_i\})=\prod_i\phi_i(\Theta_i) \tag{7}$$

and found the following self-consistent equation for the individual site wave function $\phi_0(\Theta)$

$$\left[-\frac{1}{2}E_C\left(\frac{\partial}{\partial\Theta}\right)^2-E_J\cos(\Theta-\bar{\Theta})\right]\phi_0(\Theta)=E_0\phi_0(\Theta), \tag{8}$$

where

$$\langle e^{i\Theta}\rangle=\int d\Theta\,\phi_0^*e^{i\Theta}\phi_0(\Theta)=\rho e^{i\bar{\Theta}}.$$

The amplitude ρ, determined by solving the above equation numerically is shown in Fig. 1 of Ref. 10, as a function of the ratio E_J/E_C ($\equiv$ Josephson energy/charging energy) For $E_J/E_C<0.125$ we find $\rho=0$ and hence we conclude that the system of point superconductors we have been considering do not have long range superconducting order. Clearly, it is tempting to associate E_J with the coupling between the negative-U centers in our Hubbard model and assume that it goes to zero as $c\to0$. Evidently, this would imply a critical concentration determined by $E_C=E_J(c_0)$. In short, charge fluctuations can destroy the phase coherence of superconducting order parameter if the coupling between the negative-U centers drops below certain critical value. Indeed this was one of the main point of the paper by Doniach and Inui.[1] In what follows we shall develop a strategy for investigating the possible link between the microscopic model defined by Eq. (1) and the above semiphenomenological arguments. In any case, even if such direct link does not exist we

shall take the demise of superconductivity due to phase fluctuations in granular samples as a hint that such fluctuations might play similar role in the model we are about to study.

In concluding this Introduction we note that the specific task we shall undertake is a contribution to the general problem of treating disorder and electron-electron interactions simultaneously. For a comprehensive discussion of the relevant issues in this field the reader is referred to the relatively recent review article by Belitz and Kirkpatrick.[9] We also note that many authors with interest similar to ours convert the problem into that of bosons (Cooper pairs) in a random potential and focus attention on the possibility that they might be localized.[11,12] We wish to avoid such an indirect approach and will tackle the problem head on in terms of a simple but well-defined model.

II. THE COHERENT POTENTIAL APPROXIMATION FOR THE RANDOM-U HUBBARD MODEL

The physics described by this simple model appears to be exceedingly rich. For instance, one might expect that, under some circumstances, the Cooper pairs are subject to Anderson localization[13] and hence they form a random set of Andreev scatterers for the quasiparticles.[14] Such system of scattering centers may then Anderson localize the quasiparticles themselves and turn the system into an insulator below the critical concentration c_0 for superconductivity. However, very little systematic fully microscopic work has been done on the problem and hence, as a preliminary exercise, a mean field theoretic treatment is called for even at the risk of failing to capture some of its important features. In any case, as we shall show, even such limited description turns out to be of physical interest.

Formally, the task is to find the Green's function

$$\boldsymbol{G}(i,j;\tau;\{U_i\}) = -\begin{bmatrix} \langle T\{c_{i\uparrow}(\tau)c^{+}_{i\uparrow}(0)\}\rangle & \langle T\{c_{i\uparrow}(\tau)c_{i\downarrow}(0)\}\rangle \\ \langle T\{c^{+}_{i\downarrow}(\tau)c^{+}_{i\uparrow}(0)\}\rangle & \langle T\{c_{i\downarrow}(\tau)c_{i\downarrow}(0)\}\rangle \end{bmatrix}, \tag{9}$$

where the creation and annihilation operators $c_{i\sigma}(\tau)$ and $c^{+}_{i\sigma}(\tau)$ evolve in complex time τ according the random-U Hamiltonian H in Eq. (1), T is the τ-ordering operator, $\langle\cdots\rangle$ denotes here the usual equilibrium thermal averages corresponding to H, and average the result with respect to all arrangement of the U centers each denoted by $\{U_i\}$. In short we wish to find

$$\overline{\boldsymbol{G}}(i,j;\tau) = \sum_{\{U_i\}} P(\{U_i\})\boldsymbol{G}(i,j;\tau;\{U_i\}), \tag{10}$$

where the probability distribution is assumed to be of form

$$P(\{U_i\}) = \prod_i P(U_i), \tag{11}$$

$$\text{with } P(U_i) = \begin{cases} c & \text{for} \quad U_i = U \\ 1-c & \text{for} \quad U_i = 0. \end{cases} \tag{12}$$

Note that the local order parameter defined by Eq. (3) is given by

$$\overline{\chi_i} = \overline{G}_{12}(i,i;\tau=0^{+}), \tag{13}$$

and hence the knowledge of the averaged one particle Greens functions matrix is sufficient to address the question whether or not there is superconducting long range order at a given concentration c.

As we have indicated above we shall now proceed to a mean field approximation to the above problem. This consists of two steps. Firstly, we make use of the Hartree-Fock-Gorkov decoupling scheme to find the following ''mean-field'' equation of motion:

$$\sum_l \begin{bmatrix} \left(\imath\omega_n + \mu - \frac{1}{2}U_i n_i\right)\delta_{il} + t_{il} & \Delta_i\delta_{il} \\ \Delta_i^{*}\delta_{il} & \left(\imath\omega_n - \mu + \frac{1}{2}U_i n_i\right)\delta_{il} - t_{il} \end{bmatrix} \boldsymbol{G}(l,j;\imath\omega_n) = \mathbf{1}\delta_{ij}, \tag{14}$$

where

$$n_i = \frac{2}{\beta}\sum_n e^{\imath\omega_n\delta}G_{11}(i,i;\imath\omega_n),$$

$$\chi_i = \frac{1}{\beta}\sum_n e^{\imath\omega_n\delta}G_{12}(i,i;\imath\omega_n),$$

$$\Delta_i = -U_i\chi_i,$$

ω_n is the Matsubara frequency.

Secondly, we find average of the solution to Eq. (13), namely $\boldsymbol{G}(i,j;\imath\omega_n;\{u_i\})$, over all U-configurations using the coherent potential approximation (CPA). The justification for this second step is that the CPA is well known to be a reliable mean-field theory of disorder for wave propagation in a medium described by independent random variables.[6–8,15] In what follows we shall investigate the consequences of the above theory by implementing it for a 2^d, square lattice.

To implement the CPA we rewrite Eq. (13) in the Dyson form

$$\boldsymbol{G}(i,j;\imath\omega_n)=\boldsymbol{G}^0(i,j;\imath\omega_n)+\sum_l \boldsymbol{G}^0(i,l;\imath\omega_n)\boldsymbol{V}_l\boldsymbol{G}(l,j;\imath\omega_n), \tag{15}$$

where

$$\boldsymbol{V}_l=\begin{pmatrix} \frac{1}{2}U_l n_l & -\Delta_l \\ -\Delta_l^* & -\frac{1}{2}U_l n_l \end{pmatrix}. \tag{16}$$

The CPA recipe for $\overline{\boldsymbol{G}}(i,j;\imath\omega_n)$ is to set it equal to the coherent Green's function $\boldsymbol{G}^C(i,j;\imath\omega_n)$, which is the solution of Eq. (15) for the case where the random potential $\boldsymbol{V}_l$ is replaced by the energy dependent, complex coherent potential $\boldsymbol{\Sigma}(\imath\omega_n)$, the same on every site. To determine the coherent potential (self-energy) we study, in turn a $U_i=-|U|$ impurity in the coherent lattice. On the impurity site at i we find

$$\boldsymbol{G}^\alpha(i,i;\imath\omega_n)=[1-\boldsymbol{G}^C(i,i;\imath\omega_n)\boldsymbol{V}_i^\alpha - \boldsymbol{\Sigma}(\imath\omega_n)]^{-1}\boldsymbol{G}^C(i,i;\imath\omega_n),$$

$$\text{for} \quad \alpha=0 \quad \text{and} \quad U, \tag{17}$$

where

$$\boldsymbol{V}_i^{\alpha=0} \quad \text{and} \quad \boldsymbol{V}_i^{\alpha=U}=\begin{pmatrix} \frac{1}{2}Un_i & -\Delta_i \\ -\Delta_i^* & -\frac{1}{2}Un_i \end{pmatrix}. \tag{18}$$

Then, the usual CPA condition that determines the self-energy $\boldsymbol{\Sigma}(\imath\omega_n)$ is given by

$$c\boldsymbol{G}^{(0)}(i,i;\imath\omega_n)+(1-c)\boldsymbol{G}^{(U)}(i,i;\imath\omega_n)=\boldsymbol{G}^C(i,i;\imath\omega_n). \tag{19}$$

Similar equations have been used to describe random superconductors by Lustfeld[16] and more recently by Litak *et al.*[17] The principle difference between our present concerns and that of these earlier authors is that we are focusing on the randomness of the interaction parameter U_i and not on the random site energies ϵ_i as was their aim. To put it another way, we are studying a problem analogous to that of a ''spin glass''[4] rather than that of dirty superconductors.

Equations (17), (18), and (19) together with

$$n^\alpha=\frac{2}{\beta}\sum_n \mathrm{e}^{\imath\omega_n\delta}G_{11}^\alpha(i,i;\imath\omega_n),$$

$$\chi^\alpha=\frac{2}{\beta}\sum_n \mathrm{e}^{\imath\omega_n\delta}G_{12}^\alpha(i,i;\imath\omega_n), \tag{20}$$

$$\Delta^U=-U^\alpha\chi^\alpha,$$

$$\overline{n}=cn^{(U)}+(1-c)n^{(0)},$$

$$\overline{\chi}=c\chi^{(U)}+(1-c)\chi^{(0)},$$

where $\alpha=0$ and U as before [Eq. (17)], are the fundamental equations of our theory. Manipulating the CPA equations yield the following gap equation:

$$\overline{\chi}=-\frac{U}{\beta}\sum_n e^{\imath\omega_n\delta}\left[-\frac{c}{2\imath\omega_n}\mathrm{Tr}\{\boldsymbol{G}^{(U)}\}\frac{\|\boldsymbol{G}^{(U)}\|}{\|\boldsymbol{G}^C\|} + \|\boldsymbol{G}^{(U)}\|\left(c\frac{2\imath\omega_n-\mathrm{Tr}\boldsymbol{\Sigma}}{2\imath\omega_n}\frac{\|\boldsymbol{G}^{(U)}\|}{\|\boldsymbol{G}^C\|}-1\right)\right]\overline{\chi}, \tag{21}$$

where

$$\mathrm{Tr}\{\boldsymbol{G}^\alpha\}=G_{11}^\alpha(i,i;\imath\omega_n)+G_{22}^\alpha(i,i;\imath\omega_n),$$

$$||\boldsymbol{G}^\alpha||=G_{11}^\alpha(i,i,\imath\omega_n)G_{22}^\alpha(i,i;\imath\omega_n) - G_{12}^\alpha(i,i;\imath\omega_n)G_{21}^\alpha(i,i;\imath\omega_n).$$

In what follows we present results of solving the above equations numerically for various interesting regimes. Of particular interest is the large U limit. As U_i change its values form 0 to $-|U|$ there exists a Mott-Hubbard metal-insulator transition for large enough interaction $|U|$. Another interesting feature of the problem at hand is that fluctuations of pairing potentials Δ_i, which changes randomly from 0 to Δ^U, invalidate the Anderson theorem[19–21] and hence states appear in the gap.[22]

III. ORDER PARAMETER FLUCTUATIONS

At first we have calculated T_C and $\overline{\chi}$ for zero temperature ($T=0$) by means of VCA where, as we mentioned in the Introduction, effective interaction between electrons $U_{\mathrm{eff}}=cU$. Figures 3(a) and 3(b) show the critical temperature $T_C^{(c)}$ normalized to the corresponding quantities of the clean system with U on every site, namely $T_C(c=1)$ and averaged pairing parameter $\overline{\Delta}(T=0,c=1)$, calculated for effective interaction U_{eff}, respectively, as functions of concentration c. Calculations were done for various values of the interaction parameter $U/W=-0.3, -0.5, -1.0, -2.0$, where $W=8t$ is the bandwidth and for a half filled band $n=1$. One can see that for these approximations there is no evidence of critical concentration $c_0>0$ below which the system is normal at $T=0$, i.e., no percolation.

As is clear from Eq. (14), U_i fluctuating between 0 and $-|U|$ has two distinct direct consequences. On the one hand it causes the Hartree potential $\frac{1}{2}U_i n_i$ to fluctuate. On the other it gives rise to a fluctuating pairing parameter $-\Delta_i$. As it turns out these two effects have very different influence on the solutions to Eqs. (18)–(21). Therefore, we examine them separately. As disorder was treated by CPA, at first we made calculations after neglecting Hartree potential $\frac{1}{2}U_i n_i$, in Eq. (18) and studied the case of order parameter fluctuation on their own. This means that we took the impurity potential in Eq. (18) to be

$$\boldsymbol{V}_l=\begin{pmatrix} 0 & -\Delta_l \\ -\Delta_l^* & 0 \end{pmatrix}. \tag{22}$$

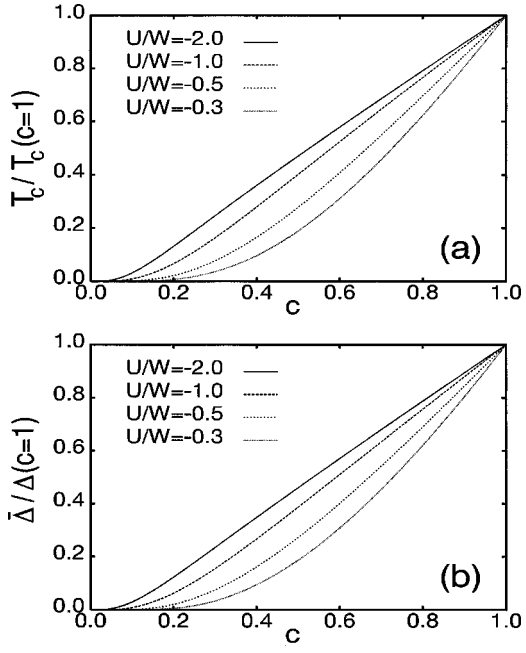

FIG. 3. The critical temperature $T_C/T_C(c=1)$ (a) and the pairing parameter $\overline{\Delta}/\Delta(c=1)$ (b) (calculated with VCA) versus concentration of negative centers c for $n=1$. Values of the interaction parameter U specified in the figures.

In Figures 4(a)–4(c) we show the critical temperature $T_C/T_C(c=1)$ (a), the order parameter (for $T=0$) $\overline{\chi}/\chi(c=1)$ (b), and the local pairing potential on U site $\Delta_U/\Delta_U(c=1)$ (c), versus concentration of negative U centers c for $n=1$. Calculations were done by means of CPA neglecting the Hartree term and using the same values of interaction parameters as in Fig. 3.

Surprisingly, our simplified CPA results agree with the VCA argument in the Introduction inasmuch as we found nonzero local order parameter on both the $U=0$ and $U<0$ sites at all concentrations $c\neq 0$. That is to say we obtained finite $\overline{\chi}\neq 0$ and T_C for any value of concentration c and interaction $U_i<0$ and no evidence of percolation. The order parameter $\overline{\chi}$ increases gradually from 0 to its maximal value with changing the concentration c. Interestingly, in the large U limit, $|U|/W>0.5$, T_C and Δ_U are nearly constant for various c and they reach large finite values for arbitrary small concentrations of negative centers c.

To further pursue the matter of percolation, as might be manifested by a critical concentration, we return to the full CPA solution. Restoring the Hartree potential, which was neglected in the above discussion, we have used the full impurity potential $\mathbf{V}_i^{\alpha=U}$ as in Eq. (18) to carry out the CPA procedure. Figures 5(a)–5(d) show the critical temperature $T_C^{(c)}/T_C(c=1)$ (a), the order parameter $\overline{\chi}/\chi(c=1)$ (b), the local pairing potential on U site $\Delta_U/\Delta_U(c=1)$ (c), and the local charge on U site n_U (d) versus concentration of negative centers c for $n=1$ and the same interactions as in Figs. 3 and 4. Here one can clearly see that all that quantities T_C, $\overline{\chi}(T=0)$ and Δ_U are tending to zero for some small enough concentration of negative U centers c_0. Below this critical concentration the system is normal. For larger interaction $(U/W=-1.0,-2.0)c_0=0.5$ and the order parameter scales

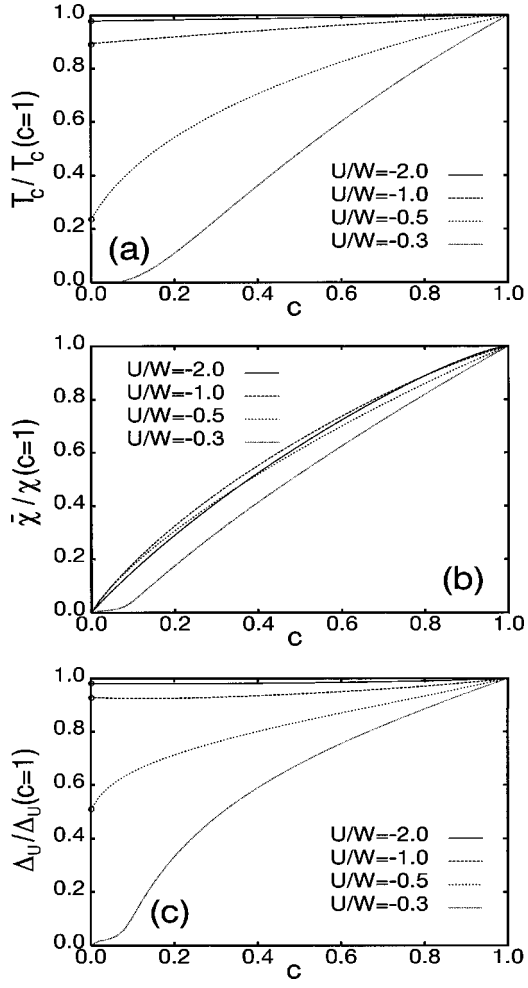

FIG. 4. The critical temperature $T_C/T_C(c=1)$ (a), the order parameter $\overline{\chi}/\chi(c=1)$ (b), and the local pairing potential on U site $\Delta_U/\Delta_U(c=1)$ (c), calculated with CPA neglecting diagonal Hartree terms, versus concentration of negative centers c for $n=1$. Values of the interaction parameter U specified in the figures.

as $\chi\approx(c-c_0)^{1/2}$. Decreasing $|U|$ we observe systematic decrease of c_0. Thus we have discovered a percolation like phenomenon.

To investigate the cause of critical concentration c_0 we have studied the density of quasiparticle states both in superconducting and in the normal states. In the latter case, for large enough interaction $|U|>0.5W$, there exists a band splitting in the system. With changing the concentration c we observe Mott metal-insulator transition. It is caused by large fluctuations of Hartree term $\frac{1}{2}U_i n_i$ [Eq. (14)] as in the original paper of Hubbard.[18] In Figs. 6(a)–6(c) we plotted the densities of states (full line) and the local density of states on U site (dashed line) for $U/W=-2.0$, $n=1$ and $T=0$ for different concentrations c: $c=0.4$ (a normal metal), $c=0.5$ (b insulator), and $c=0.6$ (c superconductor). The Fermi energy in these plots: $\epsilon_F=\mu=0$. Thus changing c from 0 to 1 system changes from normal metal [Fig. 6(a)] to a superconductor [Fig. 6(c)] through an insulator [Fig. 6(b)]. Remarkably, for a low concentration of negative centers [Fig. 6(a)] $c=0.4<c_0$ (here $c_0=0.5$) in spite of finite and relatively large value of averaged density of states at the Fermi energy $\overline{D}(0)=-1/\pi\mathrm{Im}G_{11}^C(0+\imath\delta)$, the local density of states on U

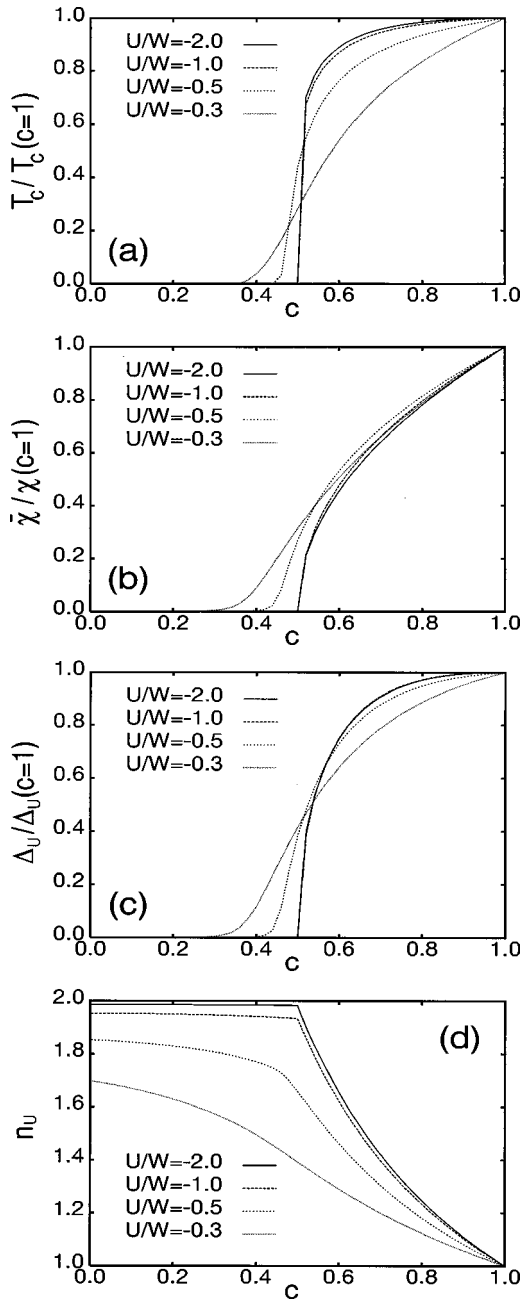

FIG. 5. The critical temperature $T_C/T_C(c=1)$ (a), the order parameter $\bar{\chi}/\chi(c=1)$ (b), the local pairing potential on U site $\Delta_U/\Delta_U(c=1)$ (c), and the local charge on U site n_U (d) calculated with CPA including diagonal Hartree terms, versus concentration of negative centers c for $n=1$. Values of the interaction parameters U specified in the figures.

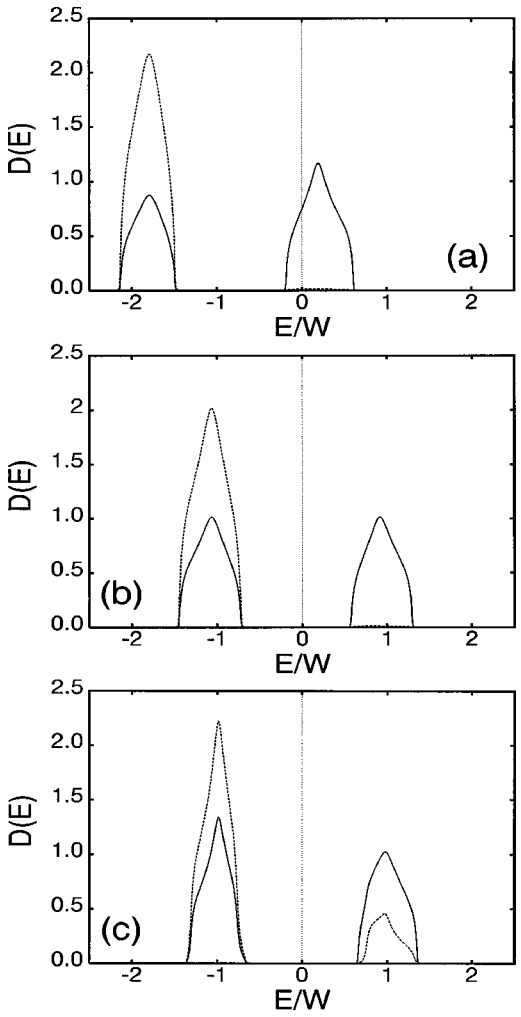

FIG. 6. The densities of states (full line) and the local density of states on U site (dashed line) for $U/W=-2.0$ and $n=1$ for different concentrations c: $c=0.4$ (a metal), $c=0.5$ (b insulator), and $c=0.6$ (c superconductor).

sites $D^U(0)=-(1/\pi)\mathrm{Im}\,G^U_{11}(0+\imath\delta)$ appears to be extremely small. Evidently the doubly occupied states form a lower ''Hubbard'' band split off from the upper band which is associated with the singly occupied sites. Below c_0 the band of doubly occupied sites are filled and hence the pairs can not move. Thus, since ϵ_F is in the gap between the bands of double and single occupancy this is an insulating state.

This effect has been further investigated for other band fillings. The transition from normal to superconducting phase occurred for each of band fillings n at some, specific, critical concentration $c_0(n)$. Figures 7(a)–7(d) show simultaneously the order parameter $\bar{\chi}$ (a), the local pairing potential on U site Δ_U (b), the local charge on U site n_U (c), and the chemical potential μ (d) plotted versus concentration c for $U/W=-2.0$, at $T=0$ and several values of n ($n=$ 1.8, 1.6, 1.4, 1.2, 1.0, 0.8, 0.6, 0.4, 0.2). Interestingly, that transition from superconducting to normal phase is accompanied by a large value of local charge occupation n_U [Fig. 7(c)] and large jump of a chemical potential μ (from one subband to another) near c_0 [Fig. 7(d)]. It appears that for c below c_0 $n_U \approx 2$. Namely, every U site is doubly occupied with a pair of electrons [Fig. 7(c)]. Because there are no empty spare U sites in the system these pairs cannot move. That is to say, they are localized on the U sites.

Similar calculations have been performed for smaller interaction $|U|(U/W=-0.5)$ The corresponding results are presented in Figs. 8(a)–8(d), respectively. Here the interaction $|U|$ is not large enough to create a band splitting effect but the tendency with $\bar{\chi}\to 0$ is still observable as concentration c is tending to some finite $c_0>0(c\to c_0)$. Here c_0 is less than in former case of larger interaction $|U|=2W$ (Fig. 7). The occupation of negative U centers is larger than n but clearly less than two electrons per site. For small enough

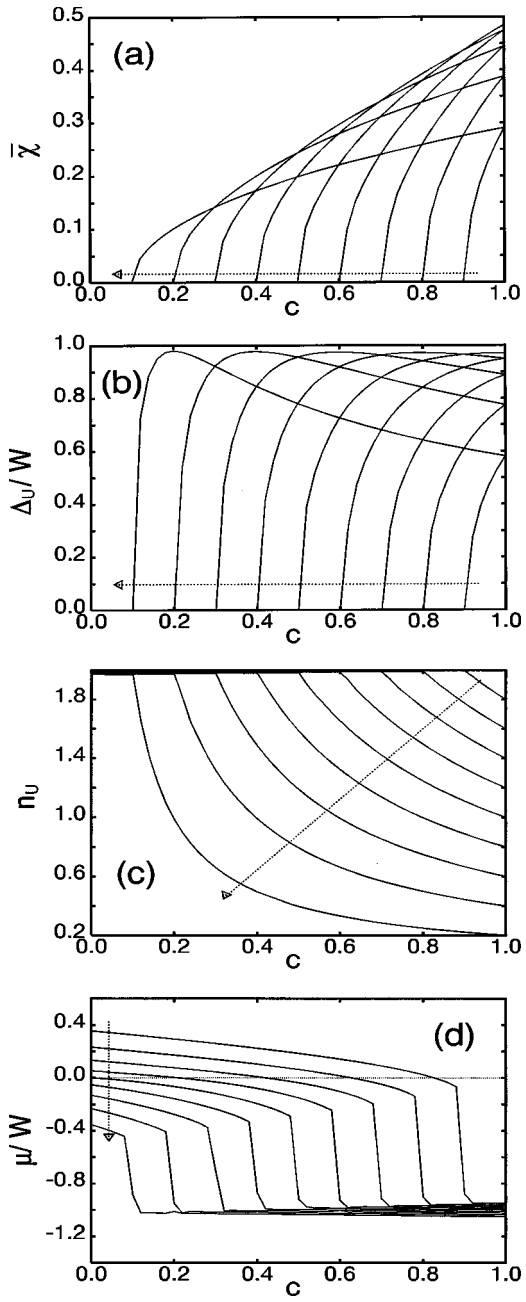

FIG. 7. The order parameter $\overline{\chi}$ (a), the local pairing potential on U site Δ_U (b), and the local charge on U site n_U (c) and the chemical potential μ (d) plotted versus concentration c for $U/W=-2.0$ and several values of n ($n=$ 1.8, 1.6, 1.4, 1.2, 1.0, 0.8, 0.6, 0.4, 0.2 — the direction of n changing is pointed out by the arrow).

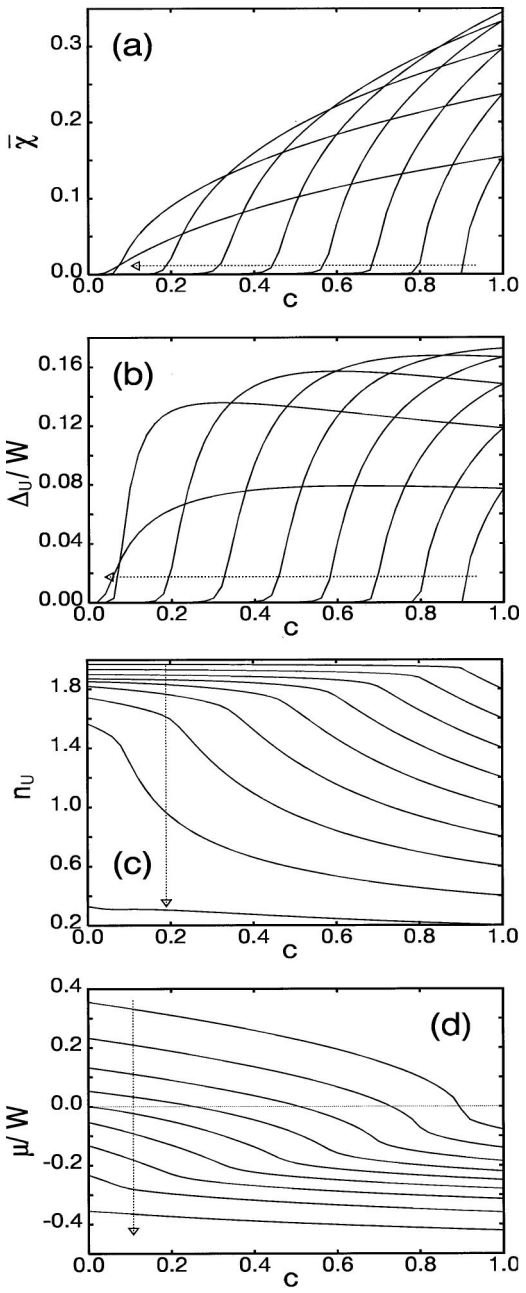

FIG. 8. The order parameter $\overline{\chi}$ (a), the local pairing potential on U site Δ_U (b), and the local charge on U site n_U (c) and the chemical potential μ (d) plotted versus concentration c for $U/W=-0.5$ and several values of n ($n=$ 1.8, 1.6, 1.4, 1.2, 1.0, 0.8, 0.6, 0.4, 0.2 — the direction of n changing is pointed out by the arrow).

band filling $n=0.2$, the order parameter $\overline{\chi}$ was finite for all c and we have not observed a percolation phenomenon. For larger band fillings we have obtained $\overline{\chi}=0$ below $c<c_0$ but instead of a square root behavior $\overline{\chi}\approx(c-c_0)^{1/2}$ for c close to c_0 for larger U [$U/W=-2.0$, Fig. 7(a)] here χ goes to zero rather in the asymptotic way [Fig. 8(a)].

To investigate the demise of the superconducting state near c_0 we have studied the density of states in the appropriate region of parameter space. Figures 9(a) and 9(b) shows the quasiparticle densities of states (a) and the local densities of states on U site (b) for $U/W=-0.5$, $n=0.4$, and three values of c specified in the figures. It is clearly visible how the superconducting gap is filled in, due to pair breaking, with c. Beginning from the clean system with interaction U on every site ($c=1$) we start with sharp edges in the quasiparticle density of states [Fig. 9(a)], then for smaller value of c ($c=0.6$) and the gap parameter Δ of the same order [Fig. 7(b)] the real gap in the quasiparticle density of states $\overline{D}(E)$ changes significantly. The gap becomes smaller with smaller c and loses its clear edges. For small enough c ($c=0.14$) it nearly disappears. Clearly, the Anderson theorem for a superconductor with nonmagnetic disorder is not satisfied in this case.[19] As is well known, according to Anderson

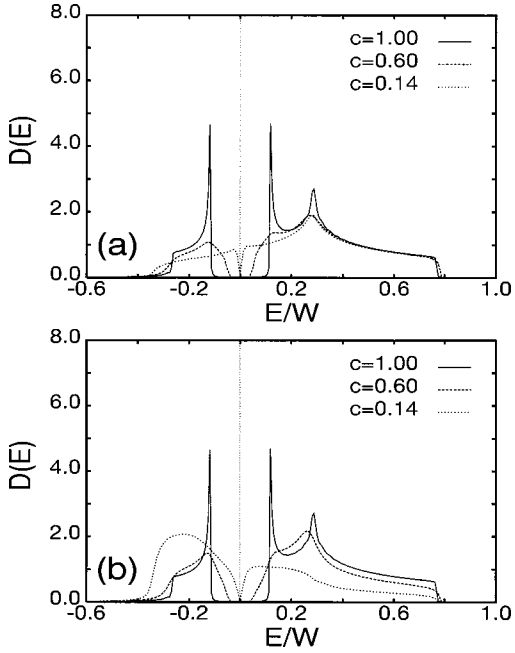

FIG. 9. The averaged quasiparticle densities of states (a) and the local densities of states on U site (b) for $U/W=-0.5$, $n=0.4$ and several values of c specified in the figures.

theorem the gap remains absolute in presence of disorder due to potential scattering provided the spatial fluctuations of Δ_i about $\overline{\Delta}$ are negligible.[20] Clearly, in the random interaction case this is not true and this kind of disorder leads to pair breaking.

Thus, on account of the large fluctuations of pairing potential Δ_i in our system, due to disorder, we observe a qualitative change in quasiparticle density of states shown in Fig. 9(a). These fluctuations lead also to complicated gap equations where T_C is determined not only by $\boldsymbol{G}^C$ but also by $\boldsymbol{\Sigma}$, $\boldsymbol{G}^U$ [Eq. (21)].

Finally, we investigated the factors which determine the critical concentration c_0. In Fig. 10 we show c_0 as a function of band filling for two interaction parameters $U/W=-2.0$ and -0.5. In both cases function can be approximated by a straight line $c_0=a+bn$. In case of $U/W=-2.0$, $a=0$ and $b=0.5$ but for $U/W=-0.5$, $a\approx 0.32$ and $b\approx 0.6$.

IV. CONCLUSIONS

We have examined the question of percolating superconductivity in the context of a random U Hubbard model. We have studied the case where U_i is $-|U|$ and 0 with probability c and $1-c$, respectively, on a lattice whose sites are labeled i using the Gorkov decoupling. Changing concentration c, we checked that simple averaging procedures such as virtual crystal approximations (VCA) do not lead to any zero temperature phase transition. Furthermore, we found that if charge fluctuations are neglected, even a full mean field theory of disorder, such as the CPA, does not predict a percolation transition. However, when the fluctuations in the Hartree potential are included on equal footing with the fluctuations in the pairing potential Δ and the problem is treated in the coherent potential approximation a percolation phenomena, with a critical concentration c_0 of the negative U centers, is discovered in our fully microscopic theory. For $c<c_0$ the lack of superconductivity is due to Mott localization of Cooper pairs and it highlights the qualitative difference between disorder in the crystal potential and the disorder in the interaction between the carriers. In short, the whole phenomenon is due to the combined effect of electron-electron interaction and disorder.[9] Having found the critical concentration c_0 we investigated its dependence on various parameters which defined the problem. In short we studied $c_0(n,U)$. For strong attractive interaction $c_0=n/2$ and $\overline{\chi}\approx(c-c_0)^{1/2}$ near c_0 but for smaller interaction $\overline{\chi}\to 0$ (as $c\to c_0$) rather in a nonpolynomial manner. Calculations have been performed by a real space recursion algorithm which we developed for disordered superconductors in a earlier publication.[23]

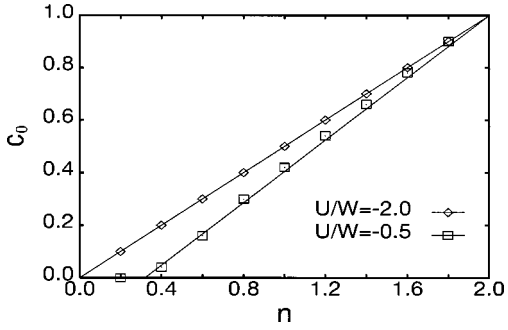

FIG. 10. The critical concentration of negative centers c versus band filling n for $U/W=-2.0$ and -0.5.

Finally, we note that the inhomogeneous conductor model, discussed in the Introduction, predicts $c_0=0.5$ for $d=2$ [Eq. (4)]. Obviously, the argument leading to that result do not engage the basic physics of the fundamental quantum phenomenon described above. Moreover, our results may be brought to correspondence with the prediction of the granular superconductor model, also mentioned in the Introduction, by associating local U site of our lattice with one grain. Then it is clear that E_J goes to zero as the distance between U centers increases. Thus one expects a minimum concentration c_0 for which $E_J/E_C<0.125$ and hence no superconductivity. Unfortunately it would be difficult to estimate c_0 since we do not know the the specific dependence of E_J on c.

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