Superconducting phases in the presence of Coulomb interaction: From weak to strong correlations

Tadeusz Domański and Karol I. Wysokiński
Institute of Physics, M. Curie Skłodowska University, ul. Radziszewskiego 10a, 20-031 Lublin, Poland
(Received 18 May 1998; revised manuscript received 8 September 1998)

We study the evolution of the superconducting phases in a model with competing short-range attractive (W) and on-site repulsive (U) interactions. The influence of the correlations on the phase diagram of s- and d-wave superconductors is studied by means of various approximations. The knowledge of the normal state correlation effects allows the tracking of the influence of U on the superconductivity in correlated systems. We have found the qualitatively different response of the superconducting phases in systems with $W<U_{cr}$, when the system ceases to superconduct for large enough U, and in the limit of strong $W>U_{cr}$, when the system remains superconducting for arbitrarily large U. [S0163-1829(99)07701-2]

I. INTRODUCTION

The discovery of the high-temperature superconductors[1] has raised a question of the operating mechanism of superconductivity. Anderson[2] was the first to propose that the single band repulsive Hubbard model in the large U limit is a proper model to describe the normal and superconducting state of the materials. Subsequent analytical[3,4] and numerical[5,6] studies led to contradicting results concerning the possibility of superconducting order out of purely repulsive interactions. The fluctuation exchange (FLEX) theory[7] leads to the sizable T_c for reasonably large electron repulsion and also to the agreement with some experimental results on high-temperature superconductors.[8] In this work we shall not take this direct contribution of on-site U term to the pairing and concentrate on the normal state modifications due to U.

The experimental data on the high-T_c superconductors seem to support applicability of the models with both repulsive and attractive interactions.[9] The simplest such model is the extended Hubbard model with on-site repulsion and intersite attraction. Its Hamiltonian can be written as

$$H=\sum_{ij\sigma} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}+\frac{1}{2}\sum_{i,j,\sigma,\sigma'} W_{ij}n_{i\sigma}n_{j\sigma'} -\mu\sum_{i\sigma} n_{i\sigma}. \tag{1}$$

Here $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator for a spin σ electron at site i, $t_{ij}=-t$ is the amplitude of an electron to hop from site j to its nearest neighbor site i, μ denotes the chemical potential. $U>0$ is the repulsive interaction between opposite spin electrons at a given site, while $W_{ij}=-|W|$ is the attraction between two electrons seating at neighboring sites.

Competition between the interactions leads to interesting phase diagram of the model. Depending on the parameters one finds magnetic, superconducting, and charge ordered phases.[10] In this work we shall be interested in evolution with increasing U of the superconducting phases only. We shall use Hartree-Fock approximation, second order perturbation theory (SOPT), Hubbard's alloy analogy approximation, and the expansion around the exact, atomic limit solution of the model.

It turns out that the response of the d-wave superconducting state to the increase of U is qualitatively different depending whether the attractive interaction $|W|$ is smaller or larger than U_{cr}, which marks the appearance of the gap in normal state spectrum.

II. THE THEORY

The off-diagonal part of the self-energy matrix $\Delta_{\mathbf{k}}$, which is the order parameter of a spin singlet pairing, is evaluated in the mean-field approximation and written as[11,12]

$$\Delta_{\mathbf{k}}=-\frac{1}{\beta N}\sum_{\mathbf{q}} (U+W_{\mathbf{k}-\mathbf{q}})\sum_{n=-\infty}^{+\infty}\frac{\Delta_{\mathbf{q}}}{|G^{\sigma}_{N}(\mathbf{k},i\omega_n)|^{-2}+(\Delta_{\mathbf{q}})^2}, \tag{2}$$

where $G^{\sigma}_{N}(\mathbf{k},i\omega_n)$ is the normal state Green's function, $i\omega_n=(2n+1)\pi i\beta^{-1}$ are fermionic Matsubara frequencies, and $\beta=(k_BT)^{-1}$ is the inverse temperature.

We take the function $G^{\sigma}_{N}(\mathbf{k},i\omega_n)$ in the standard form[12] $G^{\sigma}_{N}(\mathbf{k},i\omega_n)=[i\omega_n-\xi_{\mathbf{k}}+\tilde{\mu}-\Sigma^{\sigma}_{\mathbf{k}}(i\omega_n)]^{-1}$, where $\xi^{\sigma}_{\mathbf{k}}=\varepsilon_{\mathbf{k}}+\Sigma_{\mathbf{q}}W_{\mathbf{k}-\mathbf{q}}\langle n_{\mathbf{q}\sigma}\rangle$ and $\tilde{\mu}=\mu-zWn$ (z is the coordination number, W denotes amplitude, and $W_{\mathbf{k}}$ the Fourier transform of W_{ij}). In the following we shall neglect small modifications of the normal state spectrum due to the Fock term. $\Sigma^{\sigma}_{\mathbf{k}}(i\omega_n)$ is the frequency and wave-vector-dependent normal state self-energy. It incorporates the effects of U which influences the superconducting state via Eq. (2).

To close the system of equations one has to express the chemical potential μ through the carrier concentration n. It is given by the equation

$$n=\lim_{\delta\to 0^{+}}\frac{1}{N}\sum_{\mathbf{q},\sigma}\frac{1}{\beta}\sum_{n=-\infty}^{+\infty}G^{\sigma}_{N}(\mathbf{k},i\omega_n)\exp(i\omega_n\delta). \tag{3}$$

We have assumed spin singlet pairing. The orbital phases of interest in the context of high-temperature superconductors are s wave, extended s wave, and d wave. The experimental data seem to converge and it is believed that in these materials the order parameter has the *d*-wave symmetry.[13] Thus we shall be mainly interested in the influence of correlations on this symmetry phase.

III. NUMERICAL RESULTS AND DISCUSSION

For a purpose of numerical illustration we have assumed the electron spectrum corresponding to two-dimensional tight binding dispersion. This spectrum possesses the Van Hove singularity in the center of the band. This feature has recently been argued[14] to play the important role in the description of high-temperature superconductors. It does not play a crucial role in the present work except of increasing the value of the density of states for some band fillings. The band width $D=8t$ is taken below as the unit of energy.

Various approximations for the normal state self-energy can and have been employed here for studying the effect of U on the superconducting phases.

(1) We start with the Hartree-Fock (HF) approximation, which leads to $\Sigma^{\sigma}(i\omega_n)=Un_{-\sigma}$. The effect of U on superconducting phases in this approximation has been studied previously[10] very carefully. We thus only mention that there is no influence of U on the *d*-wave superconducting phase in this approximation.

(2) For elevated values of U the second order perturbation theory (SOPT) is a much more reliable approximation. It allows for larger values of U. The self-energy reads[15]

$$\Sigma_{\sigma}{}^{\mathrm{SOPT}}(\mathbf{k},i\omega_n)=Un_{-\sigma}+\left(\frac{U}{N}\right)^2\sum_{\mathbf{p},\mathbf{q}}\frac{f(\xi^{\sigma}_{\mathbf{k}+\mathbf{q}})f(\xi^{-\sigma}_{\mathbf{p}-\mathbf{q}})[1-f(\xi^{-\sigma}_{\mathbf{p}})]+[1-f(\xi^{\sigma}_{\mathbf{k}+\mathbf{q}})][1-f(\xi^{-\sigma}_{\mathbf{p}-\mathbf{q}})]f(\xi^{-\sigma}_{\mathbf{p}})}{i\omega_n-Un_{-\sigma}-\xi^{\sigma}_{\mathbf{k}+\mathbf{q}}-\xi^{-\sigma}_{\mathbf{p}-\mathbf{q}}+\xi^{-\sigma}_{\mathbf{p}}}. \tag{4}$$

In order to solve the gap equation (2) together with Eq. (3) we simplify further the self-energy by replacing the full wave-vector-dependent expression, Eq. (4), by **k**-averaged value. This is equivalent to the so-called ''local approximation.''[16]

Figure 1 collects the results obtained in this approximation for *d*-wave superconducting state. One can see a destructive effect of U on the *d*-wave superconductivity, particularly so near $n=1$.

(3) Alloy analogy approximation (AAA). This approximation which has been proposed by Hubbard and which is known[17] to be equivalent to the coherent potential approximation preserves at least the first six moments of the density of states in the normal phase and is thus superior to the previous one. It is an interpolation scheme which has correct limits at small and large values of U.

For the paramagnetic system $n_{\uparrow}=n_{\downarrow}=n/2$ the self-energy is calculated from the following set of self-consistent equations:

$$\frac{(1-n/2)\Sigma(z)}{1+\Sigma(z)F(z)}+\frac{(n/2)[U-\Sigma(z)]}{1-[U-\Sigma(z)]F(z)}=0, \tag{5}$$

$$F(z)=\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{z-\xi_{\mathbf{k}}+\tilde{\mu}-\Sigma(z)}. \tag{6}$$

In this approach the gap develops in the normal state spectrum for elevated values of U (i.e., for $U>U_{cr}\sim 0.5D$).

In Fig. 2 we show the dependence of the *d*-wave superconducting transition temperature on the carrier concentration n ($n<1$) for the attractive interaction $W=-0.2D$ and few values of electron repulsion. Note the strong destructive effect of U on superconducting state. Inspection of Fig. 2 shows that for these parameters the normal state density of states consists of the single band with the smeared Van Hove singularity. In this case there is a strong competition between attractive and repulsive interactions and for ($U\geqslant|W|$) the repulsion leads to a disappearance of superconducting order for any value of carrier concentration.

Qualitatively different behavior is observed (see Fig. 3) for larger values of $|W|$ ($|W|>U_{cr}$). In this case there exists a range of carrier concentrations (centered roughly around $n=0.5$) for which *d*-wave superconducting state remains intact for arbitrarily large values of U. Figure 3 illustrates the

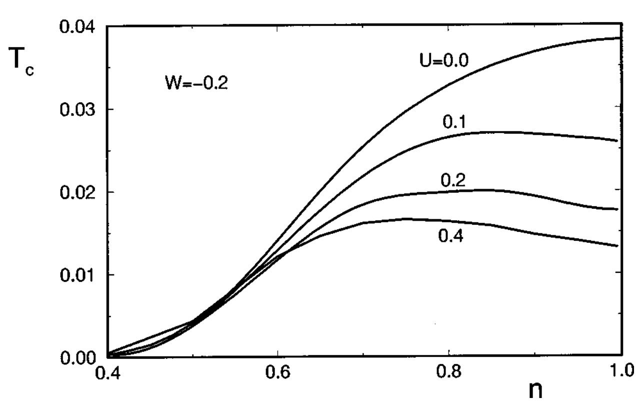

FIG. 1. $T_c^{(d)}$ vs n for $W=-0.2$ and several values of U. The on-site correlations are treated within the SOPT. HF approximation corresponds to the $U=0.0$ curve.

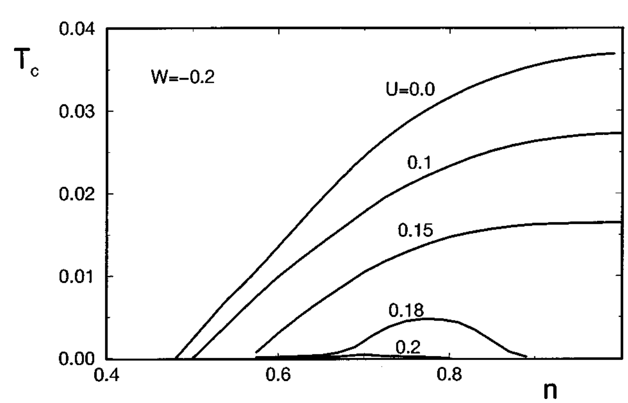

FIG. 2. $T_c(n)$ of the *d*-wave superconductor obtained in the AAA for pairing potential $W=-0.2$. Superconductivity is destroyed by strong enough repulsion U.

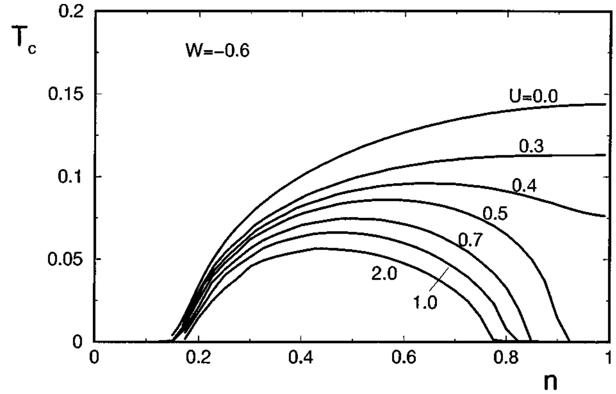

FIG. 3. The same as in Fig. 2 but for $W=-0.6$ ($|W|>U_{cr}$). Even the infinitely strong U does not destroy superconducting phase completely.

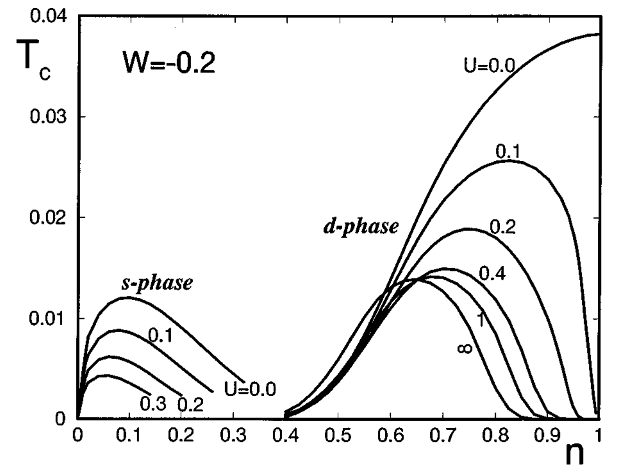

FIG. 4. $T_c^{(s)}$ and $T_c^{(d)}$ vs n obtained within the Hubbard I approximation.

evolution of the d-wave superconducting phase with increasing U and going from weak to strong correlations. In this parameter range the normal state has a band gap due to strong on-site repulsion. The main effect of U is thus connected with the modification of the spectrum which develops a gap of magnitude $\approx U$. The attractive interaction $|W|$, operating inside each of the subbands, is responsible for the pairing of electrons from the same subband. For less than half-filled band ($n<1$) the doubly occupied sites are effectively decoupled from the system and this explains an evident independence of the phase diagram on U for large U.

(4) Expansion around the atomic limit (Hubbard I approximation). The model (1) with $t_{ij}=0$ and $W_{ij}=0$ can be solved exactly. To this end one considers the local part of the Hamiltonian, i.e., $H_{\mathrm{loc}}=-\mu\Sigma_{i,\sigma}n_{i,\sigma}+U\Sigma_i n_{i\uparrow}n_{i,\downarrow}$. The (atomic) single particle Green's function is given exactly by

$$G_{ii}^{\sigma}(\omega)=\frac{1-\langle n_{i,-\sigma}\rangle}{\omega+\mu}+\frac{\langle n_{i,-\sigma}\rangle}{\omega-U+\mu}\equiv[\omega+\mu-\Sigma_{\mathrm{loc}}^{\sigma}(\omega)]^{-1}. \tag{7}$$

The kinetic hopping processes are then treated in a perturbative manner[18] (see also Ref. 19 for systematic improvements) and one finds $G_{ij}^{\sigma}(\omega)$ which when transformed to the Fourier space is characterized by two real poles, i.e., it has a form

$$G^{\sigma}(\mathbf{k},\omega)=\frac{1}{\omega+\tilde{\mu}-\xi_{\mathbf{k}}^{\sigma}-\Sigma_{\mathrm{loc}}^{\sigma}(\omega)}\equiv\frac{A_{(1)}^{\sigma}}{\omega+\tilde{\mu}-E_{(1)}^{\sigma}(\mathbf{k})}+\frac{A_{(2)}^{\sigma}}{\omega+\tilde{\mu}-E_{(2)}^{\sigma}(\mathbf{k})}. \tag{8}$$

In this approach the U term is treated exactly. The method is expected to describe the physics of the model more reliably than usual mean field theory, particularly for large and intermediate values of U.

In Fig. 4 we show the band filling dependence of the transition temperature of the s- and d-wave symmetry superconductor. We have taken $W=-0.2D$. One can see that the d-wave superconductivity persists over some range of n for arbitrarily strong correlations. The same is true for other values of attraction. A lack of the critical value of W below which strong enough correlations destroy superconductivity is due to the fact that one gets a gap in the single particle spectrum even for arbitrarily small but nonzero value of U. Thus these results have to be compared with those obtained in previous approximation for $U>U_{cr}$. Indeed, for elevated values of U both approximations lead to qualitatively similar behavior. It is worth to note that in the $U\rightarrow\infty$ limit this approximation is identical to the decoupling scheme for the Hubbard operators[20] used previously.

Three of the above discussed approximations lead to virtually the same results for the transition temperature $T_c^{(s)}$. One can note the asymmetry between electron doped (low n and s-wave) and hole doped (large n and d-wave phase) superconductors.

IV. SUMMARY AND CONCLUSIONS

In this paper we have analyzed the s- and d-wave superconducting phases of the extended Hubbard model (1) with the competing attractive and repulsive interactions neglecting all other possible instabilities of the model. We have started with the weak correlations and second order perturbation theory and found that an increasing U weakens superconductivity, particularly near $n=1$. Similar behavior is obtained within the alloy analogy approximation provided the attraction is weak. Large correlations have been found to completely destroy the superconductivity in this case. The interesting behavior has been noticed for attractive forces bigger than some critical value. In such a case there exists a range of densities for which the system remains superconducting (with d-wave symmetry of the order parameter) no matter how strong the correlations are. We have identified this critical value as being roughly equal to the value of U, for which there appears a gap in the single particle density of states. This also explains why one evidently does not get such a critical value of attraction in the Hubbard I approximation. In this approximation there is a gap in the spectrum even for arbitrarily small U and thus $U_{cr}=0$ and one virtually always ends up in the ‘‘strong attraction’’ limit $|W| > U_{cr} = 0$ regime. The degradation of superconductivity due to correlations in systems with weak attraction and its robustness against U in systems in which attraction exceeds some critical value is an interesting effect worth studying with a help of better controlled approximations with respect to both interactions U and W.

We kindly acknowledge support from the Polish Committee of Scientific Research through Grant No. 2P03B 031 11.

[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986); Rev. Mod. Phys. **60**, 585 (1988).
[2] P. W. Anderson, Science **235**, 1196 (1987).
[3] J. Beenen and D. M. Edwards, Phys. Rev. B **52**, 13 636 (1995).
[4] M. Mierzejewski and J. Zieliński, Phys. Rev. B **56**, 11 925 (1997).
[5] N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. B **50**, 7215 (1994); Phys. Rev. Lett. **73**, 748 (1994).
[6] T. Husslein, *et al.*, Phys. Rev. B **54**, 16 179 (1996).
[7] N. E. Bickers *et al.*, Phys. Rev. Lett. **62**, 961 (1989); Phys. Rev. B **46**, 8050 (1992).
[8] T. Dahm and L. Tewordt, Phys. Rev. Lett. **74**, 793 (1995); Phys. Rev. B **52**, 1297 (1995); T. Dahm, D. Manske, and L. Tewordt, J. Low Temp. Phys. **111**, 879 (1998).
[9] R. Micnas and S. Robaszkiewicz, in *High T_c Superconductivity 1996: 10 Years after the Discovery*, Vol. 343 of NATO Advanced Study Institute, Ser. E. Applied Sciences, edited by E. Kaldis *et al.* (Kluwer, Dordrecht, 1997), p. 31.
[10] R. Micnas, J. Ranninger, and S. Robaszkiewicz, Phys. Rev. B **39**, 11 653 (1989).
[11] C. Bastide, C. Lacroix, and A. da Rosa Simoes, Physica C **159**, 347 (1989).
[12] A. Romano, C. Noce, and R. Micnas, Phys. Rev. B **55**, 12 640 (1997).
[13] K. A. Kouznetsov *et al.*, Phys. Rev. Lett. **79**, 3050 (1997).
[14] R. Markiewicz, J. Phys. Chem. Solids **58**, 1173 (1997).
[15] H. Schweitzer and G. Czycholl, Z. Phys. B **83**, 93 (1991).
[16] R. Taranko, E. Taranko, and E. Malek, J. Phys. F **18**, L87 (1988).
[17] A. Gonis, *Green Functions for Ordered and Disordered Systems* (Elsevier, Amsterdam, 1992).
[18] C. Bastide and C. Lacroix, J. Phys. C **21**, 3557 (1988).
[19] W. Metzner, Phys. Rev. B **43**, 8549 (1991).
[20] T. Domański, K. I. Wysokiński, and R. Ramakumar, Phys. Rev. B **54**, 3058 (1996).