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LETTER TO THE EDITOR

An extended Hubbard model with inter-site attraction in two dimensions and high-T_c superconductivity

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Abstract. We study a simple model for superconductivity based on an extended Hubbard model with on-site repulsive and inter-site attractive interaction for arbitrary electron density. For the two-dimensional square lattice d-wave pairing is most stable for a nearly half-filled band. p-wave and then extended s-wave pairing become stable upon decreasing band filling. Competition between the various anisotropic pairings and antiferromagnetism as well as the effect of next-nearest-neighbour hopping is discussed. We relate the present model to high-T_c superconducting oxides.

In this Letter we study a simple model of narrow-band materials with local attractive interaction. We consider the extended Hubbard model with on-site repulsion and inter-site attraction

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

where t_{ij} is the transfer integral, μ the chemical potential, $n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}$, U is the on-site Coulomb repulsion and W_{ij} is the inter-site attraction; the number of electrons per site is given by

$$n = N^{-1} \sum_{i\sigma} \langle n_{i\sigma} \rangle.$$

It was shown in the past [1–4] that an effective Hamiltonian of the form of (1) can be obtained from the Hubbard Hamiltonian when the electrons are strongly coupled to phonons or other bosonic modes like excitons or plasmons. If the electron–boson interaction is sufficiently strong this can lead to a compensation of the repulsive Hubbard U interaction and on-site pairing [1]. If the interaction is weaker then we are left with on-site repulsive and short-range attractive interaction leading to inter-site pairing [2]. Both on-site and inter-site pairings can lead to superconductivity of a charged hard-core Bose gas on a lattice if the electron pairs form real bound states [4].

In this Letter we consider the case $U > 0$ and treat U and W in the weak coupling limit. Using a broken symmetry Hartree–Fock scheme we analyse the superconductivity

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due to the short-range inter-site attractive interaction for two dimensions as a function of band filling. Our analysis is similar to previous work on heavy-fermion systems which were however limited to three-dimensional systems and close to the half-filled band situation [5]. For the pure singlet superconducting state one obtains the following gap equation for $\Delta_k = (1/N)\Sigma_q V_{k,q}\langle c_{-q\downarrow} c_{q\uparrow}\rangle$

$$\Delta_k = \frac{1}{N}\sum_q V_{k,q}\frac{\Delta_q}{2E_q}\tanh\left(\frac{\beta E_q}{2}\right) \tag{2}$$

where $E_q = (\bar{\varepsilon}_q^2 + |\Delta_q|^2)^{1/2}$, $\bar{\varepsilon}_q = \varepsilon_q - \bar{\mu} + pW_q/\gamma_0$, $\varepsilon_q = -t\gamma_q$ and $\bar{\mu} = \mu - n(U/2 - W_0)$. $\beta = 1/(k_B T)$ and $\gamma_q = \Sigma_\delta e^{-iq\cdot\delta}$ is the lattice factor with $\boldsymbol{\delta}$ being the vector linking the nearest neighbours and $V_{k,q} = -U + W_{k-q}$. The Fock parameter

$$p = \frac{1}{N}\sum_q \gamma_q \langle c_{q\sigma}^+ c_{q\sigma}\rangle$$

and the chemical potential μ satisfy the following equations:

$$p = -\frac{1}{N}\sum_q \bar{\varepsilon}_q \gamma_q F_q$$

$$n - 1 = -\frac{2}{N}\sum_q \bar{\varepsilon}_q F_q \tag{3}$$

where $F_q = (2E_q)^{-1}\tanh(\beta E_q/2)$.

The pairing potential $V_{k,q}$ takes on the separable form for the square lattice and nearest-neighbour interaction and (2) can be solved by an *ansatz*: $\Delta_k = \Delta_0 + \Delta_\gamma\gamma_k + \Delta_\eta\eta_k$. The various terms in Δ_k refer to on-site s-, extended s- and d-wave pairing where $\gamma_k = 2(\cos k_x + \cos k_y)$, $\eta_k = 2(\cos k_x - \cos k_y)$.

The gap equation for triplet (equal-spin) pairing is

$$\Delta_\alpha^p = \frac{2W}{N}\sum_q \sin q_\alpha \Delta_q^p F_q \qquad \alpha = x, y \tag{4}$$

where $\Delta_q^p = \Delta_x^p \sin q_x + \Delta_y^p \sin q_y$ has a p-like character. The transition temperature for the onset of pure s-wave pairing is given by

$$\begin{pmatrix} 1 + U\varphi_1(T_c) & U\varphi_2(T_c) \\ -\dfrac{W}{4}\varphi_2(T_c) & 1 - \dfrac{W}{4}\varphi_\gamma(T_c) \end{pmatrix}\begin{pmatrix} \Delta_0 \\ \Delta_\gamma \end{pmatrix} = 0 \tag{5}$$

where

$$\varphi_1(T_c) = N^{-1}\sum_q F_q(T_c)$$

$$\varphi_2(T_c) = N^{-1}\sum_q \gamma_q F_q(T_c)$$

$$\varphi_\gamma(T_c) = N^{-1}\sum_q \gamma_q^2 F_q(T_c)$$

and $F_q(T_c) = (2\bar{\varepsilon}_q)^{-1} \tanh(\beta_c \bar{\varepsilon}_q/2)$. The equations

$$\frac{4}{W} = \frac{1}{N}\sum_q \eta_q^2 F_q(T_c)$$
$$\frac{1}{2W} = \frac{1}{N}\sum_q \sin^2 q_x F_q(T_c) \tag{6}$$

determine the onset of d-wave and p-wave pairing, respectively. Such a strict separation of the transition temperatures implies T_c for d- and p-wave pairing independent of U.

Equations (5) and (6) for the transition temperatures together with (3) for the chemical potential have been solved numerically for the square lattice (under the assumption that $p = 0$). The lattice sums were performed using exact DOS (density of states) or by direct numerical integration, thus properly taking into account the Van Hove singularity.

If $n = 1$ ($\bar{\mu} = 0$), we analyse (5) and (6) using low-temperature (weak coupling) and high-temperature expansions and obtain that the d-wave pairing gives the highest T_c while extended s-wave pairing occurs only for $W/D \geq \pi^2/8$, where $D = 4t$ is the half band width. For $U < 0$, on site s-wave pairing exists for any value of W/D. The numerical solutions for s-, p- and d-wave pairing are given in figure 1.

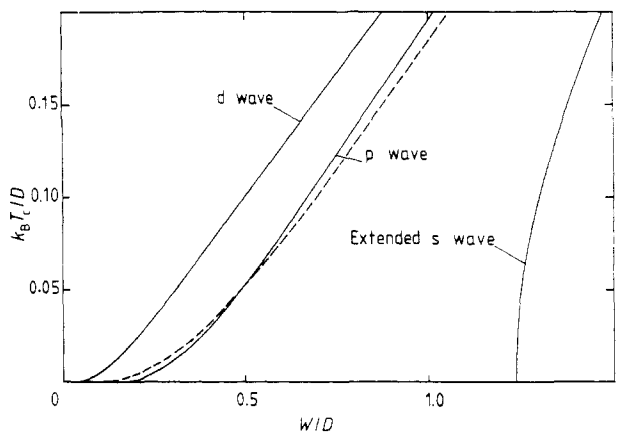

Figure 1. T_c for d-, p- and extended s-wave pairings for the square lattice and half-filled band. The broken curve indicates T_c for both on-site (s) pairing versus $-U/D$ and SDW for U/D.

For $n \neq 1$ the nature of the pairing state strongly depends on band filling. For the s-wave pairing an approximation based on a square DOS yields in the weak coupling limit

$$k_B T_c = 1.14D[n(2-n)]^{1/2} \exp\left(-\frac{1+\lambda[3(n-1)^2-1]+\alpha\lambda(n-1)^2}{2\lambda\{(n-1)^2-\alpha/4\lambda+(\alpha/4)[1+(n-1)^2]\}}\right) \tag{7}$$

where $\alpha = U/D$, $\lambda = W/D$. This indicates that the electron pairing takes place in the whole Brillouin zone with the half band width playing a role of the energy scale. For this reason the commonly used procedure of averaging the pairing potential over the Fermi surface is not applicable. One is then obliged to solve the equation for T_c numerically; results are given in figure 2. While the d-wave pairing gives the highest T_c close to $n = 1$

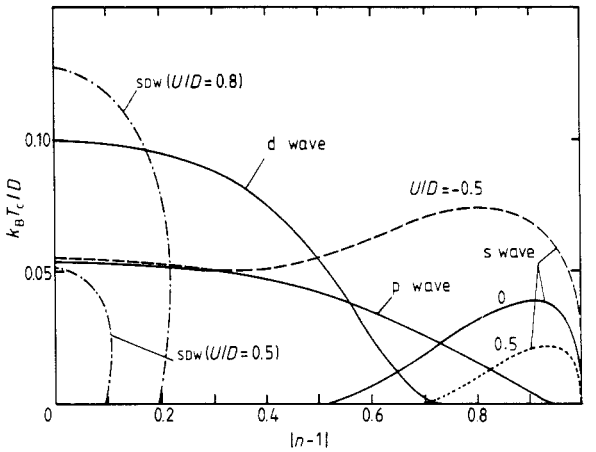

Figure 2. T_c for s-, p- and d-wave pairings for the square lattice versus electron density n for $W/D = 0.5$ and various values for U/D. T_c for SDW is indicated by chain curves.

the competing p-wave and the extended s-wave pairings can be realised for lower electron densities. T_c for s-wave pairing shows strong non-monotonic behaviour with a sharp increase for small values of n, going through a maximum upon increasing n and dropping to zero asymptotically above some value of n. Moreover, s-wave pairing is reduced by increasing on-site repulsion, while it becomes increasingly more stable upon decreasing U below zero. The concentration n_c determining the phase boundary between the d-wave and the p-wave pairing is located numerically at $0.2 < n_c < 0.52$ for $0 < W/D \leqslant 2$ and n_c decreases with decreasing T. For $U > 0$ (or small $U < 0$) one therefore expects the sequence of transitions with decreasing n: d $\rightarrow$ p $\rightarrow$ s. For larger values of negative U it is possible to have d $\rightarrow$ s transition or only s-wave state stable for any n.

What kind of superconductivity is established below T_c is an open question. Needless to say that for $n = 1$, below T_c d-wave appears with admixture of the s-component. Let us point out that for low electron densities the possibility of the formation of inter-site electron pairs and their Bose condensation should be considered [6].

As far as the SDW (spin-density wave) ordering is concerned it is clear that it can compete with anisotropic superconductivity. For $n = 1$, upon using the logarithmic approximation for the exact DOS, the temperature T_N for the onset of SDW is given by:

$$k_B T_N = 0.5D \exp[-(\pi^2 D/U - 0.601)^{1/2} + 2.205].$$

We observe that high superconducting transition temperatures can be achieved with W being much smaller than U. Moreover, we find that the pure SDW state is rather quickly destroyed by deviating from the half-filled band case even for U/D as large as 1. At $T = 0$ K, the onset of SDW occurs for $|\mu| = 4D \exp[-(\pi^2 D/U + (\ln 4)^2)^{1/2}]$. Close to $n = 1$, the SDW can dominate but d-wave pairing caused by W can still be stable. In figure 2 we mark the phase boundaries of SDW for different values of U.

We have also studied the influence of next-nearest-neighbour hopping on superconducting T_c taking $\varepsilon_k = -2t(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y$, where t_2 denotes the next-nearest-neighbour hopping integral, and results are given in figure 3. The purpose was to analyse the effect of the DOS singularity on T_c and to provide some indication as far as the pressure dependence of T_c is concerned. We find that for a definite range of n,

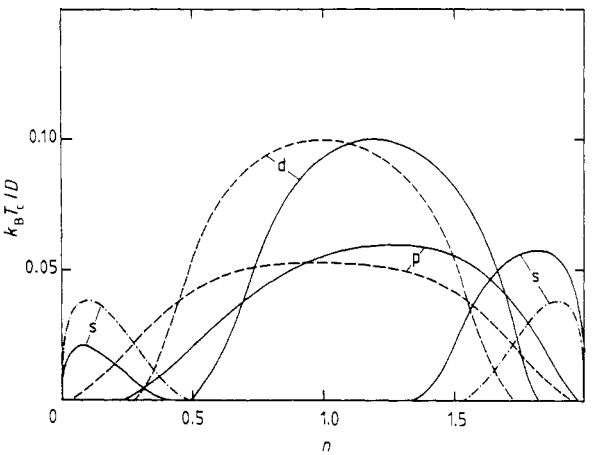

Figure 3. A comparison of T_c for s-, p- and d-wave pairing for the square lattice via electron density and for nearest- and next-nearest-neighbour hopping. ($W/D = 0.5$, $U = 0$). The full curves are plotted for $t_2/t = 0.3$ and the broken and chain curves are for $t_2 = 0$.

T_c can be substantially altered even for small t_2 and in both cases $t_2 > 0$ and $t_2 < 0$ are important.

Let us now relate the present model with the new high-T_c superconductors [7], especially La_2CuO_4-based compounds. It is well established by band structure calculations and transport measurements that these materials are essentially quasi-two-dimensional. The short coherence length in these materials is consistent with our model where pairing is due to short-range attractive interaction. Transition temperatures can be high due to the fact that pairing takes place in the whole Brillouin zone contrary to the BCS model. For example, taking a typical value of $t \sim 0.4$ eV one obtains for $n = 1$ a T_c which varies between 37 and 148 K for W between 0.11 and 0.19 eV. On the other hand for $U = 0.34$ and 0.59 eV, T_N is 186 K and 464 K, respectively. The onset of SDW for these values of U at $T = 0$ K occurs for 2–5% deviation from the half-filled band. These crude estimations are not in disagreement with the recent study of the antiferromagnetism of $La_2CuO_{4-\delta}$ [8].

The phase diagram derived in this work is reminiscent of the one observed in $(La_{1-x}Ba_x)_2CuO_{4-\delta}$ [9]. The fact that in the experimentally observed phase diagram one has a region of SDW close to the half-filled band and superconductivity appearing only below a certain critical concentration could be due to either changes in the pairing potential with Ba doping or due to antiferromagnetic spin fluctuations. Recent NMR measurements attribute the value of $2\Delta/k_BT_c \sim 1.3 \pm 0.2$ to anisotropic pairing [10]. Other evidence for anisotropic superconductivity comes from the anisotropic behaviour of H_{c2} and its positive curvature near T_c [11]. The observed isotope effect in $La_{2-x}Sr_xCuO_{4-\delta}$ [12] indicates that superconductivity is somehow related to electron–lattice coupling and tends to support our model of short-range pairing due to a polaronic mechanism.

As far as Y–Ba–Cu–O is concerned we speculate that, if at all it can be described by the present model, then it should fall into the electron density regions where s-wave pairing is predominant.

In the present work we assume that we are in the weak (or intermediate) correlation

regime ($U < 2D$). This implies a not very large increase of the effective mass of carriers and the Sommerfeld coefficient γ—which is in fact observed. Our picture of a quasi-two-dimensional system can lead to a behaviour of the resistivity in the normal state if the carrier (holes) concentration is low [13] that is linear in T.

We should point out that in the limit of strong correlations ($U \gg t$), the model (1) still gives a superconducting ground state except for the half-filled band case (the Mott insulator). Such a limit would be closer to the Anderson idea of resonating valence bond state [14] with the difference that superconducting pairing would be caused primarily by the short-range attractive interaction W.

For strictly two-dimensional systems no long-range ordered state is possible for any finite temperature. However, the Kosterlitz–Thouless-type transition is possible for the superconducting state, while this is not the case for the SDW state. The interlayer coupling will stabilise both the superconducting and the SDW states. The mean-field superconducting transition temperatures obtained in this Letter are rather accurate even in the absence of any interlayer coupling [15].

The present mean-field approach is justified for not too strong electron correlations and perhaps for not too low electron densities. It is a challenging problem to study the transition from Cooper pairs to real-space pairs when the electron density is decreased. For on-site pairing this change-over is continuous [16]. However, for inter-site pairing this remains so far an unresolved problem.

An important point (presently under investigation) is the coexistence of SDW and anisotropic superconductivity as well as the question whether the presence of antiferromagnetic spin fluctuations can enhance further the d-wave pairing especially close to $n \simeq 1$ [17].

In summary, we studied a simple model permitting us to incorporate magnetic correlations (U) and superconducting pairing (W) for systems with short coherence length (nearest-neighbour real-space pairing). Even though this model is extremely simplified as compared to the complex structure of the high-T_c oxides, our findings seem to go into the right direction in interpreting these materials.

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