Weak coupling model for s*- and d-wave superconductivity

D.van der Marel

Laboratory of Solid State Physics, Materials Science Center
University of Groningen, Nijenborgh 4, 9747 AG Groningen

The phase diagram of the unconstrained $t - J$ model is calculated using the random phase approximation. It is found that the extended $s$ and the $d_{x^2-y^2}$-channels are not degenerate near half filling. Extended $s$-pairing with a low $T_c$ occurs only for a band containing less than 0.4 electrons or holes per unit cell, whereas in a large region around half-filling $d$-wave pairing is the only stable superconducting solution. At half filling superconductivity is suppressed due to the formation of the anti-ferromagnetic Mott-Hubbard insulating state. By extending the analysis to the unconstrained $t - t' - J$ model, it is proven that, if a Fermi surface is assumed similar to the one that is known to exist in cuprous oxide superconductors, the highest superconducting $T_c$ is reached for about 0.7 electron per site, whereas the anti-ferromagnetic solution still occurs for 1 electron per site. It is shown, that the maximum $d$-wave superconducting mean field transition temperature is half the maximum value that the Neél temperature can have in the Mott-insulating state.
In spite of a huge experimental and theoretical effort to understand the superconductivity in the cuprous oxide high T\textsubscript{c} superconductors \cite{1,2}, a mechanism for superconductivity has not yet been firmly established. A lot of attention has been devoted to obtain a model for superconductivity starting from the Hubbard hamiltonian, however, there is a growing suspicion that the positive U Hubbard model alone can not give rise to superconductivity \cite{3}. A different approach has been to treat the electronic degrees of freedom and 'spin fluctuations effectively as separate channels \cite{4,5}, leading to a retarded electron-electron interaction mediated by spin-fluctuations. The latter model has proven to be more successful in the sense of providing a possible mechanism of superconductivity.

Here I will discuss pairing using an exchange-only Hamiltonian

\[
H = \sum_{k,\sigma} (\xi_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + 2 \sum_Q \sum_{k,q} J(Q) \left[ \vec{S}_{k,k+Q} \cdot \vec{S}_{q,q+Q} - \frac{1}{4} \sum_{\sigma\sigma'} c^\dagger_{k+Q\sigma} c^\dagger_{q+Q\sigma'} c_{q\sigma'} c_{k\sigma} \right]
\]  

(1)

The t – J model is studied here without the usual constraint on double occupancy of the same site as a model in its own right. In the real-space representation J couples nearest neighbouring sites on a square lattice. Hence the exchange part is of the form

\[
\frac{1}{2} (J_0 \sum_{R,\delta} \vec{S}_R \cdot \vec{S}_{R+\delta} - \frac{1}{4} n_R n_{R+\delta})
\]

where \(\delta\) runs over the four nearest neighbour sites, and the factor 1/2 compensates double counting of the interactions in the summation over \(R\). If one considers only two neighbouring spins the energy of the triplet state is 0, and of the singlet it is \(-J_0\), hence the sign convention is such, that \(J_0 > 0\) couples neighbouring spins anti-ferromagnetically.

For the dispersion of the band I will consider a nearest neighbour and a next nearest neighbour hopping term, but apart from that, it is the same hamiltonian as was used in the papers by Baskaran, Zou and Anderson (BZA) \cite{6,7}, Emery \cite{8} and by Kotliar \cite{9}. Although usually such a Hamiltonian is thought to be derived from the Hubbard model by means of a Gutzwiller projection, (which also changes the character of the fermion operators, by projecting out double occupancy of the same sites) it should be pointed out, that in the cuprous oxide systems this term may also have a different microscopic origin. As the actual bandstructure in these systems is experimentally known to be better described by the
three band model of Zaanen, Sawatzky and Allen \cite{10}, (which is again a simplified version of the real valence band structure involving 6 oxygen 2p bands and 5 copper 3d-bands for the occupied states, as well as unoccupied 3s and 3p states) a transformation to a single band hamiltonian will in principle generate both an effective Hubbard $U$ and an intersite $J$ \cite{11–13}. Examples of such transformations can be found in the work by Emery \cite{8}, and by Jansen \cite{14}. However, also other, more complicated types of interactions are generated when making transformations of this type, notably the correlated hopping term (with six operators) which, as has been shown by Hirsch, promotes superconductivity of hole-carriers \cite{15}. The interaction considered by Jansen as well as the correlated hopping term treated by Hirsch, effectively provide an on-site attraction, which, when considered on its own, promotes pairing in the (non-extended) s-wave channel. In this paper I will assume that the net on-site interaction is repulsive, which, as will be discussed below, tends to suppress superconductivity by stabilizing the anti-ferromagnetic solution.

Monthoux and Pines \cite{5} have considered the $t-t'$ bandstructure together with an interaction of the form $g(q)\vec{s}(q) \cdot \vec{S}(-q)$, where $\vec{s}(q)$ represents the valence electron spin-operator, and $\vec{S}(-q)$ is a separate spin-fluctuation operator, the properties of which are determined by the spin-susceptibility. The transport and superconducting properties are then calculated from strong-coupling theory using empirical values for the spin-susceptibility and $g(q)$. It has been shown by Monthoux et al. that the effective electron-electron Kernel arising from such a coupling becomes indeed a spin-dependent interaction \cite{16}, which could in principle be written as a frequency dependent version of Eq. \cite{1} \cite{17}. In the same paper a weak coupling analysis of such a frequency dependent Kernel was given. In the present paper the problem is further simplified by disregarding a possible frequency dependency of $J(Q)$, which, depending on the details of the microscopic origine of Eq. \cite{1}, may still be a justifyable approximation. This allows us to explore the phase diagram in somewhat more detail without having too many parameters to consider.

Apart from these general considerations I have no sound microscopic justification for using this hamiltonian. The main motivation to use it comes from the fact that, as I will show in
this paper, it appears to do a surprisingly good job as a phenomenological model consistent with at least some of the experimentally known aspects of superconductivity in these systems.

BZA \cite{7} considered pairing of the $s^*$-type near half filling, Emery considered $d_{x^2-y^2}$-pairing, and Kotliar studied both $s^*$ and $d$-type pairing. Below I will show, that the $s^*$-type pairing is not a stable solution near half filling, and is dominated by pairing of the $d$-type. As the latter again tends to be unstable with respect to the anti-ferromagnetic Mott-Hubbard insulating state at half filling, superconductivity can only exist sufficiently far away from this region. As the optimal $T_c$ would have been reached at half filling for a symmetrical band, this would lead to the conclusion that superconductivity is only a marginal effect in such a system. However, the high $T_c$ cuprates do not have a symmetrical band, and the Fermi surface is known to be distorted from the perfect square that arises from considering only nearest neighbour hopping. This actually comes to rescue: As a function of band-filling it pulls apart the regions, where anti-ferromagnetism and high $T_c$ are optimal, without having a noticeable effect on the superconducting or anti-ferromagnetic transition temperatures.

Three important trends emerge from this analysis:

(1) Given the distorted shape of the Fermi surface as it is known to occur in the cuprates, hole doping gives rise to higher $T_c$'s than electron doping.

(2) There exists a universal relation between the highest Ne`el temperature found in the phase diagram and the highest possible mean field superconducting $T_c$, with $T_N/T_c \approx 2$. That a relation of this kind should exist was already pointed out by Anderson \cite{23} shortly after the discovery by Bednorz and Müller.

(3) This implies that with reasonable values for the intersite exchange interaction, providing the correct Ne`el temperature, one automatically obtains values for the superconducting transition temperature which are (even though they are larger than the experimental values in the cuprates) definitely in the right ball-park.

The $k$-space representation of the exchange interaction is of the form of Eq.1 with
\[ J(Q) = \frac{1}{2} J_0 (\cos(Q_x a) + \cos(Q_y a)) \]  

(2)

This type of interaction favours anti-ferromagnetism if \( J_0 > 0 \), which becomes especially stable if the band is half filled. The antiferromagnetic alignment of nearest neighbours gives rise to a spin-dependent effective field, which is periodic with the wave vector \((\pi/a, \pi/a)\).

Let us now turn to the superconducting gap equations. If the interaction potential \( V_{kq} \) is of the form

\[
H^i = - \sum_{k,q} V_{k,q} c^\dagger_{k \uparrow} c^\dagger_{-q \downarrow} c_{-q \uparrow} c_{q \downarrow}
\]  

(3)

the BCS gap equation is

\[
\Delta_k = \sum_q \frac{\Delta_q V_{k,q}}{2 E_q} \tanh \left( \frac{E_q}{2 k_B T} \right)
\]  

(4)

where \( E_q \equiv \sqrt{\epsilon_q^2 + \Delta_q^2} \) as usual. If we can make the assumption, that the main contribution leading to superconductivity comes from the \( J \)-term, we see that the interaction entering the gap equations is

\[
V_{k,q} = 2 J(k-q) + 2 J(k+q)
\]  

(5)

With this substitution we obtain

\[
\Delta_k = J_0 \left[ \Psi_x^+ \cos(k_x a) + \Psi_y^+ \cos(k_y a) \right]
\]  

(6)

where I introduced the dimensionless pairing amplitudes

\[
\Psi_i^+ \equiv \sum_q E_q^{-1} \Delta_q \cos(q_i a) \tanh \left( \frac{E_q}{2 k_B T} \right)
\]  

(7)

As there are two possible order parameters \( \Psi_i^+ \), we have here two coupled equations, which can be easily disentangled with the help of symmetry selection rules. I will do this for the case where the superconductor has a four-fold rotation axis. In that case \( \Delta \) is either an odd or an even function of \( k \). In the former case, which corresponds to \( d_{xy} \) symmetry, pairing amplitudes of the form \( \Psi_i^- = \sum_q E_q^{-1} \Delta_q \sin(q_i a) \) have a finite amplitude, whereas \( \Psi_x^+ \) and \( \Psi_y^+ \)
are zero. The hamiltonian considered here does not couple to the \( d_{xy} \) pairing-channel. If \( \Delta \) is even, we have to consider two possibilities: Either \( \Psi_x^+ = \Psi_y^+ \) leading to an extended s-wave gap, or \( \Psi_x^+ = -\Psi_y^+ \) leading to a \( d_{x2-y2} \) symmetry of the gap function. The gap function corresponding to these two cases is

\[
\Delta_k = \frac{1}{2}\Delta_0 [\cos k_x a \pm \cos k_y a]
\]  

where the plus and minus sign correspond to the \( s^* \)- and \( d_{x2-y2} \)-wave types of pairing respectively, and the gap equation becomes

\[
\frac{2}{J_0} = \sum_q E_q^{-1} [\cos q_x a \pm \cos q_y a]^2 \tanh \left( \frac{E_q}{2k_B T} \right) \tag{9}
\]

This equation was also obtained by Kotliar [9]. In his analysis the constraint of no double occupancy of the same site was taken into account in an approximate way, by having \( t \) proportional to doping of the half filled band. At half filling one then effectively has \( t = 0 \), for which case, as was shown by Kotliar, the summations on the right hand side of this Eq. 4 are identical for the two types of pairing. As a result he obtained a degeneracy between the \( d \)-and \( s \)-ordered state at half filling, leading to the conclusion that a pairing of type \( s + id \) could occur. For any finite value of \( t \) this degeneracy is however lifted. In the meantime a variety of numerical and theoretical techniques have been applied to the \( t - J \) and related models, from which a tendency toward \( d_{x2-y2} \)-pairing has been found near half filling [25–29]. It is easy to show, that for the \( s^* \)-type pairing at half filling of a symmetric band, \( J_0 \) has to exceed a critical value. Let us assume that \( \epsilon = (W/4) \cdot (\cos(k_x a) + \cos(k_y a)) \). For \( T = 0 \) the gap equation becomes

\[
J_0^{-1} \sqrt{W^2/4 + \Delta_0^2} = \sum_q |\cos q_x a + \cos q_y a| = 0.811 \tag{10}
\]

hence the critical value of \( J_0 \) for \( s^* \)-pairing is at half filling \( J_0^* = 0.62W \). The reason for the appearance of a critical value is, that at half filling the \( s^* \)-type gap is exactly zero for all \( k \) at the Fermi surface. Only by mixing in states away from the Fermi level, superconductivity of this type may occur, which requires a minimum coupling strength. The \( d \)-channel is much
more effective in this sense, as $\Delta_k$ is finite at the Fermi surface except for the node-points. As a result in the $d$-channel we have $J_0^c = 0$.

The ground state energy relative to the normal state can now be determined by realizing that it is the expectation value of the reduced hamiltonian minus the non-interacting part, which is [30]

$$
\sum_k \left( |\epsilon_k| - E_k + \frac{\Delta_k^2}{2E_k} \right)
$$

where the first two terms represent the energy gained by redistributing the electrons over $k$-space in the correlated wavefunction, whereas the third term compensates double counting of the interaction. In principle one has to solve the gap equation together with a constraint on electron occupation number [31–33], however the corrections to the free energy are of the order $(\Delta_0/E_F)^2$, [34] which is small for the parameters that we will consider.

I still need to specify the electron dispersion relation before we can solve the gap equations. If one considers a tight-binding model with a single orbital per site, with only hopping between nearest and next nearest neighbours, the single particle energies are

$$
\epsilon_k = -2t \left( \cos(k_xa) + \cos(k_ya) \right) - 4t' \cos(k_xa) \cdot \cos(k_ya) - E_F
$$

The $t'$-term is due to next-nearest neighbour hopping. Let me briefly discuss some of the properties of such a band. If $t' = 0$ at half filling of the band, such a dispersion relation has the remarkable property that the Fermi surface forms a perfect square, with a diverging effective mass over the entire Fermi surface. In practice this situation will never occur, as there will always be some finite coupling between next nearest neighbours. This causes a bulging of the Fermi surface, as is shown in Fig. [4], which eventually transforms into a rotated Fermi surface if $|t'| \gg |t|$. The shape obtained for $t' = -0.7t$ is very close to what has been calculated with the local density approximation for e.g. La$_2$CuO$_4$ and YBa$_2$Cu$_3$O$_7$ [35,36]. A significant change also occurs in the density of states (DOS) at the Fermi energy, which is displayed in Fig. [2] as function of the number of electrons per unit cell. This somewhat unusual representation of the DOS is useful in the discussion below, where we
compare ground state energies of various types of ordering at a given electron density. We see, that as \( t' \) is increased, the DOS becomes a-symmetric, and the maximum is shifted to the left side of the point where the band is half filled. Of course the direction in which this occurs is dictated by the sign of \( t' \). With \( t' < 0 \) we mimic the situation encountered in the \( CuO_2 \)-planes of the high \( T_c \) cuprates.

In Fig. 3 numerical calculations of the free energy are shown as a function of occupation number for \( J_0/W = 0.6 \), where \( W = 8t \) corresponds to the bandwidth if \( t' = 0 \). For the sake of completeness also the free energy of the anti-ferromagnetically ordered state is included. This was calculated from the same hamiltonian. To stay in the same spirit as for the superconducting solutions, the random phase approximation was used. Hence the free energy was minimized together with a constraint on the electron occupation number, anticipating a finite expectation value of \( \langle c_{k+Q\uparrow}^\dagger c_{k\uparrow} \rangle = -\langle c_{-k\downarrow}^\dagger c_{-k-Q\downarrow} \rangle \) at the point \( Q = (\pi/a, \pi/a) \). We notice that the anti-ferromagnetically ordered state at half filling is always more stable than the metallic state. However, for small values of \( J_0 \) the \( d \)-wave paired superconducting state is still more favourable. This is a consequence of our choice of model Hamiltonian, which is perhaps somewhat pathological near half filling: Physically the exchange terms should arise from a strong repulsive interaction between electrons making a virtual transition to the same orbital of \( e.g. \) a transition metal atom. On the one hand this leads to exchange coupling between spins on neighbouring orbitals, while on the other hand it causes the opening of a Mott-Hubbard gap, which is much larger than the anti-ferromagnetic gap. This would strongly stabilize the anti-ferromagnetic solution. Tempting as it may be to add an on-site repulsion at this point as an additional model parameter, I will not do so: It has become clear in recent years, that a large repulsive \( U \) gives rise to very strong correlation effects, at and near half filling, which can not be properly treated with the random phase approximations made in this paper \[37\ \[39\]. For this reason, and also because fluctuations are neglected with the latter approximations, the present analysis is insufficient close to half filling. For higher doping it could have some relevance to the mechanism of superconductivity. It is important to add in this context, that the symmetry
of an additional on-site interaction is such, that it cancels out in the gap equation for the \( s^* \) and \( d \)-channels. Hence an on-site \( U \) does not affect the gap-function or the free energy for these types of superconductivity.

Although from a Maxwell construction one is lead to the conclusion that phase separation should occur in \( s^* \)- and \( d \)-ordered regions, this is strongly suppressed if the long range Coulomb interaction is taken into account. [18] Although the Coulomb term is not included explicitly in the Hamiltonian, the presence of such a term is assumed implicitly by imposing the constraint that the electronic density is macroscopically conserved. As was stressed by Emery, Kivelson and Lin [19,20], who studied the \( t-J \) model together with the constraint on no doubly occupied sites, ‘the holes are often donated by oxygen atoms which are quite mobile ... ’, providing a physical mechanism for screening of the long range Coulomb term. Putikka, Luchini and Rice [21] provided numerical evidence that, in the absence of a long range Coulomb force, phase separation occurs for \( J/t > 3.8 \) as \( n \to 0 \) and \( J/t > 1.2 \) near half filling. The present analysis does not lead to phase separation if the long range Coulomb interaction is taken into account. [22]

The phase diagram is displayed in Fig. 4. Due to electron-hole symmetry in this case, the diagram is symmetric around half occupation of the band. Roughly speaking \( s^* \)-pairing is favoured far away from half filling of the band, whereas \( d \)-wave pairing becomes the most stable solution near half filling. For \( J_0 < 0.3W \) there are regions of no superconductivity, which broaden upon decreasing \( J_0 \), and completely cover the horizontal axis for precisely \( J_0 = 0 \). This tendency towards \( d \)-wave pairing near half filling was also obtained by Littlewood [10] for the charge transfer model [10], again using a weak coupling treatment. In these calculations an inter-site exchange interaction is not introduced explicitly, and can only result indirectly from the repulsive on- and inter-site interactions which are taken into account in the model.

We see, that \( J_0 > 0.7W \) is required to find an antiferromagnetic phase near half filling. As can be seen from the free energies versus doping, the phase boundaries between \( s^* \) and \( d \), and between \( d \) and \( AF \), correspond to a discontinuous change from one type of ordering to the
other. For the $s^*-d$ boundary this discontinuity will probably be softened without loosing the superconductivity by the occurrence of an intermediate state of mixed $s + id$ character, as was proposed by Kotliar at precise half filling and $t = 0$. The phase boundary between $d$ and $AF$ is different in this respect. As both the anti-ferromagnetic and superconducting correlations occur in the same band of electrons, they will tend to suppress each other. Because finite anti-ferromagnetic correlations will occur on the superconducting side of the phase boundary and vice versa, at the boundary $T_c$ and $T_N$ should come out to be zero if such corrections are taken into account. This requires a treatment of the model hamiltonian which goes beyond the level of random phase approximations made in this paper. The fact, that the $d$-paired and anti-ferromagnetic solutions both have their optimum at half filling, is rather worrying, as in a real solid the anti-ferromagnetic solution will in practice turn out to be the more stable one, due to the opening of a Mott-Hubbard gap.

Fortunately nature does provide us with a way to make a separation in parameter space between the anti-ferromagnetic and superconducting states. As already pointed out above, in practice there will always be a finite value of $t'$. From Fig. 2 we see, that in this case the maximum value of the DOS does not occur at half filling of the band. A well-known result from BCS theory is, that a high DOS at the Fermi level enhances $T_c$. If on the other hand precisely 50 % of the states is occupied, the opening of an anti-ferromagnetic gap causes a downward shift of all occupied levels in the reduced Brillouin-zone, which is the reason why the anti-ferromagnetic solution is best stabilized at precise half filling. This effect is demonstrated in Fig. 3, where we see that indeed the lowest free energy of the $d$-paired state occurs now at 35% filling, whereas the anti-ferromagnetic solution is still at half filling. We also notice from this plot, that this a-symmetry implies that the highest $T_c$'s of a $d$-paired superconductor are to be expected on the left (‘hole-doped’) side of half-filling. Lower $T_c$’s occur on the right side.

Let us now consider the $\Delta/T_c$-ratio following from the gap equation. Within the context of BCS theory we have $\Delta_0(T) = 0$ at $T_c$, so that $T_c$ follows from
$$\frac{2}{J_0} = \sum_q \epsilon_q^{-1} \tanh \left( \frac{\epsilon_q}{2k_B T_c} \right) \left[ \cos q_x a \pm \cos q_y a \right]^2$$  \hspace{1cm} (13)

where the ± sign refers again to the two symmetries of pairing. This equation can be easily solved numerically. The result is, that for extended s-wave pairing the ratio $2\Delta_0/k_B T_c$ is 6.5, whereas for d-wave pairing it rises gradually from 4 if $J_0 \ll W$, up to 6.5 in the limit where $J_0 \gg W$. This is not sensitive to the value of the parameter $t'$. We should keep in mind here, that $\Delta_0$ is the maximum value reached by $\Delta(k)$ (respectively at the $(\pi,0)$- and $(\pi,\pi)$-point for d- and s*-pairing).

Finally it is interesting to look how the mean field estimate of $T_c$ depends on the coupling strength $J_0/W$. In Fig. 6 $T_c^{MF}/W$ is displayed as a function of $J_0/W$ for the d-wave channel. First of all we notice, that for $J_0 > W/4$ the value of $T_c^{MF}$ is about $J_0/4$. For $J_0/W << 1$ this crosses over to a quadratic dependency $T_c^{MF} = 4J_0^2/W$. For comparison a similar curve is displayed for conventional s-wave pairing, using the negative U Hubbard model in a band with a square DOS. We notice that the mean field transition temperature with the latter model becomes $T_c^{MF} = |U|/4$ for large $|U|$ (which is actually outside the range of validity of the BCS weak coupling approach [11,12]), and has the familiar BCS-like $\exp \left( -W/|U| \right)$ behaviour for small $U$. The $T_c$ for the extended s-wave pairing lies again below the negative $U$ curve, and is only finite above a threshold value of $J_0$ as discussed above.

A consequence of this is, that the model hamiltonian proposed here leads to quite reasonable values of the transition temperature, which are relatively insensitive to the value assumed for the bandwidth. If we assume that for example $J_0 = 0.1 eV$, we would find that the Neél temperature in the Mott-insulating state can not exceed the mean field value for $Z = 4$ interacting neighbours $T_N^{MF} = ZS(S+1)J_0/6 = 580 K$. If we assume that the bandwidth is smaller than about 0.5 eV, we obtain from the BCS gap equation that the d-wave transition temperature can not exceed the mean field value $T_c^{MF} = 290 K$. This demonstrates that the optimal Neél temperature and the optimal superconducting transition temperature have a ratio of about 2 for $J_0/W$ of the order 0.2 to 1. Keeping in mind, that with the mean field approach we over-estimate both $T_N$ and $T_c$, I expect that the ratio between the two should
remain relatively intact if corrections beyond the mean field approximation are included. In the limit where \( J_0/W \) is small, \( T_c \) comes out smaller, although the suppression of the transition temperature goes much slower than for conventional \( s \)-wave superconductivity. For example if the bandwidth is 1 eV we obtain \( T_c = 137 \) K, and with \( W = 2 \) eV we find that \( T_c = 74 \) K.

Finally it is possible now to draw a phase diagram in the temperature versus doping plane. Let us choose \( J_0 = 0.1eV \), which gives approximately the correct value for \( T_N \), and \( t'/t = -0.7 \) which gives approximately the right Fermi surface. To stay in the regime where \( T_N \approx 2T_c \), let us assume \( 8t = W = 0.5eV \). The latter parameter is rather small compared to the 2 to 3 eV of the bare copper-oxygen \( p_x, p_y, d_{x^2-y^2} \) anti-bonding band \[35\], and leads to a slight over-estimation of \( T_c \). Although the estimated Neél temperature can be indicated at half filling of the phase-diagram, the present analysis has no bearing on the region near half filling, which was left open for that reason. The phase diagram, displayed in Fig.\[7\], perhaps somewhat optimistically gives values of \( T_c \) above 200 K, which so far has not been found experimentally. According to the rule-of-thumb that \( T_c \) scales with \( T_N \) \[23\], one has to look for systems with relatively high Neél temperatures in order to reach room temperature superconductivity. A number of factors will lower \( T_c \) below the mean field value given here. First of all, anti-ferromagnetic correlations will occur near the Mott-insulating state, which tend to suppress the superconducting order. Very strong on-site spin correlations are known to exist due to the large on-site \( U \), but \( d \) and \( s^* \)-pairs are insensitive to this interaction channel, as can be seen from the gap equation. Second, the mean field approach links \( T_c \) directly to the energy scale of the pair-breaking, which again leads to an overestimation of \( T_c \). The reason for this, is that the long range phase-coherence can be lost in a dephasing-transition, if the phase fluctuations have a lower energy scale than the pair-breaking energy. This requires a better knowledge of the phase fluctuation spectrum of the \( d \)-wave superconducting state.

Using a weak coupling BCS treatment of the \( t-t'-J \) model, I have shown that there exists a universal ratio of 2 between the Neél temperature at half filling and the optimal mean field
superconducting transition temperature. If a realistic shape of the Fermi surface is taken, the optimal $T_c$ occurs for 0.7 electron per site, while the Mott-insulating antiferromagnetic state occurs at half filling. With these parameters, $T_c$ is shown to be lower for electron doping than for hole doping.

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[17] A small difference is the absence of the spin-independent second term of Eq. [1] in the expressions of Monthoux. It implies that in their analysis the triplet channel is repulsive, and the interaction in the $s^*$ and $d_{x^2-y^2}$ channels is scaled with a factor $3/4$ compared to our expressions. Also a repulsive interaction in the $d_{xy}$-channel emerges.

[18] The charging energy per unit volume for a small fraction of spherical $d$-type droplets
dispersed in an $s^*$-type medium is $\frac{8}{15}\pi^2 e^2 (n_d - n)^2 r^5 \cdot N/V$, where $N = \frac{n_d - n_s}{4\pi r^3} V$ is the number of droplets, $V$ is the sample volume, $n_d$, and $n_s$ are the densities of the $d$ and $s$-type ordered states, and $n$ is the average density. For $n_d$ and $n_s$ of comparable magnitude we interpret $r$ as the characteristic length scale on which phase separation occurs with a charging energy per unit volume $\frac{2\pi}{5} e^2 (n_d - n)(n - n_s)r^2$, which has the correct limiting behaviour for small $n_s$ or $n_d$ and interpolates between these two cases. In a layered electron gas one can instead consider a cylindrical shape, for which the charging energy density is $\frac{\pi}{4} e^2 (n_d - n)(n - n_s)r^2$. The $r^2$ scaling behaviour tends to reduce $r$. A lower bound occurs due to quantum size effects: Due to quantum confinement the kinetic energy of each electron increases with an amount of about $\hbar^2 \Delta k^2 / 2m^*$. For particles moving in a 2D plane $\Delta k^2 \approx \frac{2\pi}{r}$, so that the increase in energy per unit volume is $\frac{2\pi\hbar^2}{m^* r^3} (n_d - n)(n - n_s)(n_d + n_s - n)(n_d - n_s)^{-2}$, which again interpolates between the two limits where $n_d$ or $n_s$ is small.

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[22] The minimum energy due to the combined effect of the Coulomb interaction and quantum confinement occurs at a length scale $r^4 = 8a_0(n_d + n_s - n)(n_d - n_s)^{-2}$. The increase in energy per unit volume is then $\pi \text{Ry}(n_d - n)(n - n_s)(n_d - n_s)^{-1} \sqrt{(2a_0)^3(n_d + n_s - n)}$, where Ry and $a_0$ are the effective Rydberg and Bohr radius respectively. This should be smaller than the gain in free energy due to phase separation. For the parameters considered in this text, the latter is at least two orders of magnitude smaller than the former, implying that phase separation is strongly suppressed.

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FIGURES

FIG. 1. First Brillouin-zone of a square lattice, with the occupied states indicated as the shaded area. The lozenge indicates the perfectly nested Fermi surface.

FIG. 2. Density of states at the Fermi energy in units of $1/W$ as a function of electron occupation number.

FIG. 3. Free energy difference with the normal state of the $s^*$-wave (solid) and $d$-wave (long dashed) superconducting state and of the anti-ferromagnetic state (short dashed curve) with $J_0 = 0.6W$ and $t' = 0$. Energies are in units of $W$.

FIG. 4. Phase diagram in the $J_0$-$n$ plane, where $n$ is the number of electrons per unit cell.

FIG. 5. Free energy difference with the normal state of the $s^*$-wave (solid) and $d$-wave (long dashed) superconducting state and of the anti-ferromagnetic state (short dashed curve) with $J_0 = 0.6W$ and $t' = -0.7t$. Energies are in units of $W$.

FIG. 6. Solid curve: $T_c/J_0$ calculated for the $d$-wave channel of the exchange-only model with $t' = 0$ and 1 electron per site. The same curve is obtained for $t' = 0.7$ with 0.7 electron per site. Open lozenges: $T_c$ of the $s^*$-wave channel with the latter parameters. Dotted curve: $T_c/|U|$ versus $|U|/W$ for the negative $U$ Hubbard model taking a square DOS.

FIG. 7. Phase diagram in the temperature-density plane with the parameters $J_0 = 0.1eV$, $W = 8t = 0.5eV$, and $t'/t = -0.7$. The curves are interrupted in the part near the middle, where the present analysis is physically meaningless. The mean field Neél temperature at half filling, using the same value for $J_0$ as in the metallic regime, is indicated as a clover.