Pairing instabilities in the two-dimensional Hubbard model

Andrey V. Chubukov

Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801 and P. L. Kapitza Institute For Physical Problems, Russian Academy of Sciences, 117334 ul. Kosygina 2, Moscow, Russia

Jian Ping Lu

Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801 (Received 22 May 1992)

We show that for low and moderate fillings the ground state of the two-dimensional Hubbard model with positive-U and nearest-neighbor hopping is unstable with respect to d-wave pairing with d_{xy} symmetry of the gap wave function: $\Delta \sim \sin k_x \sin k_y$. The inclusion of the next-neighbor hopping may either suppress the pairing or change the symmetry of the superconducting state.

The discovery of high- T_c superconductivity stimulated a search for pairing instabilities in two-dimensional (2D) correlated electronic systems. It is now generally believed that the low- Γ behavior of cuprate superconductors may be described in terms of the simple one-band Hubbard model on a 2D square lattice which, presumably, also involves a next-nearest hopping term in order to fit the shape of a Fermi surface.¹

The nearest-neighbor Hubbard model has been extensively studied in the past few years. Both analytical²⁻⁷ and numerical⁸⁻¹¹ calculations found that at half-filling the system has long-range antiferromagnetic order. Away from half-filling, antiferromagnetic order first transforms into an incommensurate one (linearly polarized³ or spiral⁷ depending on the strength of the coupling) and then disappears above some critical doping concentration. For weak coupling, the destruction of the magnetic order occurs very near half-filling and the conventional paramagnon theory predicts the d-wave pairing with $\Delta \propto \cos k_x - \cos k_y$.⁵ Though the justification of the paramagnon theory is questionable because both Cooper and zero-sound channels contain Van Hove singularities, more sophisticated renormalization-group (RG) calculations^{2, 12} also point to the possibility for a transition into a superconducting $d_{x^2-y^2}$ state. The same type of instability was also found in recent calculations¹³ which used the phenomenological form of $\gamma(q)$ known to fit the NMR data.¹⁴ It was also argued⁴ that the renormalization of the quasiparticle self-energy may change the form of the Fermi surface in such a way that the nodes of the superconducting gap will be located in the regions of the Brillouin zone where there is no free Fermi surface. Were it the case, the pairing gap function would be nodeless over the whole Fermi surface, though, formally, the d-wave symmetry (i.e., the change in sign of Δ under a rotation to $\pi/2$) would be preserved.

While the presence of a well-defined peak at (π, π) in the polarization operator near half-filling uniquely favors $d_{x^2-y^2}$ pairing, at least for small values of the coupling, little is known about the possible pairing instability for larger doping concentrations when $\chi(\mathbf{q})$ is flat. Different numerical studies^{8,11} and low-U mean-field calculations¹⁵ did not find any evidence for superconducting instabilities in this region. Challenging these results, Baranov and Kagan¹⁶ recently developed a perturbative expansion in the filling factor, similar to that in the 3D systems,^{17,18} and found that the positive-U Hubbard model is unstable, at arbitrary small filling, against *d*-wave pairing, but with $\Delta \propto \sin k_x \sin k_y$.

In this paper, we show that (i) the d_{xy} instability is likely to be dominant for all moderate fillings, and (ii) that the inclusion of the next-nearest hopping t' leads to a very rich phase diagram where besides the d_{xy} instability one can also find the regions of the $d_{x^2-y^2}$ and *p*-wave pairing.

A standard way to search for a possible superconducting instability in the positive-U Fermi-liquid in the low density limit is to renormalize the bare vertex for the Cooper channel and check the signs of higher-momentum harmonics which are generated by the screening of the scattering amplitude due to the fermionic back-ground.^{19,17,18} In the 3D case, the polarization operator in the particle-hole channel (Fig. 1) is nonanalytic for the momentum transfer near $2k_F$, which in the real space means that the screening produces a long-range oscillating "tail" in the effective interaction between the particles on the Fermi surface (Kohn-Luttinger effect¹⁹). Combined with the obvious difference in signs between even and odd angular momentum *l* harmonics, this effect leads to an attraction in all large-l channels.¹⁹ It was later shown^{17,18} that the Kohn-Luttinger effect stretches right up to l = 1 and actually ensures the *p*-wave pairing in the 3D Fermi liquid at low density.

In two dimensions, the situation is completely different because the effective (renormalized) interaction between the two particles on the Fermi surfaces does not contain nonanalytical terms which one might expect to be responsible for attraction.^{20,16} However, this does not rule out the possibility for a superconductivity. The point is that, in the case of initial on-site repulsion, the regular qdependence in the effective bare vertex $\Gamma(\mathbf{q})$, where q is a transferred momentum, also appears only after the renor-



FIG. 1. Irreducible diagrams which contribute to the bare interaction in the Cooper channel in the second order in the perturbation theory. We use the same diagrammatic technique as in Ref. 19. The dotted line represents the interaction potential. The contributions from the first three diagrams completely cancel each other. The interaction potential on the remaining one links p to -k, which obviously ensures the additional change in the sign of all harmonics with odd angular momentum.

malization. These q-dependent terms are absent in a Fermi-gas description²⁰ when the energy spectrum is approximated by a parabola ($\epsilon_k \sim p^2/2m - \epsilon_F$), but they do appear when the higher-order terms in the expansion of ϵ_k are taken into account. Since the q dispersion in $\Gamma(\mathbf{q})$ entirely determines the possibility for the pairing instability with nonzero orbital momentum (the conventional s-wave instability is suppressed due to the first-order onsite repulsion), exact calculations are required to establish whether a particular model of interest is unstable against BCS pairing.

Given the arguments above, we will focus on the 2D Hubbard model on a square lattice

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i\downarrow} .$$
⁽¹⁾

The hopping term is chosen to be nonzero for the nearest (t) and next-nearest (t') neighbors.

The study of a superconductivity away from the Fermi-gas description requires knowledge of the possible symmetries of a gap function. For the 2D square lattice, the D_4 space group is known to contain four onedimensional (singlet) irreducible representations, A_1 and A_2 for s wave, B_1 and B_2 for d wave, and one twodimensional representation, E, which corresponds to a triplet pairing.²¹ An arbitrary eigenfunction in each representation then can be written as a product of the corresponding basic eigenfunction $[\cos k_x + \cos k_y]$ for A_1 , $\cos k_x - \cos k_y$ for B_1 , $\sin k_x \sin k_y$ for B_2 , $(\cos k_x)$ $-\cos k_y \sin k_x \sin k_y$ for A_2 , and $A \sin k_x + B \sin k_y$ for E] and a representative from a complete set of functions which have the whole D_4 symmetry. At low density, i.e., small ap_F , the polar coordinates $(|k|, \phi)$ are more convenient and the complete sequences of eigenfunctions can be rewritten as

$$A_{1}: \cos(4n\phi) ,$$

$$A_{2}: \sin[4(n+1)\phi] ,$$

$$B_{1}: \cos[(4n+2)\phi] ,$$

$$B_{2}: \sin[(4n+2)\phi] ,$$

E: $A \sin[(2n+1)\phi] + B \cos[(2n+1)\phi]$.

In the leading order in the density, the momentum transfer for the particles at the Fermi surface is the same as in the isotropic case: $q^2 = 2p_F^2[1-\cos(\phi-\phi')]$ where ϕ and ϕ' measure the directions of the momenta for incoming and outgoing particles. It then immediately follows that, to get the first (n=0) eigenfunctions in the *p*-wave, *d*-wave $(B_1 \text{ or } B_2)$, and unconventional *s*-wave (A_2) channels, one should expand the renormalized interaction $\Gamma(\mathbf{q})$, up to $O(q^2)$, $O(q^4)$, and $O(q^8)$, respectively. In what follows we will restrict with a search for *p*- and *d*-wave instabilities.

The general form of the low-q expansion of $\Gamma(\mathbf{q}) = \Gamma(q, \theta)$ is

$$\Gamma(\mathbf{q}) = A + B(qa)^{2} + (qa)^{4}(C_{1} + C_{2}\cos 4\theta) + 0[(qa)^{6}], \qquad (2)$$

where a is the lattice spacing and $\theta = (\phi + \phi')/2$. For small coupling, $A \sim U$, while both B and $C_{1,2}$ have the order of U^2/t reflecting the fact that the q dispersion in $\Gamma(\mathbf{q})$ appears only after the renormalization of the initial on-site repulsion.²² Substituting the expression for q^2 in Eq. (2), we find

$$\Gamma_{E} = 2(ap_{F})^{2}B ,$$

$$\Gamma_{B_{1}} = 2(ap_{F})^{4}(C_{1} + 3C_{2}) ,$$

$$\Gamma_{B_{2}} = 2(ap_{F})^{4}(C_{1} - 3C_{2}) .$$
(3)

Obviously, the sign of Γ ... determines the possibility for the pairing instability in the corresponding channel.²³ Note that in writing Eq. (3) we took into account the additional change in sign of the *p*-wave component imposed by the spin summation.

The coefficients in Eq. (2) were obtained analytically by calculating the renormalization of the vertex function in the particle-hole channel (Fig. 1) and expanding the electronic spectrum

$$\epsilon_k = -2[t(\cos k_x a + \cos k_y a) + 2t' \cos k_x a \cos k_y a] - \mu$$
(4)

up to the third order near its minima at k = 0. This approach is valid for $\delta = t'/t > -\frac{1}{2}$. After the lengthy calculations, we obtained that, to the leading order in (ap_F) ,

$$\Gamma_E = \lambda (ap_F)^2 \frac{t+4t'}{(t+2t')} , \qquad (5)$$

$$\Gamma_{B_1} = \frac{\lambda}{160} (ap_F)^4 \frac{13t^2 + 48tt' - 48(t')^2}{(t+2t')^2} .$$
 (6)

$$\Gamma_{B_2} = \frac{\lambda}{160} (ap_F)^4 \frac{-3t^2 - 48tt' + 208(t')^2}{(t+2t')^2} . \tag{7}$$

Here $\lambda = (1/48\pi)[u^2/(t+2t')]$ and $(ap_F)^2 = [4(t+t')+\mu]/(t+2t')]$. For t'=0, these equations coincide with the results of Baranov and Kagan.¹⁶

It follows from Eqs. (5)-(7) that if only nearestneighbor hopping is present (t'=0), the interaction is repulsive in the *p*-wave and d_{B_1} channels, but it is attractive in the d_{B_2} channel. This uniquely leads to the d_{xy} superconductivity in the nearest-neighbor Hubbard model at low density. However, the inclusion of the secondneighbor hopping term may change the type of the instability (Fig. 2). For t' > 0, the region of the d_{xy} instability stretches up to $\delta = t'/t = 0.28$. For $0.28 < \delta < 1.22$, both *p*- and *d*-wave instabilities are suppressed (there is possibly A_2 instability in this region). For larger δ , the interaction in the B_1 channel becomes attractive while that in the B_2 channel remains repulsive, and this leads to the $d_{x^2-y^2}$ superconductivity.²⁴

For negative t' (which is believed to be the case for some high- T_c compounds²⁵), the B_2 instability disappears at $\delta = -0.05$, while the B_1 channel becomes attractive for $\delta < -0.22$. However, the effective interaction in the p-wave channel also changes the sign at $\delta = -0.25$ and immediately overshadows the B_1 instability since the pwave amplitude contains fewer powers of ap_F . In the vicinity of $\delta = -\frac{1}{2}$, the expansion in powers of q breaks down since the Fermi surface, even for a small density of the carriers, stretches up to the boundary of the Brillouin zone.²⁶ A simple estimate shows that the maximum value of T_c for the *p*-wave instability which one can reach before entering into the dangerous region $|1-2\delta| \leq (ap_F)^2$ is given by $\ln[(ap_F)^2/T_c] \sim \ln^2 ap_F$. It is curious that it differs only by a preexponential factor from the expression one might obtain if the Kohn-Luttinger effect was actually present in the 2D Fermi gas.¹⁸



FIG. 2. The low-density part of the phase diagram of the 2D Hubbard model on the square lattice. n is the density of electrons and b is related to the ratio of the nearest and next-nearest hoppings by $b=2\delta/(1+2\delta)$, where $\delta=t'/t$. The hatched regions marked as B_1 , B_2 , and E correspond to the superconducting states with $d_{x^2-y^2}$, d_{xy} , and p-wave symmetry of the gap wave function, respectively. For negative b, the slope of the right boundary of the B_1 phase (dashed line) is not known exactly.

For $\delta < -\frac{1}{2}$, the minimum of the energy spectrum shifts from (0,0) to $(0,\pi)$ and $(\pi,0)$. Correspondingly, the Fermi surface of electrons forms pockets around these points. This opens an additional channel of the interaction with the momentum transfer near (π,π) . The calculations in this case require a larger amount of work and we only checked that the *p*-wave instability is suppressed for all $\delta < -\frac{1}{2}$.²⁷

The next question one should address is whether the superconducting instabilities found above are specific only for low filling or they survive in passing from low to moderate densities. To answer this question, we calculated the leading corrections to the partial amplitudes in the B_1 and B_2 channels. These corrections result from (i) a noncircular form of the Fermi surface, (ii) ap_F dependence of $C_{1,2}$ in Eq. (2), and (iii) the next terms in the low-q expansion of the effective vertex [namely, $(aq)^{6}(D_{1}+D_{2}\cos 4\theta)$]. Naively, one might expect the finite-density corrections to diminish the (absolute) values of both *d*-wave vertices, since near half-filling the shape of $\Gamma(\mathbf{q})$ with the maxima at (π,π) is compatible with $d_{x^2-y^2}$ but not d_{xy} superconductivity. However, direct calculations show that the situation is less simple. Specifically, for the nearest-neighbor Hubbard model, we combined analytical and numerical calculations and obtained

$$\Gamma_{B_1} = \Gamma_{B_1}^0 [1 + 0.53(ap_F)^2] ,$$

$$\Gamma_{B_2} = \Gamma_{B_2}^0 [1 + 0.63(ap_F)^2] ,$$
(8)

where Γ^0 stands for the leading term given by Eqs. (6) and (7). It follows from Eq. (8) that away from low density the partial amplitudes in the B_1 and B_2 channels first move apart, in contradiction with the naive expectations. This strongly indicates that for small U the B_2 instability is very likely to survive for all moderate filling factors before the polarization operator in the particle-hole channel acquires a well-defined maxima at (π,π) . The latter seems to happen rather close to the half-filling because the polarization operator at (π,π) is only logarithmically divergent at $\mu = 0$. Obviously, the critical temperature for the B_2 instability passes through a maximum at some intermediate doping concentration. Note also that the pwave amplitude only increases with the density¹⁶ $\Gamma_E = \Gamma_E^0 [1 + 0.19(ap_F)^2]$ and hence no *p*-wave instability is expected for all fillings.

For $t' \neq 0$, we addressed the question of stability of various superconducting phases by calculating numerically the positions of the critical lines for B_1 and B_2 instabilities as functions of the density. The results are presented on Fig. 2. We found that for t' > 0 the two critical lines come closer to each other probably indicating that above some critical density the region of the normal phase will disappear leaving only the crossing (i.e., first-order transition) line between the two different *d*-wave states. However, the investigation of this possibility is beyond the scope of our low density approach. For t' < 0, the calculations indicate that the width of the superconducting (B_2) region increases with ap_F complementing the results obtained for only nearest-neighbor hopping. However,

we are not able to draw definite conclusions about the slope of the B_1 instability line. It also follows from our calculations that the boundary of the *p*-wave instability terminating at $\delta = -0.25$ does not contain any significant ap_F dispersion.

Summarizing our findings, we have shown that the 2D Hubbard model with weak on-site repulsion and nearestneighbor hopping is unstable against d_{xy} pairing for all densities of carriers except very close to half-filling, where from the general arguments one should expect $d_{x^2-y^2}$ superconductivity. In the more general case of nearest- and next-nearest-neighbor hopping, the superconducting state at low density may have either B_1 or B_2 or even *p*-wave symmetry depending on the particular ratio of the hoppings. Note that the crossing between B_1 and B_2 instabilities near half-filling was tentatively found in the random-phase approximation (RPA) calculations for the nearest-neighbor Hubbard model.⁵

Of course, the superconducting instabilities found in this paper are nonuniversal in a sense that they are sensitive to the particular form of the energy spectra and also

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to the q dependence of the bare interaction U(q). However, it is worth noticing that the conclusion about d_{xy} instability for small t' remains unchanged if the screened Coulomb repulsion acts not only at a given site but also between nearest neighbors. For a more complicated form of U(q), the theory presented here will be valid if the second-order q-dependent contributions which involve $U^2(0)$ exceed the corresponding first-order terms in the expansion of U(q) in powers of q. It is also interesting to note that only d-wave pairing seems to be consistent with the recent NMR measurements of $1/T_1$ in cuprate oxide superconductors below T_c .²⁸

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- ²²It is worth noticing that, for not very small U, when Born approximation fails, the interaction potential should be replaced by the scattering amplitude T. In two dimensions, the vacuum renormalization is known to be singular in the low-density limit (Ref. 20) and the calculation of T yields universal *small* repulsion $T = -1/2 \ln(ap_F)$ independently on the actual strength of the coupling.
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