Superconductive pairing in the Hubbard model with a low occupancy

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It is shown that a D-dimensional ($D > 2$) electron system described by the Hubbard model far from the half-occupancy is unstable against the superconducting transition to a state with triplet pairing. It is shown that in the two-dimensional case there is no triplet pairing (in contrast to the case of an arbitrary value of D).

1. The possibility of nonphonon superconducting mechanisms has rekindled strong interest in the Hubbard model:

$$H=-t\sum_{\langle ij\rangle,\sigma}c_{i\sigma}{}^{+}c_{j\sigma}+U_0\sum_i n_{i\uparrow}n_{i\downarrow}.$$

In particular, many papers have been published on the D-dimensional Hubbard model with half-occupancy and also in the limit $D\to\infty$ (Refs. 1 and 2). The Fermi-liquid limit $U_0\ll t$ was considered in the two-dimensional Hubbard model near half-occupancy[3-5] and it was found that the normal Fermi system becomes unstable against the superconducting transition to a state with singlet d pairing. Here we analyze the opposite limit of low occupancy (heavy doping). In this case the normal Fermi system is also unstable against the superconducting transition (but to a state with the triple pairing when $D > 2$) and a considerable role in the appearance of the photoconductivity is played by the Kohn singularity in the polarization operator.

2. The Hubbard Hamiltonian for a simple D-dimensional "cubic" lattice considered in the momentum representation is

$$H-\mu N=\sum_{p,\sigma}\varepsilon_p c_{p,\sigma}^{+}c_{p,\sigma}+{}^1/_2U_0\sum_{pp'k\sigma\sigma'}c_{p,\sigma}^{+}c_{-p+k,\sigma'}^{+}c_{p',\sigma}c_{-p'+k,\sigma'},\tag{1}$$

where

$$\varepsilon_p=-2t(\cos p_1a+\ldots+\cos p_Da)-\mu$$

is the electron spectrum, a is the lattice constant, t is the energy of a jump, and U_0 is the Hubbard repulsion constant at one site. Far from half-occupancy we have

$$\varepsilon_p\approx\frac{p^2}{2m}-\mu^*,\qquad m=\frac{1}{2a^2t},\qquad \mu^*=\mu+2Dt=\frac{p_F{}^2}{2m}.\tag{2}$$

A low occupancy implies that $p_Fa\ll 1$. We can see that in the specified approximation the unrenormalized electron spectrum is identical with the spectrum of a free Fermi gas and the Hubbard Hamiltonian is exactly equivalent to the Hamiltonian of a slightly nonideal Fermi gas with repulsion between the particles. The corresponding gas parameter is proportional to the quantity

$$mU_0p_F{}^{D-2}=\frac{U_0}{2a^2t}p_F{}^{D-2}.$$

In this way the model of a slightly nonideal Fermi gas includes the Hubbard case with a weak interaction $U_0 < t$ and a density of order unity as well as the Hubbard case with a strong interaction $U_0 > t$, but with a low density. If $D = 3$, the role of the gas parameter f_0p_F is played by

$$\frac{mU_0}{4\pi}p_F=\frac{U_0}{8\pi a^2t}p_F,$$

and if $D = 2$, the gas parameter f_0 corresponds to

$$\frac{mU_0}{4\pi}=\frac{U_0}{8\pi a^2t}.$$

It was shown in Ref. 6 that, because of the presence of a Kohn singularity of the form $(q-2p_F)\ln|q-2p_F|$ in the effective interaction $\tilde{\Gamma}(q)$ of two Fermi particles via the Fermi background, a three-dimensional slightly nonideal Fermi gas with repulsion between the particles is unstable against the superconducting transition to a state with triplet p pairing and the transition takes place at a temperature

$$T_{c_1}\propto\mu^*\exp\left\{-\frac{5\pi^2}{8(2\ln 2-1)(f_0p_F)^2}\right\}.$$

On the other hand, it was pointed out in Ref. 7 that a strong two-dimensional Kohn singularity of the form $\mathrm{Re}(q-2p_F)^{1/2}$ in $\tilde{\Gamma}(q)$ (see also Ref. 8) does not result in the superconducting transition in a two-dimensional slightly nonideal Fermi gas with repulsion, since the value of q (composed of the momenta of the particles entering (**p**) and leaving (**p**′) the Cooper channel when these particles lie on the Fermi surface) cannot exceed $2p_F$.

3. We now consider the problem of the superconducting transition in the D-dimensional Hubbard model with low occupancy. The problem of the feasibility of the superconducting transition in the Fermi system with repulsion can be solved by calculating (in the case of a gas) the effective unrenormalized vertex for the Cooper channel $\tilde{\Gamma}(\mathbf{p},\mathbf{p}')$ to second order in perturbation theory:

$$\Gamma_D(\mathbf{p},\mathbf{p}')=U_0+U_0{}^2\Phi(\mathbf{p},\mathbf{p}').\tag{3}$$

It is very important to note that $\Phi(\mathbf{p},\mathbf{p}')$ does not represent simply a polarization loop, but a set of second-order diagrams which cannot be cut along two fermion lines directed to the same side. There are four such diagrams (see Refs. 6 and 9). After averaging over the spin indices, their sum is $\Pi(\mathbf{p}+\mathbf{p}')$ and not $\Pi(\mathbf{p}-\mathbf{p}')$, as one would find if an allowance were made for just one polarization loop:

$$\Pi(q)=\int\frac{d^Dk}{(2\pi)^D}\frac{\theta(\varepsilon_{\mathbf{k}+\mathbf{q}})-\theta(\varepsilon_{\mathbf{k}})}{\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}}.$$

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It should be noted that in the $D=3$ case this circumstance leads not to the d but to the p pairing (see Ref. 6). In the case of low occupancy $p_F a \ll 1$ we can confine ourselves to the approximation (2) for the unrenormalized electron spectrum. Then, Eq. (3) for the unrenormalized vertex of the Cooper channel $\tilde{\Gamma}_D(q)$ becomes

$$\tilde{\Gamma}_D(q)=U_0+U_0^2\Pi_D(q),$$
$$\Pi_D(q)=mp_F^{D-2}\frac{\Omega_{D-1}\Gamma^2((D+1)/2)}{\pi^D(D-1)\Gamma(D)}\,{}_2F_1\left(1,\frac{2-D}{2};\frac{3}{2};\frac{q^2}{4p_F^2}\right),$$
$$q=|\mathbf{p}+\mathbf{p}'|\leqslant 2p_F. \tag{4}$$

The polarization operator $\Pi_D(q)$ was first calculated in Ref. 10. The following notation is used in Eq. (4): $\Omega_D = 2\pi^{D/2}/\Gamma(D/2)$ is the area of a unit sphere in a D-dimensional space; ${}_2F_1(a,b;c;z)$ is the hypergeometric function. The results of Fig. 10 determine the following nature of Kohn singularity in the limit $q\to 2p_F$:

a) if $D\neq 1, 3, \ldots, 2n+1, \ldots$, then $\Pi_D(q)$ is a regular function when $q<2p_F$ and we have $\Pi_D(q)\sim(2p_F-q)^{(D-1)/2}$ when $q>2p_F$;

b) if $D=1, 3, \ldots, 2n+1, \ldots$, then $\Pi_D(q)\sim(q-2p_F)^n\ln|q-2p_F|$.

The appearance of the superconductivity is clearly related to the presence of a pole in the upper vertex $\Gamma(q)$ of the Cooper channel, which is the solution of the Bethe–Salpeter integral equation. Reduction of this equation to algebraic form is possible if use is made of the Gegenbauer polynomials $C_l^{(D-2)/2}(\cos\theta)$ which are D-dimensional analogs of the Legendre polynomials $[(q^2=2p_F^2(1+\cos\theta)]$. They satisfy the orthogonality relationships

$$\int_0^\pi C_l^{(D-2)/2}(\cos\theta)C_m^{(D-2)/2}(\cos\theta)(\sin\theta)^{D-2}\,d\theta\sim\delta_{lm}.$$

The Cooper pairing with the generalized orbital momentum l appears if the value of the corresponding partial harmonic of the unrenormalized vertex $\tilde{\Gamma}_l$ is negative and has the maximum absolute value, $\tilde{\Gamma}_0\approx U_0>0$, so that there is no s pairing. The maximum absolute value $|\tilde{\Gamma}_l|$ corresponds to $l=1$ (i.e., to the p pairing):

$$\tilde{\Gamma}_1^{(D)}=-mp_F^{D-2}\frac{2^{D-3}\Omega_D}{\pi^D(D-1)}$$
$$\times\left[\frac{(D-2)\Gamma((D+1)/2)\Gamma((D-1)/2)}{\Gamma(D+1)}\right]^2$$
$$\times{}_3F_2\left(2,\frac{D+1}{2},\frac{3D-2}{2};D+1,D+1:1\right)<0. \tag{5}$$

The other harmonics with $l\geqslant 2$ are either positive or smaller in absolute magnitude. The superconducting transition temperature is given by

$$T_{c_1}\sim\mu^*\exp\left\{-\frac{2}{|\tilde{\Gamma}_1^{(D)}|g(\mu^*)}\right\}, \tag{6}$$

where

$$g(\mu^*)=2mp_F^{D-2}\frac{\Omega_D}{(2\pi)^D}$$

is the density of states at the chemical potential (Fermi) level. If $D=3$, then Eqs. (5) and (6) are identical with the results reported in Ref. 6.

4. We conclude by considering in detail the situation when $D=2$ (see also Ref. 11). In this case it follows from Eq. (4) that in the approximation described by (2) the unrenormalized vertex for the Cooper channel is

$$\tilde{\Gamma}=U_0+m/(2\pi)U_0^2=\tilde{\Gamma}_0>0$$

and, as pointed out above, the superconducting transition does not occur. Therefore, in the case of the two-dimensional model we can expand the spectrum of cosines further (through the third term). This gives

$$\varepsilon_p\approx\frac{p^2}{2m}-\alpha(p_x^4+p_y^4)-\mu^*,\quad \alpha=\frac{a^2}{24m},$$

$$\mu^*=\mu+4t=\frac{p_F^2}{2m}. \tag{7}$$

In contrast to Eq. (2) this spectrum is not isotropic, so that $\Pi(\mathbf{q})$ may depend not only on $q=|\mathbf{q}|$, but also on the combinations q_x and q_y, which are invariant relative to the transformations of the symmetry group of the square (isomorphous with D_4). Fairly complicated calculations of $\Pi(\mathbf{q})$, involving a singular denominator, lead to the following result:

$$\Pi(\mathbf{q})=\frac{m}{2\pi}\left\{1-\mathrm{Re}\left[1-\frac{4p_F^2}{q^2}\left(1+a^2\frac{q_x^4+q_y^4}{48q^2}\right)\right]^{1/2}\right.$$
$$\left.+\frac{q^2a^2}{48}+\frac{p_F^2a^2}{8}\right\},$$
$$\mathbf{q}=\mathbf{p}+\mathbf{p}'. \tag{8}$$

It is interesting to note that $\Pi(\mathbf{q})$ in Eq. (8) has a root contribution, which would have been obtained also by expanding cosines only up to the second term (it was first calculated in Ref. 8) as well as a nonroot contribution due to the correction $\alpha(p_x^4+p_y^4)$ to the electron spectrum.

The complete system of functions factorizing the kernel of the integral Bethe–Salpeter equation should be functions of the irreducible representations of the symmetry group. In the case of the D_4 group there are five irreducible representations: four of which are one-dimensional (A_1, A_2, B_1, and B_2), corresponding to a singlet state, and one (E) is two-dimensional, corresponding to a triplet state. The one-dimensional representations include the following functions:

1) A_1 (identical): $1, \cos 4\varphi, \cos 8\varphi, \ldots$;
2) A_2: $\sin 4\varphi, \sin 8\varphi, \sin 12\varphi, \ldots$;
3) B_1: $\cos 2\varphi, \cos 6\varphi, \cos 10\varphi, \ldots$;
4) B_2: $\sin 2\varphi, \sin 6\varphi, \sin 10\varphi, \ldots$.

The two-dimensional representation E includes the following set of harmonics:

$\cos\varphi, \cos 3\varphi, \cos 5\varphi, \ldots$;
$\sin\varphi, -\sin 3\varphi, \sin 5\varphi, \ldots$.

We consider the vectors $\mathbf{p}$ and $\mathbf{p}'$ as lying on the Fermi surface and rewrite $\Pi(\mathbf{q})$ from Eq. (8) in the form of a function of the angles φ_1, φ_2 between the vectors $\mathbf{p}$ and $\mathbf{p}'$, on the one hand, and the x axis, on the other. To lowest order in the small parameter $p_F a\ll 1$, we obtain

$$\Pi(\mathbf{q})=\Pi(\varphi_1,\varphi_2)=\frac{p_F{}^2a^2}{6}+\frac{p_F{}^2a^2}{24}\cos(\varphi_1-\varphi_2).$$

Hence, in this approximation, we have

$$\tilde{\Gamma}_{A_1},\ \tilde{\Gamma}_E>0,\quad \tilde{\Gamma}_{A_2},\ \tilde{\Gamma}_{B_1},\ \tilde{\Gamma}_{B_2}=0,$$

where $\tilde{\Gamma}_\alpha$ is the irreducible unrenormalized vertex for the Cooper channel in the case of a harmonic corresponding to the irreducible representation α. Therefore, we can say that in this low-occupancy limit the singlet s pairing and the triplet pairing are impossible.[2)] The precision of the calculations reported here is insufficient to analyze the possibility of the superconducting pairing for other harmonics and the problem of the existence of superconducting phases with the order parameters transforming in accordance with the irreducible representations A_2, B_1, and B_2, remains unsolved.

We should also point out that if the correction to the spectrum of free Fermi particles had been, in contrast to Ref. 7, spherically symmetric

$$\varepsilon_p \approx \frac{p^2}{2m}-\mu^* \to \frac{p^2}{2m}-\alpha p^4-\mu^*,\qquad 0<\alpha\ll 1$$

(this is the nature of the spectrum typical of ^{3}He quasiparticles in a solution of ^{4}He), then the Fermi system would have been unstable against triplet p pairing.

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[2)] A similar result was obtained also by V. N. Popov.

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