SUPERCONDUCTIVITY IN THE HUBBARD MODEL WITH STRONG REPULSION AND WEAK INTERACTION

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Superconductivity of an electron system with strong correlations with filling close to one electron per cell is investigated. Some special variables reducing the Hubbard model to a system of holes and local spins are introduced. Various magnetic states of the model: ferromagnetic, paramagnetic and antiferromagnetic are investigated. It is shown that the tendency to pairing caused by electronic correlations is suppressed by magnetic fluctuations.

The Hubbard model describes a system of electrons on a lattice with the Hamiltonian [1,2]

$$\mathscr{H} = \sum_{n \neq n'} t_{nn'} c^{+}_{n\sigma} c_{n'\sigma} + U \sum_{n} \hat{n}_{n\uparrow} \hat{n}_{n\downarrow} + \sum_{n\sigma} \mu_{\sigma} \hat{n}_{n\sigma}, \quad (1)$$

where $c^{+}_{n\sigma}$, $c_{n\sigma}$ are the Fermi operators of electrons on the lattice site n with spin projection $\sigma = \pm\frac{1}{2} \equiv \uparrow, \downarrow$; $t_{nn'} = t_{n'n}$ is the electron hopping integral from the lattice site n to the lattice site n'; U is the constant of Coulomb repulsion on a lattice site; $\hat{n}_{n\sigma} = c^{+}_{n\sigma} c_{n\sigma}$ is the operator of electron number with spin projection σ; $\mu_{\sigma} = \sigma\omega_0 - \mu$ is the chemical potential depending on the spin projection, where ω_0 is the precession frequency of the electron spin in an external magnetic field and μ is the usual chemical potential.

We shall develop the method of strong coupling when the last two terms of the Hamiltonian (1) are taken into account very precisely. The first term is considered as a perturbation [3]. For $U \gg t$ only three states $|na\rangle = |n0\rangle$, $|n\uparrow\rangle$, $|n\downarrow\rangle$ can be conserved per lattice site and the state $|n\uparrow\downarrow\rangle$ with two electrons per lattice site can be removed or can be taken into account as a perturbation by the parameter t/U. In that case the operators $c^{+}_{n\sigma}$, $c_{n\sigma}$, $\hat{n}_{n\sigma}$ can be expressed in terms of the Hubbard operators $X^{ab}_{n} = |na\rangle\langle bn|$ [3].

The operators $X^{0\sigma}_{n}$ and $X^{\sigma 0}_{n}$ anticommute in various lattice sites, while the others just commute. The Hamiltonian (1) for $U \to \infty$ has in terms of the Hubbard operators X^{ab}_{n} the form $\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_{\mathrm{int}}$, with

$$\mathscr{H}_0 = \sum_{n\sigma} \mu_{n\sigma} X^{\sigma\sigma}_{n}, \quad \mathscr{H}_{\mathrm{int}} = \sum_{n' \neq n} t_{n'n} X^{\sigma 0}_{n} X^{0\sigma}_{n'}. \quad (2)$$

On constructing the temperature Green functions of the initial Fermi operators $c^{+}_{n\sigma}$, $c_{n\sigma}$ we replace them by the Hubbard operators $X^{\sigma 0}_{n}$, $X^{0\sigma}_{n}$ and average them over the primary density matrix $\rho_0 = \exp(-\beta\mathscr{H}_0)$ together with the temperature S-matrix

$$S_{\tau} = T_{\tau} \exp\left(- \int_0^{\beta} \mathscr{H}_{\mathrm{int}}(\tau)\, \mathrm{d}\tau \right),$$

where $\beta = 1/T$ is the inverse temperature, τ is the imaginary time, and T_{τ} is the time ordering product. One can prove Wick's theorem for the Hubbard operators X^{ab}_{n} averaged with the primary density matrix ρ_0 following the ideas of Vaks, Larkin and Pikin [4]. The basic result of Wick's theorem is formulated in terms of commutators or anticommutators alone of the operators X^{ab}_{n} between each other and the mean values of the powers of the diagonal operators X^{00}_{n}, $X^{\sigma\sigma}_{n}$ with primary density matrix ρ_0. The result of Wick's theorem can be represented in compact form if we present the operators X^{ab}_{n} in terms of the Bose and Fermi operators and the accidental field as it was in the simpler case of the SU(2) group in ref. [5]. Such a general representation was pub-

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lished in ref. [6] and will be proved in a later more detailed publication. There we shall study the case of nearly half-filling, when the Hubbard holes are the charge carriers and the chemical potential is essentially larger than the temperature $\mu \gg T$. In that case the Hubbard operators can be expressed in terms of the Fermi hole operators $h_{n\sigma}$, $h^+_{n\sigma}$ and the operators of spin one-half s_n,

$$X^{\uparrow\uparrow}+X^{\downarrow\downarrow}\equiv N=1-h^+\cdot h,$$
$$X^{00}=1-N,\quad X^{\uparrow\uparrow}-X^{\downarrow\downarrow}\equiv 2s^0_{\mathrm{T}},$$
$$X^{\uparrow\downarrow}\equiv s^+_{\mathrm{T}},\quad X^{\downarrow\uparrow}\equiv s^-_{\mathrm{T}},\quad \boldsymbol{s}_{\mathrm{T}}=\boldsymbol{s}+\tfrac{1}{2}h^+\boldsymbol{\sigma}h. \tag{3}$$

Here N is the electron number operator, s_{T} is the operator of the total spin which consists of the local spin s and the hole spin $\frac{1}{2}h^+\sigma h$ where σ are the Pauli matrices, further

$$X^{0\uparrow}=h^+_{\downarrow},\quad X^{0\downarrow}=-h^+_{\uparrow},$$
$$X^{\uparrow 0}=(\tfrac{1}{2}+s^0+h^+\cdot h)h_{\downarrow}-s^+h_{\uparrow},$$
$$X^{\downarrow 0}=-(\tfrac{1}{2}-s^0+h^+\cdot h)h_{\uparrow}+s^-h_{\downarrow}. \tag{4}$$

Formulae (3) and (4) make up the non-Hermitian representation of the graded Spl(1,2) algebra. Relations (3) and (4) do not represent the exact operator relations determined in a Hilbert space. They permit one to calculate the Green function in the framework of the temperature diagram technique. In the case of the full Hubbard model at $U\neq\infty$ one can construct the representation of the graded Spl(2,2) algebra. The total set of dynamical variables consists of electrons in lower and upper Hubbard bands, local spins and excitons that transmit electrons between the two bands. If we substitute the representation (3), (4) by X^{ab}_n in the Hamiltonian (2) we get the following effective Hamiltonian,

$$\mathscr{H}_0=\sum_{n\sigma}\mu_{-\sigma}h^+_{n\sigma}h_{n\sigma}+\omega_0\sum_n s^0_n,$$
$$\mathscr{H}_{\mathrm{int}}=\sum_{n\neq n'}t_{nn'}h^+_{n'}(-\tfrac{1}{2}-h^+_n\cdot h_n+\boldsymbol{s}_n\boldsymbol{\sigma})h_n$$
$$+\frac{4}{U}\sum_{n\neq n'}t^2_{nn'}\boldsymbol{s}_{n'}\boldsymbol{s}_n, \tag{5}$$

where summation is implied over the spin indices. The last term in $\mathscr{H}_{\mathrm{int}}$ is a correction of the order t/U to the Hamiltonian (2) that is part of the Anderson superexchange. This correction is essential for the magnetic structure of the model ground state. The ground state structure can be determined in a self-consistent field approximation when one can confine oneself to the lowest order of perturbation theory. Such an approach can be found when there are a great number of neighbours z around each lattice site. In that case the Fourier image of the hopping integral t_k satisfies two simple relations when summed over the Brillouin band,

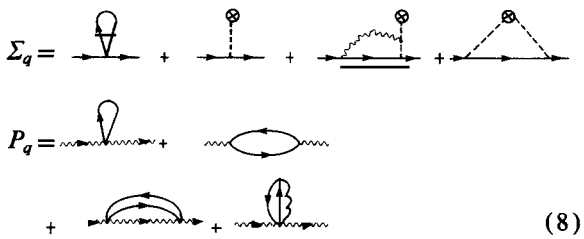
$$\sum_k t_k=0,\quad \sum_k t^2_k=t^2_0/z\ll t^2_0. \tag{6}$$

We shall also suppose that the number of holes per lattice site p is small, $p\ll 1$.

The ferromagnetic state with spins oriented in some definite directions has a simpler structure. This state is realized at a sufficiently large hole concentration $1\gg p\gg t/U$ and low temperature $T\lesssim pE_\phi$, where $E_\phi=t_0-\mu$ is the Fermi energy. Holes and magnons are collective excitations in the ferromagnetic phase [7,8]. The hole–magnon Hamiltonian can be obtained from (5) by means of the following non-Hermitian substitution of the local spins s on the Bose operators a, a^+,

$$s^0=a^+a+\phi,\quad s^-=a,$$
$$s^+=-a^+(2\phi+a^+a). \tag{7}$$

Here ϕ is the accidental field introduced in ref. [5]. At $T\to 0$, ϕ does not fluctuate and approaches $-\frac{1}{2}$ and the representation (7) turns into the well-known Dyson–Mallev representation [5]. The Feynman diagrams for the mass operators of holes Σ_q and magnons P_q,



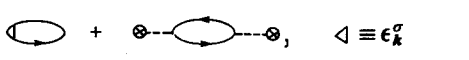
(8)

determine the dispersion laws of holes ϵ_k and magnons ω_k:

$$\epsilon^{\pm}_k=-(\tfrac{1}{2}\mp\overline{s^0}+p^{\pm})t_k+\mu^{\pm}\Rightarrow\begin{cases}-t_k+\mu\\ \qquad\qquad\text{for } T\to 0,\\ \mu\end{cases}$$

$$\omega_k = \sum_{k'} (t_{k'} - t_{k+k'})(p^+_{k'} - p^-_{k'}). \quad (9)$$

Here the solid line represents a hole, the wavy line represents a magnon, and the broken line represents the longitudinal spin component; $q=(\omega, k)$ is the four-momentum of a hole or magnon. $p^{\pm}_k$ is the hole distribution function, $p=(E_\phi z/t_0)^{3/2}/6\pi^2$. The strong splitting of the hole dispersion law according to the spin projection is implied by (9), thus the holes with only a spin projection are thermally excited. The Goldstone theorem is fulfilled for the magnon dispersion law (9). The magnetic energy of the ground state is determined by the two following diagrams,

$E=$  $\triangleleft \equiv \epsilon^q_k$ (10)

and in analytic form

$$E = \sum_{k\sigma} (\epsilon^q_k p^q_k + \overline{s^2_0}\partial p^q_k/\partial\epsilon^q_k).$$

Comparing it with the energy of the paramagnetic state one can be convinced that the ferromagnetic state has low energy and determines the Curie point of the ferromagnetic phase transition

$$T_C = E^{s/2}_\phi/4\pi^2 z^2 t_0^{3/2} \simeq E_\phi p.$$

These results are consistent with the Nagaoka theorem [9]. Due to the strong Fermi surface splitting in the ferromagnetic state superconductivity cannot be realized with any reasonable attraction mechanisms.

The paramagnetic state is realized at sufficiently high temperature

$$T \gtrsim E_\phi p$$

"above the ferromagnetic region" or

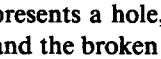
$$T \gtrsim t_0(t_0 p - U)/Up$$

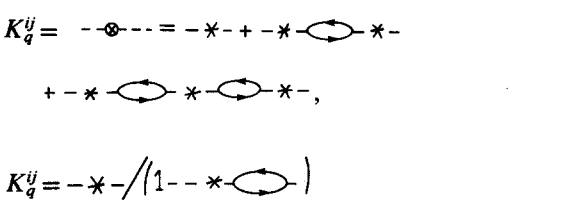
"above the antiferromagnetic region". The hole dispersion law in a paramagnetic phase is given by

$$\epsilon^{\pm}_k = -(\tfrac{1}{2}+p)t_k + \mu. \quad (11)$$

The spin correlator K^{ij}_q in the paramagnetic phase is of a quasistatical character. It can be calculated in the random phase approximation by summing the chain diagram series

$$\langle s_i(q) s_j(q')\rangle = \delta^4(q-q') K^{ij}_q,$$

$(K^{ij}_q)_0 =$  $= \tfrac{1}{4}\delta_{ij}\delta(\omega)$,

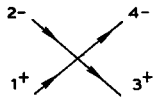
$K^{ij}_q =$ 

$$= \tfrac{1}{4}\delta_{ij}\delta(\omega)/(1 - \Pi_k/2T), \quad (12)$$

where the polarization operator Π_k has the well-known form

$$\Pi_k = \sum_{k'} \frac{t_{k'} t_{k+k'} (p_{k+k'} - p_{k'})}{-\epsilon_{k'} - \epsilon_{k+k'} + i\delta}. \quad (13)$$

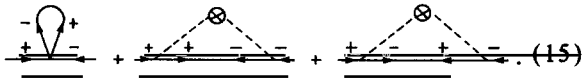
Expressions (12) and (13) for K^{ij}_q are the basic approximation with respect to the parameter $1/z$, and at $k=0$ it has the characteristic pole at the ferromagnetic transition temperature. If the Anderson superexchange interaction was taken into account in (12), then at $p<t/U$ and momentum $k=\pi(1,1,1)/a$, where a is the lattice constant, the pole connected with the antiferromagnetic phase transition appears in the spin correlator K^{ij}_q. The primary hole scattering amplitude can be easily obtained from the Hamiltonian (5),



$= -(t_{k_1} + t_{k_2}).$ (14)

This amplitude is positive for electrons (repulsion) and negative for holes (attraction). This statement was first made in refs. [10,11] and may be interpreted as an effective band narrowing when electrons approach each other, which increases the electron energy and decreases the hole energy. The kinematic hole attraction (14) makes the superconductivity discussion reasonable. This attraction surpasses the attraction caused by superexchange discussed earlier [2,16] for the parameter U/t.

The technique developed above permits one to get the Gor'kov system of equations for a normal and an anomalous Green function in terms of the hole operators $h^+_{n\sigma}$, $h_{n\sigma}$. The anomalous mass operators include three contributions in the low order of interaction,

 (15)

Here the $\pm$ signs correspond to the spin projections of the holes. The first contribution caused by the kinematic attraction of the holes and the last two are connected with the hole scattering on spin fluctuations which as shown by Abrikosov and Gor'kov [13] destroys the superconductivity. Our situation differs from that in ref. [13] in two respects: (a) we have the fluctuation of a spin lattice contrary to the case of paramagnetic impurities in ref. [13]. (b) The hole attraction is not localized on the Fermi surface. It can be shown that the superconductivity criterion [13]: the superconductivity gap Δ_s without taking into account spin fluctuation, would be larger than the energy level width on the Fermi surface $\hbar\Gamma_s$ caused by the hole scattering on the spin fluctuations, is valid in our case too. From the BCS self-consistent conditions on the gap parameter follows

$$\Delta_s = E_\phi \exp[-c(t_0/E_\phi)^{1/2}] \ll E_\phi,$$
$$E_\phi = \mu - \tfrac{1}{2}t_0, \quad c \simeq 1. \tag{16}$$

One can get expression (16) for Δ_s if we decompose

$$t_k \simeq t_0(1 - a^2k^2/z)$$

in a neighbourhood of the maximum of the Brillouin bond. The spin width of the energy level on the Fermi surface can be easily obtained form the mass operator (15)

$$\hbar\Gamma_s = 3\pi(t_0E_\phi)^{1/2}/2, \quad \Delta_s \ll \hbar\Gamma_s, \tag{17}$$

and pairing is destroyed due to the hole scattering on spin fluctuations.

The antiferromagnetic state is realized at a low hole concentration $p \lesssim t/U$ and low temperatures $T \lesssim t_0^2/U$. In that case we shall be confined to a qualitative description alone. The number of hole excitations doubles due to the decrease of the Brillouin band volume. As follows from the Hamiltonian (5) the hole hopping on a neighborhood sublattice is possible due to quantum fluctuations of the spin projection of a sublattice, the hole dispersion law has the form

$$\epsilon_k^{\pm} = \pm |t_k|/2\sqrt{2z}. \tag{18}$$

One can see that the hole four-particle interaction is attractive on the Fermi surface. However, the exchange by antiferromagnon excitations between the holes is stronger, leading to a repulsion on the Fermi surface [14]. The repulsion/attraction ratio is determined by the parameter $U/t_0\sqrt{2z}$ in the framework of the hole intermode ladder approximation. Therefore the spin fluctuation destroys the superconductivity in that case as well.

The picture developed above does not take into consideration the process of the hole spin bag formation, i.e. the construction of a ferron or magnetic polaron [15] when the hole polarizes the local spins and forms ferromagnetic regions around itself. If Coulomb hole repulsion is not considered then all holes form one big ferromagnetic drop. When the Coulomb repulsion is taken into account the number of holes in the drop is finite, but the drop forms a lattice that sticks to impurities (pinning) and the system is dielectric. The situation when a drop consists only of two holes and the two-hole drops form the Bose condensate seems to be exotic.

Let us discuss the question whether the nonphonon mechanism of superconductivity in a model of strong correlated electrons is possible in the case of weak interaction. This question seems reasonable due to the kinematic mechanism of attraction of the holes in a low Hubbard band and the electrons in an upper band due to electron–hole symmetry. The basic reasons of the pairing destruction are magnetic fluctuations that are sufficiently strong at the usual paramagnetic and antiferromagnetic phases. It is apparent that such fluctuations will be suppressed in the phase of the quantum spin liquid [2,16,17] depending on the parameters E_ϕ/t_0. Whether the pairing is conserved in that situation is an open problem.

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