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Spin fluctuations and superconducting states in the Hubbard model with a strong Coulomb repulsion

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Abstract. In the three-dimensional Hubbard model with a strong Coulomb interaction ($U \gg t$) ((t–J) model), the influence of spin fluctuations on the formation of a superconducting state is investigated. The system's magnetic susceptibility is calculated in terms of the generalized random-phase approximation, using the diagram technique for Hubbard operators. We find the magnetic phase transition lines on the (t/U, n) plane, where n is the electron concentration. Equations similar to those in the strong-coupling theory for a superconductor in the (t–J) model are derived taking into account the spin fluctuations. Equations are obtained for the superconducting transition temperatures T_c for the order parameter of s and d symmetries. Spin fluctuations are shown to suppress the superconductivity near the ferromagnetic instability of the paramagnetic phase for both s and d states. Near the antiferromagnetic instability, a sufficient enhancement of T_c is possible.

1. Introduction

Quests for non-phonon mechanisms of superconductivity in connection with the discovery of high-T_c superconductors have stimulated intense research into the mechanisms of electron pairing via spin fluctuations in metals. An interaction between the electronic and magnetic degrees of freedom in metallic systems with long-range magnetic order or under conditions close to magnetic ordering is usually studied in terms of the one-band Hubbard model [1]. The model's Hamiltonian contains only two parameters, namely the matrix element t of electron transfer from site to site, and the value of Coulomb repulsion U on one site. In two limiting cases—weak ($U \ll t$) and strong ($U \gg t$) Coulomb interactions—the exploration is possible by applying perturbation theory.

Investigations of electron pairing via spin fluctuations date back to Berk and Schrieffer [2] who analysed it in the $U \ll t$ regime. They showed that the electron interaction through spin fluctuations for a Cooper-pair singlet near the ferromagnetic instability of a metal caused a repulsion. This conclusion was confirmed later by Scalapino, Loh and Hirsch [3] for the s and d states of the order parameter. It was also shown in [3] that, if the system is near an antiferromagnetic instability, the spin fluctuations for the d state may give rise to an attraction between electrons.

Further investigation of this question is connected mainly with the limit of strong Coulomb correlations, $U \gg t$. The point [4] is that under these conditions one can exclude

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from consideration states with two electrons on one site and pass over to an effective exchange–correlation Hamiltonian with an electron interaction on neighbouring sites of value $J = t^2/U$ (the so-called (t–J) model [5]). It is in terms of this model that intensive searches for pairing correlation mechanisms have been conducted, mainly in two major directions. One direction, which is the most powerful approach, explores some novel features of statistical mechanics of the two-dimensional Hubbard model that were discovered by Anderson [6] (see [7], which reports recent developments in this area). The other direction deals with the three-dimensional Hubbard model [8–13]. We concentrate on the latter direction. The purpose of this paper is to study the mechanisms of electron pairing via spin fluctuations of a strongly correlated system near a magnetic instability, where the spin fluctuations are especially strong. In order to obtain equations similar to those used in the standard theory of strongly coupled superconductors [14, 15], one needs to exploit a perturbation theory in which the zero approximation contains the one-site Coulomb energy and the kinetic energy is taken into account as a perturbation. In this case the Hamiltonian is conveniently expressed in terms of Hubbard operators [1]; then the corresponding perturbation theory represents the diagram technique for Hubbard operators.

This technique for the general Hubbard model is expounded in a book [16] (see also all the references therein), while for the (t–J) model a very detailed treatment of it is provided in our paper [17]. The magnetic susceptibility in the (t–J) model was calculated there in an approximation in which only all the loop diagrams (exactly, the antiparallel ladders) for the electron vertex part are taken into account. The summation of this diagram is an analogue of the random-phase approximation (RPA), which is known in the theory of Fermi systems with a weak Coulomb interaction. Note that for strongly correlated systems ($U \gg t$) the RPA gives an expression for the magnetic susceptibility. This expression includes two contributions: the Pauli contribution with a weak temperature dependence, and the Curie contribution, which is proportional to $1/T$. The expression obtained in [17] for the susceptibility is used here in the derivation of superconductor equations that take into account the influence of spin fluctuations on electron pairing.

This paper is organized as follows. In section 2 we briefly discuss the principles of the diagram technique for the (t–J) model in terms of Hubbard operators, and calculate the vertex part for two electrons in the lower Hubbard band. It is shown that divergences occur in the Cooper channel, which indicate that the normal phase is unstable with respect to the formation of a superconducting order parameter of s and d symmetry. In section 3 the diagram technique is generalized in such a way that anomalous averages can be taken into account. In the next section, the equations for the matrix Green function in the Nambu representation are derived graphically, which correspond to the mean-field approximation. The equations for superconducting transition temperatures are shown to coincide with the equations that determine the poles of the vertex part in the Cooper channel. In section 5, equations for a superconductor are derived graphically taking into account the system's dynamic fluctuations and retarding effects. The kernels of the integral equations obtained are expressed through the magnetic susceptibility. In section 6, the dynamic susceptibility, which we calculated in the generalized random-phase approximation (GRPA) in [17], is discussed together with possible types of magnetic instability. In section 7 strong-coupling theory equations are solved, which involve this dynamic susceptibility, and the effects of spin fluctuations on T_c are examined in different cases.

2. Perturbation theory for the (t–J) model

In the Hubbard operator representation, the (t–J) model Hamiltonian is written as [12]

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{kin}} + \hat{H}_{\text{eff}} \tag{2.1}$$

where

$$\hat{H}_0 = \sum_{l\sigma} \varepsilon_\sigma X_l^{\sigma\sigma} \qquad \hat{H}_{\text{kin}} = t \sum_{l\Delta\sigma} X_l^{\sigma 0} X_{l+\Delta}^{0\sigma} \tag{2.2}$$

$$\hat{H}_{\text{eff}} = \kappa t \sum_{l\Delta} (X_l^{-+} X_{l+\Delta}^{+-} - X_l^{++} X_{l+\Delta}^{--}). \tag{2.3}$$

Here l numbers the lattice sites, Δ stands for nearest neighbours and $\sigma = \uparrow, \downarrow$ denotes spin projections. The operator $\hat{H}_0$ represents a one-site energy with $\varepsilon_\sigma = -\sigma h/2 - \mu$, where μ is the system's chemical potential and h is an external magnetic field. $\hat{H}_{\text{kin}}$ is the electron hopping energy from site to site, while $\hat{H}_{\text{eff}}$ is the exchange–correlation energy (J interaction). According to perturbation theory, the last two terms should be viewed as $\hat{H}_{\text{int}}$. In (2.3) the dimensionless parameter $\kappa = t/U \ll 1$ is introduced.

Thus $\hat{H}$ includes nine Hubbard operators,

$$X^{+0}, X^{0+}, X^{-0}, X^{0-} \qquad X^{+-}, X^{-+} \qquad X^{00}, X^{++}, X^{--} \tag{2.4}$$

where the first four operators are Fermi-like, X^{+-} and X^{-+} are Bose-like and the last three operators are diagonal.

Let us determine two temperature Green functions for electrons and for transverse spin components,

$$\mathcal{G}_\sigma(x, x') = -\langle T(\tilde{X}_l^{0\sigma}(\tau)\tilde{X}_{l'}^{\sigma 0}(\tau'))\rangle \tag{2.5}$$

$$D_\perp(x, x') = -\langle T(\tilde{X}_l^{+-}(\tau)\tilde{X}_{l'}^{-+}(\tau'))\rangle \tag{2.6}$$

where all the notations are standard ones [18]. Particularly, $\tilde{X}_l^{pq}(\tau)$ is the operator X_l^{pq} in the Heisenberg representation with imaginary time τ; $x = (l, \tau)$ is a four-dimensional point.

In order to calculate corrections in power series of $\hat{H}_{\text{int}}$, one must use the diagram technique for Hubbard operators. A detailed exposition of this technique for a total Hubbard Hamiltonian can be found, for example, in [16], and for the (t–J) model in our previous paper [17].

The zero approximation Green function reads

$$\mathcal{G}_\sigma^0(x, x') = G_\sigma^0(x - x')\langle F_l^{\sigma 0}\rangle_0 \tag{2.7}$$

$$D_\perp^0(x, x') = D^0(x - x')\langle B_l^{+-}\rangle_0 \tag{2.8}$$

where $F^{\sigma 0}$ and B^{+-} are linear combinations of diagonal operators:

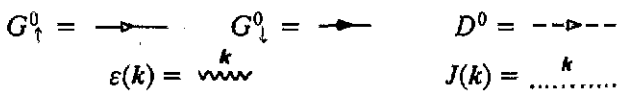
$$F^{\sigma 0} = X^{00} + X^{\sigma\sigma} \qquad B^{+-} = X^{++} - X^{--} \tag{2.9}$$

and G_σ^0 and D^0 are Fermi-like and Bose-like Green functions of the following form

$$G_\sigma^0(k; \mathrm{i}\omega_n) = 1/(\mathrm{i}\omega_n - \varepsilon_\sigma) \qquad \omega_n = (2n + 1)\pi T \tag{2.10}$$

$$D^0(k; \mathrm{i}\omega_n) = 1/(\mathrm{i}\omega_n - h) \qquad \omega_n = 2n\pi T. \tag{2.11}$$

Elements of the diagram technique are the Green lines and the interaction lines:

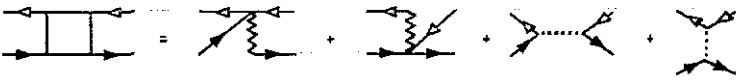


(2.12)

where

$$\varepsilon(k) = t\sum_{\Delta} e^{ik\Delta} \qquad J(k) = \kappa\varepsilon(k). \tag{2.13}$$

The Hamiltonian $\hat{H}_{\rm int} = \hat{H}_{\rm kin} + \hat{H}_{\rm eff}$ generates a lot of vertices, at which different numbers of fermion and boson lines converge. All possible types of vertices for the (t–J) model Hamiltonian are enumerated in [17]. Taking into account the subsequent concrete approximations, we consider only those vertices that have no boson lines. There are only four bare vertices of that type:



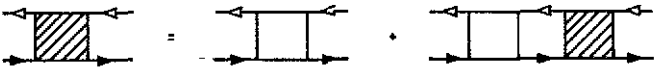
(2.14)

Here and henceforth the electron Green lines mean electron propagators corresponding to the lower Hubbard band, which are treated in the Hubbard-I approximation [1]; thus, the analytical expressions corresponding to the electron Green lines are

$$G^0_\sigma(k) = 1/[i\omega_n - E_\sigma(k)] \qquad E_\sigma(k) = \langle F^{\sigma 0}\rangle\varepsilon(k) + \varepsilon_\sigma. \tag{2.15}$$

Here $k = (k, i\omega_n)$ is a four-momentum.

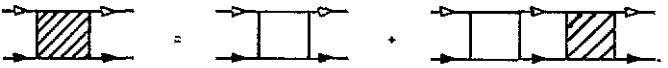
In [17], the Green function (2.6) for the transverse spin components (dynamic susceptibility) was calculated in an approximation that corresponds to the summation of diagrams with antiparallel ladders. All of these diagrams are taken into account by the Bethe–Salpeter equation for the electron four-leg diagram:



(2.16)

We have already shown (see section 6 in [17] that instabilities with respect to magnetic ordering may occur in this particle–hole channel.

We now consider a four-leg diagram in the particle–particle channel, having defined this diagram by a Bethe–Salpeter equation of the following type:

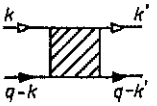


(2.17)

where the bare vertex consisting of graphs (2.14) must be written as:

(2.18)

We introduce the analytical notation for the vertex part



$$= \Gamma_c(k, q-k; q-k', k') \tag{2.19}$$

and thus the q have the meaning of the total four-momentum of colliding particles. The

Cooper channel equation (2.17) (i.e. with $q = 0$) is not difficult to solve. For a simple cubic lattice, the solution has the form

$$\Gamma_c(k, -k; -k', k') = 4t \sum_{\alpha\beta} (1 + \kappa \cos k_\alpha) A_{\alpha\beta} \cos k'_\beta \tag{2.20}$$

where

$$A_{\alpha\beta} = \frac{(1 - 2F - \kappa K_1 - \kappa K_2)\delta_{\alpha\beta} + (F + \kappa K_2)(1 - \delta_{\alpha\beta})}{(1 - \kappa K_1 + \kappa K_2)(1 - \kappa K_1 - 2\kappa K_2 - 3F)} \tag{2.21}$$

and F, K_1 and K_2 are determined by the relations

$$\begin{Bmatrix} F \\ K_1 \\ K_2 \end{Bmatrix} = \frac{2t}{N} \sum_k \begin{Bmatrix} \cos k_x \\ \cos^2 k_x \\ \cos k_x \cos k_y \end{Bmatrix} \frac{\tanh[E(k)/2T]}{E(k)}. \tag{2.22}$$

Here

$$E(k) = (1 - n/2)\varepsilon(k) - \mu \tag{2.23}$$

is the electron energy in the lower Hubbard band in the paramagnetic phase of a metal (see the expression for $E_\sigma(k)$ in (2.15)).

The poles of the vertex part (2.20) determine the temperature T_c at which the normal phase of a metal loses stability. The poles are found from the equations

$$1 = \frac{2t}{N} \sum_k [\gamma(k) + \tfrac{1}{3}\kappa\gamma^2(k)] \frac{\tanh[E(k)/2T_c]}{E(k)} \tag{2.24}$$

$$1 = \kappa t \frac{1}{N} \sum_k (\cos k_x - \cos k_y)^2 \frac{\tanh[E(k)/2T_c]}{E(k)} \tag{2.25}$$

which determine the stability boundaries with respect to the occurrence of the s and d symmetry order parameters, respectively. Here

$$\gamma(k) = \cos k_x + \cos k_y + \cos k_z. \tag{2.26}$$

Note that in the limit $U \to \infty$, equation (2.24) goes into the equation obtained for the first time by Zaitsev and Ivanov [8, 9], who interpreted T_c as a superconducting transition temperature and called the electron pairing mechanism coming from $\hat{H}_{\text{kin}}$ a kinematic mechanism. Further investigation has shown, however, that the energy of a phase with spontaneously broken symmetry is higher than that of a normal phase, so the kinematic mechanism cannot give rise to a superconducting state [13]. But in equation (2.25) for the d symmetry of the order parameter the kinematic interaction disappears and contains the contribution of $\hat{H}_{\text{eff}}$ only. This circumstance was noted for the first time in [12].

Since the kinematic mechanism does not form a superconducting state, we shall in the following take into account the perturbation theory of the J interaction only. The role of $\hat{H}_{\text{kin}}$ reduces to forming electron propagators and will be taken into account in full measure when we allow for the spin fluctuations, i.e. in the calculation of the system's magnetic susceptibility [17].

3. Perturbation theory with anomalous averages

The superconducting order parameter in the (t–J) model can be easily introduced with the help of the Nambu representation. We consider the four-component column and row

$$\psi = \begin{pmatrix} X^{0+} \\ X^{0-} \\ X^{+0} \\ X^{-0} \end{pmatrix} \qquad \bar{\psi} = (X^{+0} \quad X^{-0} \quad X^{0+} \quad X^{0-}) \tag{3.1}$$

and combine them into the Green function

$$\mathcal{G}(x, x') = -\langle T(\tilde{\psi}(x)\bar{\tilde{\psi}}(x'))\rangle. \tag{3.2}$$

Wick's theorem for Hubbard operators [16] exploits the idea of a pairing of two operators under the symbol of averaging, the first operator being a creation operator and the other an annihilation operator.

In the matrix $\psi(x)\bar{\psi}(x')$, we can separate out pairings that are normal ones:

$$\overbrace{X^{0\sigma}(x)X^{\sigma 0}(x')} = -G^0_\sigma(x-x')F^{\sigma 0}(x') \qquad \overbrace{X^{0\sigma}(x)X^{\bar{\sigma}0}(x')} = -G^0_\sigma(x-x')X^{\bar{\sigma}\sigma}(x'). \tag{3.3}$$

In addition to these pairings, we need to take into account the anomalous pairing of two annihilation or two creation operators; for example,

$$\overbrace{X^{0\sigma}(x)X^{0\sigma}(x')} = -F_{\sigma\sigma}(x-x')F^{\sigma 0}(x') - F_{\sigma\bar{\sigma}}(x-x')X^{\bar{\sigma}\sigma}(x'). \tag{3.4}$$

In relations (3.3) and (3.4), the quantities $F^{\sigma 0}(x)$ and $X^{\bar{\sigma}\sigma}(x)$ are also operators and take part in further pairings. The entire set of relations of type (3.3) and (3.4) may be expressed in matrix form:

$$\psi_\alpha(x)\bar{\psi}_{\alpha'}(x') = -\sum_{\alpha_1} g^0_{\alpha\alpha_1}(x-x')\hat{B}_{\alpha_1\alpha'}(x') \tag{3.5}$$

where the indices α and α' number the components in the Nambu columns and rows, and g^0 and $\hat{B}$ are 4×4 matrices:

$$g^0 = \begin{pmatrix} G^0_\uparrow & 0 & F_{\uparrow\uparrow} & F_{\uparrow\downarrow} \\ 0 & G^0_\downarrow & F_{\downarrow\uparrow} & F_{\downarrow\downarrow} \\ F^+_{\uparrow\uparrow} & F^+_{\uparrow\downarrow} & \bar{G}^0_\uparrow & 0 \\ F^+_{\downarrow\uparrow} & F^+_{\downarrow\downarrow} & 0 & \bar{G}^0_\downarrow \end{pmatrix} \qquad \hat{B} = \begin{pmatrix} F^{+0} & X^{-+} & 0 & 0 \\ X^{+-} & F^{-0} & 0 & 0 \\ 0 & 0 & F^{+0} & X^{+-} \\ 0 & 0 & X^{-+} & F^{-0} \end{pmatrix}. \tag{3.6}$$

Each element in the matrix g^0 depends on the argument $x - x'$; $G^0_\sigma(x-x')$ corresponds to the Green function (2.15), and $\bar{G}^0_\sigma(x-x') = -G^0_\sigma(x-x')$. The quantity $F_{\sigma\sigma'}$ represents the anomalous Green function and must be determined from the self-consistency equations.

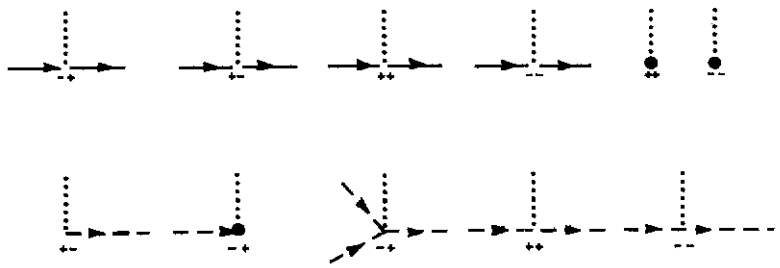


Figure 1.

Equation (3.5) determines the pairing of Fermi-like operators between each other. The pairing of Fermi-like operators with Bose-like operators can be determined similarly. The complete set of these pairings is expressed by the matrix equality

$$\overbrace{\psi_\alpha(x)X^{\sigma\sigma'}(x')} = \sum_{\alpha_1\alpha_1'} g^0_{\alpha\alpha_1}(x-x')\xi^{\sigma\sigma'}_{\alpha_1\alpha_1'}\psi_{\alpha_1'}(x'). \tag{3.7}$$

Here $\xi^{\sigma\sigma'}$ are numerical 4×4 matrices:

$$\xi^{++} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \xi^{--} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \xi^{+-} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{3.8}$$

(a matrix ξ^{-+} is Hermitian-conjugate to ξ^{+-}).

In addition, we write formulae for the pairing of Bose-like operators between each other and also with diagonal operators. We have

$$\overbrace{X^{+-}(x)X^{-+}(x')} = -D^0(x-x')B^{+-}(x') \tag{3.9}$$

$$\overbrace{X^{+-}(x)B^{+-}(x')} = 2D^0(x-x')X^{+-}(x') \tag{3.10}$$

$$\overbrace{X^{+-}(x)\hat{B}^0_{\alpha\alpha'}(x')} = D^0(x-x')\eta_{\alpha\alpha'}X^{+-}(x'). \tag{3.11}$$

In the last relation, $\hat{B}^0_{\alpha\alpha'}$ is the diagonal part of the matrix $\hat{B}_{\alpha\alpha'}$ determined in (3.6) and $\eta_{\alpha\alpha'}$ is a diagonal matrix:

$$\eta_{\alpha\alpha'} = \mathrm{diag}(1,-1,1,-1). \tag{3.12}$$

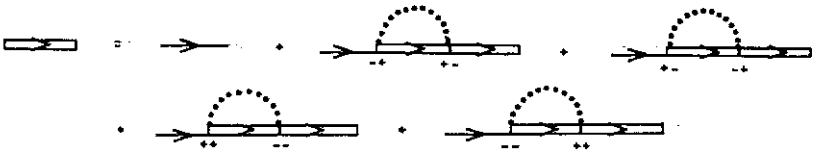
Thus, in calculating the perturbation theory series in powers of $\hat{H}_{\mathrm{eff}}$ for different Green functions, a diagram technique arises, whose possible vertices are all presented in figure 1.

The full line with the arrow represents the matrix Green function g^0 from (3.6), the broken line the boson Green function D^0, and the dotted line the J interaction (in keeping with the rules (2.12)). In writing an analytical expression corresponding to a diagram, it is necessary to write for each vertex the corresponding matrix, ξ^{+-}, ξ^{-+}, ξ^{++} or ξ^{--}. As is clear from the Hamiltonian $\hat{H}_{\mathrm{eff}}$ (2.3), the dotted line can connect vertices

(−+) with (+−) and (++) with (−−) and the diagram signs depend on the number of lines of both types.

4. The mean-field approximation

Using the graphs depicted in figure 1, one can readily construct graphical series for the electron Green function. Of the first-order graphs, we take those which contain no boson lines. Evidently, there are four such graphs. If we replace the zero-approximation Green line (corresponding to the propagator in the lower Hubbard band) by a thick line, then we obtain a self-consistent equation for the electron Green function



(4.1)

Obviously, this equation corresponds to the mean-field approximation.

In the momentum representation, this graphical equation corresponds to a 4×4 matrix equation,

$$g(k; i\omega_n) = g^0(k; i\omega_n) + g^0(k; i\omega_n)\,\Sigma_{MF}(k; i\omega_n)g(k; i\omega_n) \tag{4.2}$$

where

$$\Sigma_{MF}(k; i\omega_n) = \frac{1}{N}\sum_{k_1 n_1} J(k-k_1)[\xi^{++}g(k_1; i\omega_{n_1})\xi^{--} + \xi^{--}g(k_1; i\omega_{n_1})\xi^{++} - \xi^{+-}g(k_1; i\omega_{n_1})\xi^{-+} - \xi^{-+}g(k_1; i\omega_{n_1})\xi^{+-}]. \tag{4.3}$$

The off-diagonal matrix elements of the zero-approximation Green function g^0 in (4.2) are equal to zero and the diagonal elements are (see formula (3.6))

$$G^0(k; i\omega_n) = 1/[i\omega_n - E(k)] \qquad \bar{G}^0(k; i\omega_n) = 1/[i\omega_n + E(k)].$$

We denote the matrix element of the Green function $g(k; i\omega_n)$ by the symbol $g_{\alpha\beta}(k; i\omega_n)$ ($\alpha, \beta = 1, 2, 3, 4$). Then, using the self-consistent equations (4.2) and (4.3), we can readily set up a closed equation for the quantity

$$\Delta(k) = \frac{1}{N}\sum_{k_1 n_1} J(k-k_1)[g_{23}(k_1; i\omega_{n_1}) - g_{14}(k_1; i\omega_{n_1})]$$

which is a superconducting order parameter. This equation has the form of a gap equation of the Bardeen–Cooper–Schrieffer (BCS) theory with the matrix element depending on momenta:

$$\Delta(k) = \frac{1}{N}\sum_{k_1} J(k-k_1)\Delta(k_1)\frac{\tanh[\zeta(k_1)/2T_c]}{\zeta(k_1)} \tag{4.4}$$

where

$$\zeta(k) = [E^2(k) + |\Delta(k)|^2]^{1/2}. \tag{4.5}$$

Thus, indeed, equation (4.1) really corresponds to the mean-field approximation.

From this, one should expect that equation (4.4) linearized with respect to $\Delta(\boldsymbol{k})$ should determine the superconducting transition temperatures coinciding with the equations (2.24) and (2.25) for the vertex part poles in the Cooper channel [18]. In fact, owing to the factorization of the kernel

$$J(\boldsymbol{k}-\boldsymbol{k}_1) = 2\kappa t \sum_{\alpha=x,y,z} (\cos k_\alpha \cos k_{1\alpha} + \sin k_\alpha \sin k_{1\alpha}) \tag{4.6}$$

(for the case of the simple cubic (SC) lattice) the integral linearized equation (4.4) reduces to a system of six linear algebraic equations. The conditions for these equations to have non-trivial solutions are the equations

$$1 = 2\kappa t \frac{1}{N} \sum_{\boldsymbol{k}} \psi_l^2(\boldsymbol{k}) \frac{\tanh[E(\boldsymbol{k})/2T_c]}{E(\boldsymbol{k})} \tag{4.7}$$

which determine the transition temperatures T_c. Here the ψ_l are the basis functions of the irreducible representations of the crystal's cubic group. They correspond to s, p and d type symmetries:

$$\psi_s(\boldsymbol{k}) = (1/\sqrt{3})(\cos k_x + \cos k_y + \cos k_z)$$

$$\psi_{p_1}(\boldsymbol{k}) = \sin k_x \qquad \psi_{p_2}(\boldsymbol{k}) = \sin k_y \qquad \psi_{p_3}(\boldsymbol{k}) = \sin k_z \tag{4.8}$$

$$\psi_{d_1}(\boldsymbol{k}) = (1/\sqrt{2})(\cos k_x - \cos k_y) \qquad \psi_{d_2}(\boldsymbol{k}) = (1/\sqrt{6})(\cos k_x + \cos k_y - 2\cos k_z).$$

These functions are constructed on the states within the first coordination sphere (the number of nearest neighbours $Z = 6$) and take into account the necessary degeneration. Equation (4.7) together with (4.8) coincides formally with the equations that hold in resonating valence bond theory [5, 6]. The dependence on the order parameter momentum is determined by the basis function (4.8) according to the relation

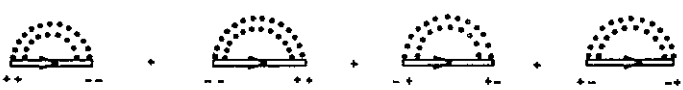
$$\Delta_l(\boldsymbol{k}) = \psi_l(\boldsymbol{k})\Delta_l \qquad l = \mathrm{s, p, d.} \tag{4.9}$$

Since the function $\psi_p(\boldsymbol{k})$ is odd, the corresponding superconducting order parameter is a triplet, while for s and d symmetry it is a singlet.

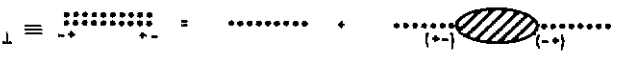
Numerical solution of equation (4.7) for a SC lattice shows that T_c is very small for s symmetry and is $<10^{-5} \times 2t$, while for d symmetry it is sufficiently large and can reach the value $T_c \simeq 10^{-3} \times 2t$.

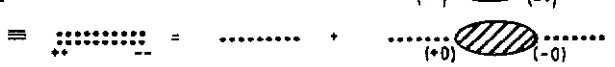
5. Allowance for spin fluctuations: strong-coupling theory equations

The graphical derivation of the mean-field equations provides a basis for including fluctuations into the theory. For this purpose, we introduce the thickening of the interaction lines in the graphs (4.1), using the established rules of the diagram technique. Thus we represent the self-energy part as

$\Sigma =$  (5.1)

Here the thick dotted line represents two types of effective interaction, which can be depicted graphically as

$J_\perp \equiv$  (5.2)

$J_\parallel \equiv$ 

where the shaded objects are the following Green functions:

 $\equiv D_\perp = -\langle T(\tilde{X}^{+-}\tilde{X}^{-+})\rangle$ (5.3)

 $\equiv D^{+-} = \langle T(\tilde{F}^{+0}\tilde{F}^{-0})\rangle.$ (5.4)

As is clear from the definition (2.6), $D_\perp$ is a Green function of the transverse spin components; D^{+-} is expressed via the density–density Green function, because, according to (2.9)

$$F^{\sigma 0} = X^{00} + X^{\sigma\sigma} = 1 - n_{\bar{\sigma}} \tag{5.5}$$

with $n_\uparrow$ and $n_\downarrow$ being the operators of the number of electron states on a site with a definite spin projection.

Explicit expressions for the Green functions $D_\perp(k; i\omega_n)$ and $D^{+-}(k; i\omega_n)$ will be given in the next section. Now we write the analytical form of equation (5.1). According to the diagram technique rules formulated in section 3,

$$\Sigma(k) = \frac{1}{N}\sum_{k_1}[-J_\perp(k-k_1)\xi^{-+}g(k_1)\xi^{+-} - J_\perp(k-k_1)\xi^{+-}g(k_1)\xi^{-+}$$
$$+ J_\parallel(k-k_1)\xi^{++}g(k_1)\xi^{--} + J_\parallel(k-k_1)\xi^{--}g(k_1)\xi^{++}]. \tag{5.6}$$

Formally, this equation is of the same type as that in the theory of strongly coupled superconductors [14, 15]; therefore, in constructing the theory, we shall use known methods.

First, we use the spectral representation for the electron Green function $g(k)$ and for the functions $J_\perp$ and $J_\parallel$:

$$g(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dz\, \frac{a(k; z)}{i\omega_n - z} \qquad J_{\perp,\parallel}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dz\, \frac{b_{\perp,\parallel}(k; z)}{i\omega_n - z}. \tag{5.7}$$

Here the discrete frequency ω_n is odd in the first integral and even in the second integral. These relations enable us to perform a summation over the frequencies ω_{n_1} on the right-hand side of equation (5.6) and then to pass from the temperature Green function $g(k; i\omega_{n_1})$ to the retarding function $g(k; \omega)$ with the help of the analytical continuation $i\omega_n \to \omega + i\delta$, and the expression for the spectral density

$$a(k, z) = -2\,\mathrm{Im}\, g(k; z).$$

Then we pass over to the following expression for $\Sigma(k; \omega)$:

$$\Sigma(k; \omega) = -\frac{1}{N}\sum_{k_1}\int \frac{dz\, dz'}{(2\pi)^2}\frac{\tanh(z'/2T) + \coth(z/2T)}{\omega - z - z' + i\delta}[b_\perp(k-k_1; z)\xi^{-+}$$
$$\times \mathrm{Im}\, g(k_1; z')\xi^{+-} - b_\perp(k_1 - k; -z)\xi^{+-}$$
$$\times \mathrm{Im}\, g(k_1; z')\xi^{+-} - b_\parallel(k-k_1; z)\xi^{++}$$
$$\times \mathrm{Im}\, g(k_1; z')\xi^{--} + b_\parallel(k_1 - k; -z)\xi^{--}\,\mathrm{Im}\, g(k_1; z')\xi^{++}]. \tag{5.8}$$

The quantity Σ is a 4×4 matrix, which we derive from the following expansion in Pauli matrices τ_α ($\alpha = 0, 1, 2, 3$):

$$\Sigma(k) = [1 - Z(k)]\omega\tau_0 \times \tau_0 + \theta(k)\tau_3 \times \tau_0 - \varphi(k)\tau_2 \times \tau_2. \tag{5.9}$$

The matrix equation (5.8) splits into the following system of equations for the quantities Z, θ and φ:

$$(1 - Z(k; \omega)]\omega = \frac{1}{N}\sum_{k_1}\int \frac{dz'}{2\pi}\mathcal{K}_\perp(k - k_1; \omega z') \operatorname{Im}\frac{z' Z(k_1; z')}{D(k_1; z')} \tag{5.10}$$

$$\theta(k; \omega) = \frac{1}{N}\sum_{k_1}\int \frac{dz'}{2\pi}\mathcal{K}_\perp(k - k_1; \omega z') \operatorname{Im}\frac{E(k_1) + \theta(k_1; z')}{D(k_1; z')} \tag{5.11}$$

$$\varphi(k; \omega) = \frac{1}{N}\sum_{k_1}\int \frac{dz'}{2\pi}(\mathcal{K}_\perp(k - k_1; \omega z') + \mathcal{K}_\parallel(k - k_1; \omega z')) \operatorname{Im}\frac{\varphi(k_1; z')}{D(k_1; z')} \tag{5.12}$$

where

$$D(k; \omega) = \omega^2 Z^2(k; \omega) - [E(k) + \theta(k; \omega)]^2 - \varphi^2(k; \omega). \tag{5.13}$$

This is a system of coupled non-linear integral equations with the kernels

$$\mathcal{K}_{\perp,\parallel}(k - k'; \omega z') = -\int_{-\infty}^{\infty}\frac{dz}{2\pi}\frac{\tanh(z'/2T) + \coth(z/2T)}{\omega - z - z' + i\delta} b_{\perp,\parallel}(k - k'; z). \tag{5.14}$$

In the standard superconducting theory, the quantity $\theta(k)$ is usually neglected in the equations for $Z(k)$ and $\varphi(k)$, their kernels being averaged over the momenta k and k_1 lying on the Fermi surface. After that, the integration over momentum k_1 reduces to an integration over the electron energy $E(k_1)$, and the equations become integrals only over frequency. Such an approximation is possible if the kernels depend weakly on the wavevector direction. This is not so in our case because the quantities $J_\perp(k - k_1)$ and $J_\parallel(k - k_1)$ depend greatly on the vector $k - k_1$, and it is impossible to pass from integration over the three-dimensional vector k_1 to integration over the one-dimensional variable $E(k_1)$. Thus, equations (5.10)–(5.12) remain integral over frequency z' and momentum k_1.

In order to get analytical results, we pass to the weak-coupling limit. In this case, T_c must be much less than the limiting frequency ω_m of the spectrum of the collective modes determined by the poles of the function $J_{\perp,\parallel}(k; \omega)$. In this situation, the kernels (5.14) can be approximated thus

$$\mathcal{K}_{\perp,\parallel}(k - k'; \omega z') \simeq -\lambda_{\perp,\parallel}(k - k')\tanh(z'/2T) \tag{5.15}$$

where

$$\lambda_{\perp,\parallel}(k - k') = -\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dz}{z} b_{\perp,\parallel}(k - k'; z) = \operatorname{Re} J_{\perp,\parallel}(k - k'; 0). \tag{5.16}$$

Then $Z(k) \to 1$ and the function $\varphi(k; \omega) \equiv \Delta(k)$ for the order parameter ceases to

depend on frequency, and equation (5.12) reduces to a BCS theory equation with the matrix element depending on momenta:

$$\Delta(k) = \frac{1}{N}\sum_{k_1} V(k-k_1)\Delta(k_1)\frac{\tanh[\zeta(k_1)/2T]}{\zeta(k_1)} \tag{5.17}$$

where

$$V(k) = \tfrac{1}{2}\,\mathrm{Re}\,J_\perp(k;0) + \tfrac{1}{2}\,\mathrm{Re}\,J_\parallel(k;0). \tag{5.18}$$

Now the problem reduces to one of calculating the value of $V(k)$.

6. Calculation of an effective pairing interaction

According to the graphical definitions (5.1), the effective interactions $J_\perp$ and $J_\parallel$ are expressed via two Green functions, $D_\perp$ and D^{+-}:

$$J_\perp(k) = J(k) + J^2(k)D_\perp(k) \qquad J_\parallel(k) = J(k) + J^2(k)D^{+-}(k). \tag{6.1}$$

The Green function of the transverse spin components $D_\perp$, defined by relation (5.3), was calculated in our previous paper [17] with the help of the GRPA:

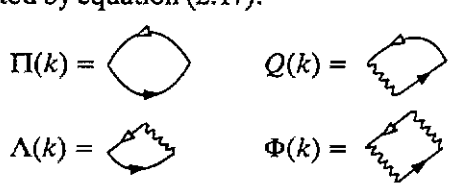
$$D_\perp(k) = -\frac{\chi_0(k)}{[1-\Lambda(k)][1-Q(k)] + \chi_0(k)[\Phi(k)+J(k)]} \equiv -\chi(k) \tag{6.2}$$

where

$$\chi_0(k) = (nn_0/2T)\delta_{\omega_n,0} - \Pi(k). \tag{6.3}$$

The bare dynamic susceptibility $\chi_0(k)$ (after the analytical continuation $i\omega_n \to \omega + i\delta$) simultaneously displays features of localized and itinerant models. The expression (6.2) itself is the system's dynamic susceptibility in the paramagnetic phase of a metal. The result (6.2) can be considered as a generalization of the known result of the RPA in the regime $U \ll t$ [19] for the regime $U \gg t$.

The quantities Π, Q, Λ and Φ denote four types of loops that appear in the graphical series generated by equation (2.17):



(6.4)

These loops are determined by the expressions

$$\begin{Bmatrix}\Pi(k)\\ Q(k)\\ \Lambda(k)\\ \Phi(k)\end{Bmatrix} = \frac{1}{N}\sum_{k_1}\begin{Bmatrix}1\\ \varepsilon(k_1)\\ \varepsilon(k_1-k)\\ \varepsilon(k_1)\varepsilon(k_1-k)\end{Bmatrix}\frac{f[E(k_1-k)]-f[E(k_1)]}{i\omega_n + E(k_1-k) - E(k_1)} \tag{6.5}$$

where $f(E)$ is the Fermi distribution function. In the formula (6.3), n_0 is a parameter determined by the formula

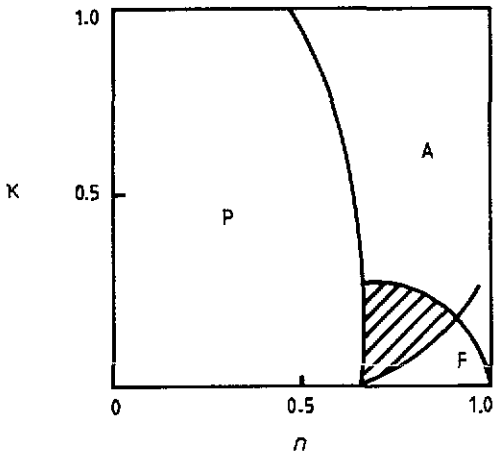


Figure 2.

$$n_0 = 2\,e^{\mu/T}/(1 + 2\,e^{\mu/T}). \tag{6.6}$$

This parameter increases sharply from 0 to 1 if the chemical potential reverses sign, i.e. if the electron concentration n is varied. In order to calculate the value of $D^{+-}(k)$, it is convenient to introduce the density–density Green function

$$D^N(x, x') = \langle T(\tilde{N}_l(\tau)\tilde{N}_{l'}(\tau'))\rangle \tag{6.7}$$

where $N_l = F_l^{+0} + F_l^{-0}$. In the same GRPA as that used in order to derive the expression (6.2), we find

$$\tfrac{1}{2}D^N(k) = \frac{\chi_0^N(k)}{[1 + \Lambda(k)][1 + Q(k)] + \chi_0^N(k)[\Phi(k) - J(k)]} \equiv \chi^N(k) \tag{6.8}$$

where

$$\chi_0^N(k) = [nn_0(1 - n_0)/2T]\delta_{\omega_n,0} - \Pi(k). \tag{6.9}$$

Now it is easy to obtain expressions for the functions $D_\perp$ and D^{+-} via the dynamic magnetic susceptibility $\chi(k)$ and the dielectric susceptibility $\chi^N(k)$:

$$D_\perp(k) = -\chi(k) \qquad D^{+-}(k) = -\tfrac{1}{2}\chi(k) + \tfrac{1}{2}\chi^N(k). \tag{6.10}$$

Finally, using the relations (5.18), (6.1) and (6.10), we obtain the final expression for the effective pairing interaction

$$V(k) = J(k) - \tfrac{3}{4}J^2(k)\,\mathrm{Re}\,\chi(k; 0) - \tfrac{1}{4}J^2(k)\,\mathrm{Re}\,\chi^N(k; 0). \tag{6.11}$$

This must be substituted into equation (5.17) for the superconducting order parameter.

We quote the necessary information, obtained in [17], about the magnetic susceptibility. The poles of the function $\chi(k; 0)$ determine the stability boundary of the paramagnetic phase with respect to magnetic ordering: ferromagnetic state (F) with $k = 0$ and antiferromagnetic state (A) with $k \approx k_0 = (\pi, \pi, \pi)/a$. The phase diagram for the magnetic phases was constructed on the (κ, n) plane [17]. It is reproduced in figure 2 for the SC lattice.

Magnetic phases occur mainly in the concentration interval $\frac{2}{3} < n < 1$. The critical concentration $n_c = \frac{2}{3}$ corresponds to sign reversal of the chemical potential, thus $T = 0$ and $n > n_c$. In the shaded region of the diagram, the system's magnetic states are unknown. It may be a heterogeneous phase consisting of ferro- and antiferromagnetic phase regions, as was shown, for example, in the limit of small hole concentrations, $(1 - n) \ll 1$.

The formula (6.2) for the magnetic susceptibility is valid in a wide concentration interval; the only exceptions are the vicinities of $n = 0$ and $n = 1$, where one must use the gas approximation for electrons or holes.

We note that near the intercept of the boundary lines of the A and F phases (for the SC lattice, the point of intersection, n, is 0.91), another magnetic phase can form, which is neither ferromagnetic nor antiferromagnetic. Since the problem of two interacting order parameters was not considered, we exclude from consideration the vicinity of this point. Thus, the right-hand boundary of the shaded region of the diagram determines the conditional boundary of validity of the expression (6.2).

With $T = 0$ and $\mu > 0$, the localized contribution to the bare susceptibility $\chi_0(k)$ in (6.3) predominates, and the formula (6.2) results in the following expression for the static magnetic susceptibility:

$$\chi(k; 0) \simeq 1/[\Phi(k; 0) + J(k)]. \tag{6.12}$$

Near the ferromagnetic instability, the main contribution is made by long-wave fluctuations, and (6.12) can be written as

$$\chi(k; 0) = 1/(\alpha_F + \beta_F k^2) \qquad \alpha_F = \Phi(0; 0) + J(0) \tag{6.13}$$

where $\alpha_F > 0$, $\beta_F > 0$ and α_F is small. Near the antiferromagnetic instability,

$$\chi(k; 0) = 1/[\alpha_A + \beta_A(k - k_0)^2] \qquad \alpha_A = \Phi(k_0; 0) + J(k_0). \tag{6.14}$$

The last two expressions determine the characteristic sizes k_m and k_{mA} of the fluctuation distribution in k-space with

$$k_m = (\alpha_F/\beta_F)^{1/2} \qquad k_{mA} = (\alpha_A/\beta_A)^{1/2}. \tag{6.15}$$

An investigation of the dielectric susceptibility $\chi^N(k)$, determined in (6.8), shows that with $k = 0$ it has no poles. With $k = k_0$, a pole occurs when

$$n = 0.88 + 0.14\,\kappa. \tag{6.16}$$

The existence of this pole indicates the instability of the initial phase with respect to the formation of charge density waves. However, it is clear from (6.16) that the line of this instability on the phase diagram (κ, n) (see [17]) lies outside the concentration interval we study, so we can neglect the last term in (6.11). Thus, the first term there takes into account the mean-field effects while the second term takes into account the spin fluctuation contribution. We now study the role of spin fluctuations in the formation of the superconducting state.

7. The role of spin fluctuations in the formation of the superconducting state

We consider the linearized equation (5.17) for the superconducting order parameter

$$\Delta(k) = \frac{1}{N}\sum_{k_1} J(k - k_1)\Delta(k_1)\frac{\tanh[E(k_1)/2T]}{E(k_1)}$$
$$- \frac{3}{4N}\sum_{k_1} J^2(k - k_1)\chi(k - k_1; 0)\Delta(k_1)\frac{\tanh[E(k_1)/2T]}{E(k_1)}. \tag{7.1}$$

The quantity $\chi(k - k_1; 0)$ has a sharp peak in the vicinity of $k - k_1 = 0$ near the ferromagnetic transition and a peak in the vicinity of $k - k_1 = k_0$ near the antiferromagnetic transition. The conditions $\alpha_F = 0$ and $\alpha_A = 0$ should determine the Curie and Néel temperatures T_K and T_N of the magnetic phase transition as functions of the parameters κ and n. As equations (5.17) and (7.1) use the magnetic susceptibility of the paramagnetic phase, they are valid for those regions of (κ, n, T) parameter space where T exceeds the magnetic transition temperature; thus, the T_c that occur owing to the correlation mechanism must satisfy the conduction $T_c > T_K$ (or T_N). For further analyses, we assume this condition to be valid.

In order to reveal the qualitative role of the fluctuation term in equation (7.1), we approximate $\chi(k; 0)$ by a narrow rectangular peak of width $2k_m$ with centre at $k = 0$ if the system lies near the ferromagnetic transition, and by a peak of width $2k_{mA}$ with centre at $k = k_0$ if the system lies near the antiferromagnetic transition. The quantities k_m and k_{mA} are viewed as small as desired, in order to neglect the momentum dependence of $J^2(k - k_1)$ in the second term in (7.1). This is possible because the quantity $\chi(k - k_1; 0)$ determines, in fact, the momentum distribution in space. So we can bring the quantity $J^2(k - k_1)$ outside of the summation for this quantity to have a zero argument. The result is an integral equation with a fluctuation term whose kernel is localized in k-space.

We start by examining the case where the system is near the ferromagnetic instability. In the second term in (7.1), the main contribution to the sum over k_1 comes from the narrow shell near the Fermi surface with width $2k_m$. In this situation, taking into account the kernel $J(k - k_1)$ factorization for the SC lattice (see (4.6)) in the first term, the integral equation (7.1) can be reduced approximately to a system of algebraic equations. To this end, we rewrite (7.1) as

$$\Delta(k) = 2\kappa t \sum_\beta \cos k_\beta A_\beta - \tfrac{3}{4}(\kappa t z/\alpha_F)B \tag{7.2}$$

where the notations are

$$A_\beta = \frac{1}{N}\sum_{k_1} \cos k_{1\beta}\, \Delta(k_1) \frac{\tanh[E(k_1)/2T]}{E(k_1)} \tag{7.3}$$

$$B = \frac{1}{N}\sum_{k_1}{}' \Delta(k_1) \frac{\tanh[E(k_1)/2T]}{E(k_1)}. \tag{7.4}$$

The prime over the last sum means summation over the narrow shell near the Fermi surface of width $2k_m$. Excluding the quantity B in (7.2), we obtain the following system of equations for A_α:

$$A_\alpha = 2\kappa \sum_\beta \left(K_{\alpha\beta} - \frac{3}{16}\frac{t\kappa^2 z^2}{\alpha_F} \frac{F\mathcal{F}}{1 + \frac{3}{8}(t\kappa^2 z^2/\alpha_F)\mathcal{G}} \right) A_\beta. \tag{7.5}$$

Here the following notations are introduced:

$$K_{\alpha\beta} = 2t\frac{1}{N}\sum_k \frac{\cos k_\alpha \cos k_\beta}{2E(k)} \tanh\left(\frac{E(k)}{2T}\right) \qquad F = \frac{2t}{3}\frac{1}{N}\sum_k \frac{\gamma(k)}{E(k)} \tanh\left(\frac{E(k)}{2T}\right) \tag{7.6}$$

$$\mathcal{F} = \frac{2t}{3}\frac{1}{N}\sum_k{}' \frac{\gamma(k)}{E(k)} \tanh\left(\frac{E(k)}{2T}\right) \qquad \mathcal{G} = 2t\frac{1}{N}\sum_k{}' \frac{1}{E(k)} \tanh\left(\frac{E(k)}{2T}\right). \tag{7.7}$$

Equating to zero the determinant of the system (7.5) leads to two equations for T_c for s and d symmetries of the order parameter. In the case of s symmetry the equation reads

$$1 = 2Kt\frac{1}{N}\sum_k [\tfrac{1}{2}\gamma^2(k) - \nu_s\gamma(k)]\frac{\tanh[E(k)/2T_c]}{E(k)} \tag{7.8}$$

where

$$\nu_s = \frac{3}{8}\frac{tK^2z^2}{\alpha_F}\frac{\mathcal{F}}{1+\frac{3}{8}(tK^2z^2/\alpha_F)\mathcal{G}}. \tag{7.9}$$

The equation for T_c for d symmetry coincides with equation (4.7) of the mean-field approximation, because the fluctuation contributions cancel out in this case. This result for the d symmetry is a consequence of the fact that the magnetic susceptibility in the second term of (7.1) is approximated by a very narrow peak.

The quantities $\mathcal{F}$ and $\mathcal{G}$ are positive with $\varepsilon_F > 0$; thus, the factor ν_s, which defines the intensity of the fluctuation contribution to the pairing interaction, is also positive. It is clear from equation (7.8) that fluctuations suppress superconductivity. As the ferromagnetic transition is approached $\alpha_F \to 0$ and ν_s increases, but the increase of ν_s is limited by the denominator in the expression (7.9). In the limit $\alpha_F \to 0$, ν_s reaches a maximum value:

$$\nu_{s\max} = \mathcal{F}/\mathcal{G} = (\tfrac{3}{2}n - 1)/(1 - n/2). \tag{7.10}$$

To obtain the last expression, we use the relations

$$\mathcal{G} = 4t\rho_0(\tilde{\varepsilon}_F)\ln(2\gamma\omega_m/\pi T_c) \qquad \mathcal{F} = \tfrac{3}{2}\tilde{\varepsilon}_F\rho_0(\tilde{\varepsilon}_F)\ln(2\gamma\omega_m/\pi T_c) \tag{7.11}$$

in which $\rho_0(\varepsilon)$ is the electron density of states in the bare band, $\tilde{\varepsilon}_F = \varepsilon_F(1 - n/2)^{-1}$, and the Fermi energy [8] is

$$\varepsilon_F = \tfrac{1}{2}W(\tfrac{3}{2}n - 1) \tag{7.12}$$

where $W = 2zt$ is the width of the bare band. In the concentration interval $\frac{2}{3} < n < 1$ with $\varepsilon_F > 0$, $\nu_{s\max}$ varies from 0 to 1.

We now consider the system near the antiferromagnetic transition, when $\chi(k; 0)$ has a sharp maximum in the vicinity of $k = k_0$. Since the susceptibility here is centred at the point k_0, we arrive at the result that if the momentum k in the second term of equation (7.1) lies in the narrow layer near the Fermi surface of width $2k_{mA}$, then this layer contains the vector $k_1 + k_0$ rather than the momentum k_1, in contrast with the ferromagnetic instability case. Put another way, the vector k_1 lies in the layer near the Fermi surface, which is displaced by the vector k_0. In the final analysis, this leads to sign reversal of the fluctuation term in the equation for T_c:

$$1 = 2Kt\frac{1}{N}\sum_k [\tfrac{1}{2}\gamma^2(k) + \nu_s^A\gamma(k)]\frac{\tanh[E(k)/2T_c]}{E(k)}. \tag{7.13}$$

The fluctuation contribution intensity is determined by the factor

$$\nu_s^A = \frac{3}{8}\frac{tK^2z^2}{\alpha_A}\frac{\mathcal{F}^A}{1+\frac{3}{8}(tK^2z^2/\alpha_A)\mathcal{G}^A} \tag{7.14}$$

where

$$\mathcal{F}^A = \frac{1}{N}{\sum_k}' \gamma(k)\frac{\tanh\{[(1-n/2)\varepsilon(k)+\mu]/2T_c\}}{(1-n/2)\varepsilon(k)+\mu}. \tag{7.15}$$

We obtain a similar result for $\mathcal{G}^A$. The prime means that the summation in (7.15) is

performed over a narrow layer near the Fermi energy of width $2k_{mA}$. Integrating over energy, we find

$$\mathcal{F}^A = \frac{2}{3}\frac{\frac{3}{2}n-1}{(1-n/2)^2} \qquad \mathcal{G}^A = \frac{1}{6(1-n/2)^2}\frac{\omega_m}{\varepsilon_F}. \tag{7.16}$$

These formulae are obtained in a model with a constant density of states. $\rho_0(\varepsilon) = 1/W$. The quantity $\omega_m = v_F k_{mA}$ is the limiting frequency of the spin fluctuation spectrum (v_F is the electron velocity on the Fermi surface). In deriving formulae (7.16), we assume that $\varepsilon_F \gg \omega_m$.

We see that the antiferromagnetic fluctuations bring about an additional electron attraction; however, the fluctuation contribution intensity ν_s^A is also limited, because of the denominator in the expression (7.14). From (7.14) and (7.16), we arrive at the result that

$$\nu_{s\max}^A = 4(\tfrac{3}{2}n-1)\varepsilon_F/\omega_m \tag{7.17}$$

so $\nu_{s\max}^A$ lies in the interval from 0 to $2\varepsilon_F/\omega_m$.

With the d symmetry of the order parameter, the fluctuation contribution in the equation for T_c cancels out, too, just as in the case of an antiferromagnetic instability.

Equations (7.8) and (7.13) can be explicitly solved for T_c if the rectangular band model with constant density of states is used. In the logarithmic approximation, we have

$$T_c = \frac{\gamma}{\pi}[2n(1-n)]^{1/2} W \exp\left(-\frac{(1-n/2)^3}{(\frac{3}{2}n-1)^2\kappa \mp (\frac{3}{2}n-1)(1-n/2)^2\kappa\nu_s}\right). \tag{7.18}$$

The '$-$' sign in the denominator corresponds to ferromagnetic instability, the '$+$' sign to antiferromagnetic instability. Near the left-hand and right-hand boundaries of the concentration interval $\frac{2}{3} < n < 1$, T_c is small; the expression (7.18) has a maximum inside this interval. In the physically interesting case of the antiferromagnetic instability, T_c may be sufficiently great inside this interval, because of the large pre-exponential factor. However, the fluctuation part of the pairing interaction cannot be greater than 1, because of the small parameter κ.

It is clear from the formula (7.18) that T_c in a narrow concentration interval is very sensitive to the quantity ν_s and can reach values of $\sim(10^{-3}$ to $10^{-2})W$, with the values of ν_s not exceeding 1. Near the ferromagnetic instability, T_c is several orders of magnitude lower. The formula (7.18) defines the tendency of T_c to increase sharply with increasing concentration n and fluctuation contribution intensity ν_s.

Recall also that the formula (7.18) for T_c does not take into account the contribution of the kinematic mechanism [8]. The authors of [8] think that this contribution is dominant (only for the s symmetry order parameter; in the case of d symmetry, the fluctuation contribution cancels out in the equation for T_c). In our view, the kinematic mechanism is overestimated in [8, 9], because these authors did not take into account the fluctuation effect in the consideration of the kinematic term in perturbation theory. It is known that the Hubbard model in the limit $U \to \infty$ indicates strong tendencies for ferromagnetic ordering, tendencies that must weaken the pairing effect of the kinematic mechanism. Allowance for the corresponding fluctuation corrections (at least in the limit $U \to \infty$), which are contained in the part $\hat{H}_{kin}$ of the Hamiltonian, is a separate, very complicated, problem of the competition between the ferromagnetic and superconducting order parameters.

Now we pass on to the case of a d symmetry order parameter. Since in the limit of a very narrow peak in $\chi(k; 0)$, the fluctuation contribution has cancelled out in the equation

for T_c, we need to weaken this condition and thus preserve the momentum dependence of the quantity $J^2(k-k_1)$ in the next term of equation (7.1). For the SC lattice, this leads to the following approximate equation for T_c (in the case of antiferromagnetic instability):

$$1 = 2\kappa t \frac{1}{N}\sum_k [1 + \nu_d^{\perp A}(\cos k_x + \cos k_y) + \nu_d^{\parallel A} \cos k_z]\psi_d^2(k) \frac{\tanh[E(k)/2T_c]}{E(k)}. \tag{7.19}$$

The resulting equation contains two parameters characterizing the fluctuation contribution intensities:

$$\begin{Bmatrix} \nu_d^{\perp A} \\ \nu_d^{\parallel A} \end{Bmatrix} = 6(\kappa t)^2 \frac{1}{N}\sum_k{}' \begin{Bmatrix} \cos k_x + \cos k_y \\ \cos k_z \end{Bmatrix} \psi_d^2(k)\chi(k_F - k; 0) \frac{\tanh[E(k+k_0)/2T_c]}{E(k+k_0)} \tag{7.20}$$

where

$$E(k + k_0) = -(1 - n/2)\varepsilon(k) - \mu. \tag{7.21}$$

(In the paramagnetic phase of a metal, the z dimension differs in the basis function $\psi_d(k)$ of the superconducting order parameter.) The summation in (7.20) is limited by the layer near the Fermi surface of width $2k_{mA}$. The factors $\cos k_\alpha\ \psi_d^2(k)$ can be transformed into the product of d symmetry basis functions constructed on sites that follow the first coordination sphere. We can pass from equation (7.19) to equation (4.7) by neglecting basis functions of the d-like state.

The calculation of T_c from equation (7.19) demands numerical computations, as in the case of the mean-field approximation. In such computations, it would certainly be better to use the more general equation (7.1) rather than equation (7.19), in which rough approximations were made. To us, it was important to solve the question concerning the d state in principle and to see that in this case also the spin fluctuations lead to an increase of T_c ($\nu_d^{\perp A} > 0$ and $\nu_d^{\parallel A} > 0$ with $\varepsilon_F > 0$).

8. Conclusions

Let us sum up some results of the investigation. In contrast to the case of a weak Coulomb interaction [3], two contributions to the electron pairing interaction arise in the (t–J) model. The first contribution is of a statistical nature and is allowed by the mean-field approximation. The other contribution is a dynamic one and occurs owing to the interaction of electrons with spin fluctuations. In some regions of electron concentrations, the fluctuation contribution may be sufficiently large. It increases sharply near the magnetic phase transitions and, in the case of a ferromagnetic instability, fluctuations cause an electron repulsion; in the case of an antiferromagnetic instability, they cause an attraction, as was the case in the regime $U \ll t$.

Although the equations for a superconductor are derived in the spirit of strong-coupling theory [14], we consider the weak-coupling limit only in order to obtain analytical results, in which the equation for the superconducting order parameter reduces to the equation of the BCS theory with a strong momentum dependence of the electron pairing matrix element. Within the framework of this approximation, we have derived equations and formulae for T_c. The general equations obtained for a superconductor are in the spirit of the theory of strongly coupled superconductors with bare electron–boson vertices. A more accurate equation is

$\Sigma =$  (8.1)

for it has exact electron–boson vertices. However, using the above vertices in equation (7.1) is a very complicated problem. Generally, a number of questions touched upon in the paper remain open, because they demand numerical solutions of the equations obtained here and in [17]. These aspects include the concentration dependence and the value of T_c in real cases, where $\chi(k; 0)$ cannot be approximated by a narrow peak. Other problems are the calculation of the Curie temperature T_K and the Néel temperature T_N with respect to the parameters κ and n, and a comparison with the values of T_c. Only such numerical analyses permit one to find such regions on the (κ, n) plane where T_c greatly exceeds T_K and T_N, and where the developed theory can be applied.

Other important issues in the problem of superconductivity in a strongly correlated system include the question about the damping of electron states formed by the Hubbard-1 approximation. In a model with localized magnetic moments (s–d exchange model), such damping causes a strong suppression of the magnetic moment in the paramagnetic phase of a metal. The problem is to ascertain the role of electron damping due to real processes of electron-spin fluctuation interaction in a superconductor with a pairing interaction via virtual exchange by spin fluctuations. The general investigation that we have carried out in this paper gives hopeful predictions in the question of the possible role of spin fluctuations in the formation of high-T_c superconductivity in strongly correlated systems.

Note added in proof. Some problems listed in section 8 have been resolved by us and will be published. More accurate use of the GRPA approximation results in the essential renormalization of the vertices when parameter J in leading terms is replaced with t.

References

[1] Hubbard J 1963 *Proc. R. Soc.* A **276** 238
[2] Berk N F and Schrieffer J R 1966 *Phys. Rev. Lett.* **17** 433
[3] Scalapino D J, Loh E and Hirsch J E 1987 *Phys. Rev.* B **35** 6694
[4] Gros C, Joint R and Rice T M 1987 *Phys. Rev.* B **36** 381
[5] Baskaran G, Zou Z and Anderson P W 1987 *Solid State Commun.* **63** 973
[6] Anderson P W 1987 *Science* **235** 1196
[7] Chen Y H, Wilczek F, Witten E and Halperin B I 1989 *Int. J. Mod. Phys.* B **3** 1001
[8] Zaitsev R O and Ivanov V A 1988 *Int. J. Mod. Phys.* B **5** 153
[9] Zaitsev R O and Ivanov V A 1987 *Fiz. Tverd. Tela* **29** 2554, 3111
[10] Takahashi I 1988 *Physica* B **149** 69
[11] Kotliar G and Lin J 1988 *Phys. Rev. Lett.* **61** 1784
[12] Plakida N M, Yushankhai V Yu and Stasyuk I V 1989 *Physica* C **160** 80
[13] Zaborov A V and Sadovski M V 1988 Nearest neighbour pairing in Hubbard model *Series of Preprints* Problems of high-T_c superconductivity (Ural Division of USSR Academy of Science)
[14] Eliasberg G M 1960 *Sov. Phys.–JETP* **38** 966, **39** 1437
[15] Vonsovski S V, Izyumov Yu A and Kurmaev E Z 1982 *Superconductivity of Transition Metals, their Alloys and Compounds* (Berlin: Springer) p 34
[16] Izyumov Yu A and Scryabin Yu N 1988 *Statistical Mechanics of Magnetically Ordered Systems* (New York: Consultants' Bureau) p 72
[17] Izyumov Yu A and Letfulov B M 1990 *J. Phys.: Condens. Matter* **2** 8905
[18] Abrikosov A A, Gorkov L P and Dzyaloshinski I E 1975 *Methods of Quantum Field Theory in Statistical Physics* (New York: Dover)
[19] Izuyama T, Kim D J and Kubo R 1963 *J. Phys. Soc. Japan* **18** 1025