

Superconductivity in the Hubbard model with strong repulsion, a small number of carriers, and a large coordinate number

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The problem of the superconductivity of a system of electrons on a lattice with strong single-site correlations (a system described by the Hubbard Hamiltonian) is studied. In the framework of the strong-coupling method special variables are introduced that reduce the Hubbard variables to a system of Bose and Fermi operators and random fields. In the case when the occupancy is close to one electron per site and each site has a large number of neighbors the Hubbard model reduces to a system of weakly interacting electrons (holes) and local spins. Different magnetic phases of the system (ferromagnetic, paramagnetic, and antiferromagnetic) are investigated. It is shown that the pairing tendency due to electron correlations is suppressed by paramagnetic fluctuations and enhanced by antiferromagnetic fluctuations.

1. INTRODUCTION

The discovery of high-temperature superconductivity in metal-oxide compounds^{1,2} has become a powerful stimulus to the study of nonphonon models of superconductivity. The Hubbard model^{3,4} and its various generalizations and modifications is the most popular model of such a kind. There are both objective and subjective reasons for the great attention paid by theorists to the Hubbard model. The objective reasons are connected with the fact that the Hubbard model correctly describes the nature of the dielectric state (Mott insulator) in lanthanum and yttrium systems for stoichiometric compounds, the antiferromagnetic structure of their ground state, and the destruction of the antiferromagnetism by doping. This makes it natural to seek the causes of the superconductivity within the framework of this model, without introducing further interactions. The subjective reasons are connected with the fact that the Hubbard model offers possibilities for the construction of dynamical approximation schemes of various kinds.⁴⁻⁸ A definite role has been played by Anderson's criticism of the traditional phonon model and by his advocacy of the Hubbard model.⁹ It is now difficult to give a list of references to papers in this direction that is in any sense complete.

In the present paper we develop an approach to the Hubbard model that is based on the temperature diagram technique for the Hubbard operators. The starting point of this approach is a realization of Wick's theorem for Hubbard operators by means of a representation of the Hubbard operators in terms of Bose and Fermi operators and random fields with specified correlation properties. Such a realization is obtained for the Hubbard-operator algebra $Pl(1, 2)$ for the case of infinite repulsion, and for the algebra $Pl(2, 2)$ for the complete model. In the case of the algebra $Pl(1, 2)$ the Hubbard operators are expressed in terms of the Fermi operators of the electrons in the lower Hubbard band, the Bose operators corresponding to the spin degrees of freedom, and two random fields, corresponding to the spin fluctuations and charge fluctuations. In the case of the complete $Pl(2, 2)$ algebra, to these degrees of freedom one adds the Fermi operators of the electrons in the upper Hubbard band, the exciton Bose operators that take electrons from the lower to the upper Hubbard sub-band, and also an appropriate

random field. The resulting representations of the algebras $Pl(1, 2)$ and $Pl(2, 2)$ make it possible to write the Hamiltonian of the model in terms of the Bose and Fermi operators and the random fields in the limit $U \gg t$, where U is the energy of the Coulomb repulsion at a site and t is the electron-hopping integral between neighboring sites. This Hamiltonian is the starting point for the analysis of the magnetic structure of the ground state and the question of the superconductivity.

This analysis can be carried out when two small parameters are present: p (the number of charge carriers per lattice site minus one, i.e., the small number of carriers in the Hubbard band), and $1/z$, where z is the number of nearest neighbors of a given site. It is everywhere assumed that the lattice is alternating.¹⁰ In the case of a small number of carriers (electrons in the upper Hubbard band or holes in the lower Hubbard band), the initial Hamiltonian reduces to a system of electrons (holes) and local spins at the sites.

The analysis of the ferromagnetic state of the model is the simplest. This state is realized in the Hubbard model for $1 \gg p \gg t/U$ and temperatures $T < p^{1/3}tz^2$, and is consistent with Nagaoka's theorem.¹⁰ The ferromagnetic state is energetically favored, since the strong dependence of the dispersion law on the sign of the spin projection leads to strong narrowing of one spin sub-band and substantial broadening of the other. The bottom of the latter band is lowered, and the electrons (holes) at the bottom of the band lower their energy. It is this energy which makes the ferromagnetic state energetically favored. Indirect exchange between local spins via polarization of the charge carriers also reduces the energy of the ferromagnetic state. The elementary excitations in the ferromagnetic phase are electrons (holes), with the same sign of the projection of the spin along the direction of the magnetization, and magnons, whose dispersion law satisfies Goldstone's theorem. Because of the strong splitting of the Fermi surface in the ferromagnetic state, superconductivity is not realized in this state for any reasonable mechanism of attraction.

The paramagnetic state is realized at sufficiently high temperatures $T > p^{1/3}tz^2$, "under the ferromagnetic region," or $T \gtrsim zt(t - pU/2)/U$, "above the antiferromagnetic region." The elementary excitations are electrons (holes) that are degenerate with respect to spin. An important role is

played by fluctuations of the local spins, the excitations of which propagate in a diffusive manner.^{11,12} In the lower Hubbard band the scattering amplitude is positive for electrons (repulsion) and negative for holes (attraction), while in the upper Hubbard band it is the opposite. This fact was first obtained in Refs. 6 and 13, and can be interpreted as an effective narrowing of the band as the electrons approach each other, increasing the energy of the electrons and lowering the energy of the holes in the lower Hubbard band.

The kinematic attraction of the holes makes a discussion of the question of superconductivity timely. This attraction is greater by a factor of U/t than the previously discussed attraction due to the superexchange interaction.¹⁴⁻¹⁶ However, superconductivity against the background of the paramagnetic state does not arise: In this case, spin fluctuations destroy the superconductivity in accordance with the Abrikosov-Gor'kov mechanism.¹⁷ This result contradicts the assertion made in the sequence of papers Refs. 6, 13, and 18 that superconductivity appears. The error made in these papers is due to an incorrect calculation of the spin correlator in the paramagnetic phase.

The antiferromagnetic state is realized for small hole concentrations $p < t/U$ and low temperatures $T < zt(t - pU/2)/U$. In view of the doubling of the lattice constant, the volume of the Brillouin zone is halved and the number of hole modes becomes equal to four. Two modes are spin-degenerate. The kinematic interaction of the holes is attractive on the Fermi surface. The exchange of antiferromagnons is stronger and does not lead to suppression of superconductivity. This picture does not take into account the formation of magnetic polarons,^{15,19} which, for a sufficiently small ratio t/U , are charge carriers in the antiferromagnetic state. Below, we give a quantitative account of the physical picture given above.

2. DIAGRAM TECHNIQUE AND REPRESENTATION OF THE HUBBARD OPERATORS

The Hubbard model describes a system of electrons on a lattice, with the Hamiltonian⁴

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

Here $c_{n\sigma}^+$ and $c_{n\sigma}$ are the Fermi operators of an electron at the n th lattice site and with spin projection $\sigma = \pm 1/2 \equiv \uparrow, \downarrow$; $t_{nn'}$ is the electron-tunneling integral from site n to site n' , with $t_{nn'} = t_{n'n}$; $\hat{n}_{n\sigma} = c_{n\sigma}^+ c_{n\sigma}$ is the operator of the number of electrons at site n with spin projection σ ; $\mu_{n\sigma} = \mu - \sigma\omega_0$ is the spin-dependent chemical potential, where ω_0 is the precession frequency of the electron spin in the external magnetic field B and μ is the intrinsically chemical potential. Our task is to develop the strong-coupling method, in which the second and third terms in the Hamiltonian (1) are taken into account exactly and the first term can be treated as a perturbation.⁴

Such a strong-coupling method has been developed earlier in the theory of magnetism^{20,21} and is based on the introduction of Hubbard operators and the construction of the theory in terms of them. For this, we note that at lattice site n there are four possible states $|na\rangle = |n0\rangle, |n\uparrow\rangle, |n\downarrow\rangle, |n\uparrow\downarrow\rangle$, where $|n0\rangle$ is the state without electrons, $|n\sigma\rangle$ is a state with one electron, and $|n\uparrow\downarrow\rangle \equiv |n2\rangle$ is the state with two electrons at the site. The Hubbard operators, defined as

$X_n^{ab} = |na\rangle\langle bn|$, and the electron operators are easily expressed in terms of these: $c_{n1} = X_n^{01} - X_n^{12}$, $c_{n1} = X_n^{01} + X_n^{12}$, $c_{n1}^+ = X_n^{10} - X_n^{21}$, $c_{n1}^+ = X_n^{10} + X_n^{21}$, $\hat{n}_{n\sigma} = X_n^{\sigma\sigma} + X_n^{22}$. Here the operators $X_n^{0\sigma}, X_n^{\sigma 0}, X_n^{\sigma\sigma}$, and $X_n^{2\sigma}$ on different sites anticommute, and the other Hubbard operators commute. In terms of the Hubbard operators, the Hamiltonian (1) has the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int}, \quad \mathcal{H}_0 = - \sum_{n\sigma} \mu_{n\sigma} X_n^{\sigma\sigma} + (U + 2\mu) \sum_n X_n^{22},$$

$$\mathcal{H}_{int} = \sum_{n \neq n', \sigma} t_{nn'} (X_n^{\sigma 0} + 2\sigma X_n^{2, -\sigma}) (X_{n'}^{0\sigma} + 2\sigma X_{n'}^{-\sigma 2}). \quad (2)$$

For $U \gg t$ the contribution of the operators $X_n^{2, -\sigma}$ and $X_n^{-\sigma 2}$ is small in zeroth order and below will be taken into account in perturbation theory in the parameter t/U . In the construction of the temperature Green functions from the initial operators $c_{n\sigma}^+$ and $c_{n'\sigma'}$ one can express the latter in terms of the Hubbard operators $X_n^{0\sigma}, X_n^{\sigma 0}, X_n^{2\sigma}$, and $X_n^{\sigma 2}$ and then average over the bare density matrix $\bar{\rho}_0 = \exp(-[SB:\beta\mathcal{H}_0])$ together with the temperature S matrix

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

where $\beta = 1/T$ is the inverse temperature, τ is the imaginary time, and T_τ is a τ -ordered exponential.²² As a result, the need arises to calculate the following averages:

$$Y_k = \text{Sp} (X_{n_1}^{a_1 b_1} X_{n_2}^{a_2 b_2} \dots X_{n_k}^{a_k b_k} \bar{\rho}_0) / \text{Sp} (\bar{\rho}_0). \quad (3)$$

The method of calculating such averages is usually called Wick's theorem for Hubbard operators.⁴ To formulate Wick's theorem in the case of the operator algebra

$$[X_n^{ab}, X_m^{cd}]_{\pm} = \delta_{nm} (\delta_{ba} X_n^{cd} \pm \delta_{ad} X_n^{cb}), \quad (4)$$

(here the plus sign is for Hubbard Fermi operators, and the minus sign for Hubbard Bose operators), we order the indices $a, b = 1, 2, \dots, N$ in some way that makes it possible to divide the algebra of the X operators into three subalgebras—a Cartan subalgebra X^0 , including all the diagonal Bose operators X_n^{aa} , a subalgebra X^- , including the operators X_n^{ab} for $a < b$, and a subalgebra X^+ , including the operators X_n^{ab} for $a > b$. We note that X^0 and $X^\pm$ are graded Lie subalgebras with respect to the operations of commutation and anticommutation, and the following relations are fulfilled:

$$[X^0, X^0] = 0, \quad [X^-, X^0] = X^-, \quad [X^+, X^0] = X^+,$$

$$[X^-, X^-] = X^-, \quad [X^+, X^+] = X^+, \quad [X^+, X^-] = X^-. \quad (5)$$

The division into the subalgebras X^+ and X^- is not unique and depends on the way in which the indices a and b are ordered.

Using the commutation relations between the elements of the subalgebra X^- and the elements of the complete algebra X , we can reduce the average (3) to the trace of just the elements of the Cartan subalgebra X^0 (Ref. 4):

$$I_{n_1 a_1, \dots, n_p a_p}^p(y_1, \dots, y_p) = \sum C_p \text{Sp} (X_{n_1}^{a_1 a_1} X_{n_2}^{a_2 a_2} \dots X_{n_p}^{a_p a_p} \bar{\rho}_0), \quad (6)$$

Here the parameters y_a are determined by the expansion of

the Hamiltonian in the elements of the Cartan subalgebra:

$$\beta \mathcal{H}_0 = - \sum_{n,a} y_a X_n^{aa}, \quad \rho_0 = \exp(-\beta \mathcal{H}_0) / \text{Sp}[\exp(-\beta \mathcal{H}_0)]. \quad (7)$$

For the single-site averages $I_{a_1, \dots, a_p}(y_1, \dots, y_N)$ from (6) it is easy to obtain the recursion relation

$$I_{a_1, \dots, a_p}^p(y) = \partial I_{a_1, \dots, a_{p-1}}^{p-1} / \partial y_p + I_{a_1, \dots, a_{p-1}}^{p-1} I_{a_p}, \quad (8)$$

and the quantities I_a are determined as follows:

$$I_a = \partial F(y) / \partial y_a, \quad F(y) = \ln \{ \text{Sp}[\exp(-\beta \mathcal{H}_0)] \}, \quad (9)$$

where $F(y)$, obviously, is the thermodynamic potential.

From the relations (8) and (9) there follows the diagrammatic "cross technique"⁴ for calculating the averages $I_{n_1 a_1, \dots, n_p a_p}^p(y_1, \dots, y_N)$ (6):

$$\langle X_n^{aa} \rangle = \begin{array}{c} \times \\ | \\ \bullet \end{array} = I_a = \partial F(y) / \partial y_a \equiv K_a, \quad (10)$$

$$\langle X_{n_1}^{a_1 a_1} X_{n_2}^{a_2 a_2} \rangle = \begin{array}{cc} \times & \times \\ | & | \\ \bullet & \bullet \end{array} + \begin{array}{cc} \times & \times \\ \diagdown & \diagup \\ \bullet & \bullet \end{array} = I_{a_1} I_{a_2} + K_{n_1 a_1, n_2 a_2}^2, \quad (11)$$

$$K_{n_1 a_1, n_2 a_2}^2 = \delta_{n_1 n_2} \partial^2 F(y) / \partial y_{a_1} \partial y_{a_2},$$

$$\langle X_{n_1}^{a_1 a_1} X_{n_2}^{a_2 a_2} X_{n_3}^{a_3 a_3} \rangle = \begin{array}{ccc} \times & \times & \times \\ | & | & | \\ \bullet & \bullet & \bullet \end{array} + \begin{array}{ccc} \times & \times & \times \\ \diagdown & & \diagup \\ \bullet & & \bullet \end{array} + \begin{array}{ccc} \times & \times & \times \\ & \diagdown & \diagup \\ & \bullet & \bullet \end{array} + \begin{array}{ccc} \times & \times & \times \\ & \diagdown & \diagup \\ & \bullet & \bullet \end{array} + \begin{array}{ccc} \times & \times & \times \\ & \diagdown & \diagup \\ & \bullet & \bullet \end{array}, \quad (12)$$

$$\begin{array}{ccc} \times & & \times \\ \diagdown & & \diagup \\ \bullet & & \bullet \end{array} \equiv K_{n_1 a_1, n_2 a_2, n_3 a_3}^{(3)} = \delta_{n_1 n_2 n_3} \partial^3 F(y) / \partial y_{a_1} \partial y_{a_2} \partial y_{a_3}. \quad (13)$$

The examples (10)–(13) show that the averages $I_{n_1 a_1, \dots, n_p a_p}^p(y)$ are calculated by expanding in the irreducible cumulants $K_{n_1 a_1, \dots, n_p a_p}$ and the irreducible cumulant has the very simple form

$$K_{n_1 a_1, \dots, n_p a_p}^p(y) = \delta_{n_1, \dots, n_p} \partial^p F(y) / \partial y_{a_1} \dots \partial y_{a_p}. \quad (14)$$

It may be said that, when they are averaged with the bare density matrix ρ_0 , the diagonal Hubbard operators behave like random fields whose irreducible cumulants are specified by the relations (14). Thus, the Wick theorem^{4,20,23} that makes it possible to calculate the averages Y_k (3) has been completely formulated.²¹ At this stage, however, the diagrammatic rules of correspondence for the analytical expressions cannot be formulated simply. To formulate such rules we shall express the Hubbard operators X_n^{ab} in terms of the Bose operators, Fermi operators, and random fields whose averages are specified by irreducible cumulants of the type (14). Such a representation for the spin operators in the group $SU(2)$ was obtained in Ref. 21.

The idea of the derivation of such a representation is the following. For the validity of the Wick theorem the explicit form of the X operators is not important. Only the correct commutation relations between the operators of the subalgebra X^- and the elements of the complete algebra X , and also the correct values of the averages of products of elements of the Cartan subalgebra X^0 over the bare density matrix ρ_0 , are important. Following the example of the group $SU(2)$, as the elements of the subalgebra X^- we must choose simply

Bose or Fermi operators with certain complications. As the elements of the subalgebra X^0 we must choose expressions of the particle-number type (bilinear in the Bose and Fermi operators), while the elements of the subalgebra X^+ should be obtained from the condition that the algebra $X(4)$ be closed. This program can indeed be realized.

For $U/t \rightarrow \infty$ and when the occupancy at each lattice site is less than unity, only the three states $|n0\rangle$, $|n\uparrow\rangle$, and $|n\downarrow\rangle$ are important and it is necessary to construct a representation of the algebra $Pl(1, 2)$. The representation has the following form in terms of the spinor field ψ_σ , ψ_σ^+ , the Bose field a^+ , a , and the random fields Φ , Ω :

$$X^{\uparrow\uparrow} + X^{\downarrow\downarrow} = N = (\psi^+ \psi) + \Omega, \quad X^{00} = 1 - N, \quad (15a)$$

$$(X^{\uparrow\downarrow} - X^{\downarrow\uparrow})/2 = s_T^0, \quad X^{\uparrow\downarrow} = s_T^+, \quad X^{\downarrow\uparrow} = s_T^-.$$

Here N is the electron-number operator, and the quantities $s_x^T = s_T^+ + s_T^-$, $s_y^T = -i(s_T^+ - s_T^-)$, and $s_z^T = s_T^0$ form the total-spin vector, which can be written in the form

$$s^T = s + (\psi^+ \sigma \psi)/2, \quad (15b)$$

where σ are the Pauli matrices and the operators s are expressed in terms of a^+ , a , and Φ by a relation analogous to that obtained in Ref. 21 for the group $SU(2)$:

$$s^- = -a, \quad s^0 = a^+ a + \Phi, \quad s^+ = -a^+ (a^+ a + 2\Phi). \quad (15c)$$

For the operators $X^{0\sigma}$ and $X^{\sigma 0}$ we have

$$X^{0\sigma} = \psi_\sigma, \quad X^{\sigma 0} = \{ \psi^+ [1 - (\psi^+ \psi) - \Omega/2 + (s\sigma)] \}_\sigma. \quad (15d)$$

To calculate the cumulants of the random fields Ω and Φ it is sufficient to give the thermodynamic potential $F(x, y)$, where $x = \beta\mu \equiv \omega_\Phi$ and $y = -\beta\omega_0 \equiv \omega_\Omega$:

$$F(x, y) = \ln \left\{ \frac{[1 + \exp(x+y/2) + \exp(x-y/2)](1 - \exp y)}{[1 + \exp(x+y/2)][1 + \exp(x-y/2)]} \right\} \quad (16)$$

and the cumulants for the fields Ω and Φ are calculated from formula (14) if it is assumed that x is conjugate to Ω and y to Φ . The expression in (16) for the partition function is easily obtained from the condition that the averages of the operators N and s_T^0 , written in terms of the operators $X^{\uparrow\downarrow}$ and $X^{\downarrow\uparrow}$, coincide with their averages written in terms of the operators $\psi_\sigma^+ \psi_\sigma$ and $a^+ a$ and the random fields Ω and Φ . The fields Ω and Φ incorporate the difference of the averages (over the bare density matrix ρ_0) of $X^{\uparrow\downarrow} - X^{\downarrow\uparrow}$ and $\psi^+ \psi$ for the operator N and of $(X^{\uparrow\downarrow} - X^{\downarrow\uparrow})/2$ and $(\psi^+ \psi - \psi_1^+ \psi_1)/2 + a^+ a$ for s_T^0 . The relations (15) realize a certain non-Hermitian representation of the algebra $Pl(1, 2)$ for any values of the fields Ω and Φ , and should not be regarded as operator identities, defined in some Hilbert space, but only as relations that permit one to calculate Green functions in the framework of the temperature diagram technique. The fluctuation properties of the fields Ω and Φ ensure the correct values of the averages in the Cartan subalgebra X^0 .

In the case of the complete Hubbard model for $U \neq \infty$ it is possible to construct for the complete algebra $Pl(2, 2)$ a representation that contains [in addition to the operators in the case of the algebra $Pl(1, 2)$] Fermi operators φ_σ^+ , φ_σ of electrons in the upper Hubbard band, exciton operators that carry electrons from the lower to the upper Hubbard band

and vice versa, and also the random field Ξ that controls the number of electrons in the upper Hubbard sub-band. A representation of the algebra $Pl(2, 2)$ is given in Appendix A.

3. THE EFFECTIVE HAMILTONIAN OF THE MODEL. THE CASE OF SMALL OCCUPANCY

For $U \gg t$ the operators X_n^{22} , $X_n^{2\sigma}$, and $X_n^{\sigma 2}$ in the Hamiltonian (2) can be omitted, since the states $|n2\rangle$ are empty. Substituting the representation (15) for the X operators into (2), we obtain

$$\mathcal{H}_0 = - \sum_{n\sigma} \mu_\sigma \psi_{n\sigma}^\dagger \psi_{n\sigma} + \sum_n [\omega_0 a_n^\dagger a_n - \mu \Omega_n + \omega_0 \Phi_n], \quad (17a)$$

$$\mathcal{H}_{int} = \sum_{n \neq n'} t_{nn'} \psi_n^\dagger [1 - \Omega_n/2 - (\psi_n^\dagger \psi_n) + (s_n \sigma)] \psi_{n'}. \quad (17b)$$

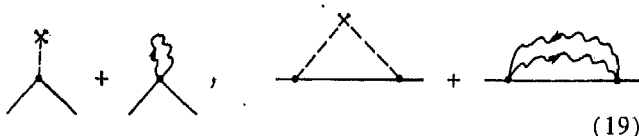
The Hamiltonian (17) describes a system of electrons with four-particle interaction, interacting with a random field Ω and a system of local spins s (15c). We note that the Hamiltonian (17b) is non-Hermitian. However, there is no inconsistency in this. It specifies the rules for calculations in the framework of the diagram technique, and must not be regarded as an operator defined in a certain Hilbert space. In the case when the number of electrons at each site is small and the temperature T is small in comparison with the chemical potential, further simplifications are possible. We note that the magnitude of the chemical potential is fixed by the condition (see Fig. 1)

$$t_{nn}=0 \text{ or } \sum_k t_k=0, \quad \sum_k t_k^2 = t_0^2/z = zt^2, \quad (18)$$

where the summation over k runs over the Brillouin zone, t_k is the Fourier transform of $t_{nn'}$, and the last of the three relations (18) is the definition of the number z of neighbors. In the case when $T, \omega_0 \ll |\mu|$ with $\mu < 0$ (see Fig. 1), the thermodynamic potential F (16) is equal to $\ln(1 - \exp y)$, does not depend on the parameter x , and differs in sign from the free energy of an oscillator with frequency ω_0 . It is obvious that in this situation all the cumulants of the field Ω are equal to zero, and Ω can also be set equal to zero.

One can also convince oneself that the spin-spin s - d in-

teraction [the last term in $\mathcal{H}_{int}$ (17b)] does not have any effect on the dynamics of the electrons and can be omitted. In fact, cumulants of the field Φ and loops of Bose operators $a^\dagger a$ always appear together:



$$(19)$$

and cancel each other. The Hamiltonian $\mathcal{H}_{int}$ (17b) is reduced in this case to the form

$$\mathcal{H}_{int} = \sum_{n \neq n'} t_{nn'} [(\psi_n^\dagger \psi_{n'}) - (\psi_n^\dagger (\psi_n^\dagger \psi_n) \psi_{n'})] \quad (20)$$

and describes a system of electrons with dispersion law $t_k - \mu$. To convince ourselves of this, we shall consider the Green function (GF) of the initial electron operators $c_{n\sigma}^\dagger, c_{n\sigma}$:

$$G_{\sigma\sigma'}(\tau, n) = \text{Sp} \{ T_\tau [c_{n\sigma}(\tau) c_{n\sigma'}^\dagger(0) S_\tau] / \text{Sp} (S_\tau \rho_0) \}, \quad (21a)$$

$$G_{\sigma\sigma'}(i\xi, k) = \sum_n \int_0^\beta \exp(-i\xi\tau - ikr_n) G_{\sigma\sigma'}(\tau, n) d\tau. \quad (21b)$$

Here τ is the temperature time, r_n is the position vector of the cell with label n , $c_{n\sigma}^\dagger(\tau)$ and $c_{n\sigma}(\tau)$ are operators in the interaction picture, and S_τ is the temperature S -matrix.²² By replacing the operators $c_{n\sigma}^\dagger$ and $c_{n\sigma}$ by the X operators $X_n^{\sigma\sigma}$ and $X_n^{\sigma\sigma}$ (omitting $X_n^{\sigma 2}$ and $X_n^{2\sigma}$) and replacing $X_n^{\sigma\sigma}$ and $X_n^{\sigma\sigma}$ by the operators $\psi_{n\sigma}^\dagger$ and $\psi_{n\sigma}$ in accordance with the relation (15d) with the contributions of Ω and s omitted, we obtain in place of (21a) the expression

$$G_{\sigma\sigma'}(\tau, n) = \text{Sp} \{ T_\tau (\psi_{n\sigma}^\dagger(\tau) [1 - \psi_{n-\sigma}^\dagger(\tau) \psi_{n-\sigma}(\tau)] \psi_{n\sigma'}(0) \rho_0) \}. \quad (22)$$

On the basis of Eq. (22) for the GF $G_{\sigma\sigma'}(\tau, n)$ we can construct a perturbation-theory series in $\mathcal{H}_{int}$ (20) and perform the classification and summation of the diagrams. The classification of the diagrams is performed naturally using the principle of one-particle irreducibility, i.e., by distinguishing blocks that cannot be separated by cutting one ψ -field line:

$$G_q = E_q + E_q \Sigma_q + E_q \Sigma_q \Sigma_q + \dots + E_q \Sigma_q \Sigma_q \Sigma_q + \dots \quad (23)$$

Here E_q and Σ_q are the end operator and mass operator, and $q = (i\xi, k)$ is the four-momentum. The sequence (23) is easily summed and leads to the following representation for the GF G_q :

$$G_q = E_q (g_{0q}^{-1} - \Sigma_q)^{-1} = E_q g_q.$$

This representation differs from the usual Dyson representation by the presence of the end operator E_q . The poles of the GF G_q are determined by the poles of the propagator g_q , which coincides with the GF of the operators $\psi^\dagger, \psi$. Consequently, the poles of g_q determine the excitation spectrum, and the end operator E_q specifies the residue of the GF of the initial fields $c_{n\sigma}^\dagger, c_{n\sigma}$. In lowest order of perturbation theory the diagrams for the operators Σ_q and E_q have the form

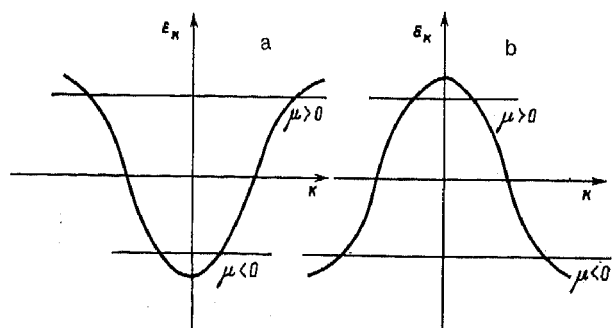


FIG. 1. Electron-dispersion law $\varepsilon_k = ct_k$; c is a constant of order unity and the horizontal lines are the position of the chemical potential; $\mu - t_{\min} = E_F$ is the Fermi energy for $\mu < 0$ (the electron case), and $t_{\max} - \mu = E_F$ is the Fermi energy for $\mu > 0$ (the hole case). Here, a) $t_0 < 0, t_{\min} = t_0, t_{\max} = t_{k_B}$; b) $t_0 > 0, t_{\min} = t_{k_B}, t_{\max} = t_0$, where k_B is the momentum at the Brillouin-zone boundary. In the case of hopping to nearest-neighbor sites the cases (a) and (b) can be reduced to each other by a redefinition of the quasimomentum, and therefore the article will consider the case (b) with $t_0 > 0$.

$$\begin{aligned} \Sigma_q &= \text{diagram 1} + \text{diagram 2} + \text{diagram 3}, \\ \varepsilon_q &= 1 - \text{diagram 4} + \text{diagram 5}, \end{aligned} \quad (24)$$

where the cross denotes the hopping integral t_k , a circle corresponds to the end vertex, which is equal to 1, and a point corresponds to the bare four-fermion vertex

$$F_{k_1 k_2; k_3 k_4} = \text{diagram 6} = -(t_{k_3}^+ t_{k_4}^-). \quad (25)$$

It follows from the construction given above that the electron-dispersion law ε_k in lowest order both in the interaction and in the parameter p (the number of electrons per unit cell) has the form $t_k - \mu$. The electron-scattering amplitude in lowest order in p is determined by the sequence of diagrams

$$\text{diagram 7a} + \text{diagram 7b} + \dots + \text{diagram 7c} + \dots \quad (26)$$

In leading order in $1/z$ the diagram (26a) is the leading diagram and the scattering amplitude is given by the relation (25). The smallness of the diagram (26b) is easily established by performing the summation over the frequencies, expanding the denominator in a series in t_{k_1} and t_{k_2} , where k_1 and k_2 are the momenta of the intermediate lines, and integrating over the loop momentum using the relation (18). We note that we can sum the series (26) in explicit form, obtaining for the scattering amplitude $F(E, \mathbf{k})$

$$F(E, \mathbf{k}_1, \mathbf{k}_2; \mathbf{k}_3, \mathbf{k}_4) = -(t_{k_3} + t_{k_4}) / \left[1 + \sum_{k'} \frac{t_{k'} + t_{k-k'}}{E - \varepsilon_{k'} - \varepsilon_{k-k'} - i\delta} \right]. \quad (27)$$

Here $E = \varepsilon_{k_1} + \varepsilon_{k_2} = \varepsilon_{k_3} + \varepsilon_{k_4}$ and $\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$ are the energy and momentum of the colliding particles. The relations obtained fully determine the character of the state in the case of small occupancy and strong attraction: The electron gas is paramagnetic, and the dispersion law and scattering amplitude are of order t and do not depend on U . These results can also be obtained in the gas approximation by other, more direct methods.²⁴

4. THE FERROMAGNETIC STATE FOR OCCUPANCY CLOSE TO UNITY

The Hubbard Hamiltonian (1) possesses electron-hole symmetry: It preserves its functional form when the electron operators are replaced by hole operators. After the Mott transition (the formation of two Hubbard sub-bands and a forbidden band between them) the electron-hole symmetry is preserved: There is complete similarity between the properties of electrons in the upper Hubbard band and those of holes in the lower Hubbard sub-band. For definiteness, we shall discuss holes in the lower Hubbard sub-band. The chemical potential μ in this case is positive, and in the case of importance to us ($T \ll \mu$, $\omega_0 \ll 2\mu$) the expression for the thermodynamic potential F is simplified:

$$F(x, y) = -x + \ln \{ [2 \operatorname{ch}(y/2)] (1 - \exp y) \}. \quad (28)$$

It follows from the expression (28) for F that the field Ω does not fluctuate and is equal to -1 , while the correlators of the field Φ coincide exactly with the corresponding correlators for spin $s = 1/2$. Consequently, we can write the effective Hamiltonian in the lower Hubbard band when it is almost completely filled in terms of the hole operators h_n^+ and h_n

$$h_n^+ = \tau \psi_n, \quad h_n = \psi_n^+ \tau, \quad \tau = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (29)$$

and the operators of spins s for $s = 1/2$:

$$\mathcal{H}_0 = \sum_{n\sigma} \mu_{-\sigma} h_{n\sigma}^+ h_{n\sigma} + \omega_0 \sum_n s_n^z, \quad (30a)$$

$$\begin{aligned} \mathcal{H}_{\text{int}} &= \sum_{n \neq n'} t_{n'n} h_{n'}^+ [-1/2 - (h_n^+ h_n) + (s_n \sigma)] h_n \\ &+ \frac{4}{U} \sum_{n \neq n'} |t_{nn'}|^2 s_n s_{n'}. \end{aligned} \quad (30b)$$

The last term in $\mathcal{H}_{\text{int}}$ (30b) is a correction of order t/U to the first contribution and is a part of the Anderson superexchange²⁵ that is important for the establishment of antiferromagnetic order when the occupancy is close to unity. It is derived in Appendix A.

The principal properties of the ferromagnetic state, and the region of temperature and hole concentration (on the low-concentration side) in which it is realized, can be established in the self-consistent field approximation, which is valid in the parameter $1/z$. We shall assume that the ferromagnetic state is realized, and determine in this state the spectrum of the holes and magnons and also the correlators of the longitudinal components of the spin. We then find the free energy of the magnetic state and determine the region in which it exists. The hole-magnon Hamiltonian is obtained from (30b), if the spin operators are replaced by the Bose operators a^+ , a and the random field Φ in accordance with (15c) (Ref. 21). As $T \rightarrow 0$ the quantity $\Phi \rightarrow -1/2$, and we obtain the well known Dyson-Maleev representation. The Feynman diagrams for the mass operator Σ_q of the holes, the mass operator P_q of the magnons, and the end operator E_q of the holes have the form

$$\Sigma_q = \text{diagram 8a1} + \text{diagram 8a2} + \text{diagram 8a3} + \text{diagram 8a4} + \text{diagram 8a5} + \text{diagram 8a6} + \text{diagram 8a7} + \text{diagram 8a8} \quad (31a)$$

$$P_q = \text{diagram 8b1} + \text{diagram 8b2} + \text{diagram 8b3} + \text{diagram 8b4} + \text{diagram 8b5} + \text{diagram 8b6} + \text{diagram 8b7} + \text{diagram 8b8} \quad (31b)$$

$$E_q = -1/2 + \text{diagram 8c1} + \text{diagram 8c2} + \text{diagram 8c3} + \text{diagram 8c4} + \text{diagram 8c5} + \text{diagram 8c6} + \text{diagram 8c7} + \text{diagram 8c8} \quad (31c)$$

The end operator E_q relates the Green functions of the initial electrons ($c_{n\sigma}^+$, $c_{n\sigma}$) to the GF of the Hubbard holes:

$$(G_q)_e = \tau (G_{-q})_h E_{-q} \tau. \quad (32)$$

$$\begin{aligned}
 & \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3}, \quad \text{Diagram 4} = \text{Diagram 5} + \text{Diagram 6} + \dots, \\
 & \text{Diagram 7} = \text{Diagram 8} + \text{Diagram 9} + \dots, \\
 & \text{Diagram 10} = \text{Diagram 11} + \text{Diagram 12} + \dots,
 \end{aligned}
 \tag{33}$$

(34a)

(34b)

In lowest order in $1/z$ it is sufficient to sum the sequence (34a) and the analogous sequences for higher correlators. As a result of summation of the Taylor series for the dressed correlators of the field Φ one can use Eq. (14) with the thermodynamic potential determined by Eq. (28), if the bare frequency ω_0 is replaced by the renormalized frequency

here $p_k^\pm$ are the Fermi distribution functions of holes with spin projection $\pm 1/2$, and the quantity y in this case becomes equal to $-\beta\omega_R$. The quantity x changes analogously ($x \rightarrow \beta\mu_R$), where μ_R is the renormalized chemical potential

the field Ω in this case remains equal to -1 . We can now let $\omega_0 \rightarrow 0$ and obtain the following self-consistent equation for the average value of the spin s :

Here m is the average number of magnons at the given temperature, and m_k is the Bose distribution function of the magnons. In order to "close" the relations (35) and (37), we supplement them with the dispersion laws $\varepsilon_k^\pm$ and ω_k of the holes and magnons, respectively:⁸

$$\omega_k = \sum_{k'} (t_{k'} - t_{k+k'}) (p_{k'}^+ - p_{k'}^-). \quad (38b)$$

$$t_k = t(z - k^2 a^2), \quad tz = t_0, \quad (39)$$
$$\bar{s} = -\frac{1}{2} \text{th } \beta \omega_R \simeq -\frac{\bar{s}\beta}{2} \sum_k t_k \frac{\partial p_k}{\partial \epsilon_k} \frac{\partial \epsilon_k}{\partial \bar{s}}. \quad (40)$$
$$T_K = - \sum_k t_k^2 \partial p_k / \partial \epsilon_k \approx 2\pi^2 z^2 (E_F t)^{1/2}. \quad (41)$$

We shall discuss the question of the magnetic energy of the ground state. The energy contribution linear in the hole concentration is determined by the following two diagrams:

and has the analytical form

Here the first contribution is the kinetic energy of the holes, and the second is the energy of the indirect exchange interaction of the holes with each other. At low temperatures the second contribution is the main one, and the energy gain of the ferromagnetic state is equal to $z^2(E_F t)^{1/2}/16\pi^2$ per unit cell of the crystal. The interaction of the holes is due to the second term in the Hamiltonian (30b). Only holes with opposite spin projections interact, and the interaction is attractive. However, because of the strong splitting of the Fermi surface, superconductivity cannot be realized in the ferromagnetic state.

5. THE PARAMAGNETIC STATE OF THE HOLE SUBSYSTEM

The paramagnetic state is realized at sufficiently high temperatures $T > T_C = z^2(E_F t)^{1/2}/2\pi^2$ above the ferromagnetic region, or at $T > zt(t - pU/2)/U$ above the antiferromagnetic region. In this state the local spins s_n at the sites are disordered ($\overline{s_n} = 0$), and the structure of the paramagnetic state can be investigated in the leading approximation in the parameter $1/z$. It follows from the Hamiltonian (30b) that the hole-dispersion law has the form

$$\varepsilon_k^\pm = -(\frac{1}{2} + p)t_k + \mu, \quad (43)$$

and E_q is equal to $-1/2 - p$. To find the spin correlators in the paramagnetic phase one can develop a diagram technique for expanding the averages $\langle s_{n_1}^{i_1} \dots s_{n_m}^{i_m} \rangle$ in irreducible cumulants, as in the expansion (12) for averages from the Cartan subalgebra. In the given case there are no simple formulas for the bare irreducible cumulants, but the diagram technique itself works fully. In particular, the lowest bare correlators for spin 1/2 are equal to

$$\begin{aligned} \text{Diagram 1} &= 0, & \text{Diagram 2} &= \frac{1}{4} \delta_{nm} \delta_{ij}, & \text{Diagram 3} &= \frac{i}{8} \varepsilon_{ijkl} \delta_{nmp}, \\ \text{Diagram 4} &= -\frac{1}{8} \delta_{il} \delta_{jm} \delta_{nmp}, \end{aligned} \quad (44)$$

where i, j, l , and k are vector indices, and n, m, p , and r are site labels. All the correlators are static, i.e., proportional to $\delta(\omega_1) \dots \delta(\omega_n)$, where $\omega_1, \dots, \omega_n$ are the frequencies flowing into the lines. Consequently, effects of the spin-diffusion type^{11,12} are absent in the framework of this cumulant diagram technique and are nonperturbative effects.

The finite width of the spin correlators does not affect a number of phenomena (such as the scattering of holes by paramagnetic fluctuations) that are determined by integrals over the frequency. The usefulness of the cumulant diagram technique is connected with the fact that the contribution of higher correlators to integral quantities of the mass-operator type is small in the parameter $1/z$. In the calculation of the pair spin correlator K_q^{ij} it is sufficient to sum the sequence of the chain diagrams, which is of leading order in the parameter $1/z$:

$$\begin{aligned} K_q^{ij} \delta^4(q - q') &= \langle s_i(q) s_j(q') \rangle \equiv \text{Diagram 1} + \text{Diagram 2} + \dots \\ &= \text{Diagram 3} + \text{Diagram 4} + \dots \\ K_q^{ij} &= \text{Diagram 3} / (1 - \text{Diagram 4}) = \frac{1}{4} \delta_{ij} \delta(\omega) / (1 - \Pi_k/4T), \end{aligned} \quad (45)$$

where the polarization operator Π_k has the well known form

$$\Pi_k^F = 2 \sum_{k'} t_{k'} t_{k+k'} (p_{k+k'} - p_{k'}) / (\varepsilon_{k'} - \varepsilon_{k+k'} + i\delta). \quad (46)$$

The expressions (45), (46) for K_q^{ij} display a characteristic pole for $k = 0$ at the temperature of the transition to the ferromagnetic state. If we take into account the Anderson superexchange [the last term in the Hamiltonian (30b)], the polarization operator Π_k acquires an additional contri-

bution Π_k^{af} , equal to

$$\Pi_k^{af} = 4 \sum_n \exp(ik \cdot r_n) |t_{n0}|^2 / U. \quad (47)$$

On the boundary of the Brillouin zone, $\exp(ik \cdot r_n) = -1$, and for $p = 0$ the correlator K_q^{ij} possesses a pole at $T = zt^2/U$. This pole corresponds to a transition to the antiferromagnetic state with increase of the lattice constant. The pole of the spin correlator K_k at $k = 0$ determines the phase-transition line between the paramagnetic and the ferromagnetic phase:

$$T_{p,f}(p) = -zt^2/U + 3^{1/2} z^2 p^{1/2} t / 4\pi^{1/2}, \quad (47a)$$

while the pole of the spin correlator K_k at $k = \pi(1, 1, 1)/a$ determines the phase-transition line between the paramagnetic and the antiferromagnetic phase:

$$T_{p,af}(p) = zt(t - pU/2)/U. \quad (47b)$$

The phase-transition lines $T_{p,f}(p)$ and $T_{p,af}(p)$ are depicted in Fig. 2.

The hole-dispersion law $\varepsilon_k^\pm$ (43) and the spin correlator K_q^{ij} (45)–(47) determine the principal excitations in the paramagnetic phase, and we can turn to the discussion of the question of superconductivity. The bare amplitude for scattering of holes with opposite spin projections is determined by the relation (25). It is negative for holes, corresponding to attraction. This fact was first obtained in Refs. 6 and 13, and can be interpreted as an effective narrowing of the band as the electrons approach each other, so that the energy of the electrons is increased and the energy of the holes is lowered. The kinematic attraction (25) makes a discussion of the question of superconductivity timely. The attraction is renormalized slightly in leading order in $1/z$ on account of the summation of the diagrams (25), and is determined by the relation (27), but the fact of the attraction is not changed by this. We note that the kinematic attraction (25) is greater by a factor of U/t than the previously discussed attraction arising from the superexchange interaction.^{14,15}

In discussion of the possibility of the realization of su-

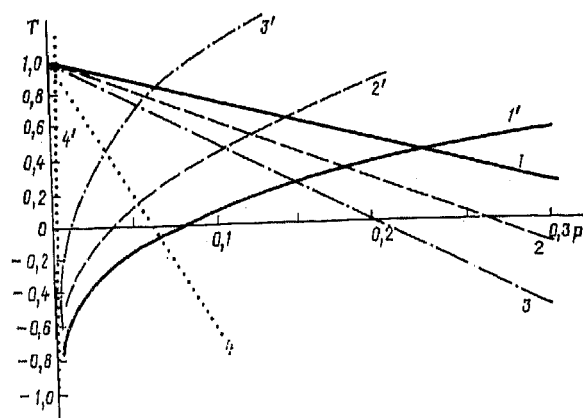


FIG. 2. Lines of phase transitions between the paramagnetic and the antiferromagnetic phase: $T_{p,af}(p)$ is the series of curves 1–4, and $T_{p,f}$ is the series of curves 1'–4'. The solid, dotted, dashed-dotted, and dashed curves correspond to different values of the ratio t/U , equal to 0.2, 0.15, 0.1, and 0.05, respectively. The hole concentration per lattice site is plotted along the horizontal axis, and the temperature in units of zt^2/U is plotted along the vertical axis.

perconductivity it is necessary first to decide whether the superconductivity is formed on account of Bose condensation of local pairs or whether a BCS-type state with anomalous averages is realized. The analysis of the poles of the scattering amplitude (27) for $\varepsilon_k = -t_k + \mu$ and $\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 = 0$ can be reduced easily to the analysis of the roots of the equation

$$1+2 \int \frac{\varepsilon \rho(\varepsilon) d\varepsilon}{E-2\mu+\varepsilon} = 0, \quad \rho(\varepsilon) = \sum_b \delta(\varepsilon - t_b); \quad (48)$$

here $\rho(\varepsilon)$ is the spectral density of states. Equation (48) is easily reduced to an algebraic equation for simple models of the density of states: $\rho(\varepsilon) = 1/2t_0$ or $\rho(\varepsilon) = 3(t_0^2 - \varepsilon^2)/4t_0^3$. One can convince oneself that in each case there is one root for $E - 2\mu$, equal to $0.46t_0$ or $0.43t_0$, respectively, which corresponds to a resonance in the hole conduction band. There are no bound states below the bottom of the hole band, so that local pairs do not arise.

To analyze the possibility that a superconducting state of the BCS type is realized, we shall consider the system of Gor'kov equations²⁶ for the normal and the anomalous Green functions of the initial Fermi operators $c_{n\sigma}^+$, $c_{n\sigma}$. By means of the relations (15d) and (29) the Green functions of the operators $c_{n\sigma}^+$, $c_{n\sigma}$ can be reduced to Green functions of the operators $h_{n\sigma}^+$, $h_{n\sigma}$. It is convenient to make use of the Nambu formalism,²⁷ introducing two-component field operators $C_n = (c_{n1}, c_{n1}^+)$, $C_n^+ = (c_{n1}^+, c_{n1})$ for the physical electrons and $H_n = (h_{n1}, h_{n1}^+)$, $H_n^+ = (h_{n1}^+, h_{n1})$ for our holes. Introducing into the Hamiltonian $\mathcal{H}(1)$ the anomalous terms c^+c , cc and defining matrix Green functions in terms of operators $C_n^i C_n^{+i}$ by relations of the type (21), we can use Eqs. (15d) and (29) to express the matrix Green function $\hat{G}_q$ of the initial fields c_n in terms of the matrix Green function $\hat{g}_q$ of the fields H_n by means of the matrix end operators:

$$\hat{G}_q = \begin{pmatrix} G_{\dagger q} & F_q^+ \\ F_q & G_{\downarrow -q} \end{pmatrix} = \hat{E}_q + \hat{g}_q \hat{E}_q, \quad \hat{g}_q = \begin{pmatrix} g_{\dagger q} & f_q^+ \\ f_q & g_{\downarrow -q} \end{pmatrix}, \quad (49a)$$

$$E_q^+ = \begin{pmatrix} 0 & 1 \\ -(1+p)/2 & 0 \end{pmatrix}, \quad E_q^- = \begin{pmatrix} 0 & -1 \\ (1+p)/2 & 0 \end{pmatrix}. \quad (49b)$$

The expressions given above for the end operators are obtained for $p \ll 1$ in leading order in $1/z$, i.e., in the leading loop approximation. It follows from the relations (49) that the Green function $\hat{G}_q$ of the physical electrons is proportional to the Green function $\hat{g}_q$ of our holes, and the question of the superconductivity can be resolved in terms of the hole Green function $\hat{g}_q$. We note that the Green functions F_q and F_q^+ are mutually adjoint, whereas the Green functions f_q and f_q^+ satisfy the simple relation

$$(1+p)^2(f_q)^* = 4f_q^+. \quad (50)$$

The hole Green functions $\hat{g}_q$ satisfy the usual (in the theory of superconductivity) matrix Dyson equation

$$(\hat{g}_{0q}^{-1} - \hat{\Sigma}_q) \hat{g}_q = \hat{1}, \quad g_{0q}^{-1} = i\xi - \varepsilon_h \sigma_3; \quad (51)$$

here σ_3 is a Pauli matrix. In lowest order in p and $1/z$ there are two diagrams for the mass operator $\hat{\Sigma}_\sigma$:

$$\Sigma_A = \text{diagram with a loop on a line}, \quad \Sigma_B = \text{diagram with a triangle on a line} \quad (52)$$

The first diagram in (52) gives the correction of order p to the hole-dispersion law and contains the kinematic attraction of holes that stimulates the appearance of superconductivity. The second diagram in (52) describes the scattering of holes by paramagnetic spin fluctuations. This interaction is analogous to the scattering by paramagnetic impurities that was considered by Abrikosov and Gor'kov,¹⁷ which destroys the superconductivity. Our task is to solve Eq. (51) with $\hat{\Sigma}_q$ (52) and to elucidate the condition for the appearance of superconductivity. For this we give the explicit form of $\hat{\Sigma}_q$ (52):

$$\hat{\Sigma}_g = \Sigma_g^m + \sigma_3 \Sigma_g^p + \sigma_+ \oplus_g^- + \sigma_- \oplus_g^+; \quad (53)$$

here $\Sigma_q^{n,p}$ are the normal mass operators and $\Theta_q^\pm$ are the anomalous mass operators. Each of the mass operators Σ and Θ is equal to a sum of a kinematic and a spin contribution ($\Sigma = \Sigma^k + \Sigma^s$ and $\Theta = \Theta^k + \Theta^s$), which have the form

$$\Sigma_q^{m,p,h} = - \sum_{\mathbf{k}, \mathbf{k}'} (t_{\mathbf{k}} + t_{\mathbf{k}'}) g_{\mathbf{k}, \mathbf{k}'}^{m,p}, \quad (54a)$$

$$\Theta_q^h = -2t_k \sum_{\mathbf{E}'\mathbf{k}'} f_{\mathbf{E}'\mathbf{k}'}, \quad \Theta_q^{+h} = -2 \sum_{\mathbf{E}'\mathbf{k}'} t_{\mathbf{k}'} f_{\mathbf{E}'\mathbf{k}'}^+, \quad (54b)$$

$$\Sigma_q^{m,ps} = 3 \sum_{k'} t_k t_{k'} K_{k-k'} g_{kk'}^{p,m}, \quad (54c)$$

$$\Theta_q^- = -3 \sum_{k'} t_k^2 K_{k-k'} f_{\frac{1}{2}k'}, \quad \Theta_q^+ = 3 \sum_{k'} t_k^2 K_{k-k'} f_{\frac{1}{2}k'}^+, \quad (54d)$$

Here $g_q^{p,m} = (g_{1,q} \pm g_{1,-q})/2$, and K_k is the static spin correlator (45). Solving the algebraic equation (51), we obtain an expression for the function $\hat{g}_q$ in terms of the mass operators:

$$\begin{aligned} g_q^m &= (i\xi - \Sigma_q^m)/D_q, \quad g_q^p = (\epsilon_k + \Sigma_q^p)/D_q, \quad f_q^\pm = \Theta^\pm/D_q, \\ D_q &= (i\xi - \Sigma_q^m)^2 - (\epsilon_k + \Sigma_q)^2 - \Theta_q^+ \Theta_q^-, \end{aligned} \quad (55)$$

By substituting the expression (55) for the GF $\hat{g}_q$ and Eqs. (54) for the mass operator, we obtain a closed system of equations for the mass operator and for elucidation of the possibility of superconducting solutions. Remaining at the qualitative level, we can make use of the criterion of Ref. 17 for the existence of superconductivity: The superconducting gap Δ_s^0 with neglect of spin fluctuations should be greater than the width $\hbar\Gamma_s$ (of the energy level at the Fermi surface) due to electron scattering by spin fluctuations. For this we find the superconducting gap $\Delta_s^0 = (\Theta_0^+ \Theta_0^k)^{1/2}$, where $\Theta_0^{\pm k}$ are the anomalous kinematic mass operators at zero momentum. Omitting the mass operator $\Sigma_q^{a,m}$ in the expression (55) for $f_q^{\pm}$, substituting $f_q^{\pm}$ into the relation (54b), summing over the frequencies ξ , and using the smallness of the Fermi momentum k_F in comparison with the momentum π/a at the Brillouin-zone boundary, we obtain the BCS self-consistency condition for the gap:^{22,27}

$$1 = t_0 \sum_k E_k^{-1} \operatorname{th}(\beta E_k/2), \quad E_k^2 = \varepsilon_k^2 + \Delta_s^2. \quad (56)$$

Confining ourselves to the case of zero temperature, we obtain

$$1 = 2t_0 \int_{-t_0}^{t_0} \frac{\rho(\varepsilon) d\varepsilon}{[(t_0 - \varepsilon - 2\tilde{E}_F)^2 + 4\Delta_s^2]^{1/2}}, \quad \tilde{E}_F = t_0/2 - \mu. \quad (57)$$

This integral over ε is calculated by dividing the range into

two regions $t_0 - \varepsilon \leq 2\tilde{E}_F$ and $t_0 - \varepsilon \gg 2\tilde{E}_F$. In the first region the spectral density of states $\rho(\varepsilon)$ is equal to $[(zt - \varepsilon)/t]^{1/2}/4\pi^2 t$, while in the second it depends on the chosen model of the density of states. Performing the integration over the first region and replacing the contribution of the second by a constant, we obtain

$$\Delta_s^0 = \tilde{E}_F \exp[-c_1/t_0 \rho(t_0 - 2\tilde{E}_F)] = \tilde{E}_F \exp[-c_2(t/\tilde{E}_F)^{1/2}]. \quad (58)$$

Here c_1 and c_2 are constants of order unity. The spin-relaxation frequency Γ_s is determined by the imaginary part of the mass operator for $i\xi = \varepsilon_k$ and has the form

$$\Gamma_s = 12\pi \sum_{\mathbf{k}'} t_{\mathbf{k}\mathbf{k}'} K_{\mathbf{k}-\mathbf{k}'} \delta(t_{\mathbf{k}} - t_{\mathbf{k}'}). \quad (59)$$

Using the smallness of the Fermi momentum ($k_F a \ll 1$), we obtain for Γ_s the following integral representation:

$$\Gamma_s = \frac{3z^2 t a k_F}{4\pi} \int_0^1 dy^2 \left[1 + \frac{zt^2}{UT} - \frac{z^2 t k_F a}{4\pi^2 T} - \left(\frac{1}{2} + \frac{1-y^2}{4y} \ln \left| \frac{1+y}{1-y} \right| \right)^{-1} \right]. \quad (60)$$

For $U/t \rightarrow \infty$, when the paramagnetic state is above the ferromagnetic region, the integral in Eq. (60) is strictly greater than unity. For a certain finite value of U/t , as follows from the diagrams of Fig. 2, the parameter zt^2/UT cannot be greater than 2 and the integral (60) cannot be greater than $1/3$. Consequently,

$$\hbar \Gamma_s > (z^2/4\pi) (2\tilde{E}_F t)^{1/2}.$$

The other contributions to the mass operator (52) are small on the Fermi surface in the parameters p and $T/z^2 t$ in comparison with those taken into account.

Comparing Γ_s (60) and Δ_s^0 (58), it is easy to arrive at the conclusion that $\Gamma_s \gg \Delta_s^0$, i.e., that the spin fluctuations destroy the superconductivity. This result contradicts the assertion in the sequence of papers Refs. 6, 13, and 18 that superconductivity is realized in the paramagnetic phase on account of the kinematic attraction. In these papers the spin correlator in the paramagnetic phase was calculated incorrectly: The contribution of the fluctuations of the local spins was omitted and a contribution to the electron spin fluctuations that is small in the parameter p was taken into account, leading to the conclusion that spin fluctuations are suppressed at $T \ll \tilde{E}_F$. The spin-correlator width due to the flipping of a local spin by holes has order of magnitude $4z^2 \tilde{E}_F T/\pi^3 t$. Despite the fact that $\tilde{E}_F < \hbar \Gamma_s$, the renormalization of the interaction vertices is small in the parameters p and $1/z$, and can be disregarded in the rigorous self-consistent solution (given in Appendix B) of Eqs. (54) and (55) in the strong-coupling region.

6. THE ANTIFERROMAGNETIC STATE FOR OCCUPANCY CLOSE TO UNITY

The antiferromagnetic state is realized for low hole concentrations $p < t/U$ and low temperatures $T \lesssim zt^2/U$. The physical reason for the antiferromagnetism lies in Anderson superexchange;²⁵ the idea of such superexchange was first put forward by Kramers in the 1930's (Ref. 19). As follows from the calculation given in Appendix A, the reason for the

superexchange lies in virtual transitions of electrons from the almost filled lower Hubbard band to the upper band on account of the s - d interaction of the spin of the electrons with local spins at the sites.

First we shall describe qualitative ideas about the nature of the charge carriers in the antiferromagnetic state for $t \ll U$. Because of the doubling of the lattice constant and the halving of the volume of the Brillouin zone, two hole bands, degenerate with respect to the spin projection, arise. The width of these bands is substantially smaller than the width of the bands in the ferromagnetic and paramagnetic phases. In fact, hopping of a hole to a nearest-neighbor site is possible only on account of quantum fluctuations of the spin at that site, while hopping to the next sites within the same magnetic sublattice has a substantially lower probability than hopping to a nearest-neighbor site in the paramagnetic or ferromagnetic phase.

The narrowing of the hole band in the antiferromagnetic phase leads to the formation, from the hole, of a magnetic polaron^{15,19} for $t \ll U$. The formation of a ferromagnetic region around the hole leads to a loss of superexchange energy of the order of t^2/U to the binding, but at the same time the hole gains potential energy on account of the broadening of its band. One can convince oneself that it is advantageous for two holes to form a ferromagnetic pocket. If we disregard the Coulomb repulsion of the holes, they all gather into one ferromagnetic droplet. When the Coulomb repulsion is taken into account the droplet size is finite, but the droplets form a lattice that is pinned to the impurities, and the system is an insulator.¹⁹ The situation when the droplets each consist of only two holes, and form a Bose condensate, is exotic.

In this section we shall discuss the question of the possibility of superconductivity of "bare" holes, not surrounded by a ferromagnetic region. Such holes can exist for a not too small ratio t/U . We shall confine ourselves to the case when the temperature T is equal to zero. The starting point is the Hamiltonian (30) for the hole-spin system. Assuming the lattice to be alternating,¹⁰ we determine the state of the spin subsystem. For sublattice 1 we shall use the representation (15c), and for sublattice 2 we shall use the analogous representation with the axis of quantization in the opposite direction:

$$s_1^- = a_1, \quad s_1^0 = \Phi_1 + a_1^+ a_1, \quad s_1^+ = -a_1^+ (2\Phi_1 + a_1^+ a_1), \quad (61a)$$

$$s_2^- = a_2, \quad s_2^0 = -\Phi_2 - a_2^+ a_2, \quad s_2^+ = -a_2^+ (2\Phi_2 + a_2^+ a_2); \quad (61b)$$

here a_1^+ , a_1 , a_2^+ , and a_2 are Bose operators. At $T = 0$ we have $\Phi_1 = \Phi_2 = -1/2$ and we obtain an effective Bose Hamiltonian, the quadratic part of which has the form

$$\mathcal{H}_{af}^0 = \sum_{\mathbf{k}\alpha\beta} T_{\alpha\beta}(\mathbf{k}) s_{\alpha\mathbf{k}} s_{\beta}(-\mathbf{k}) \approx \frac{1}{2} \sum_{\mathbf{k}} T(\mathbf{k}) (a_{1\mathbf{k}}^+ a_{1\mathbf{k}} + a_{2\mathbf{k}}^+ a_{2\mathbf{k}}) + P_{\mathbf{k}} (a_{1\mathbf{k}}^+ a_{2\mathbf{k}} + a_{1\mathbf{k}} a_{2\mathbf{k}}). \quad (62)$$

Here $T_{\alpha\beta}(\mathbf{k})$ is the Fourier transform of the Anderson superexchange:

$$T_{\alpha\beta}(\mathbf{k}) = 4U^{-1} \sum_{\mathbf{m}} |t(\mathbf{r}_m + a(\alpha - \beta)\mathbf{e}_0/2)|^2 \times \exp[i\mathbf{k}\mathbf{r}_m + i\mathbf{k}\mathbf{e}_0(\alpha - \beta)a/2], \quad (63)$$

where $\mathbf{r}_m$ are vectors of elementary translations of the antiferromagnetic crystal; the indices $\alpha, \beta = \pm 1$ label the magnetic sublattices; $\mathbf{e}_0$ is the unit vector in the direction

between the two sites in the unit cell; $T_k = T_{11}(k) - T_{11}(0) + [T_{1,-1}(0) + T_{-1,1}(0)]/2$ and $P_k = [T_{1,-1}(k) + T_{-1,1}(k)]/2$.

The Hamiltonian (62) can be diagonalized by means of the u, v transformation⁴

$$a_{1k} = u_k b_k + v_k c_k^+, \quad a_{2k} = u_k c_k + v_k b_k^+, \quad (64)$$

where c_k, c_k^+, b_k , and b_k^+ are Bose creation and annihilation operators for antimagnons. The coefficients u_k and v_k satisfy the relation $u_k^2 - v_k^2 = 1$ and have the form

$$u_k = [\beta_k/2\alpha_k]^{1/2}, \quad v_k = -P_k/[2\alpha_k\beta_k]^{1/2}, \quad (65)$$

$$\alpha_k = (T_k^2 - P_k^2)^{1/2}, \quad \beta_k = T_k + \alpha_k.$$

The antimagnons b, c possess the same dispersion law ω_k which, for small k , has an acoustic character:

$$\omega_k = (T_k^2 - P_k^2)^{1/2} \approx c_s k, \quad c_s = 4a(2z)^{1/2}t^2/U. \quad (66)$$

In order to find the dispersion law of the holes and their wave functions in the antiferromagnetic state, we go over to the self-consistent field approximation in respect of the spins s_n . For this it is necessary to find the average value of the zeroth component of the spin at a site:

$$\bar{s}_1^0 = -\bar{s}_2^0 = -1/2 + \langle a_1^+ a_1 \rangle = -1/2 + \sum_k |v_k|^2 = -\frac{1}{2} (1 - 1/2z). \quad (67)$$

Substituting $\bar{s}^0$ (67) into the Hamiltonian (30), we obtain the quadratic Hamiltonian of the holes:

$$\mathcal{H}_{af}^h = -\frac{1}{2} \sum_{\alpha\beta\sigma k} t_{\beta\alpha}(k) h_{k\beta\sigma}^+ [1 - 2\alpha\sigma(1 - 1/2z)] h_{k\alpha\sigma}. \quad (68)$$

Here $t_{\beta\alpha}(k)$ is determined by the relation (63), if $4|t_{mn}|^2/U$ is replaced by t_{mn}^+ ; $h_{k\alpha\sigma}^+$ and $h_{k\alpha\sigma}$ are hole wave functions with spin projection σ at site α in the unit cell. From (68) it is easy to find the hole-dispersion law $\varepsilon^\pm(k)$ for arbitrary $t_{\alpha\beta}(k)$. We shall confine ourselves to the case $|t_{11}(k)| \ll |t_{1,-1}(k)|/z$, i.e., hopping to a nearest-neighbor site is dominant. In this case, for the dispersion law $\varepsilon_k^\pm$ we have

$$\varepsilon_k^\pm = \pm \eta^2 |t_k|, \quad t_k = t_{1,-1}(k), \quad \eta = (1/4z)^{1/2}. \quad (69)$$

The hole wave functions $e_\sigma^\nu(k)$, where σ is the spin projection and $\nu = \pm 1$ labels the solutions, have the form

$$2^{1/2} e_{\pm}^\pm = (2^{1/2} \tilde{e}_{\pm}^\pm)^* = (\eta^{-1} e^{i\varphi}, \pm \eta), \quad (70)$$

$$2^{1/2} e_{\pm}^\pm = (2^{1/2} \tilde{e}_{\pm}^\pm)^* = (\eta e^{i\varphi}, \pm \eta^{-1});$$

here $\tilde{e}_\sigma^\nu$ is the solution of the conjugate problem; the spin projection σ is the quantum number that labels the solutions; φ is the phase of the matrix element t_k . Using the hole wave functions (70), we can easily obtain the effective interaction Hamiltonian for the hole operators $p_{\sigma k}^{*\nu}$ and $p_{\sigma k}^\nu$:

$$\mathcal{H}_{af}^{hh} = (1/4\eta^2) \sum_{\alpha\beta\gamma\delta} (|t_{k1}| A_{\alpha\beta\gamma\delta} + |t_{k2}| D_{\alpha\beta\gamma\delta}) p_{\gamma k_1}^{*\alpha} p_{\delta k_2}^{*\beta} p_{\gamma k_1}^\gamma p_{\delta k_2}^\delta, \quad (71)$$

where the matrices A, B, C and D have the form

$$A = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad (72)$$

$$C = \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}, \quad D = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

It follows from the Hamiltonian (71) that holes from the lower band attract each other, while holes from the upper band repel each other. Here there is a strong interaction mixing the hole bands. To answer the question of the sign and magnitude of the interaction on the Fermi surface it is necessary to solve the equations of the ladder approximation for the scattering amplitude $T_{k_1 k_3, k_2 k_4}^{\alpha\gamma, \beta\delta}$:

$$T_{k_1 k_3, k_2 k_4}^{\alpha\gamma, \beta\delta} = F_{k_1 k_3}^{\alpha\gamma, \alpha_1 \gamma_1} \left[\delta_{\alpha_1 \beta} \delta_{\gamma_1 \delta} + \sum_{k'} \frac{T_{k_1 k_3, k_2 k_4}^{\alpha_1 \gamma_1, \beta \delta}}{E - \varepsilon_{k_1}^{\alpha_1} - \varepsilon_{k_2}^{\gamma_1} - \varepsilon_{k_3}^{\beta} - \varepsilon_{k_4}^{\delta}} \right], \quad (73)$$

here $k = k_1 + k_3 = k_2 + k_4$; $E = \varepsilon_{k_1}^{\alpha} + \varepsilon_{k_3}^{\gamma} = \varepsilon_{k_2}^{\beta} + \varepsilon_{k_4}^{\delta}$, $F_{k_1 k_3}^{\alpha\gamma, \beta\delta} = \eta^{-2} (|t_{k_1}| A_{\alpha\beta} B_{\gamma\delta} + |t_{k_3}| D_{\alpha\beta} C_{\gamma\delta})/4$ is the Born scattering amplitude.

It is natural to seek the solution of Eq. (73) in the form $T_{k_1 k_3, k_2 k_4} = F_{k_1 k_3} U(k, E)$, where summation over index pairs $\alpha\gamma$ is assumed. For U we obtain the following solution:

$$U(k, E) = \left[1 - \sum_{k'} F_{k', k-k'} / (E - \varepsilon_{k'} - \varepsilon_{k-k'}) \right]^{-1}, \quad (74)$$

and the matter reduces to the inversion of a 4×4 matrix, which does not present a problem. The poles of $U(k, E)$ give the spectrum of the bound states, and one can convince oneself that if $\rho(\varepsilon) = \text{const}$, $E = \pm 0.834 \eta^2 t_0$, and the bottom of the band corresponds to $E_{\min} = -\eta^2 t_0$, then bound states of holes are absent, i.e., the situation is analogous to the paramagnetic case.

For simplicity, we shall not give the complete expression for the scattering amplitude, but confine ourselves to the case $k = 0, E = 0$:

$$T_{k_1, -k_1, k_2, -k_2}^{\alpha\gamma, \beta\delta}(E)|_{E=0} = 2^{-1} \eta^2 |t_{k_1}| \begin{pmatrix} 1 & 0 & 0 & 1 \\ -1 & 0 & 0 & -1 \end{pmatrix}^{\alpha, \beta\delta}, \quad (75)$$

i.e., T does not depend on the index γ . It follows from (73) that the scattering amplitude of holes in the lower band is positive, but the force of attraction is suppressed by a factor of $2\eta^4 = 1/2z$ in comparison with that for the bare Hamiltonian (71).

To answer the question of the sign of the total interaction at the Fermi surface, it is necessary to consider the sign and magnitude of the interaction due to the exchange of antimagnons. It has been known for a long time²⁸ that the exchange of antimagnons induces repulsion in an s state and attraction in a p state. Our situation differs from the usual situation in that the initial Hamiltonian (30) is non-Hermitian, and therefore a separate analysis is required. Using the hole wave functions (70), we obtain from the Hamiltonian (30) the following spin-hole Hamiltonian for the holes in the lower hole band:

$$\mathcal{H}_{af}^{sp} = \frac{1}{2} \sum_{k=k'+k''} |t_k| \{ \eta^{-2} [s_+^0(k') p_+^+(k) p_+(k'') - s_-^0(k') p_+^-(k) p_-(k'')] + [s_+^+(k') + s_-^+(k')] p_+^+(k) p_+(k'') + [s_+^-(k') + s_-^-(k')] p_+^-(k) p_-(k'') \}. \quad (76)$$

Here the subscript on the spin operators labels the sublattice. Substituting the representations (61) and (64) into (76), we obtain the following effective Hamiltonian $\mathcal{H}_{af}^{sp} = \mathcal{H}_{af}^{sp1} + \mathcal{H}_{af}^{sp2}$:

$$\mathcal{H}_{af}^{sp1} = \frac{1}{2} \sum_{\mathbf{k}=\mathbf{k}'+\mathbf{k}''} |t_{\mathbf{k}}| (u_{\mathbf{k}'} + v_{\mathbf{k}'}) [(b_{\mathbf{k}'} + c_{\mathbf{k}'}) p_{\uparrow}(\mathbf{k}) p_{\uparrow}(\mathbf{k}'') + (b_{\mathbf{k}'} + c_{\mathbf{k}'} +) p_{\uparrow}(\mathbf{k}) p_{\uparrow}(\mathbf{k}'')], \quad (77)$$

$$\mathcal{H}_{af}^{sp2} = 2^{-1} \eta^{-2} \sum_{\mathbf{k}=\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}'} |t_{\mathbf{k}}| [(u_1 v_2 b_1 + c_2 + u_1 u_2 b_1 + b_2 + v_1 v_2 c_1 + c_2 + v_1 u_2 b_1 c_2) p_{\uparrow}(\mathbf{k}) p_{\uparrow}(\mathbf{k}'') + (u_1 v_2 c_1 + b_2 + v_1 v_2 b_1 + b_2 + u_1 u_2 c_1 + c_2 + v_1 u_2 b_1 c_2) p_{\uparrow}(\mathbf{k}) p_{\uparrow}(\mathbf{k}'')]. \quad (78)$$

We do not give the Hamiltonian with three operators b and c , since its contribution to the hole scattering is small in the parameter $1/z$. The hole-scattering amplitudes for the exchange of one and two antimagnons have the form

$$F_1 = 2^{-1} t_{\mathbf{k}_1} t_{\mathbf{k}_2} \omega_{\mathbf{k}_1 - \mathbf{k}_2} (u_{\mathbf{k}_1 - \mathbf{k}_2} + v_{\mathbf{k}_1 - \mathbf{k}_2})^2 / [(\varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_2})^2 - \omega_{\mathbf{k}_1 - \mathbf{k}_2}], \quad (79)$$

$$F_2 = 2^{-1} \eta^{-1} t_{\mathbf{k}_1} t_{\mathbf{k}_2} \sum_{\mathbf{k}'} (\omega_{\mathbf{k}'} + \omega_{\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}'}) u_{\mathbf{k}'} v_{\mathbf{k}'} u_{\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}'} v_{\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}'} \times [(\varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_2})^2 - (\omega_{\mathbf{k}'} + \omega_{\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}'})^2]^{-1}. \quad (80)$$

For small momenta $\mathbf{k}_1, \dots, \mathbf{k}_4$ and for energies $\varepsilon_{\mathbf{k}_1}, \dots, \varepsilon_{\mathbf{k}_4}$ on the Fermi surface, taking into account the expressions (65), (66) for $\omega_{\mathbf{k}}$, $u_{\mathbf{k}}$, and $v_{\mathbf{k}}$, we obtain

$$F_1 = zt/4\lambda = zU/16, \quad \lambda = 4t/U, \quad (81)$$

$$F_2 = -4^{-1} \eta^{-1} \sum_{\mathbf{k}'} \omega_{\mathbf{k}'}^{-1} (u_{\mathbf{k}'} v_{\mathbf{k}'})^2 \approx -zt/4\lambda = -zU/16. \quad (82)$$

It follows from the estimates (82) and (81) that exchange of one antimagnon induces repulsion, while exchange of two induces attraction. The attractions and repulsions cancel each other on the Fermi surface, but, because the region of attraction in frequency is greater by a factor of $(k_F a)^{-1}$ (see Fig. 3), it is not ruled out that superconductivity can be realized in this situation.

Two limiting cases are possible. In the first, the characteristic one-magnon exchange energy $\omega_F = 4(2z)^{1/2} k_F t^2 / U$ and two-magnon exchange energy $2\Omega = 8zt^2 / U$ are smaller than the Fermi energy $E_F^a = k_F^2 a^2 t / 2z^{1/2}$. In this case the kinematic interaction is unimportant near the Fermi surface, since it is weaker than the antimagnon interaction by a factor of $4t/z^{3/2} U$. The condition for realization of this case

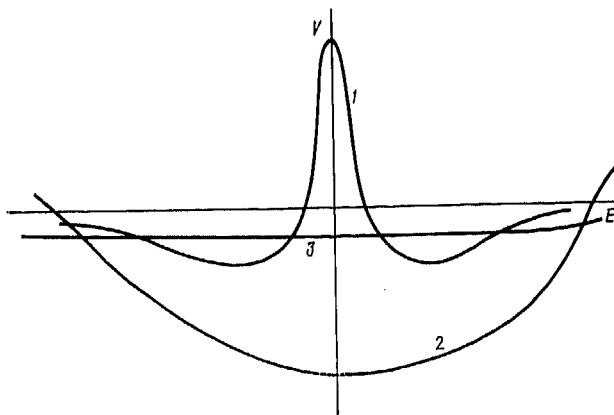


FIG. 3. Qualitative behavior of different interactions of holes in the vicinity of the Fermi surface. Curve 1 corresponds to one-antimagnon exchange, curve 2 to two-antimagnon exchange, and curve 3 to the kinematic attraction.

is $\omega_F \ll E_F^a$ or $t/U \ll k_F a / 8\sqrt{2}z \approx 2.5 \times 10^{-3}$ for $k_F a \approx 1/z$ and $z = 6$. It is clear that for such a small ratio t/U the charge carriers are magnetic polarons¹⁹ or RVB droplets.²⁹ In particular, for $\omega_F \ll 2\Omega$ the ratio $t/U \lesssim 10^{-4}$ and the bottom of the magnetic-polaron band in the three-dimensional case for $z = 6$ lies at $E = -5t$, while the bottom of the hole band lies at $E = -1.2t$.

The conclusion reached in Ref. 30, on the basis of the potential shown in Fig. 3, that superconductivity can be realized in the antiferromagnetic phase pertains to the case of very small t/U , when the holes are unstable against the formation of magnetic polarons.

In the second case, the magnon-exchange energy is greater than the Fermi energy: $2\Omega \gg \omega_F \gg E_F^a$ or $1 \gg t/U \gg k_F a / 8\sqrt{2}z$. In this case, the contributions of the one-magnon and two-magnon exchange to the interaction of the holes cancel. But this does not mean that the kinematic interaction (75) leads to superconductivity. Because of the large force of the magnon interaction (81), (82), corrections in the parameters t/U , $k_F a$, and $1/z$ are important in this case. The calculation of these corrections lies outside the scope of this paper.

We note that a superconductivity mechanism due to two-phonon exchange was proposed in Ref. 31. The contribution of one-phonon exchange in this case is suppressed because of the strong dispersion of the dielectric permittivity.

CONCLUSION

In this paper a diagram technique for the strong-coupling method in the Hubbard model has been developed systematically. This diagram technique differs from that of Refs. 6 and 4 in that it is possible to introduce physically illustrative dynamical variables and investigate the structure of an arbitrary order of perturbation theory. We have studied the structure of the simplest types of ground states and the elementary excitations in the Hubbard model with a carrier concentration close to one per lattice site. The use of the small parameters t/U , p , and $1/z$ has made it possible to investigate the ferromagnetic, paramagnetic, and antiferromagnetic states of the system. The tendency to superconductivity is due to the kinematic attraction of holes, but spin fluctuations destroy the superconductivity in the paramagnetic phase and substantially alter the character of the interaction of the holes in the antiferromagnetic phase.

We note that in this paper we have not taken into account the long-range Coulomb interaction, which for $p \ll 1$ makes the application of perturbation theory to the hole gas difficult and hinders the appearance of superconductivity. The methods and results of this paper differ substantially from those in the well known sequence of papers (Refs. 16 and 32). This is connected with the fact that our work has used the parameter $1/z$, while Refs. 16 and 32 essentially used the parameter $1/N$, where N is the number of one-electron states per lattice site. In the framework of the approach developed, the most urgent task is to analyze the spin-liquid state,^{16,32} in which the spin fluctuations are suppressed by a factor of at least E_F/t_0 in comparison with the paramagnetic case. It is of interest to consider the more realistic

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APPENDIX A

Below we give a representation of the algebra $PI(2, 2)$ of the operators X^{ab} of the complete Hubbard model in terms of the Fermi fields ψ_σ^+ , ψ_σ , φ_σ^+ , φ_σ of the electrons in the lower and upper Hubbard bands, the Bose fields a^+ , a , α^+ , α of the magnons and excitons, and the random fields Ω , Φ , Ξ . The elements of the Cartan subalgebra and the spin operators have the form

$$X^{11} + X^{22} = N = (\psi^+ \psi) - (\varphi^+ \varphi) + \Omega, \quad X^{22} = (\varphi^+ \varphi) + \alpha^+ \alpha + \Xi,$$

$$X^{00} = 1 - N - X^{22}, \quad s_x = s + \frac{1}{2} \psi^+ \sigma \psi - \frac{1}{2} \varphi^+ \sigma \varphi, \quad (A1)$$

$$s^0 = a^+ a + \Phi, \quad s^- = a, \quad s^+ = -a^+ (a^+ a + 2\Phi).$$

From the Fermi operators $X^{0\sigma}$, $X^{\sigma 0}$, $X^{2\sigma}$, $X^{\sigma 2}$ it is convenient to organize two spinors $\mu_\sigma = X^{0\sigma}$, $\nu_\sigma = (-X^{12}, X^{12})$, $\mu_\sigma^+ = X^{\sigma 0}$, $\nu_\sigma^+ = (-X^{21}, X^{21})$; then

$$F(x, y, z) = \ln \left\{ \frac{(1 + e^{x-y/2} + e^{x+y/2} + e^z)(1 + e^{x+y/2-z})(1 + e^{x-y/2-z})(1 - e^y)(1 - e^z)}{[1 + \exp(x+y/2)][1 + \exp(x-y/2)]} \right\}. \quad (A4)$$

The cumulants of the fields Ω , Φ , Ξ are equal to the derivatives of F with respect to the parameters x , y , z . Substituting the representation (A1)–(A3) of the operators X^{ab} into the Hamiltonian (2), we obtain the Hamiltonian of the complete Hubbard model in our variables:

$$\mathcal{H}_0 = \sum_n [-\mu_0 \psi_{n0}^+ \psi_{n0} + (U - \mu_0) \varphi_{n0}^+ \varphi_{n0} + U \alpha_n^+ \alpha_n + \omega_0 \alpha_n^+ a_n], \quad (A5)$$

$$\begin{aligned} \mathcal{H}_{int} = \sum_{n \neq n'} t_{nn'} \{ & \psi_n^+ [1 - \Xi_n - \Omega_n/2 - (\psi_n^+ \psi_n) - \alpha_n^+ \alpha_n] \chi_{n'} + \\ & + \varphi_n^+ [\Xi_n + \Omega_n/2 + (\varphi_n^+ \varphi_n)] \chi_{n'} + \\ & + s_n (\psi_n^+ - \varphi_n^+) \sigma \chi_{n'} + \alpha_n^+ (\varphi_n^+ \psi_n) \tau \chi_{n'} + \\ & + \frac{1}{2} (\varphi_n^+ \sigma \varphi_n) (\psi_n^+ \sigma \chi_{n'}) - \frac{1}{2} (\varphi_n^+ \varphi_n) (\psi_n^+ \chi_{n'}) \}, \\ \chi_{n'} = & \psi_{n'} + \varphi_{n'} - \alpha_{n'} \tau \psi_{n'}^+, \end{aligned} \quad (A6)$$

For $-z = \beta U \gg 1$, which is practically always fulfilled, the expression (A4) for the free energy F goes over into the expression (16) for F , and the field Ξ can be set equal to zero. For $U \gg t$ the Hamiltonian (A6) can be used to obtain corrections to the Hamiltonian for $U/t = \infty$. Such corrections are important for us when the occupancy is close to unity. They have the structure $\psi_1^+ \psi_2$, $s_1 \cdot s_2$, $s_1 \cdot (\psi_2^+ \sigma \psi_3)$, and $(\psi_1^+ \psi_2)(\psi_3^+ \psi_4)$. For us, only the $s_1 \cdot s_2$ contribution is important, since the Hubbard Hamiltonian is degenerate in the limit $U/t = \infty$ and for occupancy close to unity. This contribution is determined by the following diagram:

$$\delta \mathcal{H}^{ss} = \text{diagram} = \frac{t}{U} \sum_{n \neq n'} |t_{nn'}|^2 \varepsilon_n s_{n'}$$

and represents indirect exchange via electrons of the almost completely filled lower Hubbard sub-band, or part of the Anderson superexchange²⁵ responsible for the interaction of

$$\mu = \psi, \quad \nu = \varphi - \alpha \tau \psi^+,$$

$$\begin{aligned} \mu^+ = \psi^+ \left[1 - \Xi - \Omega/2 - (\psi^+ \psi) - \alpha^+ \alpha - \frac{1}{2} (\varphi^+ \varphi) \right. \\ \left. + \frac{1}{2} (\varphi^+ \sigma \varphi) \sigma + (s\sigma) \right] - \alpha^+ \tau \varphi, \end{aligned}$$

$$\nu^+ = \varphi^+ [\Xi + \Omega/2 + (\varphi^+ \varphi) - (s\sigma)] - \alpha^+ \tau \psi, \quad (A2)$$

where

$$\tau = i\sigma y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

is the metric spin matrix and

$$X^{02} = \alpha, \quad X^{20} = \alpha^+ (1 - 2\Xi - \Omega - (\varphi^+ \varphi) - \alpha^+ \alpha) - \psi^+ \tau \nu^+. \quad (A3)$$

To calculate the cumulants of the random fields Ω , Φ , Ξ , we give the thermodynamic potential F as a function of the parameters $x \equiv \omega_\Omega = \beta\mu$, $y \equiv \omega_\Phi = -\beta\omega_0$, $z \equiv -\beta U$:

local spins. The remaining corrections of order t/U are unimportant for us, since they are corrections to contributions already present.

APPENDIX B

In this appendix we shall prove that Eqs. (54), (55) have no superconducting solution in the weak-coupling regime ($\Theta, \Theta^+ \ll \tilde{E}_F$ for $\Theta, \Theta^+ \neq 0$). Such a proof is carried through most simply by replacing the dressed spin correlator K_k by the bare spin correlator, which only reduces the spin fluctuations and facilitates the appearance of superconductivity. After this replacement the dependence on k in Eqs. (54), (55) is contained only in the form t_k , and, therefore, introducing the variable $\varepsilon = t_k$, we can consider all the mass operators as functions of ε and ξ and replace sums over k by sums over ε :

$$\sum_k f(t_k) = \frac{a^3}{(2\pi)^3} \int f(t_k) dk = \int_{-\varepsilon_0}^{\varepsilon_0} f(\varepsilon) \rho(\varepsilon) d\varepsilon = \sum_\varepsilon f(\varepsilon). \quad (B1)$$

Next, one can convince oneself that in the equations for the mass operator $\Sigma_{\varepsilon, \xi}^m$, $\Theta_{\varepsilon, \xi}^\pm$ values $t_0 - \varepsilon \ll t_0$ and $\xi \approx |\Theta| \ll t_0$ are important, while in the mass operator $\Sigma_{\varepsilon, \xi}^p$ values $t_0 - \varepsilon \approx t_0$ and $\xi \approx t_0$ are important. Since for large $t_0 - \varepsilon$ and ξ the presence of the superconducting gap is unimportant and $\Sigma_{\varepsilon, \xi}^p$ describes the renormalization of the hole-dispersion law ε_k , this renormalization is small in the parameter $1/z$ and can be omitted. This situation is analogous to the proof of Anderson's theorem.^{22,27} Introducing the notation

$$\Sigma_q^{ms} = -i\xi \sigma(\xi),$$

$$\Theta_\pm = \Theta(\xi) = \Theta^k + \Theta^*(\xi) = 4[\Theta^+(\xi)]^* = 4[\Theta^{k*} + \Theta^{*+}(\xi)], \quad (B2)$$

we obtain

$$\sigma(\xi) = \frac{3}{4} t_0^2 \sum_{\varepsilon} [1 + \sigma(\xi)] / D^2(\varepsilon, \xi), \quad (\text{B3})$$

$$\theta^h = 2t_0 \sum_{\varepsilon, \xi} [\theta^h + \theta^s(\xi)] / D^2(\varepsilon, \xi), \quad (\text{B4})$$

$$\theta^s(\xi) = -\frac{3}{4} \sum_{\varepsilon} [\theta^h + \theta^s(\xi)] / D^2(\varepsilon, \xi), \quad (\text{B5})$$

$$D^2(\varepsilon, \xi) = \xi^2 [1 + \sigma(\xi)]^2 + \frac{1}{4} (t_0 - \varepsilon + 2\tilde{E}_F)^2 + \frac{1}{4} |\theta(\xi)|^2. \quad (\text{B6})$$

In the derivation of (B2)–(B4) we have omitted the contribution Σ'' (52) of the scattering of holes by holes to the normal mass operators, since it is small in the parameter p , and also, in the numerators of the sums (B3)–(B5), the variable ε is replaced by t_0 with logarithmic accuracy in Θ/t_0 . Equations (B3)–(B5) are reduced to a single nonlinear algebraic equation. We introduce the function $A(\xi)$:

$$A(\xi) = (3t_0^2/4) \sum_{\varepsilon} D^{-2}(\varepsilon, \xi); \quad (\text{B7})$$

then it follows from (B3) and (B5) that

$$\sigma(\xi) = A(\xi) / [1 - A(\xi)], \quad \theta^s(\xi) = -\theta^h A(\xi) / [1 + A(\xi)]. \quad (\text{B8})$$

Substituting (B8) into (B7) and performing the summation over ε , we obtain a relation for $A(\xi)$:

$$A(\xi) = \frac{3z^2}{2\pi} (2\tilde{E}_F t)^{1/2} \{4[1 - A(\xi)]^{-2} \xi^2 + [1 + A(\xi)]^{-2} |\theta^h|^2\}^{-1/2}, \quad (\text{B9})$$

and also a self-consistency condition for the parameter θ^h , which follows from (B4):

$$1 = 8t_0 \sum_{\varepsilon, \xi} [1 + A(\xi)]^{-1} / \{4[1 - A(\xi)]^{-2} \xi^2 + (t_0 - 2\tilde{E}_F - \varepsilon)^2 + [1 + A(\xi)]^{-2} |\theta^h|^2\}. \quad (\text{B10})$$

Equation (B9) is easily solved by the method of iterations. Using the smallness of θ^h :

$$|\theta^h| \ll \eta = 3z^2 (2\tilde{E}_F t)^{1/2} / 4\pi,$$

we obtain

$$A(\xi) = \eta [1 - \xi \theta^h / (\eta + \xi) (2\eta + \xi)] / (\eta + \xi). \quad (\text{B11})$$

In the absence of spin fluctuations, $A(\xi) = 0$ and the denominator of (B10) for $\xi \rightarrow 0$ and $\varepsilon \rightarrow t_0 - 2\tilde{E}_F$ is proportional to $|\theta^h|^2 \equiv \Delta_s^2$; this leads to the estimate $(\tilde{E}_F/t_0) \ln(\tilde{E}_F/|\theta^h|)$ for the magnitude of the right-hand

side of (B10) and to the solution (58) for the gap. Since $A(\xi)$ (B11) for $\xi \rightarrow 0$ is equal to $1 - \xi/\eta$, the right-hand side of the self-consistency condition (B10) ceases to depend on θ^h and is of the order of $(\tilde{E}_F/t_0) \ln(\tilde{E}_F/t_0)$, so that the self-consistency condition for the gap does not have a trivial solution with $\theta^h \neq 0$.

- ¹ J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
- ² C. W. Chu, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, and Y. Q. Wang, Phys. Rev. Lett. **58**, 405 (1987).
- ³ J. Hubbard, Proc. R. Soc. London Ser. A **276**, 238 (1963).
- ⁴ Yu. A. Izyumov and Yu. N. Seryabin, *Statistical Mechanics of Magnetically Disordered Systems* [in Russian], Nauka, Moscow (1987).
- ⁵ W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
- ⁶ R. O. Zaitsev, Zh. Eksp. Teor. Fiz. **70**, 1100 (1976) [Sov. Phys. JETP **43**, 574 (1976)].
- ⁷ T. M. Rice, J. Magn. Mater. **76**, 542 (1988).
- ⁸ E. G. Batyev, Zh. Eksp. Teor. Fiz. **82**, 1990 (1982) [Sov. Phys. JETP **55**, 1144 (1982)].
- ⁹ P. W. Anderson, Science **235**, 1196 (1987).
- ¹⁰ Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
- ¹¹ S. V. Maleev, Zh. Eksp. Teor. Fiz. **66**, 1809 (1974) [Sov. Phys. JETP **39**, 889 (1974)].
- ¹² I. V. Kolokolov and E. B. Podivilov, Zh. Eksp. Teor. Fiz. **95**, 211 (1989) [Sov. Phys. JETP **68**, 119 (1989)].
- ¹³ R. O. Zaitsev and V. A. Ivanov, Fiz. Tverd. Tela **29**, 3111 (1987) [Sov. Phys. Solid State **29**, 1784 (1987)].
- ¹⁴ Z. Zou and P. W. Anderson, Phys. Rev. B **37**, 627 (1988).
- ¹⁵ J. R. Schrieffer, X. G. Wen, and S.-C. Zhang, Phys. Rev. Lett. **60**, 944 (1988).
- ¹⁶ G. Baskaran and P. W. Anderson, Phys. Rev. B **37**, 580 (1988).
- ¹⁷ A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys. JETP **12**, 1243 (1961)].
- ¹⁸ R. O. Zaitsev, Phys. Lett. **134A**, 199 (1988).
- ¹⁹ E. L. Nagaev, *Physics of Magnetic Semiconductors* [in Russian], Nauka, Moscow (1979).
- ²⁰ V. G. Vaks, A. I. Larkin, and S. A. Pikin, Zh. Eksp. Teor. Fiz. **53**, 281 (1967) [Sov. Phys. JETP **26**, 188 (1968)].
- ²¹ V. I. Belinicher and V. S. L'vov, Zh. Eksp. Teor. Fiz. **86**, 967 (1984) [Sov. Phys. JETP **59**, 564 (1984)].
- ²² A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N. J., 1963) [Russ. original, Nauka, Moscow, 1962].
- ²³ S. V. Tyablikov and V. A. Moskalenko, Dokl. Akad. Nauk SSSR **158**, 839 (1964) [Sov. Phys. Dokl. **9**, 891 (1965)].
- ²⁴ V. M. Galitskii, Zh. Eksp. Teor. Fiz. **34**, 151 (1958) [Sov. Phys. JETP **7**, 104 (1958)].
- ²⁵ P. W. Anderson, Phys. Rev. **86**, 694 (1952).
- ²⁶ L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **34**, 735 (1958) [Sov. Phys. JETP **7**, 505 (1958)].
- ²⁷ R. D. Parks (ed.), *Superconductivity* (Marcel Dekker, N. Y., 1969).
- ²⁸ B. V. Kärpenko, Fiz. Met. Metalloved. **9**, 794 (1960); **10**, 301 (1960).
- ²⁹ T. K. Lee, F. C. Zhang, and L. N. Chang, J. Phys. C **21**, L225 (1988).
- ³⁰ V. I. Belinicher, Preprint No. 42, Institute of Semiconductor Physics, Siberian Branch of the USSR Academy of Sciences (1989).
- ³¹ Yu. V. Kopae, Pis'ma Zh. Eksp. Teor. Fiz. **47**, 628 (1988) [JETP Lett. **47**, 726 (1988)].
- ³² P. B. Wiegman, Phys. Rev. Lett. **60**, 821 (1988).
- ³³ V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).

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