Magnetic structures in the Hubbard model with nearly half-filled band for nonalternating lattices

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(Submitted 16 May 1980)
Zh. Eksp. Teor. Fiz. **79**, 1942–1953 (November 1980)

We consider the magnetic ordering due to finite concentration of vacancies for a Fermi crystal with a planar triangular lattice and an hcp lattice. It is shown that for these lattices the ground state corresponds to an unsaturated ferromagnet with a moment equal to 1/3 and 1/4 of the saturation moment, respectively.

PACS numbers: 75.10.Jm

1. INTRODUCTION

The magnetic properties of quantum Fermi crystals have been the subject of many recent studies.[1] These crystals include either the solid phases of He^3 or the planar structures produced when He^3 atoms are adsorbed on various substrates. It was observed in experiment[2] that on a graphite surface the He^3 atoms form a regular triangular $\sqrt{3}\times\sqrt{3}$ lattice. Such a structure exists at densities $n=(0.585$ to $1.05)n_0$ (n_0 is the density corresponding to one He^3 atom for three minima of the potential relief of the substrate.)

The magnetism of He^3 is of the exchange type, since it is determined by the spin of the He^3 nucleus, and the dipole moment is therefore extremely small and cannot play a significant role at the transition temperature $T_c\sim 1$ mK. The constant J_0 for direct exchange of the positions of two atoms in the crystal, however, is quite small, and the reciprocal time τ^{-1} in which the atom jumps over to a new position in the liquid is quite large. The large value of τ^{-1} is due to the fact that the He^3 atoms are not closely packed in the liquid, and the number of vacancies is appreciable. Therefore in the crystalline structures the probability of an atom hopping over to a vacancy position, if the latter exists, should be of the same order. At sufficient vacancy density the magnetic properties of such crystals depend on the indirect exchange connected with the presence of vacancies, since the motion of the vacancies causes rearrangement of the atoms.

For solid He^3, which forms a bcc lattice, estimates yield $J_0\approx 1$ mK and $\tau^{-1}\sim 10$ K. For a planar structure and for an hcp structure, which He^3 can form at sufficiently high pressures, the values of J_0 and τ^{-1} are unknown. However, the inequality

$$J_0\ll\tau^{-1} \tag{1}$$

itself should remain in force. The inequality (11) makes it possible, in the presence of a sufficient vacancy density, to neglect the direct exchange and describe the system by the Hubbard model with infinite repulsion of the particles at one and the same lattice site.

A finite vacancy density can be due to various causes. The formation of a localized vacancy in both a two-dimensional and in a three-dimensional crystal calls for expenditure of some positive energy. If the vacancion band is wide enough, however, the energy of a delocalized vacancy can become negative. In this case, according to Andreev and Lifshitz,[3] a restructuring of the ground state takes place in a three-dimensional crystal, and zero vacancions can be produced. The vacancies can also be produced in a nonequilibrium fashion. A two-dimensional lattice liquid with enough vacancies can be produced on the surface of the graphite by the He^3 atoms if the degree of coverage is small. The situation with a small but finite vacancy density can be of interest also for magnetic dielectrics. In the Hubbard model with infinite repulsion this situation correspond to a nearly half-filled band.

The present paper is devoted to a study of the magnetic properties of such a model, neglecting all other types of exchange at low temperatures. Such a model was first considered by Nagaoka.[4] He found the ground states on the lattices that can be broken up into two sublattices, such that the site of one sublattice can have only sites of the other as nearest neighbors (only the nearest-neighbor approximation is considered). Lattices that admit of such a subdivision will be called alternating.

It is easy to show that for alternating lattices the ground state is ferromagnetic with a maximum possible summary spin. As for nonalternating lattices, Nagaoka has demonstrated that their ground state is not a ferromagnetic state with maximum summary spin.

One of us has recently proposed a method for the construction of the ground state of nonalternating lattices.[5] It was shown that a finite vacancy density on a planar triangular lattice leads to a special ferromagnetic structure with a magnetic moment equal to 1/3 of the saturation moment. It must be noted that the calculations of the ground state for an fcc lattice were made by Zaitsev,[6] but the results he obtained for the magnetic structure are incorrect, and the very value of energy of the ground state, assumed to be antiferromagnetic, agrees with the value of the energy in the ferromagnetic case.

The purpose of the present paper is a detailed calculation of the wave function and the ground-state energy for a planar triangular lattice. In addition, we refine here the previously developed method[5] as applied to an hcp lattice and establish in fact, for the first time ever, the form of the magnetic ordering in such a lattice and calculate the ground-state energy.

We confine ourselves to the case of one vacancy at

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$T=0$ in the absence of direct exchange, i.e., to the Hubbard model with infinite repulsion for nearly half-filled band. At a low finite density, the type of the magnetic ordering should not change.

2. VARIATIONAL PRINCIPLE. CONSTRUCTION OF GROUND STATE WAVE FUNCTION

The Hubbard model is described by the Hamiltonian

$$H=-\sum_{i,j}\Omega_{ij}(a_i^+a_j+b_i^+b_j)+I\sum_i n_i^a n_i^b, \qquad n_i^a=a_i^+a_i, \quad n_i^b=b_i^+b_i, \tag{2}$$

where a_i^+, a_i; b_i^+, b_i are respectively the creation and annihilation operators of particles with up and down spin; Ω_{ij} is the matrix element of the transition of a particle from site i to site j, and I the repulsion potential between two particles on one site. We confine ourselves to the nearest-neighbor approximation and write for two neighboring sites $\Omega_{ij}=\Omega>0$. The choice of the sign is connected with the fact that Ω_{ij} is in fact the overlap integral of two wave functions for a crystal with vacancy positions at the sites i and j (see, e.g., Ref. 7), and therefore its sign should coincide with the sign of the corresponding matrix element for the hop-over of a particle in a two-well potential.

In the limit $I\to\infty$ of interest to us, each site can be occupied not more than once, and therefore the model can be described by a purely tunnel Hamiltonian

$$H=-\sum_{i,j}\Omega_{ij}(a_i^+a_j+b_i^+b_j), \tag{3}$$

with the usual anticommutation relations replaced by the following:

$$\begin{gathered}\{a_i^+, a_j\}_+=\delta_{ij}(1-n_i^b), \quad \{b_i^+, b_j\}_+=\delta_{ij}(1-n_i^a),\\ \{a_i, b_j\}_+=\{a_i^+, b_j^+\}_+=0,\\ \{a_i^+, b_j\}_+=\delta_{ij}a_i^+b_i, \quad \{b_i^+, a_j\}_+=\delta_{ij}b_i^+a_i,\\ a_ib_i=b_ia_i=a_i^+b_i^+=b_i^+a_i^+=0.\end{gathered} \tag{4}$$

The relations (4) are connected with the fact that the Hamiltonian (3) acts only on a space of states in which no more than one particle is located on each lattice site. It is convenient to choose as the basis vectors of the states in this space a set of states with specified vacancy coordinates and with a definite projection of the particle spin on the z axis at each occupied lattice site. These vectors are completely determined by the numbers of the unoccupied sites and by the spin configuration, i.e., by the numbers of the sites occupied by particles with down spin. For one vacancy, we denote the basis state by the vector $|i, \{\alpha_i\}\rangle$, where i is the number of the unoccupied site, and the symbol $\{\alpha_i\}$ denotes all the indices $(j_1, j_2, \ldots, j_m)$ that number the sites with the inverted spins.

The state $|i, \{\alpha_i\}\rangle$ can be obtained from the state $|\Psi_f\rangle$ in which each site is occupied by a spin-up particle

$$|i, \{\alpha_i\}\rangle=a_i\prod_{\alpha\in j_1,\ldots,j_m} b_\alpha^+a_\alpha|\Psi_f\rangle. \tag{5}$$

Using the properties of the operators (4), it is easy to determine the result of the action of the Hamiltonian (3) on the state (5):

$$H|i, \{\alpha_i\}\rangle=\sum_k\Omega_{ik}a_k\prod b_\alpha^+a_\alpha|\Psi_f\rangle+\sum_k\Omega_{ik}b_k(b_i^+a_i)\prod b_\alpha^+a_\alpha|\Psi_f\rangle$$
$$=\sum_k\Omega_{ik}|k, \{\alpha_k^i\}\rangle, \tag{6}$$

where the configuration $\{\alpha_k^i\}$ is obtained from the configuration $\{\alpha_i\}$ by moving the particle k, without changing the projection of its spin, to the location of the vacancy i. We see thus that the Hamiltonian (3) describes the hopping of a vacancy to neighboring sites of a Nagaoma "superlattice"[4] defined by the set of indices i and $\{\alpha_i\}$.

We now expand the eigenstate of the Hamiltonian (3) in the set (5):

$$|\Psi\rangle=\sum_i\sum_{\{\alpha_i\}}\Phi(\mathbf{r}_i, \{\alpha_i\})|i, \{\alpha_i\}\rangle. \tag{7}$$

The equation for the wave function $\Phi(\mathbf{r}_i, \{\alpha_i\})$ is obtained by substituting the expansion (7) in the Schrödinger equation and using the property (6):

$$E\Phi(\mathbf{r}_i, \{\alpha_i\})=\sum_k\Omega_{ik}\Phi(\mathbf{r}_k, \{\alpha_k^i\}). \tag{8}$$

For a numerical calculation of the wave function of the ground state we use the Schrödinger variational principle:

$$\begin{aligned}E_0&=\min\{\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle\}\\ &=Z\Omega+\min\Big\{-\sum_{i,\{\alpha_i\}}\sum_k\Omega_{ik}[\Phi(\mathbf{r}_i, \{\alpha_i\})-\Phi(\mathbf{r}_k, \{\alpha_k^i\})]^2\\ &\quad\times\Big[2\sum_{i,\{\alpha_i\}}\Phi^2(\mathbf{r}_i, \{\alpha_i\})\Big]^{-1}\Big\}\\ &=\min\Big\{\sum_{i,\{\alpha_i\}}[\Phi(\mathbf{r}_i, \{\alpha_i\})\sum_k\Omega_{ik}\Phi(\mathbf{r}_k, \{\alpha_k^i\})]\\ &\quad\times\Big[\sum_{i,\{\alpha_i\}}\Phi^2(\mathbf{r}_i, \{\alpha_i\})\Big]^{-1}\Big\},\end{aligned} \tag{9}$$

where E_0 is the energy of the ground state. (The function Φ is chosen to be real.)

We shall show first how to obtain from (9) the known result concerning the ground state on alternating lattices. To this end we sum the obvious inequality.

$$2\Omega_{ik}\Phi(\mathbf{r}_i, \{\alpha_i\})\Phi(\mathbf{r}_k, \{\alpha_k^i\})\geqslant-\Omega_{ik}[\Phi^2(\mathbf{r}_i, \{\alpha_i\})+\Phi^2(\mathbf{r}_k, \{\alpha_k^i\})] \tag{10}$$

over $i, \{\alpha_i\}$, and k and obtain as a result

$$N\geqslant-Z\Omega D, \tag{11}$$

where N and D are respectively the numerator and denominator of the fraction in the right-hand side of (9), and Z is the number of nearest neighbors. If it is possible to construct a function such that the inequality (11) turns into an equality, then this means that a ground state with energy $E=-Z\Omega$ has been found. But (11) become an equality only if (10) becomes an equality for any two neighbors on the superlattice. For alternating lattices this condition can be satisfied if the wave function $\Phi(\mathbf{r}_i, \{\alpha_i\})$ does not depend at all on the spin configuration $\{\alpha_i\}$, and the dependence on the position of the vacancy reduces to a reversal of the sign on going from one sublattice to the other. It should be noted that there is no alternative, since for both planar

and three-dimensional lattices all the sites of the superlattice are interconnected (see Ref. 4). The independence of the wave function of the spin configuration means that the crystal in the ground state is a saturated ferromagnet.

The situation is different with nonalternating lattices, since it is impossible to effect for them the indicated alternation of the sign of the wave function. The inequality (11) is in this case rigorous. The principle of constructing the ground state consists in the fact that on the superlattice the wave function is concentrated near those points that have the largest number of neighbors that are not neighbors to one another (for alternating lattices this is true for any point). These points should form a periodic lattice for the vacancy positions.

Actually, when constructing the ground state we make use of the fact that on nonalternating lattices the state with the maximum summary spin and with the minimum energy turns out to be degenerate. In the situation with spins-up of all particles, this degeneracy makes it possible to construct, generally speaking various states with periodic wave function having a different number of zeros.

Let us consider some such state. Since the vacancy is not located on a site corresponding to a zero of the wave functions, it is possible to reverse the spins of the particle on these sites without changing the energy. The result is two sublattices with oppositely directed spins. For convenience, we shall refer to the sublattices with up- and down-spins as A and B, respectively. The wave function corresponding to the case when the vacancy is permitted to be only on the sublattice A is the zeroth approximation. When such a function is substituted in the functional (9) we obtain the same energy as in the purely ferromagnetic situation, but of course, it is no longer a solution of Eq. (8). If we now consider wave functions that take on nonzero values on those sublattice sites which correspond to vacancy position on the subllatice B, as well as to more complicated spin configurations, then obviously the energy will be lower.

The sublattices A and B must be chosen that each sublattice site corresponding to the zeroth approximation have the maximum number of neighbors that are not neighbors to one another. It will be shown in the next section that this requirement makes the choice of the zeroth approximation for a triangular lattice perfectly unique. In the case of an hcp lattice, some refinements are needed.

Triangular lattice

The minimum energy at the maximum total spin corresponds to the minima of the vacancy spectrum

$$\varepsilon(\mathbf{k})=2\Omega(\cos \mathbf{k}\tau_1+\cos \mathbf{k}\tau_2+\cos \mathbf{k}(\tau_1+\tau_2)), \tag{12}$$

where $\tau_1=(1,0)$, $\tau_2=(-\frac{1}{2},\sqrt{3}/2)$ are the principal periods of the lattice [the unit of length is everywhere the distance between the neighboring lattice sites; the spectrum (12) can be easily obtained if it is recognized that the wave function depends only on the position of the vacancy and if one goes over to Fourier components in Eq. (8)].

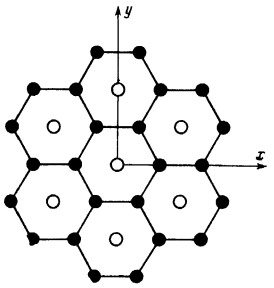

FIG. 1. Magnetic-ordering structure in the ground state on a triangular lattice. ●) Sites with up spins, ○) with down spins.

The energy $\varepsilon(\mathbf{k})$ has the minimum value -3Ω at two points belonging to one Brillouin zone

$$\mathbf{k}_1=\tfrac{4}{3}\pi(1,0), \quad \mathbf{k}_2=\tfrac{4}{3}\pi(\tfrac{1}{2},-\sqrt{3}/2).$$

This double degeneracy makes it possible to construct a state with a wave function that vanishes on centers of hexagons and reverses sign on going from neighbor on a hexagonal lattice (see Fig. 1). We note that such a wave function has the maximum number of zeros. By reversing the spins at the centers of the hexagons we obtain the zeroth approximation. The nearest neighbors of each sublattice site corresponding to the zeroth approximation are not at all neighbors to one another.

It is very important to take the symmetry into account in the numerical calculation, for this decreases significantly the number of nonequivalent spin configurations. Since the spins on the sublattice B are reversed, we are interested only in those symmetry elements that transform the sublattices A and B into themselves. That subgroup of the entire crystal triangular-lattice group consisting of such elements will be called the symmetry group of the magnetic structure. The symmetry group of the magnetic structure is determined by the elements

$$T_1,\ T_2,\ C_6,\ \sigma_x, \tag{13}$$

where T_1 and T_2 are translations by the vectors

$$\mathbf{T}_1=(\tfrac{3}{2},-\sqrt{3}/2), \quad \mathbf{T}_2=(0,\sqrt{3}),$$

C_6 is a rotation through an angle $\pi/3$ about the origin, and σ_x is replacement of y by $-y$ (see Fig. 1). The remaining elements of this group can be represented in the form of products of the elements (13) raised to the corresponding powers. In the higher approximations the wave function will effect the same one-dimensional irreducible representation of the magnetic-structure symmetry group as the zeroth-approximation function. The latter is determined by the characters of the elements (13)

$$\chi(C_6)=-1, \quad \chi(T_1)=\chi(T_2)=\chi(\sigma_x)=1. \tag{14}$$

The concrete application of the group premises is described in Sec. 3 of this paper.

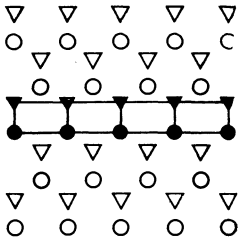

FIG. 2. ○ and ▽) Sites of two neighboring basal planes of hcp lattice, ● and ▼) sites on which the wave function with maximum number of zeros does not vanish.

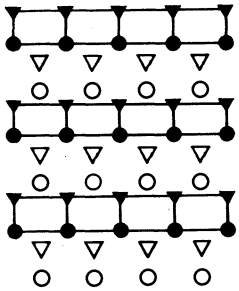

FIG. 3. One of the possible magnetic structures on an hcp lattice.

Hexagonal close packed structure

For the hcp structure in the situation with maximum summary spin there are two branches of the vacancy spectrum, since the unit cell contains two sites. We are interested in the lower branch:

$$\varepsilon(\mathbf{k})=\Omega\{2\lambda(\mathbf{k})-[2(1+\cos\mathbf{k}\tau_3)(3+2\lambda(\mathbf{k}))]^{1/2}\},$$
$$\lambda(k)=\cos\mathbf{k}\tau_1+\cos\mathbf{k}\tau_2+\cos\mathbf{k}(\tau_1+\tau_2), \qquad (15)$$

where $\tau_1=(-1,0,0)$ and $\tau_2=(\frac{1}{2},-\sqrt{3}/2,0)$ are the principal lattice periods in the basis plane, $\tau_3=(0,0\,2\sqrt{2/3})$ is the period in the perpendicular direction. It is easy to determine from (15) that the minimum energy $\varepsilon=-4\Omega$ corresponds to values $\mathbf{k}\cdot\tau_3=0$ and $\lambda(\mathbf{k})=-1$.

The Brillouin zone contains this a whole equal-energy line that gives the minimum energy. The infinite-fold degeneracy make it possible to construct a wave function (this will be the wave function with the maximum number of zeros) which does not become equal to zero only on one straight line in each basal plane. All the lines are parallel and are so arranged that for two lines on neighboring basal planes each site of one line has one nieghbor on the other (see Fig. 2). The wave functions on the nonzero sites has a constant modulus and reverses sign on going from neighbor to neighbor. In contrast to the triangular lattice, the wave function with the maximum number of zeros does not determine the magnetic ordering. This is clearly already from the fact that if all the spins are reversed at the sites corresponding to the zeros of such a wave function, the structure will not be periodic.

It is possible to construct for an hcp lattice a periodic structure such that all the neighbors of the superlattice points corresponding to the zeroth approximation are not neighbors of one another. It is easily understood that the zeroth approximation should be realized by a structure in which each site of sublattice A has as its neighbors only four sites of the same sublattice. In this case, for any point of the sublattice corresponding to the zeroth approximation, only those neighbors which are obtained when the vacancies hop over from sublattice A to sublattice B (such configurations are in accord with the approximation) will be neighbors of one another. There are, however, many such periodic structures. It is possible, for example, to arrange in each basal plane an alternation of parallel lines with non-inverted and inverted spins. The result is a system of corrugated surfaces, on each of which the spins are ferromagnetically ordered, but on the neighboring surfaces the spin projections are opposite (Fig. 3). It is possible to insert between two surfaces with non-inverted spins several surfaces with inverted ones. Other more complicated structures are also possible.

It is remarkable that for all such structures, the number of ineffective bonds per site of sublattice A between the configurations corresponding to the first approximation is the same. Therefore the choice of the magnetic structure cannot be based on the first approximation. It is easily seen that the second-approximation energy will be minimal in the case of a minimal number of ineffective bonds between the superlattice sites on which a vacancy can land in the second approximation (such sites are obtained if the vacancies are allowed to make two steps from sublattice A in any direction), the energy will also be lower if the number of the number of the configurations obtained in the second approximation per site of sublattice A is minimal. The last requirement leads to a decrease of the denominator of the functional (9) without reducing the number of effective bonds in the numerator.

An analysis of the different structures shows that these requirements are satisfied by only one structure, shown in Fig. 4. In each basal plane the sites of sublattice A are at the vertices of a hexagon. The bonds between the hexagons are effected via neighboring basal planes. The unit magnetic cell of this zeroth-approximation structure contains 32 sites (16 each in the neighboring basal planes). Twelve of these belong to sublattice A. From the results of a numerical calcula-

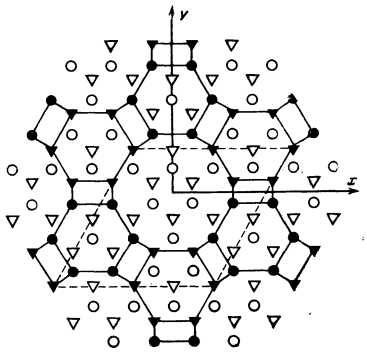

FIG. 4. Structure of magnetic ordering in the ground state on the hcp lattice. ● and ▼) Sites with up spins, ○ and ▽) with down spins. The dashed lines enclose the unit cell. The coordinate plane xy coincides with basal plane, marked by circles. The z axis is perpendicular to the xy plane.

tion of the wave function in the higher approximations (see Sec. 4 of the present paper) it is seen that the average magnetizations if sublattices A and B remain the same as in the zeroth approximation. This leads to an unsaturated ferromagnet with a total magnetic moment equal to $\frac{1}{4}$ of the saturation moment.

Numerical calculations were made also for several other magnetic-ordering structures. In all cases the energy turned out to be higher than for the structure shown in Fig. 4. This confirms the correctness of the principles used to construct the ground state.

The spatial symmetry group of the magnetic structure is determined for an hcp lattice by the following elements (see Fig. 4):

$$T_1,\ T_2,\ T_z,\ \sigma_{yz},\ \sigma_{xy},\ C_6^z, \tag{16}$$

where T_1, T_2, and T_3 are translations by the vectors

$$\mathbf{T}_1=(4,\ 0,\ 0),\quad \mathbf{T}_2=(2,\ 2\sqrt{3},\ 0),\quad \mathbf{T}_z=(0,\ 0,\ 2\sqrt{2/3}),$$

σ_{yz} and σ_{xy} are simple reflections in the planes yz and xy, C_6^z is a crew axis of sixth order (rotation through an angle $\pi/3$ about the z axis with subsequent translation by $\mathbf{T}_z/2$). The other symmetry elements can be obtained by taking the product of the operations (16) raised to the corresponding powers. For example, $T_z^{-1}(C_6^z)^2\sigma_{yz}$ gives the slip plane.

We note that the symmetry group of the magnetic structure contains the same rotation elements as the crystal group of the hcp lattice. The irreducible representation is determined from the zeroth-approximation wave function and is given by the characters of the elements (16):

$$\chi(T_1)=\chi(T_2)=\chi(T_z)=\chi(\sigma_{xy})=\chi(C_6^z)=1;\quad \chi(\sigma_{yz})=-1\ . \tag{17}$$

3. DESCRIPTION OF THE CALCULATION PROCEDURE

We note first that the translational symmetry allows us, when summing over the index i in the numerator and denominator of (9), to confine ourselves to one unit magnetic cell. (We agree the vacancy position to determine the assignment to a particular cell). In addition, there is no need to consider separately the equivalent sites of the superlattice, i.e., sites that can be transformed by rotations and reflections from the symmetry group of the magnetic structure. Consequently the summation in (9) can be additionally confined to nonequivalent configurations only. Allowance for the equivalent sites of the superlattice reduces to multiplication of each term of the sum over i and $\{\alpha_i\}$ by a weight equal to the number of equivalent configurations per cell. There exist, however, configurations that go over into themselves upon transformation with negative character. The amplitudes corresponding to them are zero and can be completely disregarded in the functional (9).

Assume now that in a ceratin approximation, n out of all the superlattice sites on which vacancies are allowed to exist are nonequivalent with amplitudes $\Phi_0, \Phi_1, \ldots, \Phi_{n-1}$. When account is taken of everything said above, the functional (9) takes then the form

$$E_0=\min\Omega\left\{\left(\sum_{k=0}^{n-1}P_k\beta_k\Phi_k\sum_z{}'\Phi_{k+z}\beta_{k+z}\right)\left(\sum_{k=0}^{n-1}\Phi_k^2P_k\beta_k\right)^{-1}\right\}. \tag{18}$$

Here P_k is the weight of the k-th configuration, Φ_{k+z} is the amplitude of the neighbor, and we have introduced a parameter β that vanishes if the corresponding configuration goes over into itself under some transformation with negative character, and is equal to unity in the opposite case. The summation over the nearest neighbors is restricted to those superlattice sites on which a vacancy can be located in the chosen approximation. Each neighbor amplitude Φ_{k+z} is expressed in terms of one of the chosen amplitudes:

$$\Phi_{k+z}=\chi(G^j_{k+z})\Phi_j,\quad j\leqslant n-1, \tag{19}$$

where $\chi(G^j_{k+z})$ is the character of the element (this can be also an identity transformation) that transforms a configuration with amplitude Φ_{k+z} into an equivalent one with amplitude Φ_j.

The following remark must be made concerning (19). Two equivalent configurations Ψ_a and Ψ_b can be made to go into one another either by one or by several transformations. In the latter case we have

$$\Psi_a=G_1\Psi_b,\quad \Psi_a=G_2\Psi_b,\ldots,\quad G_1\neq G_2,$$

whence

$$\Psi_a=G_1G_2^{-1}\Psi_a,\quad \Psi_b=G_2^{-1}G_1\Psi_b.$$

In the one-dimensional representation realized by the wave function $\Phi(\mathbf{r}_i,\{\alpha_i\})$ the characters of all the elements are equal to ±1. If the characters of the elements G_1 and G_2 are of opposite sign, then

$$\chi(G_1G_2^{-1})=\chi(G_1)\chi(G_2^{-1})=\chi(G_1)\chi(G_2)=-1.$$

Consequently, the configurations Φ_a and Ψ_b go over into one another via transformations with negative characters. Such configurations, however, are excluded from the functional (18). Therefore in the case of several transformations it is immaterial which element is contained in (19). We shall henceforth call Φ_j the neighbor of Φ_k, bearing (19) in mind.

It follows from (18) and (19) that to construct the functional the procedure to be followed is:

1. Construct the number all the nonequivalent configurations in the chosen approximation.

2. Determine the configurations that go over into one another under transformations with negative character, and find the values of β_k for the different configurations.

3. Find the weights P_k for the configurations with $\beta_k\neq0$

4. Determine for each configuration with $\beta_k\neq0$ the nearest neighbors and the sign with which the corresponding amplitude enters.

The foregoing procedure was effected with a computer. Each configuration was specified by the coordinates of the vacancy and of the spoiled lattice sites, i.e., the sites of sublattice A with spins down and the sites of sublattice B with spins up. The initial configuration corresponding to the zeroth approximation

was set manually. The remaining configurations were constructed by special programs (different for the two considered lattices), which generated the configurations obtained when vacancies hop from site to site. The number of the approximate corresponded to the number of steps made by the vacancy from the initial point in various directions. To determine the equivalent configurations the programs included special symmetry blocks to realize various rotations and reflections. For a triangular lattice, the capability of the computer made it possible to construct a functional in the fifth approximation, and in the third approximation for the hcp lattice. The obtained functionals were minimized by the standard steepest-descent method. The amplitude Φ_0 corresponding to the zeroth approximation was fixed at $\Phi_0 = 1$.

4. CALCULATION RESULTS

The energy values obtained by minimizing the functional (18) for magnetic-ordering structures corresponding to the ground state (Fig. 1 for a triangular lattice and Fig. 4 for hcp lattice) are given in Table I. This table gives also for each approximation the number of nonequivalent superlattice sites on which a vacancy can be located.

In the case of a triangular lattice, good convergence of the energy is seen. For an hcp lattice the accuracy attained in the energy calculation was lower, since we confined ourselves to the third approximation. It is seen from Table I, however, that for like approximations the energies obtained for the different lattices have approximately the same relative accuracy.

By way of illustration of the correctness of the choice of the ground-state magnetic structure, we present the results of a variational calculation of the energy for an antiferromagnetic structure on an hcp lattice (Fig. 3):

Approximation:	0	1	2	3
E/Ω:	−4	−5.13	−5.37	−5.44

In first approximation, the antiferromagnetic ordering and the structure corresponding to the ground state give energies that agree to two significant figures. This means that in both situations the number of ineffective bonds per site of sublattice A is the same. In the succeeding approximations, as seen from the tables, the antiferromagnetic structure gives a higher energy.

Calculation shows that the wave function of the ground state is concentrated near the basic configuration, i.e., superlattice sites corresponding to the zeroth approximation, and decreases rapidly for more complicated configurations. (The character of the decrease of the amplitudes as a function of the number of steps made by the vacancy with basic configuration is illustrated by Table II.) In view of the large number of points it is impossible to present here all the calculated values of the wave function. We give for the configurations of each step only severeal of the amplitudes with the maximum absolute value. The data of Table II correspond to calculation in fifth order for a triangular lattice and third order for the hcp lattice. Judging from these data, the amplitudes decrease exponentially. We note that there is a considerable spread of the amplitudes for one and the same step, such that some of them differ by one or two orders of magnitude.

TABLE I. Results of variational calculation of ground-state energy.

	Lattice type	Approximation					
		0	1	2	3	4	5
Number of nonequivalent configurations	Triangular	1	2	5	13	48	167
	Hcp	1	7	43	294	–	–
E/Ω	Triangular	−3	−3.79	−4.00	−4.04	−4.06	−4.07
	Hcp	−4	−5.13	−5.46	−5.54	–	–

TABLE I. Values of amplitudes.

Lattice type	Step				
	1	2	3	4	5
Triangular	$-3.6\cdot10^{-1}$	$1.4\cdot10^{-1}$	$-6.0\cdot10^{-2}$	$2.3\cdot10^{-2}$	$-6.4\cdot10^{-3}$
	–	$9.2\cdot10^{-2}$	$-4.8\cdot10^{-2}$	$2.1\cdot10^{-2}$	$-5.6\cdot10^{-3}$
	–	$3.9\cdot10^{-2}$	$-3.8\cdot10^{-2}$	$2.1\cdot10^{-2}$	$-5.5\cdot10^{-3}$
Hcp	$-2.2\cdot10^{-1}$	$1.2\cdot10^{-1}$	$-3.2\cdot10^{-2}$	–	–
	$-2.2\cdot10^{-1}$	$1.0\cdot10^{-1}$	$-3.1\cdot10^{-2}$	–	–
	$-2.1\cdot10^{-1}$	$7.9\cdot10^{-2}$	$-2.0\cdot10^{-2}$	–	–

The probability that a vacancy is located on sublattice A and at the same time a basis configuration is realized equal to Φ_0^2/d, where d is the single-site normalization sum, i.e., the denominator of the functional (18) per site of sublattice A. We present the results of the calculation of d for $\Phi_0 = 1$ in various approximations:

Approximation:	0	1	2	3	4	5
Triangular lattice:	1	1.22	1.41	1.49	1.55	1.60
Hcp :	1	1.16	1.35	1.46	–	–

These data seem to indicate convergence of the normalization sum; this means that the vacancy has a noticeable probability of being located on superlattice sites near the basic configuration, and the magnetic structure can be spoiled only in a microscopic region around the vacancy. Therefore the average magnetizations of the sublattices A and B will be opposite. From these data we obtain an estimate of the probability of finding a vacancy on sublattice A with reversed spins

$$W_{tr}^0 \approx 0.6, \quad W_{hcp}^0 \approx 0.7,$$

i.e., the highest probability is that of locating the vacancy on sublattice A. This allows us the estimate the effective masses of the vacancy by considering the motion only over this sublattice. In this approximation the band spectrum can be easily calculated at for small wave vectors it takes the form

$$E_{tr}(\mathbf{k}) \approx E_0 + {}^3/_4 \Omega k^2 a^2,$$
$$E_{Hcp}(\mathbf{k}) \approx E_0 + {}^2/_3 \Omega k_\perp^2 a^2 + {}^8/_{13} \Omega k_\parallel^2 a^2,$$

where a is the distance between nearest neighbors on the initial lattice, and $k_\perp$ and $k_\parallel$ are the wave-vector components normal and tangential to the basal plane of the hcp lattice, respectively.

We have thus shown that, neglecting all types of exchange except the one due to a small but finite vacancy density, the magnetic ordering of quantum Fermi crystals with planar triangular or three-dimensional hcp lattice correspond to an unsaturated ferromagnet. In

the case of the triangular and hcp lattices the summary magnetic moments are equal respectively to 1/3 and 1/4 of the saturation moment. The vacancies are preferentially concentrated on a ceratin magnetic sublattice and upset the initial symmetrical density distribution in the vacancy-free crystal.

We note that our results present a rigorous variational estimate of the ground-state energy in the Hubbard model with inifinite repulsion and with nearly half-filled band for these lattices. The authors thank V. L. Pokrovskiĭ for helpful discussions.

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Translated by J. G. Adashko

Onset of inhomogeneous magnetic ordering of the spins in a superconductor

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(Submitted 29 April 1980)
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The relative role of the magnetic dipole and of the indirect exchange interaction of localized spins in the onset of magnetic ordering in a superconductor is investigated. It is assumed that in the absence of superconductivity the ordering in the spin system would be ferromagnetic. It is shown that even weak exchange exerts a substantial influence on the value of the wave vector of the magnetic structure produced in the superconductor.

PACS numbers: 74.30.Ci, 75.30.Et

The question of coexistence of magnetism and superconductivity is presently attracting increased interest in connection with the synthesis of superconducting compounds with a regular arrangement of magnetic atoms. Many compounds of this type have been synthesized by now[1-3] and their number continues to increase rapidly. There is at present no doubt that antiferromagnetism has little effect on superconductivity, and approximately ten compounds of the $GdMo_6S_8$ type are known, in which coexistence of superconductivity and antiferromagnetism has been found to take place.[1-3] A situation of much greater interest is one in which, in the absence of superconducting pairing, the localized moments should become ferromagnetically ordered when the temperature is lowered. This case is realized in the compounds $ErRh_4B_4$ and $HoMo_6S_8$, which become first magnetically disordered superconductors at a point T_{c1}, and then go over into a ferromagnetic superconducting phase at a point $T_{c2} < T_{c1}$. This situation is the subject of our study.

The magnetic ordering of the considered compounds can be brought about by two main types of interaction: magnetic dipole interaction of localized moments, and indirect exchange via the conduction electrons. Spin ordering in a superconductor in the model with indirect exchange interaction was considered in Ref. 4 and in detail in Ref. 5. It was shown there that in the region where superconductivity and magnetism coexist there is realized a helicoidal ordering of the localized spoins with wave vector **Q**. and near the point of onset of magnetic ordering.

$$Q \approx (k_F^2 \xi_0^{-1})^{1/3},$$

where ξ_0 the superconducting correlation length. The model with magnetic dipole interaction was investigated in Refs. 6 and 7. In this case the magnetic ordering in the superconductor is likewise helicoidal with wave vector

$$Q \approx (k_F/\lambda_L)^{1/2},$$

where λ_L is the London penetration depth. In real systems, the magnetic-dipole and the exchange interactions act simultaneously, and we investigate in this article their relative contributions to the structure of the inhomogeneous magnetic ordering in the superconducting phase.

We note first that a weak magnetic dipole interaction or an interaction of the order of the exchange interaction does not alter the results obtained in Refs. 4 and 5 for the case of pure exchange interaction. The situation is different in the case of weak exchange interaction against the background of the magnetic dipole interac-

 0038-5646/80/110987-03$02.40