Magnetic properties of a vacancy in a quantum Fermi crystal with a flat triangular lattice

S. V. Iordanskiĭ
L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences

(Submitted 13 February 1979)

Pis'ma Zh. Eksp. Teor. Fiz. **29**, No. 6, 361–364 (20 March 1979)

It is shown that the finite concentration of vacancies on a flat, triangular lattice of Fermi atoms produces a specific ferromagnetic structure with a magnetic moment equal to 1/3 that of saturation.

PACS numbers: 61.70.Bv, 75.10.Jm

The direct exchange of the positions of two atoms is greatly complicated in the He^3 quantum Fermi crystal (the corresponding exchange integral $J \sim 1$ mK), whereas the width of the vacancy band is $t \sim 10$ K. The direct exchange, therefore, can be neglected and the system in the presence of vacancies can be described by the Hubbard model with an infinite repulsion at the same lattice point. When there are a few vacancies the band is filled slightly less than half. The delocalized vacancies rearrange the atoms, producing exchange forces and magnetic effects associated with them.

This problem was initially examined by Nagaoka.[1] He showed that the ground state in the crystals, whose lattices can be broken down into two sublattices so that each point of one sublattice has for its nearest neighbors (the approximation of the nearest neighbors is examined) only the points of the other sublattice, is the ferromagnetic state with the maximum spin of the whole crystal $S_{max} = 1/2\, N$ (N is the number of crystal atoms). Such lattices are called cleavable lattices. The properties of the vacancy in the bcc He_3 phase, which is a cleavable lattice, was examined in Ref. 2.

At sufficient pressure, however, He forms a hexagonal close-packed lattice, which is noncleavable. The He_3 atoms at the surface of different adsorbents[3] usually form a flat triangular lattice, which is also noncleavable. The surface magnetic properties of He_3 have recently been investigated experimentally.[4] Guer[5] hypothesized that the observed effects could be attributed to the vacancies in the surface layer.

In this paper, we examine the magnetic properties of a vacancy in a triangular flat lattice. The approach apparently is the same for all noncleavable lattices, although the difficulty of the calculations may differ.

We chose a basal plane in the wave-function space, in which each lattice point is occupied by a single atom; according to Ref. 1

$$\Psi(i, a_i) = (-1)^i c^+_{1\sigma_1} \ldots c^+_{i-1\,\sigma_{i-1}} c^+_{i+1\,\sigma_{i+1}} \ldots c^+_{N\sigma_N} |0\rangle, \quad (1)$$

where $c^+_{j\sigma_j}$ and $c_{j\sigma_j}$ are the creation and annihilation operators of particles at the lattice point j with the spin projection σ_j on the given axis, $|0\rangle$ is the particle-free state (vacuum), i denotes the location of the vacancy in the lattice, and α_i is a generalized index which gives the projection of the spins at all the lattice points except the unoccupied point. The wave function in this basal plane is defined by the $\Phi(i,\alpha_i)$ coefficients and the performance of the ordinary jump Hamiltonian $\hat{H}$ is determined by

$$\hat{H}\Phi(i, a_i) = t \sum_z \Phi(i + z, a_i^{i+z}) \quad (t > 0), \quad (2)$$

where z are the nearest neighbors, the configurations of the spins α_i^{i+z} is determined from the α_i configuration by transferring the atom with spin α_{i+z} to the point i. Thus, we have a problem of jumps of the nearest neighbors in the "superlattice" (i,α_i).

If we subtract from $\hat{H}$ the diagonal matrix $z\hat{I}$, then the search for the energy E_0 of the ground state is equivalent to determining the minimum of the functional

$$\mathcal{E} = (E_0 - z) = min\left\{ - t \frac{\sum_{i, a_i} (\Phi(i, a_i) - \Phi(i + z, a_i^{i+z})^2}{\sum_{i, a_i} \Phi^2(i, a_i)} \right\}. \quad (3)$$

In contrast to the ordinary difference Schrödinger equation, this expression corresponds to the changed sign of the kinetic energy, so that the lesser energy corresponds to the states with greater gradients.

The state with the maximum gradient can be easily constructed for cleavable lattices, if we assign the value $(+1)$ to the wave function in one sublattice and (-1) in the other, irrespective of the spin configuration, which corresponds to the ferromagnetic state with a maximum spin. Thus each bond in the lattice gives the same contribution equal to -4.

In the spin-independent noncleavable lattices a fraction of the bonds are ineffective and their contribution is greater than (-4); the relevant lower state (for a maximum spin), which is obtained according to the ordinary band scheme, does not correspond to the ground state, which was illustrated by Nagaoka for the bcc and hcp structures. The point is that at the expense of the spin variable a fraction of the ineffective bands can be forced to work, thus the energy can be lowered substantially if the neighbors in the sample lattice (ignoring the spin) would no longer remain such in the superlattice. There is an advantage even in the case of a single reversed spin.

Since this cannot be done at all the points in the superlattice, the wave function is concentrated near those points where this is possible.

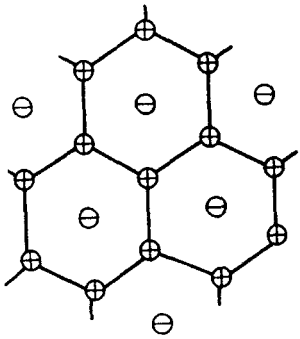

FIG. 1.

The actual construction of the trial functions uses the degeneration of the lowest state with a maximum spin. Let us construct a function with the largest number of zero points in the lattice for the lowest state with a maximum spin. Since the direction of the spin at the three points where the function vanishes is unimportant, we assume that it is opposite to that of the other points. If the $\Phi(i,\alpha_i)$ function is assumed to be nonvanishing in the configurations obtained when the vacancy enters the lattice points with initially reversed spin, then we can minimize the energy accordingly.

For the triangular lattice we have a basal configuration in which the atoms with a plus spin (+) are distributed around the perimeter of the hexagons and the atoms with a minus spin (−) are situated at their center, as shown in Fig. 1. The wave function has a maximum modulus for such a spin configurations and vacancy which is situated at the site of one of the + atoms. The calculation shows that the probability of finding the vacancy at the site of the − atom and one − atom at the perimeter of the hexagon is less than 1/10th that of the optimal configuration and decreases sharply for more complex distortions. The calculations gives the energy of the ground state per vacancy:

$$E_0 < -4.3t \qquad (E_0(S_{max}) = -3t). \tag{4}$$

Thus, the ground state of the He_3 atoms in the triangular lattice in the presence of finite concentration of vacancies corresponds to the unsaturated ferromagnet with the magnetic moment equal to 1/3 that of saturation. The vacancy sites form a honeycomb sublattice in the triangular lattice, i.e., the spatial symmetry is violated.

It can easily be seen that the excitations corresponding to the transition of the vacancy to a higher energy state must form a band. The effective mass can be estimated fairly accurately if we examine the motion of the vacancy only in the ferromagnetic "honeycomb" sublattice:

$$E(k) \approx -4.3 + \frac{9}{4} t k^2, \tag{5}$$

where α is the edge of the original triangular lattice.

In case of a single vacancy per crystal or an unspecified number of them we

cannot speak of a transition of the entire crystal to the corresponding magnetic state. The entropy[2] or energy considerations at a finite value of the direct-exchange constant J show that the proposed structure occurs in a certain finite volume in which the vacancy is localized. The relevant calculations, which differ very little from the quadratic lattice,[6] give for the localization radius

$$R \sim a(t/T)^{1/4} \quad (T >> J); \qquad R \sim a(t/J)^{1/4} \quad (J >> T). \tag{6}$$

The author wishes to thank I.E. Dzyaloshinskiĭ and L.P. Pitaevski for a useful discussion.

[1]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[2]A.F. Andreev, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 608 (1976) [JETP Lett. **24**, 564 (1976)].
[3]M. Nielsen, J.P. McTague, and W. Ellenson, J. de Phys. **38**, C4-13 (1977).
[4]A.I. Ahonen, T.A. Alvesalo, T. Haavosoja, and M.C. Veuro, J. de Phys. **39**, C6-285 (1978).
[5]R.P. Guer, PRL **39**, 1091 (1977).
[6]M.V. Feĭgel'man, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 491 (1978) [JETP Lett. **27**, 462 (1978)].