Two-dimensional quantum crystal with ground-state vacancies—He^3 on graphite

M. V. Feĭgel'man

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
(Submitted 22 March 1978)
Pis'ma Zh. Eksp. Teor. Fiz. **27**, No. 9, 491–493 (5 May 1978)

The existence of a two-dimensional crystal with vacancies in the ground state is demonstrated. The contribution made by the vacancies to the heat capacity and to the paramagnetic susceptibility is calculated. The existence of a phase transition, namely condensation of vacancies into a ferromagnetic drop, is demonstrated.

PACS numbers: 67.80.Jd, 67.80.Mg

Various structures produced in submonolayer films of helium adsorbed on a surface of graphite have been extensively investigated in recent years.[1–3] In addition to the two-dimensional analogs of ordinary phases, a crystal was obtained constituting a triangular regular superlattice of structure $\sqrt{3}\times\sqrt{3}$ on the graphite lattice. At stoichiometric concentration n_c of the helium atoms, there is one atom for three minima of the potential relief. This matched crystal (MC) exists at densities $n=(0.85–1.05)n_c$.[3] A constant period of the crystal lattice at different densities can be ensured by stratification or by the appearance of vacancies (or extra atoms). Since the MC is compressed, as are all other solid phases of helium, one can expect the second of these situations to be realized in a density interval of the same of magnitude. We then have a quantum crystal with a vacancy concentration $x_v=(n_c-n)/n_c \lesssim 0.1$. in the ground state. The properties of such crystals were discussed by Andreev and Lifshitz.[4] In particular, the MC of He^4 with $x_v \neq 0$ should be superfluid.

In this paper we consider those He^3 MC properties which are connected with the structure of magnetic vacancies. This question was considered in[11], but the result turned out to be qualitatively incorrect, since the inhomogeneous states (fluctuons) were not considered. At low temperatures the vacancies in He^3 are delocalized (band width $\Delta \sim 10$ K). This lead to the appearance of indirect exchange with $J_{\text{eff}} \sim \Delta \gg J_0 \sim 1$ mK. This problem reduces to the degenerate Hubbard model first considered by Nagaoka.[5] As applied to flat lattices, the methods of[5] give the ferromagnetic ground states for quadratic and hexagonal lattices. For a triangular lattice the structure of the ground state is unknown, but it can be shown that it is not ferromagnetic. We shall therefore have henceforth a hexagonal He^3 lattice in mind. Possible methods of obtaining this lattice will be indicated below. Of course, Δ and J_0 in a planar lattice will not be the same in bcc He^3, but the essential inequality $\Delta \gg J_0$ is preserved. As shown by Andreev,[6] at $J_0 \ll T \ll \Delta$ there is produced around the vacancy a ferromagnetically ordered region of the fluctuon type[7] with a radius $R \gg a$. For a planar lattice, a variational method[6] yields

$$R/a = (\hbar^2 y^2/2\pi \ln 2ma^2 T)^{1/4}; \qquad F_{\text{vac}} = x_v\left(\frac{\hbar^2}{ma^2}\right)^{1/2} T^{1/2}(\pi \ln 2)^{1/2} y, \tag{1}$$

where $m \sim \hbar^2/\Delta a^2$ is the effective mass of the vacancion, and $y = 2.45$ is the first root of the function $J_0(z)$. $F_{\rm vac}$ is the free energy of the fluctuons per helium atom. With each fluctuon is connected a large magnetic moment $\mu' = (\pi R^2/a^2)\mu_{\rm He^3} \sim (\Delta/T)^{1/2}\mu_{\rm He^3}$. Therefore the presence of vacancies influences noticeably the paramagnetic susceptibility of the crystal:

$$\chi \sim \frac{\mu_{eff}^2}{T} = \frac{\mu_{\rm He^3}^2}{T}\left(1 + x_v \frac{\Delta}{T}\right) . \qquad (2)$$

In addition, at low temperatures the vacancies make an appreciable contribution to the heat capacity:

$$C_{\rm vac} = -T\frac{\partial^2 F_{\rm vac}}{\partial T^2} \sim x_v \left(\frac{\Delta}{T}\right)^{1/2} . \qquad (3)$$

The foregoing analysis does not take into account the interaction between fluctuons and the possibility of their condensation. Let us find now the energy of a state in which all the vacancies are in a single ferromagnetically ordered (F) region. At $T \ll \Delta$ we have a degenerate Fermi gas of vacancions. Neglecting first the elastic repulsion, we obtain the concentration $x(T)$ of the vacancies in the region of F, and the free energy $\tilde{F}_{\rm vac}(T)$ of the vacancies per helium atom (we recall that the total number of vacancies is constant in our case):

$$x(T) = \left(\frac{ma^2 T \ln 2)}{\pi\hbar^2}\right)^{1/2}; \qquad \tilde{F}_{\rm vac}(T) = \left(\frac{\hbar^2}{ma^2}\right)^{1/2} T^{1/2} (\pi \ln 2)^{1/2} \sqrt{2}\, x_v . \qquad (4)$$

Comparing (1) and (4) we see that the condensation of the fluctuons lowers the energy. Of course, this calculation is sensible only at such small $x(T)$ that the elastic interaction of the vacancies can be neglected. We can state, however, that if the temperature T_c is such that $\tilde{F}_{\rm vac} + \tilde{F}^{\rm el}_{\rm vac} = F_{\rm vac}$, then a first-order phase transition will take place with condensation of the vacancies into an F drop. With further lowering of the temperature, the F region will increase. We estimate T_c by calculating the correction of first-order in the interaction to the energy of the degenerate Fermi gas with repulsion. By virtue of the elastic isotropy of the hexagonal lattice, the interaction of the vacancies is

$$W(r) = W\frac{a^4}{r^4} e^{-\kappa r},$$

where $W \sim Mc^2$ (M is the mass of the atom and c is the speed of sound), $\kappa \approx (\omega_0/a)\,\omega_{\rm Debye}$ (the exponential factor is due to the presence of a gap $\hbar\omega_0$ in the phonon spectrum of the matched crystal). Since the vacancies in the F region are fermions with fixed spin projection, there is no s scattering, and p scattering must be taken into account. As a result (assuming $\omega_0 \ll \omega_{\rm Debye}$) we get

$$x(T_c) \sim \Delta/_W \ll 1, \qquad T_c \sim \Delta(\Delta/w)^2. \qquad (5)$$

At $x_v \gtrsim x(T_c)$ it is necessary to take into account the interaction of the fluctuons also in the "gas" phase before the transition, and this can change the character of the transition.

We indicate in conclusion that a hexagonal lattice can be obtained either by replacing 1/3 of the He atoms from a triangular lattice by Cs atoms that form a 3×3 lattice (this structure should be realized as a result of the strong dipole repulsion of Cs on graphite[8]) or by adsorption of He on graphite coated with a monolayer of Ne.[9,10]

The author thanks S.V. Iordanskiĭ, A.É. Meĭerovich, V.L. Pokrovskiĭ, and G.V. Uĭmin for valuable discussions during all stages of the work.

[1]M. Bretz *et al.*, Phys. Rev. A **8**, 1589 (1973); R. Elgin and D. Goodstein, Phys. Rev. A **9**, 2657 (1974); M. Bretz, Phys. Rev. Lett. **38**, 501 (1977); S. Hering, S. Van Sciver, and O. Vilches, J. Low Temp. Phys. **25**, 793 (1976)].

[2]R. Rollefson, Phys. Rev. Lett. **29**, 410 (1972); B. Cowan *et al.*, Phys. Rev. Lett. **38**, 165 (1977).

[3]M. Nielsen, J. McTague, and W. Ellenson, J. Phys. (Paris) **38**, C4-1 (1977)].

[4]A.F. Andreev and I.M. Lifshitz, Zh. Eksp. Teor. Fiz. **56**, 2057 (1969) [Sov. Phys. JETP **29**, 1107 (1969)].

[5]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[6]A.F. Andreev, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 608 (1976) [JETP Lett. **24**, 564 (1976)].

[7]M.A. Krivoglaz, Usp. Fiz. Nauk **111**, 617 (1973) [Sov. Phys. Usp. **16**, 856 (1974)]; E.L. Nechaev, Usp. Fiz. Nauk **117**, 437 (1975) [Sov. Phys. Usp. **18**, 863 (1975)].

[8]I. Lander and I. Morrison, Surf. Sci. **6**, 1 (1967).

[9]G. Huff and I. Dash, J. Low Temp. Phys. **24**, 155 (1976).

[10]A. Novaco, Phys. Rev. B **15**, 5217 (1977).

[11]R. Cuyer, Phys. Rev. Lett. **39**, 1091 (1977).