Structure of vacancies in solid He³

A F Andreev

Institute of Physics Problems, USSR Academy of Sciences (Submitted November 2, 1976)
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It is shown that a macroscopic ferromagnetic region, in which the nuclear spins of the atoms are fully polarized, should be produced around a vacancy in an He³ crystal.

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The behavior of vacancies in He³ crystals has substantial singularities connected with the presence of nuclear spins in the He³ atoms. ^[1-3] If all the nuclear spins are parallel, then the crystal is ideally periodic and, owing to the quantum-tunneling effect, the vacancy is transformed into a quasiparticle with energy band width $\Delta \sim 10\,^{\circ}\text{K}$. The minimum possible vacancy energy ϵ_0 corresponding to the bottom of the band is lower than the energy of the localized vacancy by an amount on the order of Δ . Actually, however, the nuclear spins are disordered down to temperatures on the order of the exchange interaction $J \sim 10^{-3}\,^{\circ}\text{K}$, so that the crystal is not periodic. The energy of the vacancy is practically always higher than ϵ_0 in this case^[3,4] by an amount on the order of Δ . Thus, ^[3] the polarization of the nuclear spins can be accompanied by an appreciable decrease of the vacancy energy.

The resultant situation is analogous in many respects to the known problems of the behavior of the electron in liquid helium^[5] or of "fluctuons" in solids. ^[6,7] It is easily seen that each vacancy should produce in the crystal a macroscopic region in which the nuclear spins are polarized, as a result of which quantum delocalization of the vacancies takes place in this entire region.

Let the crystal temperature T satisfy the condition $J \ll T \ll \Delta$. In this case the principal role is played by the vacancy-energy region near the bottom of the band, where the energy spectrum is quadratic, $\epsilon(p) = \epsilon_0 + p^2/2M$. Here p is the quasimomentum, M is the effective mass of the vacancy and is of the order of $\hbar^2/a^2\Delta$, and a is the interatomic distance. We assume that all the nuclear spins are polarized inside a sphere of radius R and disordered outside this sphere. Then the Hamiltonian of the vacancy within the sphere is equal to $\epsilon(p)$, and at the boundary of the sphere the wave function should be equal to zero, inasmuch as in the disordered state the vacancy has a rather large excess energy. The energy of the ground state of the vacancy is in this case equal to

$$E = \epsilon_{o} + \frac{\pi^2}{2} \frac{\hbar^2}{MR^2} . \tag{1}$$

The radius R of the ferromagnetic sphere should be determined from the condition that the free energy of the system F = E - TS be minimal (S is the crystal-entropy change due to the ordering of the spins in the volume of the sphere). It is clear that $S = -N \ln 2$ where N is the number of He^3 atoms in the volume of the sphere. The free energy is equal to

$$F = \epsilon_0 + \frac{\pi^2}{2} \frac{\hbar^2}{MR^2} + \pi T \frac{4\pi}{3} R^3 \ln 2, \qquad (2)$$

where n is the number of He³ atoms per unit volume of the crystal. From the condition that this expression be a minimum, we obtain the radius of the sphere

$$R = \left(\frac{\pi\hbar^2}{4MnT\ln 2}\right)^{1/5} \tag{3}$$

The number of particles N in the volume of the sphere is of the order of $(\Delta/T)^{3/5}$, which is much larger than unity. The magnetic moment \mathcal{N} of the ferromagnetic regions lining the vacancy is thus equal to

$$\mathcal{M} = N\mu = \mu n \frac{4\pi}{3} \left(\frac{\pi}{4 \ln 2} \frac{\hbar^2}{M_B T} \right)^{3/5}$$
,

where μ is the magnetic moment of the He³ nucleus. The temperature dependence of the equilibrium number of vacancies N_v in the crystal is determined by the expression $\exp(-F/T)$, where F is obtained by substituting (3) in formula (2). We have

$$N_{v} \sim \exp \left\{ -\frac{\epsilon_{o}}{T} - \frac{5}{6} \left(\frac{\pi^{2} \hbar^{2}}{M} \right)^{3/5} (4\pi n \ln 2)^{2/5} T^{-3/5} \right\},\,$$

which differs substantially from the ordinary simple exponential relation of the type $\exp(-\cos t/T)$.

The discussed effect should therefore manifest itself experimentally in all phenomena determined by vacancies (mobilities of the charges and impurities, heat capacity, direct measurement of the number of vacancies with the aid of x rays). The large ferromagnetic moment of the vacancy should, of course, greatly influence also the magnetic properties of He^3 crystals.

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