# Vacancy mobility in crystalline $He^3$

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The temperature dependence is determined for the diffusion coefficient of a vacancy captured in $He^3$ by a region of ferromagnetically ordered spins.

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Vacancies that are delocalized at low temperatures in crystalline $He^3$ give rise to indirect exchange, since the circuiting of the vacancy around a closed path is equivalent to a permutation of atoms, and consequently, an important role in the calculation of the energy is played by the symmetry of the wave function, i.e., its dependence on the spins. Actually the direct exchange in $He^3$ is extremely small, $J \sim 10^{-3}$ K, whereas the vacancy mobility is quite large. According to various estimates, the corresponding width of the band is $\Delta \sim 10$ K, so that there exists a temperature region where direct exchange can be neglected.

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This problem, which reduces to a degenerate Hubbard model, was first considered in[1], where it was shown that for bcc and simple cubic lattices the holes lead to polarization of the particles, so that the ground state is a ferromagnetic state. For hcp and fcc lattices, the ground state is antiferromagnetic. Application of this model to crystalline $He^3$ was considered in[2-4].

Andreev[4] considered a spin structure of the fluctuon type[5] near a vacancy in bcc $He^3$, in the limit when $J \ll T \ll \Delta$.

In the present article we estimate the mobility of such a formation.

The spin structure near the vacancy can be obtained from the free-energy functional,[5] which takes in the present case the form

$$F = \int \{ (\Delta a^2/2) |\nabla\psi|^2 + U(|\psi|^2, n_{\mathbf{k}}) - TS(|\psi|^2, n_{\mathbf{k}}) \} d^3r. \tag{1}$$

The first two terms represent here respectively the kinetic energy of the vacancy localized in the region of the ordered spins ($a$ is the lattice constant), and the interaction energy of the spins and vacancies, which is proportional to the energy density of the spin waves. The last term gives the entropy of the system. We shall use the spin-wave approximation, introducing the local density $n_k(r)$ of the number of spin waves ($\mathbf{k}$ is the spin-wave momentum).

The interaction and the energy of the spin waves will be determined by an indirect method, in which we take into account the effective direct exchange with a constant $J_{eff} \sim \Delta a^3 |\psi|^2$ ($a^3|\psi|^2$ is the local concentration of the vacancies). This approach is valid when the number of spin waves is small.[1]

Analysis of the corresponding Euler-Lagrange equations leads to the following form of $\psi$:

$$\psi = R^{-1/2} r^{-1} \sin(\pi r/R) \qquad r < R - \delta R,$$

$$\frac{d\psi}{dr} \approx -\frac{1}{a}\sqrt{\frac{U(\psi) - U(0)}{\Delta} - \frac{E}{\Delta}\psi^2}, \quad r > R - \delta R,$$

$$E \sim \Delta (T/\Delta)^{2/5} \quad R \sim a(T/\Delta)^{1/5} \quad \delta R \sim a(T/\Delta)^{2/25}. \tag{2}$$

Of greatest importance for us is that the derivative remains continuous on going from the first region, where the spins are fully ordered, into the second region, so that even at $J_{eff} \sim T$, we have $d\psi/dr \sim \psi(0)/R$, and only later, after the number of the flipped spins is saturated, it assumes an exponential behavior. Formulas (2) agree with the results of[4].

The mobility of such a formation is determined by the transport of the flipped spins through the ordered region, since the absence of direct exchange forbids transport outside the fluctuons. Considering the motion of the fluctuon "center" $\rho = (\int M^z \mathbf{r} d^3r)(\int M^z d^3r)^{-1}$, where $M^z(\mathbf{r})$ is the spin density, we easily obtain a formula of the Kubo type for the diffusion coefficient of the fluctuon

$$D = \frac{\int \langle j_x^z(t, \mathbf{r}) j_x^z(0, \mathbf{r}') \rangle dt\, d^3r\, d^3r'}{(\int M^z d^3r)^2}. \tag{3}$$

The quantity in the angle brackets denotes the correlator of the spin current $j_x^z$ which transports $M^z$ in the $x$ direction. The determination of the diffusion coefficient by this formula is a rather complicated task because of the inhomogeneity of the structure and the need for considering a region with a large concentration of flipped spins.

Spin waves with orbital number $l \sim 1$ and $\varepsilon \sim T$ propagate freely inside the fluctuon, and their reciprocal wavelength is $k \sim 1/R$ (see[6]). On the other hand, waves with $l \gg 1$ and $\varepsilon \sim T$, are concentrated in a "crust" with thickness on the order of $a$, where the effective exchange integral is $J_{eff} \sim T$, and determine the dissipative processes.

To estimate the diffusion coefficient, we use a simpler method of calculating the mobility and the corresponding energy dissipation.[5]

If the fluctuon moves as a unit with low velocity $v$, then a resistance force is produced together with an energy dissipation $Q = \eta v^2$ ($\eta$ is the mobility). Calculating the energy dissipation we obtain

$$Q = -T \int \frac{\delta^2 6}{\delta n_{\mathbf{k}}^2} \delta n_{\mathbf{k}} (\mathbf{v}\vec{\nabla}) n_{\mathbf{k}} \, d^3k \, d^3r$$

if we use the approximation of spin-wave gas [$6(n_k)$ is the entropy of the ideal gas]. The main contribution to this integral is made by the "crust" region with large density of flipped spins, where the thermal pulse of the waves is $k_T \sim 1/a$. In order of magnitude, the change of the distribution function as the result of the motion is $\delta_{n_{\mathbf{k}}} \sim \tau(\mathbf{v} \cdot \nabla) n_{\mathbf{k}}$, where $\tau \sim T^{-1}$ is the characteristic relaxation time in the "crust." Estimating from formulas (3) the value of $dn_{\mathbf{k}}/dr$ and taking into account the volume $R^2 a$ of the "crust" we obtain, using the Einstein relation

$$D = T/\eta \sim (k T a^2/\hbar)(T/\Delta)^{2/5} \tag{4}$$

This result, according to formula (3), corresponds to currents in the "crust" of the fluctuon, where $\langle jj \rangle \sim T^2 a^{-4}$, with a correlation time $T^{-1}$ and a correlation radius of the order of $R$. The large correlation radius is due to the fact that during the time $T^{-1}$ the fluctuations manage to exchange spin waves that penetrate through the thickness of the fluctuon. Actually, we make no essential use of the spin-wave model, and it is to be hoped that the result (4) is independent of this model in order of magnitude.

Thus, the diffusion coefficient turns out to be large in comparison with the value ($a^2 J$) determined by direct exchange in a region of not too low temperatures, and small in comparison with the corresponding value ($\Delta a^2$) determined from the hopping probability of the vacancy itself. An appreciable decrease in the velocity of the vacancies captured by fluctuons should diminish their role in the transport of extraneous particles, such as ions.

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