Vacancy Formation Energy in Solid ^{3}He: NMR Studies

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Introduction

Following the discovery of a giant quantum plasticity in solid ^{4}He [1], there is renewed interest in understanding the fundamental crystal properties of other quantum solids, and notably solid ^{3}He which has a larger zero point kinetic energy than solid ^{4}He and for which quantum effects are more pronounced. Vacancy motion in solid ^{3}He has been studied by NMR experiments elsewhere [2,3] and those experiments have shown that the vacancy-atom tunneling frequency is very high, typically $\omega_V \sim (1-4)10^{10}$ s^{-1} [4].The vacancies are therefore delocalized and form an energy band with a width $\Delta = 4\sqrt{(z-1)}\hbar\omega_V$ [3] of the order of a few K centered at the vacancy formation energy Φ_F. The formation energies as measured by x-ray studies range from 1 to 14 K, and are a strong function of the density of the solid. This observation raises fundamental questions about the ground state of solid ^{3}He, because the bandwidth of the vacancies $z\omega_V$ becomes comparable to the formation energy and if the gap closes. the ground state would be renormalized to result in a finite number of ground state vacancies, i.e. the number of atoms would be less than the number of lattice sites.

Results and Discussion

One of the difficulties in interpreting the experimental data has been the apparent difference in formation energies as reported by x-ray measurements [5] and by NMR measurements [3]. It is believed that this difference is due to the difference in the theoretical analyses of the different sets of experiments, and in particular in the expressions used for the density of states for the vacancies which is critical for estimating the vacancy formation energy. The NMR analyses start with a formation energy Φ_F and the calculated bandwidth Δ. The number of vacancies at temperature *T*, following Guyer [6], is given by $x_V = (3T/\pi\Delta)\exp[-(\Phi_F - \Delta/2)/T]$ where Φ_F and Δ are expressed in Kelvin. On the other hand the best fit to the thermodynamic data is given by a density of states $\rho(E) = \frac{1}{2}\Phi_B^{-1/3}(E-\Phi_B)^2$ [7] where Φ_B is the lowest energy of the vacancy band. The number of vacancies in this case is given by $x_V = (\frac{T}{\Phi_B})^3\exp[-\Phi_B/T]$. The NMR analyses report Φ_F , the true formation energy, whereas the typical exponential slope of both the NMR data and the x-ray data is given by Φ_B which is reported by the analyses of the x-ray data. We have reanalyzed the NMR data in terms of the lowest vacancy energy at the bottom of the vacancy band and as shown in Fig. 1 find that there is strong agreement with the x-ray data.

Conclusions

Careful analyses of the NMR and x-ray data for the quantum diffusion of vacancies in solid ^{3}He show that there is a sharp decrease of the vacancy formation energy near V_m=24.8 cm^3/mole close to the melting curve at low temperatures.

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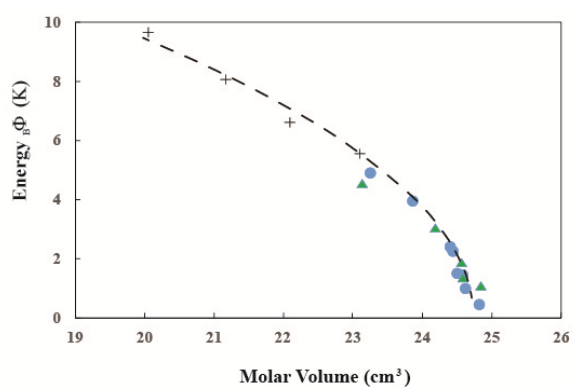

Fig.1 Variation of the vacancy formation energy in solid 3He as a function of molar volume. Plusses, NMR at high density; circles, NMR at low density (high V_m); triangles, x-ray data.

References

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