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MOMENTUM DISTRIBUTIONS IN hcp, bcc, AND LIQUID ⁴HE

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MOMENTUM DISTRIBUTIONS IN hcp, bcc, AND LIQUID ⁴HE

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Using Deep Inelastic Neutron Scattering we have measured the nuclear momentum distribution in hcp, bcc and liquid ⁴He at constant density over a temperature range 0.96K < T < 4.0K. We find no temperature dependence of the momentum distribution in the hcp solid or the liquid. We also find no difference between the hcp, bcc and liquid phases. The average kinetic energy per atom is lower than the best present theories predict.

The development of spallation neutron sources has recently provided enough flux at high energies to make it possible now to measure directly nuclear momentum distributions in some of the more weakly bound systems.(1) Some of the most interesting systems that can be studied, due to their quantum nature, are the solid heliums. They have a very rich phase diagram and small changes in pressure and temperature are sufficient to cause transitions between many different solid and liquid phases.

In ⁴He, the bcc phase exists only in a narrow region between the hcp and liquid phases. The bcc phase is very small(2), being only 50 mK wide in temperature and .07 MPa wide in pressure at its widest. This allows the unique opportunity to measure the hcp and bcc solids and the normal liquid at nearly constant external conditions (P,V,T). In fact, by proper choice of the starting point we may hold the density constant and change phases by varying the temperature by a small amount.

At present, the best calculations of the momentum distributions are obtained from Green's Function Monte Carlo techniques. These calculations(3) indicate that the momentum distribution is Gaussian in both the solid and liquid. Calculations on both fcc and hcp lattices show no differences due to the lattice types and indicate that the momentum distribution is isotropic in both cases. We will later compare our results to these calculations.

To directly measure the nuclear momentum distribution using neutron scattering we must obtain large enough momentum transfer, Q, so that we observe only incoherent single particle scattering from the N isolated atoms of mass M in the sample. In this case the dynamic structure factor is(4)

$$S(Q,E) = \int n(\vec{p}) \delta(E - \frac{\hbar^2 Q^2}{2M} - \frac{\hbar \vec{Q} \cdot \vec{p}}{M}) d^3 \vec{p} \quad (1)$$

where $n(\vec{p})$ is the momentum distribution of the scatterers and the δ -function conserves energy and momentum in the collision. The scattering peak will be centered about an energy transfer

$$E_r = \frac{\hbar^2 Q^2}{2M} \quad (2)$$

known as the recoil energy.

An isotropic Gaussian momentum distribution has the form

$$n(\vec{p}) = C \exp(-p^2/\hbar^2 A) \quad (3)$$

where A characterizes the width of the momentum distribution. Using the impulse approximation leads to the dynamic structure factor

$$S(Q,E) = C' \exp\left[-\frac{(E - E_r)^2}{\hbar^4 Q^2 A/M^2}\right] \quad (4)$$

which is itself a Gaussian of variance

$$\sigma^2 = \frac{\hbar^4 Q^2 A}{2M^2} \quad (5)$$

The impulse approximation, eq. 1, makes predictions of the variation of recoil energy, E_r , and width, σ_Q , with Q that are confirmed by our results.

Our measurements were carried out on the Low Resolution Medium Energy Chopper Spectrometer (LRMECS) at the Intense Pulsed Neutron Source at Argonne National Laboratory. An incident energy of 498 meV was used. This gives useful momentum transfers ranging from 5 \AA^{-1} to 23 \AA^{-1} when collected for scattering angles ranging from 30°

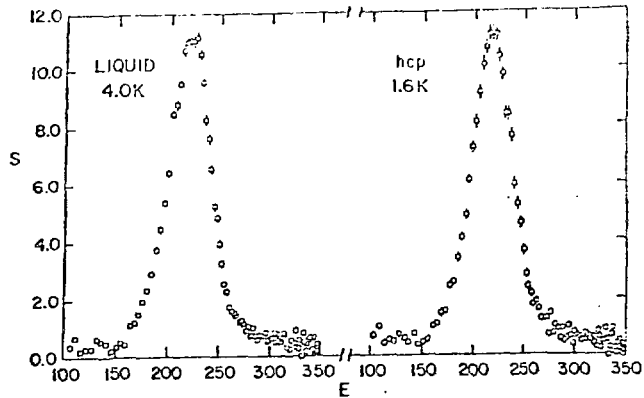


Figure 1. Dynamic structure factor for liquid and solid ${}^4\text{He}$ at $\phi = 96.9^\circ$

to 120° . The He sample was contained in an aluminum cylinder 1.25 cm ID x 10 cm long with a 0.3 cm wall thickness which was attached to a ${}^3\text{He}$ refrigerator.

The ${}^4\text{He}$ sample on which these measurements were made was held at a constant molar volume of $21.7 \text{ cm}^3/\text{mole}$. The hcp-bcc transition was at 1.72 K. Data were collected at 0.96 K (hcp), 1.60 K (hcp), 1.70 K (bcc), 1.80 K (liquid) and 4.00 K (liquid). In situ diffraction measurement made at 1.70 K to ensure that the sample was in the bcc phase. The measured dynamic structure at 1.60 K and 4.00 K is shown in figure 1. Gaussian fits of these results confirm what is obvious in the figure. The scattering at 1.6 K and 4.0 K is nearly identical. Intercomparison of all data sets indicates within present statistics and resolution, there is no dependence of the nuclear momentum distribution on either temperature or phase of the isochoric sample.

The absence of temperature dependence in both the liquid and the hcp solid indicates that the measurements sampled essentially ground state momentum distributions. In this case we can compare our results to the GFMC theories for both the liquid and solid. The kinetic energy per atom is given by

$$KE = \frac{3\hbar^2}{4M} A \quad (6)$$

Our measurements give a value of $KE = 19.5 \text{ K}$, while the GFMC results (3) were 23.4 K and 22.4 K, for the solid and liquid respectively.

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REFERENCES

- (1) For a review see the proceedings of the Los Alamos conference on "High Energy Excitations in Condensed Matter" to be published.
- (2) E. R. Gully, *J. Low Temp. Physics* **11**, 33 (1973); E. R. Gully and R. L. Mills, *Annals of Physics* **8**, 1 (1959).
- (3) P. A. Whitlock, D. M. Ceperly, C. V. Chester, and M. H. Kalos, *Phys. Rev.* **B19**, 5598 (1979).
- (4) P. C. Hohenberg and P. M. Platzman, *Phys. Rev.* **152**, 198 (1966).