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ANHARMONIC PHONONS AND LATTICE SPECIFIC HEAT IN bcc ^{3}He

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The phonon spectrum of bcc ^{3}He has been calculated including the leading anharmonic corrections to the self-consistent harmonic approximation. For small wave vectors an anomalous dispersion is found causing a maximum in $\Theta_D(T)$ in agreement with experiments.

Heat-capacity,[1,2] strain-gauge,[3] and thermal-conductivity[4] measurements indicate that $\Theta_D(T)$ for ^{3}He increases for $T \leq 0.5$ K, goes through a maximum, and shows the usual decrease only for $T > 0.5$ K. Varma[5] suggested that this anomaly might be the result of a T^{-2} contribution to C_v caused by a phonon-induced four-spin interaction. In Ref. 3, however, any such contribution was subtracted but the anomaly persisted, indicating that it might be due to the lattice only.[6]

We have calculated the phonon spectrum of bcc ^{3}He, including the leading correction[7] to the self-consistent harmonic approximation.[8] This term is almost identical to the expression, quadratic in the third-order coupling parameters, known from standard anharmonic perturbation theory. Only the third-order coupling parameters are replaced by the third derivatives of the averaged potential,

$$\langle V(R^i)\rangle = (|\det\tau^i|/\pi^3)^{1/2}\int d^3r\, V(r) \times \exp[-\textstyle\sum_{\alpha\beta}\tau_{\alpha\beta}{}^i(r_\alpha - R_\alpha{}^i)(r_\beta - R_\beta{}^i)], \quad (1)$$

where the tensor τ^i is the inverse of the static displacement correlation function.

Since Eq. (1) diverges for a Lennard-Jones interaction we have replaced $V(r)$ by a Brueckner scattering matrix.[9] This procedure is debatable since certain correlations are counted twice, but it should be reliable enough for the present

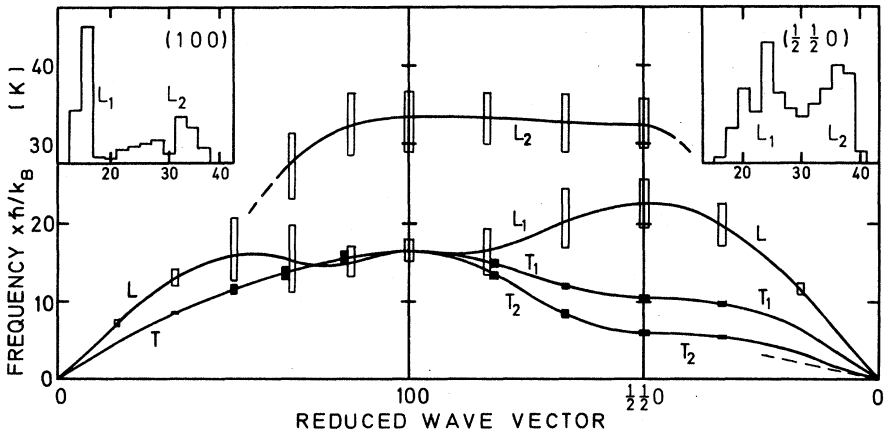

FIG. 1. Anharmonic phonon spectrum for bcc ^{3}He at 24 cm^3/mole. The bars indicate the width. Dashed line denotes sound velocity for lowest transverse branch. Inserts show two longitudinal-phonon lines at the zone boundary.

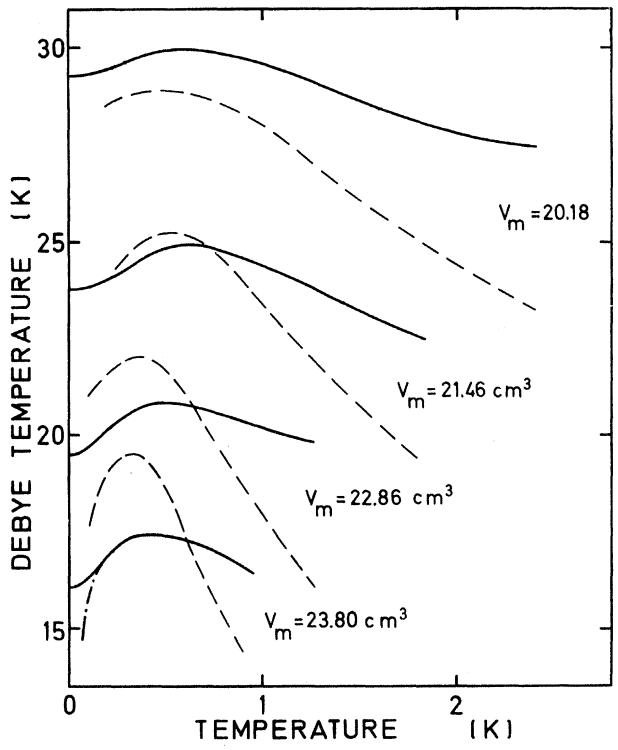

FIG. 2. Debye temperature for bcc ^{3}He. Solid curve, theory; dashed curve, Ref. 2. At the theoretical curve for 23.8 cm^3/mole the spin contribution is indicated. At higher densities it is considerably smaller.

purpose. Numerical solutions were found for a crystal of 432 particles[10] at four densities.

To calculate τ^i and for the intermediate propagators the anharmonic phonons were used self-consistently. Figure 1 shows the dispersion curves in two principal directions. In contrast to an earlier similar calculation,[11] all sound velocities are real at all densities. This is due to the fact that in Glyde and Cowley[11] τ^i was replaced by a scalar. We find, also in disagreement with Ref. 11, that the phonons are well defined only for $\hbar\omega/k_B \leq 15$ K. Above 15 K the phonon lines are rather broad, and sometimes two peaks appear.

For small wave vectors an anomalous dispersion is found, i.e., the sound velocity increases with decreasing wavelength. This is most pronounced in the (110) direction. (We also find a remarkable anisotropy.) This anomalous dispersion causes an increasing $\Theta_D(T)$ in exactly the same way as the normal dispersion causes the usual decrease at higher temperatures. Since our calculation also shows a normal dispersion at higher frequencies, a maximum in $\Theta_D(T)$ is expected. To calculate $\Theta_D(T)$, we have neglected the damping and have used the standard expression known for the specific heat of noninteracting excitations. The resulting $\Theta_D(T)$ actually shows in Fig. 2 a maximum at a position and of a magnitude consistent with experiments.[1,2] The discrepancies at temperatures above the maximum are probably due to lifetime effects or to the formation of defects.[1,2]

In the hcp phase at higher densities, anharmonicities are less important and probably not strong enough to overcome the normal dispersion. No anomaly in $\Theta_D(T)$ is therefore expected for hcp ^{3}He or ^{4}He.

Dispersion curves for bcc ^{4}He showing an even larger anisotropy and anomalous dispersion will be published elsewhere, together with details of the present calculation.

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