

COMMENTS AND ADDENDA

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Lattice Dynamics of He³ and He⁴ at High Pressures*G. G. Chell, V. V. Goldman, M. L. Klein,[†] and G. K. Horton

Department of Physics, Rutgers University, New Brunswick, New Jersey 08903

(Received 8 July 1969)

In a recent paper with a similar title, Morley and Kliewer (MK) have calculated phonon energies of He³ and He⁴ in the lowest-order self-consistent approximation. Using a fcc model, we have estimated the leading correction to MK's phonon energies. This correction is found to be substantial and of the correct sign and magnitude required to remove the discrepancy between MK Debye temperatures and the experimental values.

In a paper with a similar title, Morley and Kliewer¹ (MK) used Koehler's² formulation of the lowest-order self-consistent theory to calculate phonon spectra of hcp He³ and He⁴. The calculations were carried out at volumes of 10, 12, 14, and 16 cm³ mole⁻¹, and short-range correlations were ignored. From the dispersion law, detailed frequency spectra were constructed, and Debye temperatures obtained. The locations of critical points were also listed in detail. MK found a large disagreement between theoretical and experimental Debye temperatures. In this comment we estimate the contribution of the leading correction to the lowest-order self-consistent phonon theory.

We³ have recently introduced an improved self-consistent approximation (based on a simplified version of Choquard's⁴ formulation of lattice dynamics) which we applied to certain properties of fcc noble-gas solids. Koehler⁵ carried out a similar approximation in the calculations of phonon energies of Ne. One of the main conclusions of this work was that cubic anharmonic terms should not be ignored in any meaningful calculation. We have independently⁶ calculated phonon energies of fcc noble-gas crystals, and our results will be published elsewhere. In order to estimate the corrections to be expected to the phonon energies found by Morley and Kliewer, we

have calculated the contribution from cubic anharmonic terms at the 10 cm³ mole⁻¹ volume. At this volume the omission of short-range correlations is realistic. We can justify this statement by looking at the radial integrands in the second- and third-order self-consistent force constants. If there is a region, well into the hard core, in which the integrand vanishes, then the integrals, and so the force constants, are independent of the cutoff chosen. MK (Fig. 2 of their paper) have shown that such a region exists for the self-consistent second-order force constants and we have verified a similar result for the third-order force constants (at 10 cm³/mole). We thus have a compelling argument for the omission of short-range correlations in solid He at 10 cm³/mole. For the purpose of this Comment we have followed Cowley⁷ and Koehler⁵ and identified the physical phonon energy Ω as

$$\Omega^2(qj) = \omega_{sc}^2(qj) - 2\omega_{sc}(qj)\Delta(\Omega qj),$$

where Δ contains the effect of the cubic anharmonic terms. Phonon energies obtained from this formula with $\Delta = 0$ provide an upper bound. It is probable that if Δ contains only cubic terms, the phonon energies so obtained are a lower estimate. We have obtained numerical results for a fcc structure, using the same interatomic potential as Morley and Kliewer. We believe that the salient

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features of our results will carry over to a hcp calculation (see Ref. 8). Selected but typical values of $[\omega_{sc}(qj) - \Omega(qj)]/\omega(qj)$ are shown in Table I.

It is clear that corrections to the lowest-order self-consistent phonon energies are substantial. Furthermore, they are of the correct sign and magnitude required to remove the discrepancies between theory and experiment in the Debye temperatures shown in Fig. 11 of Morley and Kliewer.

Our results are compatible with Horner's estimate⁹ of cubic anharmonic effects in Debye temperatures of bcc He³.

We must conclude that the results of Morley and Kliewer for the phonon energies of He³ and He⁴

TABLE I. Phonon energy changes for fcc helium at 10 cm³ mole⁻¹ (lattice constant $a=4.0497$ Å).

$\frac{2\pi}{a}$	q	j	He ⁴	He ³
			$(\omega - \Omega)/\omega$	$(\omega - \Omega)/\omega$
$\frac{2\pi}{a}$	(0, 0, 0.5)	L	0.36	0.40
		T	0.36	0.41
$\frac{2\pi}{a}$	(0, 0, 1.0)	L	0.27	0.28
		T	0.28	0.31

probably require substantial correction, even at 10 cm³/mole.

*We thank the U. S. Air Force Office of Scientific Research for supporting this work under Grant No. AFSOR 1372-68.

†Permanent address: Division of Pure Chemistry, National Research Council, Ottawa 2, Canada.

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