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COMMENTS AND ADDENDA

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Lattice Dynamics of He^3 and He^4 at High Pressures*

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In a recent paper with a similar title, Morley and Kliewer (MK) have calculated phonon energies of He^3 and He^4 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 Kliewer[1] (MK) used Koehler's[2] formulation of the lowest-order self-consistent theory to calculated phonon spectra of hcp He^3 and He^4. The calculations were carried out at volumes of 10, 12, 14, and 16 cm^3 $mole^{-1}$, 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.

We[3] have recently introduced an improved self-consistent approximation (based on a simplified version of Choquard's[4] formulation of lattice dynamics) which we applied to certain properties of fcc noble-gas solids. Koehler[5] 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 independently[6] 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 cm^3 $mole^{-1}$ 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 10cm^3/mole). We thus have a compelling argument for the omission of short-range correlations in solid He at 10 cm^3/mole. For the purpose of this Comment we have followed Cowley[7] and Koehler[5] and identified the physical phonon energy Ω as

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

wnere 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 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 estimate[9] of cubic anharmonic effects in Debye temperatures of bcc He^3.

We must conclude that the results of Morley and Kliewer for the phonon energies of He^3 and He^4 probably require substantial correction, even at 10 cm^3/mole.

TABLE I. Phonon energy changes for fcc helium at 10 cm^3 $mole^{-1}$ (lattice constant $a = 4.0497$ Å).

	q	j	He^4 $(\omega - \Omega)/\omega$	He^3 $(\omega - \Omega)/\omega$
$\frac{2\pi}{a}$	(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

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Compton Profile of LiH

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Self-consistent electron wave functions were calculated previously for the LiH crystal in the cell approximation in connection with a study of positron annihilation in diatomic crystals. The Compton profile of LiH derived from these wave functions is compared with recent measurements. It is concluded that the self-consistent cell approximation to the electronic structure in LiH accounts for the principal features of the x-ray structure factors, the Compton profile, and the positron annihilation spectra.

In a previous paper,[1] the angular correlation between the photons created by positron-electron pairs annihilating in a lattice with a basis was derived in various approximations. The results were applied to LiH. Self-consistent electron wave functions with exchange were calculated. The x-ray structure factors of LiH based on these wave functions agree with experiment.[2] The positron wave function was calculated in the same approximation after appropriate changes in the crystal potential, which amount to omitting the exchange and pseudopotentials. The resulting characteristics of positron annihilation in LiH agree with the momentum distribution of the annihilating positron-electron pairs as deduced from angular-correlation measurements[3] and with positron-lifetime measurements.[4]

A further test of the theory is the prediction of the Compton profile. It is equal to the angular correlation of the γ quanta emitted in the positron-annihilation process in the approximation of a plane positron wave function. We have deduced this