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

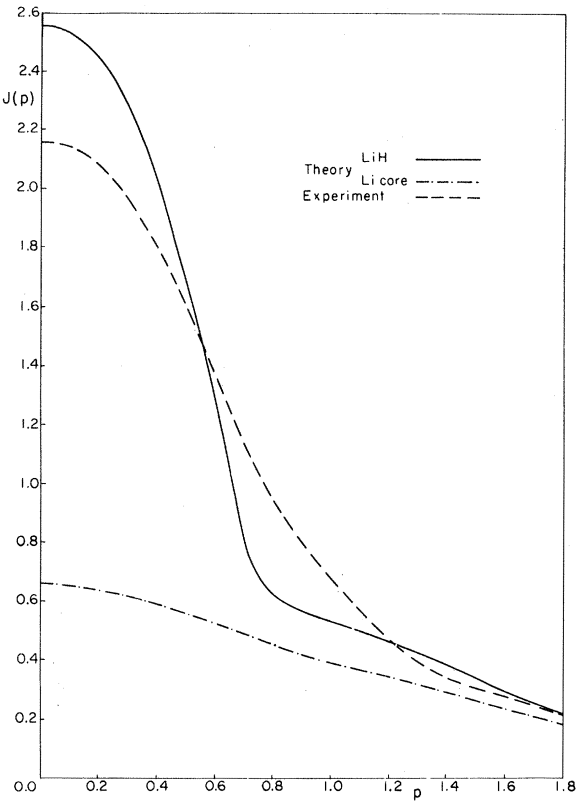

FIG. 1. Compton profile, Eq. (1), of LiH normalized to four electrons per unit cell. Experimental curve is taken from Ref. 5.

profile from the electron wave functions calculated earlier. Figure 1 shows the function

$$J(p)=\int_p^\infty D(p_1)p_1^{-1}\,dp_1\,, \tag{1}$$

where $D(p)$ is the momentum distribution of the electrons,

$$D(p)=\int d\Omega p^2\rho(\vec{p})\,. \tag{2}$$

Ω is the solid angle for p and

$$\rho(\vec{p})=\sum_{j=1}^{N}\left|\int_{\text{crystal}}\psi_-(\vec{x}_1,\ldots,\vec{x}_j,\ \ldots,\vec{x}_N)\,e^{i\vec{p}\cdot\vec{x}_j}\times d^3x_1\cdots d^3x_j\cdots d^3x_N\right|^2 \tag{3}$$

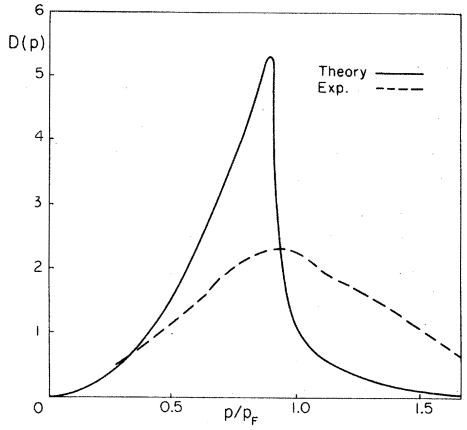

FIG. 2. Momentum distribution, Eq. (2), of the two valence electrons in the unit cell of LiH. Experimental curve is taken from Ref. 5.

is the electron momentum density of the N electrons in the crystal. The theory is compared with the experimental curve of Phillips and Weiss.[5]

A more sensitive test of the theory is given in Fig. 2, where the momentum distribution $D(p)$ for the two valence electrons in the LiH unit cell is shown with the derivative of the experimental curve of $J(p)$, after subtraction of the core electron contribution, on a scale p/p_F, where $p_F=0.8$ a.u. is the Fermi momentum of two free valence electrons in the unit cell. $D(p)$ has a pronounced maximum at $p/p_F=0.88$. After a precipitous drop, it trails off and becomes small for $p/p_F>1$. The experimental peak, by comparison, is broadened, but it is centered accurately on the theoretical Compton edge located near $p/p_F=1$.

In conclusion, the self-consistent wave functions calculated earlier for LiH in the cell approximation contain the dominant characteristics of the electronic structure of this crystal as probed by the angular correlation in positron annihilations, the positron lifetime, the x-ray structure factors, and the Compton profile.

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