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The ground state energy, pressure and compressibility of solid ^3He at high pressures.

Abstract. The ground state energy, pressure and compressibility of solid ^3He were calculated in the molar volume range 12 to 18 cm³ using the improved selfconsistent phonon theory of Goldman *et al.* A soft core potential due to Beck was used and relatively good agreement was obtained with experiment for the pressure and compressibility.

In a recent paper (Chell 1970, to be referred to as I) we calculated the compressibility of solid ^3He and ^4He in the molar volume range 12 to 18 cm³. Selfconsistent phonon theory (SCP) was used and short range correlations (src) were omitted. A nearest neighbour interaction, face centred cubic model was used. We gave reasons for believing that for isotropic crystal properties this model reproduces the main features of a hexagonal close packed model. In this letter we wish to report on the extension of the calculations for solid ^3He .

First, instead of the Lennard-Jones (12-6) (L-J) potential a new potential, $\phi(r)$, due to Beck (1968) was used in the calculations where

$$\phi(r) = A \exp(-\alpha r - \beta r^6) - \frac{0.869}{(r^2 + a^2)^3} \left(1 + \frac{2.709 + a^2}{r^2 + a^2} \right)$$

with $\alpha = 0.675 \text{ \AA}^{-1}$, $a = 4.390 \text{ \AA}^{-1}$, $\beta = 3.746 \times 10^{-4} \text{ \AA}^{-6}$ and $A = 398.7 \text{ eV}$.

This potential has several advantages over the L-J potential. It has a nonsingular core at the origin which made accurate calculations possible over the complete molar volume range considered. The difficulties arising from the singular core in the L-J potential have been discussed in I.

The ground state energy of body centred cubic ^3He has been computed by Glyde (1971) using both the Beck and L-J potentials. The former gave a lower ground state energy than did the latter. Lastly, but not least, the Beck potential was fitted to experimental and theoretically determined potentials down to an internuclear separation of 0.5 Å and thus reproduces the repulsive part of the He-He potential more accurately than the L-J. Secondly, the calculations were extended to include all neighbour interactions, a necessary step if the ground state energy is to be determined accurately over the volume range considered. Thirdly, the leading second order correction, ΔF , to the first order SCP energy, F_{sc} , was included in the calculations using the improved selfconsistent approximation (ISC) introduced by Goldman *et al.* (1968). In this letter the notation and definitions of I and Goldman *et al.* (1968) are used wherever possible. We have

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The exact effective wave function ϕ_k is then used as a trial function in the variational formula (4). The two $T\{\}$ terms cancel each other and (4) becomes simply $E_X \leq \mathcal{E}_X$. $\mathcal{E}_X$ is first expressed in terms of $a_q(k)$ ($q \neq 0$), deleting third and higher order terms. The result is $E_X^0 + E_A + E_B$ with

$$E_A = -2\Omega \sum_{kk'}^{\text{occ}} \sum_q' a_q^*(k) a_q(k') \{v(k+k'+q) + v(k-k')\} \quad (8)$$

$$E_B = -2\Omega \sum_{kk'}^{\text{occ}} \sum_q' |a_q(k)|^2 \{v(k+k'+q) - v(k-k')\}.$$

The approximation (7) is then substituted in equation (8), the resulting expression being exact up to $O(\lambda^2)$. $\mathcal{E}_X$ then has the form (5), with the same E_X^0 . The inequality (4) (with $\psi_k \equiv \phi_k$) must be true for every value of λ and n_q/λ . We then get the important result

$$X(q) \leq X_I(q) \equiv -\frac{\pi_{AB}(q)}{\pi_0(q)^2} \quad (9)$$

with

$$\pi_{AB} = \pi_A + \pi_B$$

and

$$\begin{aligned} \pi_A &= \left[\frac{4m}{\hbar^2} \right]^2 \sum_{kk'}^{\text{occ}} \frac{v(k+k'+q) + v(k-k')}{(q^2 + 2q \cdot k)(q^2 + 2q \cdot k')} \\ \pi_B &= \left[\frac{4m}{\hbar^2} \right]^2 \sum_{kk'}^{\text{occ}} \frac{v(k+k'+q) - v(k-k')}{(q^2 + 2q \cdot k)^2} \end{aligned} \quad (10)$$

The integrals $\pi_{A,B}$ are identical to the two first order polarization graphs (exchange and self energy graphs). The numerical values of $\pi_{AB}(q)/\pi_{AB}(0)$ were given by Geldart and Taylor (1970) for $q \leq 2k_F$. Their method is used in I to obtain π_{AB} in the range $q > 2k_F$. The screening function π_I corresponding to X_I is identical to the expression proposed by Geldart and Taylor, who use first order perturbation theory, with an arbitrary interpolation procedure to include the effect of the higher HF graphs. This interpolation is done here in a natural way when solving the HFKS equations.

Another advantage of the present variational method is that it leads to the useful inequality (9). Bounds for $\epsilon(q)$ and $\tilde{\epsilon}(q)$ follow from the exact formulas (1) and (2)

$$\epsilon(q) \geq \epsilon_I(q) \quad (11)$$

$$\tilde{\epsilon}(q) < \tilde{\epsilon}_I(q) \quad (12)$$

where ϵ_I and $\tilde{\epsilon}_I$ are given in terms of X_I by the same formulas.

The behaviour of $X_I(q)$ is established in I. $X_I(<0)$ is exact when $q \rightarrow 0$ and $q \rightarrow \infty$, and presents a sharp minimum for $q \sim 1.9 k_F$. The exact $X(q)$ has necessarily the same behaviour, in qualitative disagreement with the approximations proposed by Hubbard (1957), Kleinman (1967) and many other authors. The very interesting method of Singwi *et al.* (1968), also used by Shaw (1970), leads to an incorrect behaviour in the range $q < 2k_F$, when applied in the HF framework (formula (22) of Singwi *et al.*). Herman *et al.* (1969) introduced an inhomogeneity correction to V_{XKS} in a semiempirical way. It is shown in I that the corresponding effective exchange interaction is in qualitative agreement with our results in the range $q < 2k_F$ but is quite wrong, of course, when $q \geq 2k_F$, which is a quite significant range in solid state calculations.