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Theory of the Compressibility of Solid He^4 and He^3 at 0°K*

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A quantum mechanical variational method is used to calculate several properties of a close-packed lattice phase of solid He^4 and He^3 at 0°K. The method consists in expressing the expectation value of the interatomic potential energy, with respect to a Heitler-London trial wave function, as a series of powers of the mean square deviation of an atom from its lattice site. Due to the small mass of a helium atom this mean square deviation is relatively large and the series converges slowly. Three sets of numerical results are obtained by truncating the series after the first, second, and third term, respectively. A comparison of these results with the experimental data shows that the final results, i.e., after minimizing $\langle H\rangle$ with respect to the variational parameter, converge much faster than the expectation value series itself. The results include values for: cohesive energy, sound velocity, compressibility, Debye temperature, and Grüneisen constant. The calculations are repeated for a body-centered cubic lattice, and no indication of a crystallographic phase transition is found.

I. INTRODUCTION

IT should be possible to derive the properties of the gaseous, liquid, and solid phases of either helium isotope from the solutions of a Schrödinger equation:

$$(H/\epsilon)\Psi\equiv\left[-\lambda^2\sum_{i=1}^{N}\nabla_i^2+\tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}v(x_{ij})\right]\Psi=(E/\epsilon)\Psi, \quad (1)$$

where $v(x_{ij})\equiv V(r_{ij}/\sigma)/\epsilon$ is a given two-body interatomic potential, $\lambda^2\equiv\hbar^2/2M\epsilon\sigma^2$, ϵ and σ are energy and length scale factors, M is the mass of a helium atom, and ∇_i^2 is the Laplacian with respect to $\mathbf{x}_i\equiv\mathbf{r}_i/\sigma$. In the present paper we restrict the discussion to a 12-6 Mie-Lennard-Jones potential, i.e.,

$$v(x_{ij})=4(x_{ij}^{-12}-x_{ij}^{-6}). \quad (2)$$

Properties such as superfluidity[1] of liquid He^4 and nuclear magnetic susceptibility of liquid[2] or solid[3] He^3 depend in a crucial way on the required symmetry or antisymmetry of the wave function Ψ. On the other hand, at least in the solid phases, the appropriate exchange integrals are small compared to the cohesive energy[3] even at low (~30 atm) pressures, and hence we can expect that an unsymmetrized wave function will provide a good description of cohesive properties of the solid phases, especially at not too low pressures. This fact is gratifying since the first difficulty in obtaining approximate solutions of Eq. (1), on basis of an independent-particle model, is connected with the strong singularity of the interatomic potential $v(x_{ij})$ at the origin. The easiest way to remove this difficulty is to use single-particle trial wave functions localized about lattice sites, i.e., Heitler-London orbitals, which do not overlap.[4,5] However, such orbitals have zero-exchange integrals and consequently they cannot be used to discuss effects which depend on nuclear wave function symmetry. Another difficulty in solving Eq. (1) (by any method of approximation, independent-particle model or not) comes from the large value of λ for helium [$\lambda(He^4)=0.302$, $\lambda(He^3)=0.347$]. Such large values of λ imply a large zero-point kinetic energy, and lead to the following consequences. (a) The two atom equation [$N=2$ in Eq. (1)] has no negative eigenvalue,[6] i.e., a diatomic helium molecule is not stable, in contrast to the heavier inert gases.[6] (b) Even though the lowest

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* Contribution No. 913. Work was performed in the Ames Laboratory of the U. S. Atomic Energy Commission.

[1] N. Bogoliubov, J. Phys. (U.S.S.R.) **11**, 23 (1947).

[2] A. A. Abrikosov and I. M. Khalatnikov, *Reports on Progress in Physics* (The Physical Society, London, 1959), Vol. 22, p. 329.

[3] N. Bernardes and H. Primakoff, Phys. Rev. **119**, 968 (1960).

[4] N. Bernardes, Phys. Rev. **112**, 1534 (1958), and Nuovo cimento **11**, 628 (1959).

[5] N. Bernardes, Phys. Rev. **120**, 807 (1960).

[6] N. Bernardes and H. Primakoff, J. Chem. Phys. **30**, 691 (1959).

state of the many-atom problem ($N\gg 1$) in Eq. (1) has a negative eigenvalue, this ground state corresponds to a liquid rather than to a solid (liquid He^3 and He^4 do not solidify unless under a pressure of at least 30 atm) again in contrast to the heavier inert gases which solidify without any external pressure.

For small values of λ approximate solutions of Eq. (1) can be obtained rather easily,[4,5] and the ground-state (cohesive) energy per atom can be expressed as a sum of three terms: (1) a classical potential energy E_{st} determined by the average positions of all the atoms, (2) a correction ΔU to the potential energy due to zero-point motion, and (3) the kinetic energy K associated with this zero-point motion. In units of ϵ, E_{st} is of the order of $z/2$ (z the number of nearest neighbors) and both ΔU and K are of the order of λ.[5] Also δ^2, the position mean square deviation, is of the order of λ^5 (in units of σ^2). In the case of solid helium ($\lambda\approx 0.3$) all these terms (K, ΔU, and δ) become of the order of unity and cannot be regarded as small corrections.

Our present method consists in expressing ΔU as a power series in δ^2 which can be regarded as a variational parameter. For a given volume one minimizes $\Delta U+K$ ($K\propto\delta^{-2}$) with respect to δ, and thus δ is obtained as a function of the volume. In Sec. II we present a discussion of the evaluation of ΔU as a power series. In Sec. III the method is applied to a close-packed lattice and the results are compared with the experimental data for He^4. In Sec. IV the calculations are repeated for a body-centered cubic lattice and we also discuss the possibility of a crystallographic phase transition between these two lattices; no indication of such transition is found from these calculations, the close-packed lattice being more stable with respect to a bcc lattice, at low temperatures and all pressures.

II. QUANTUM MECHANICAL EQUATIONS

As an approximate trial variation solution Φ of Eq. (1) with a 12–6 potential, Eq. (2), we take

$$\Phi(\mathbf{x}_1,\mathbf{x}_2\cdots\mathbf{x}_N)=\prod_{i=1}^{N}\varphi_i(\mathbf{x}_i-\mathbf{X}_i),\tag{3}$$

where for simplicity we choose[4,5]

$$\varphi_i(\xi_i)=(\pi/2a^3)^{\frac{1}{2}}\sin|\pi\sigma\xi_i/a|/|\pi\sigma\xi_i/a|\quad\text{for}\quad\xi_i<a,$$

and

$$\varphi_i(\xi_i)=0\quad\text{for}\quad\xi_i\geqslant a.\tag{4}$$

The vectors $\mathbf{X}_i$ describe a given lattice, and a is a variational parameter proportional to the root mean square deviation of an atom from its lattice site.

TABLE I. Lattice summation constants.[a]

	C_6	C_8	C_{10}	C_{12}	C_{14}	C_{16}	C_{18}
Close-packed lattice	14.45	12.80	12.31	12.13	12.06	12.03	12.01
Body-centered cubic lattice	12.25	10.36	9.56	9.11	8.82	8.61	8.45

[a] Values from reference 7.

The expectation value $\langle H\rangle\equiv\int\Phi^*H\Phi$ of the Hamiltonian contained in Eqs. (1) and (2) is given by[4,5]

$$\begin{aligned}\langle H/N\epsilon\rangle\equiv E^*&=E_{st}^*+\lambda^2\alpha^{-2}+(A_1\alpha^2+A_2\alpha^4+A_3\alpha^6\cdots)\\&\equiv E_{st}^*(V)+K^*(V,\lambda,\alpha)+\Delta U^*(V,\alpha),\end{aligned}\tag{5}$$

where $\alpha\equiv a/\pi\sigma$, E_{st}^* is the static interatomic potential energy given by[4,5]

$$E_{st}^*=4\times\tfrac{1}{2}(C_{12}X^{-12}-C_6X^{-6}),\tag{6}$$

where X is the nearest neighbor distance (in units of σ), and the C's are tabulated constants[7] whose values depend only on the type of lattice. The coefficients in the power series for ΔU^* depend on the even moments of the square of the single-particle wave function φ_i, and in the present case, Eq. (4), they have the following values[4]:

$$A_1=\pi^2(24.9C_{14}X^{-14}-5.66C_8X^{-8}),\tag{7a}$$

$$A_2=\pi^4(198C_{16}X^{-16}-13.8C_{10}X^{-10}),\tag{7b}$$

$$A_3=\pi^6(1{,}280C_{18}X^{-18}-33.5C_{12}X^{-12}).\tag{7c}$$

Table I lists the values[7] of the C's for a close-packed (c.p.), either hexagonal or cubic, and for a body-centered cubic (bcc) lattice which will be used in the subsequent sections. Table II shows the values of the parameters[8] ϵ, σ and their various dimensionless combinations appropriate to He^3 and He^4.

According to the variational theorem an approximate value for the lowest eigenvalue of Eq. (1), and the corresponding eigenfunction Eqs. (3) and (4), can be obtained by minimizing the right-hand side of Eq. (5) (regarded as a function of the volume V and of α) with respect to the variational parameter α, i.e., the optimum value $\alpha_0(V)$ of α is given by

$$[\partial E^*(\alpha,V)/\partial\alpha]_{\alpha=\alpha_0}=0.\tag{8}$$

In view of Eq. (5), Eq. (8) is an algebraic equation of the fourth degree in α^2 if all the terms A_1, A_2, and A_3 in ΔU^* are kept. If A_3 or A_3 and A_2 in Eq. (5) are neglected Eq. (8) becomes, respectively, a quadratic

TABLE II. Interatomic potential parameters for helium.[a]

	ϵ(in °K)	σ(in A)	$N\sigma^3$(cm^3/mole)	ϵ/σ^3 (in atm)	$\lambda\equiv(\hbar^2/2M\epsilon\sigma^2)^{\frac{1}{2}}$
He^3	10.2	2.56	10	83.4	0.347
He^4	10.2	2.56	10	83.4	0.302

[a] Values from reference 8.

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[7] J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954).

[8] J. de Boer, in *Progress in Low-Temperature Physics*, edited by C. J. Gorter (North-Holland Publishing Company, Amsterdam, 1957), Vol. II, p. 1.

or linear equation in α^2. In what follows, a subscript n indicates the highest power of α^2 kept in Eq. (5), i.e., that A_{n+1} in Eq. (5) has been neglected. In Sec. III we discuss the case of a close-packed lattice for He^3 and He^4 in three successive approximations: $n=1$, 2, and 3, respectively. One expects that our approximate results should improve by keeping higher and higher powers of α^2 in Eq. (5). An idea of the rate of convergence of our approximations can be obtained by comparing our results in Sec. III for the cases $n=1$, 2, and 3. In Sec. IV we discuss the case of a face-centered cubic lattice again for He^3 and He^4 for $n=3$.

III. RESULTS AND DISCUSSION FOR A CLOSE-PACKED LATTICE

For a close-packed lattice the relation between the volume per atom V/N and the nearest neighbor distance $R\equiv\sigma X$ is $V^*2^{-\frac{1}{2}}X^3$ where $V^*\equiv V/N\sigma^3$. Using the values of the constants C shown in Table I we can write Eqs. (7a-c) for c.p. lattice as:

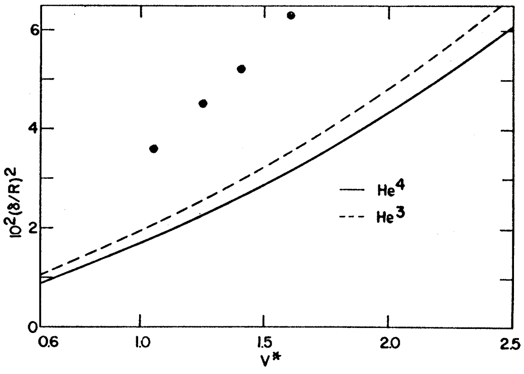

FIG. 1. Mean square deviation in a close-packed lattice, in units of the square of the nearest neighbor distance. The black circles correspond to values calculated for He^4 from calorimetric data.[9]

$$A_1=10^2(5.90V^{*-14/3}-2.84V^{*-8/3}), \quad (9a)$$

$$A_2=10^3(36.7V^{*-16/3}-5.23V^{*-10/3}), \quad (9b)$$

$$A_3=10^4(184V^{*-6}-9.8V^{*-4}). \quad (9c)$$

In view of Eq. (5), Eq. (8) becomes in three different approximations, $n=1$, 2, and 3 (see above),

$$3A_3z_3^4+2A_2z_3^3+A_1z_3^2-\lambda^2=0, \quad n=3 \quad (10a)$$

$$2A_2z_2^3+A_1z_2^2-\lambda^2=0, \quad n=2 \quad (10b)$$

$$A_1z_1^2-\lambda^2=0, \quad n=1 \quad (10c)$$

where $z(V^*)\equiv\alpha^2(V^*)$.

The range of validity of a given approximation, $n=1$, 2, or 3, is limited by the value of the volume for which A_1, A_2, or A_3, respectively, become zero. For a close-packed lattice these limits are: $V^*=1.44$ for $n=1$, $V^*=2.65$ for $n=2$, and $V^*=4.33$ for $n=3$.

For small values of λ the quadratic approximation $n=1$ is satisfactory.[4,5] In the case of helium, $\lambda\approx1$, this quadratic approximation is poor except at high densities ($V^*\ll1$). For instance, the equations in the quadratic approximation become meaningless for $V^*<1.44$ while the observed density of solid helium at low pressures ($p\approx30$ atm) corresponds to $V^*\cong2$.

TABLE III. Optimal values of the variational parameter, $z\equiv\alpha^2$ for a close-packed lattice for He^4.

z/V^*	0.6	0.8	1.0	1.5	2.0	2.5	3.0
10^2z_1	0.34	0.72	4.5				
10^2z_2	0.32	0.61	0.98	2.6	6.0		
10^2z_3	0.31	0.55	0.86	1.7	3.3	5.4	8.2

Equations (10a)-(10c) can be solved numerically, and Tables III and IV list typical values of the roots which make the right-hand side of Eq. (5) a minimum for the case of He^4 [$\lambda(He^4)=0.302$] and He^3 [$\lambda(He^3)=0.347$], respectively.

The mean square deviation δ^2 of an atom from its lattice site, $\delta^2\equiv\int\varphi_i^*\xi_i^2\varphi_i$, is given by[5]

$$\delta^{*2}\equiv(\delta/\sigma)^2=2.79\alpha^2=2.79z, \quad (11)$$

or, in terms of the nearest neighbor distance $R\equiv\sigma X$ for a close-packed lattice,

$$(\delta/R)^2=2.79z2^{-\frac{1}{3}}/V^{*\frac{2}{3}}=2.21zV^{*-\frac{2}{3}}. \quad (12)$$

Figure 1 shows the mean square deviation for He^3 and He^4 as functions of the volume as given by Eq. (12) and Tables III and IV, together with values obtained from calorimetric data for He^4.[9] One should not attribute much significance to a comparison between theory and experiment here, since the "experimental" values refer to the melting curve rather than the 0°K and they were obtained[9] on basis of a Debye harmonic model which certainly is a poor approximation for solid helium at low pressures. Previous estimates of δ/R^3 for solid helium compare favorably with our present results.

The cohesive energy can be calculated as a function of V^* when the values of $z\equiv\alpha^2$ listed in Tables III and IV are substituted in Eq. (5). Figure 2 shows the results for $E^*\equiv K^*+\Delta U^*$ for the case of He^4 corresponding to three approximations: $n=1$, 2, and 3, and ΔE_3 for He^3. Figure 3 shows the results for ΔE_3^* and E_3^* for He^3 and He^4, and Fig. 4 shows in greater detail the cohesive energies in two approximations, $n=2$ and 3,

TABLE IV. Optimal values of the variational parameter, $z\equiv\alpha^2$, for a close-packed lattice for He^3.

z/V^*	0.6	0.8	1.0	1.5	2.0	2.5	3.0
10^2z_1	0.45	0.96	6.0				
10^2z_2	···	···	1.1	2.9	6.4		
10^2z_3	0.33	0.59	0.92	1.9	3.6	5.7	8.6

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[9] C. Domb and J. S. Dugdale, in *Progress in Low-Temperature Physics*, edited by C. J. Gorter (North-Holland Publishing Company, Amsterdam, 1957), Vol. II, p. 338.

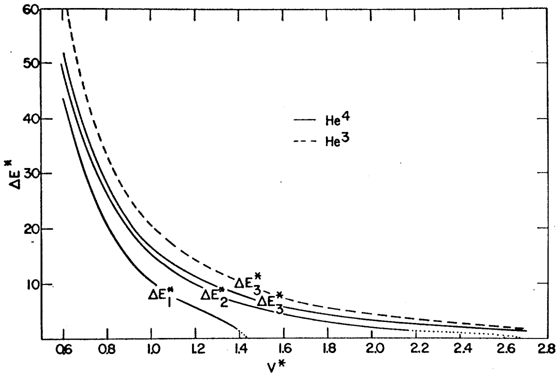

FIG. 2. Zero-point energy in a close-packed lattice. The indices 1, 2, 3 indicate the highest power of the mean square deviation kept in the zero-point potential energy of interaction.

for both He^3 and He^4 for large values of V^*, i.e., at low pressures.

A direct comparison of the results contained in Figs. 2–4 with experiment is not possible. Nevertheless, the cohesive energy of solid helium at the lowest pressures ($P=30$ atm for He^3 and 25 atm for He^4) can be obtained from the known cohesive energy of the liquid, its compressibility, and the volume change during melting. The cohesive energies of liquid and solid He^4 at a pressure of 25 atm are shown in Fig. 4. Even though our approximations become steadily worse at larger volumes, our values for E_3^* seem to be in fair agreement with experiment. One should note that our cohesive energies at low pressures are obtained as small differences between large numbers. For instance, for He^4 at $V^*=2.4$ (see Fig. 3), $E_3^*=E_{st}^*+\Delta E_3^*=-2.3+1.9=-0.4$.

A more meaningful comparison with experimental data can be obtained for the compressibilities which can be measured directly. Figure 5 shows the results for the pressure ($P^*\equiv -dE^*/dV^*$) as a function of volume for both He^3 and He^4 together with the high-pressure experimental data[10] for He^4. Figure 6 shows the same[9] at lower pressures. The agreement in the case of He^4 seems to be rather good and even at low pressures (see Fig. 6, $P<10^3$ atm) the approximations $n=1$, 2, and 3 seem to be converging to the experimental values. Unfortunately, no data are available for solid He^3.

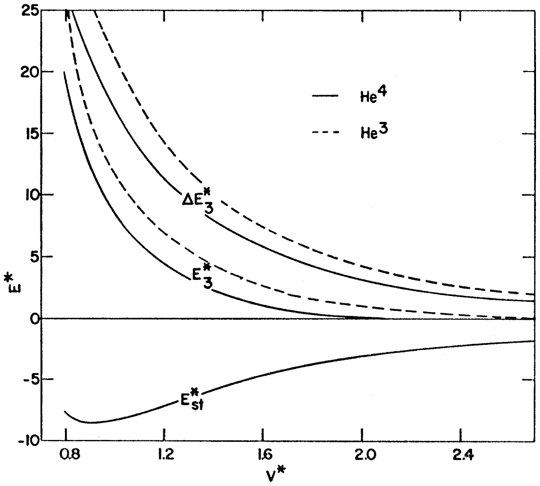

FIG. 3. Cohesive and zero-point energies of solid helium as functions of volume for a close-packed lattice.

A Debye temperature, $\theta\equiv\epsilon\theta^*$, can be obtained in two different ways as follows. One may assume the results of a Debye model for the zero-point motion energy and define

$$\theta_1^*\equiv(8/9)\Delta E^*, \tag{13}$$

or one may assume: (1) isotropy, (2) Cauchy relation, and (3) elastic continuum model, in which case it follows that[5]

$$\theta_2^*\equiv 4.7\lambda V^{*\frac{1}{3}}(\partial P^*/\partial V^*)^{\frac{1}{2}}. \tag{14}$$

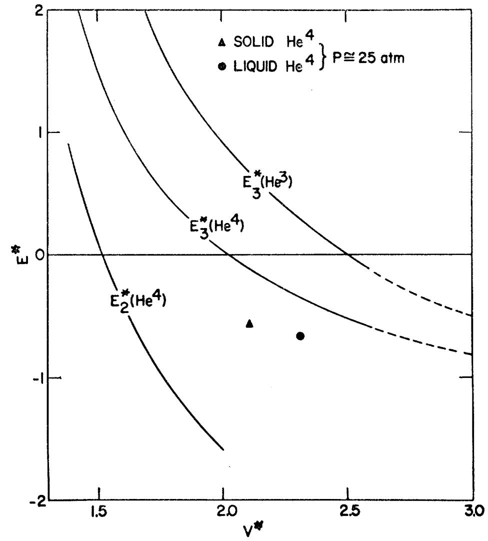

FIG. 4. Cohesive energy of solid helium at low pressures. The experimental points for liquid and solid He^4 are from reference 8.

Figure 7 shows θ_1^* and θ_2^* as functions of the volume for both He^3 and He^4. The two definitions, Eqs. (13) and (14) lead to values differing by as much as a factor of 2, which is to be expected since, on one hand due to strong anharmonicity Eq. (13) may not hold, and on the other, assumptions (1)–(3) leading to Eq. (14) may likewise not be satisfied in the case of solid helium. Figure 7 also shows values for solid He^4 obtained[8] from calorimetric data (black circles), as well as values calculated by Dugdale[11] (open circles) from Stewart's compressibility data.[10]

The value of an average Grüneisen constant, defined as $-\partial\ln\theta^*/\partial\ln V^*$, varies in the neighborhood of 2

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[10] J. W. Stewart, J. Chem. Phys. Solids **1**, 146 (1956).

[11] J. S. Dugdale, Suppl. Nuovo cimento **9**, 30 (1958).

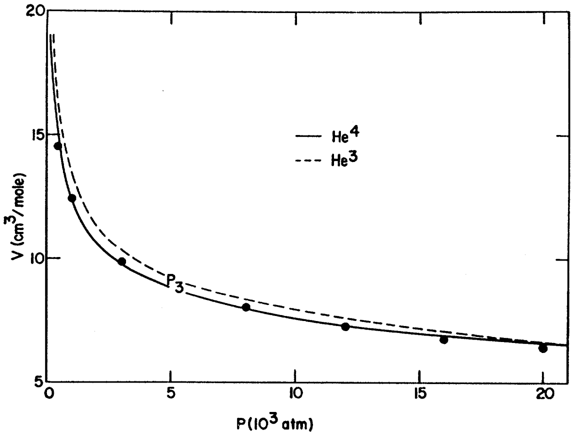

FIG. 5. Volume as a function of pressure for a close-packed lattice.

for volumes $1<V^*<3$ for both He^3 and He^4 and for either definition of θ^*. These values are in good agreement with the values calculated by Dugdale[11] from compressibility data.

IV. RESULTS AND DISCUSSION FOR A BCC LATTICE

It has been reported[12,13] that both solid He^4 and He^3 undergo phase transitions under pressures of the order of 10^3 and 10^2 atm, respectively. In the case of He^4 it has been suggested[12] that the transition is a crystallographic phase change from fcc to hcp lattice. On the other hand, Schuch *et al.*,[13] on the basis of x-ray data, claim that in the case of solid He^3 the crystallographic change at 100–150 atm involves a transition from a bcc to a hcp lattice. For $V^*\lesssim 1.5$ the classical interatomic potential energy of a bcc static lattice is practically the same as that of the static hcp lattice, but especially in He^3 zero-point motion energies are so large that a safe conclusion about relative stability of different lattice cannot be drawn without a quantitative analysis of zero-point motion effects. In this section we present results for a bcc lattice, and a comparison of these results with those of the previous section shows that, with the present model, the close-packed lattice is more stable at all volumes of interest ($V^*\lesssim 3$).

The calculations for a bcc proceed exactly in the same fashion as those presented in Sec. III. Equations (3)–(6) still persist. In Eqs. (7a)–(7c) only the lattice summation constants C are slightly changed (see Table I), and the relation between volume and nearest neighbor distance is changed to $V^*=2^2 3^{-\frac{3}{2}}X^3=0.770X^3$ appropriate to a bcc lattice. In Eqs. (5), (7), (9), and (10) we change the notation, replacing $A_{1,2,3}$ by $B_{1,2,3}$ and α by β. Thus we can write

$$E^*\equiv E_{st}^*+K^*+\Delta U^*=E_{st}^*+\lambda^2\beta^{-2} + (B_1\beta^2+B_2\beta^4+B_3\beta^6+\cdots), \quad (15)$$

$$B_1=10^2(6.36V^{*-14/3}-2.88V^{*-8/3}), \quad (16a)$$

$$B_2=10^3(41.0V^{*-16/3}-5.37V^{*-10/3}), \quad (16b)$$

$$B_3=10^4(214V^{*-6}-10.3V^{*-4}). \quad (16c)$$

Thus the variational theorem gives

$$3B_3y_3^4+2B_2y_3^3+B_1y_3^2-\lambda^2=0, \quad n=3, \quad (17)$$

where $y(V^*)\equiv\beta^2(V^*)$ and we have disregarded the lower order approximations, $n=1$, 2, Eqs. (10b) and (10c).

TABLE V. Optimal values of the variational parameter, $y\equiv\beta^2$, for the body-centered cubic lattice.

$10^2y_3/V^*$	0.5	0.9	1.4	2.0	2.4	3.0
He^4	0.20	0.66	1.56	3.1	4.5	7.65
He^3	0.22	0.73	1.7	3.35	4.85	8.05

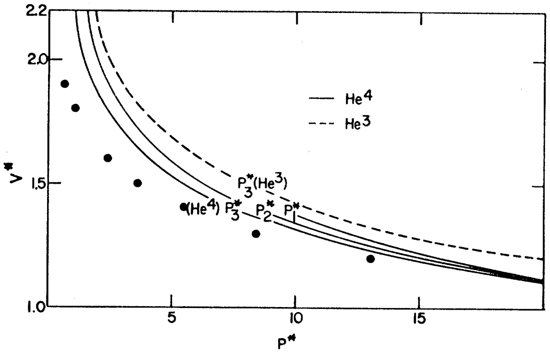

FIG. 6. Volume as a function of pressure for a close-packed lattice. The units of pressure and volume are: $\epsilon/\sigma^3\cong 83.4$ atm, $N\sigma^3\cong 10$ cm³/mole.

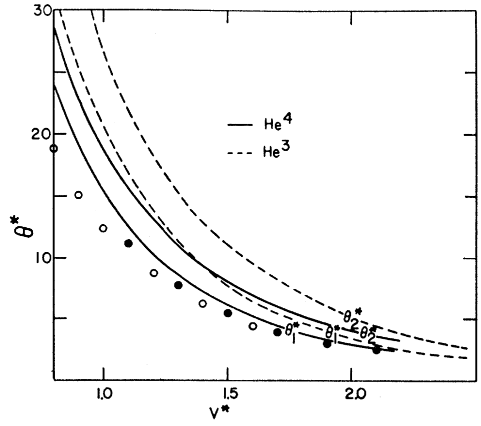

FIG. 7. Debye temperature for a close-packed lattice. θ_1^* is defined from the zero-point energy and θ_2^* from the compressibility. The circles represent values for He^4: black circles[8] from calorimetric data,[9,12] open circles from compressibility data.[10,11]

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[12] J. S. Dugdale and F. Simon, Proc. Roy. Soc. (London) **A218**, 291 (1953).

[13] A. F. Schuch, E. R. Grilly, and R. L. Mills, Phys. Rev. **110**, 775 (1958).

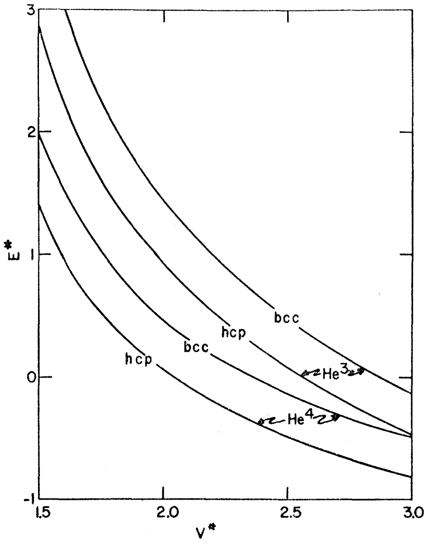

FIG. 8. Cohesive energies of hcp and bcc lattices as functions of volume at 0°K. In the present approximation the hcp lattice is more stable at all pressures for either He^3 or He^4.

Table V shows the roots of Eq. (17) for several volumes for both He^3 and He^4. Comparing Tables III and IV with V we see that for either He^3 or He^4 the mean square deviation in a bcc lattice is always less than that in a close-packed lattice.

The cohesive energy of a bcc lattice can be calculated from Eqs. (15) and (16) and Table V. In Fig. 8 we show the results (in the approximation $n=3$) for both He^3 and He^4 for the cases of a bcc and a close-packed lattice. Figure 9 shows the He^3 Debye temperature $\theta_1{}^*$ [see Eq. (13)] for both a hcp and a bcc lattice. For volumes $V^*\gtrsim 1.5$ the static energies of these two lattices are practically the same and hence all the difference in cohesive energy comes from the difference in zero-point energy. In our approximation we find that the zero-point energy (i.e., the Debye temperature in a simple Debye model) is larger for a bcc lattice for all volumes for both He^3 and He^4. From Fig. 8 we see that at 0°K the close-packed lattice seems to be more stable, compared to a bcc lattice, at all volumes, and hence no crystallographic transition would be expected. At higher temperatures the situation seems to be the same, at least in the temperature region where the lattice specific heat is proportional to $T^3[C_{\text{lattice}}{}^*=\gamma(T/\theta)^3]$. The reason is that for a given temperature and volume the free energies $[F^*=E^*(T=0)-(\gamma T^*/12)(T/\theta)^3]$ will satisfy the inequality $F_\alpha{}^*(T)<F_\beta{}^*(T)$ if (a) $E_\alpha{}^*(T=0)<E_\beta{}^*(T=0)$ and (b) $\theta_\alpha<\theta_\beta$, which are just the results we find. Thus, our present model does not explain the crystallographic transition observed in solid He^3.[13] It should be emphasized that all the previous remarks and conclusions were based on a simple (Heitler-London) model along with the assumption that the system of nuclear spins does not undergo any drastic change (in free energy) during the crystallographic transition, and these may not be adequate for solid He^3.

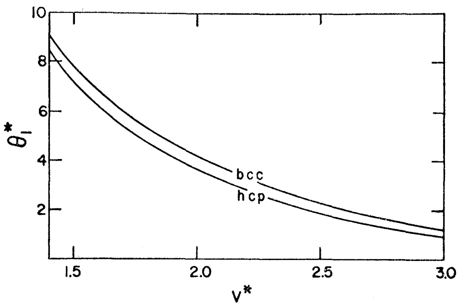

FIG. 9. He^3 Debye temperature for both a hcp and bcc lattice.

V. CONCLUSIONS

From the results of Sec. III and the comparison with the experimental data for solid He^4 we may conclude that a simple Heitler-London model and a 12–6 potential can account for the properties of, at least, solid He^4 for which experimental data are available. Not much is known about the cohesive and thermal properties of solid He^3. But, except for properties, like nuclear magnetic susceptibility, which depend on the antisymmetry of the wave function, one may expect that our present results describe the properties of this isotope to a good accuracy. It is true that at low pressures one may obtain significant improvement over the present results by keeping higher powers of α^2 in Eq. (5).[14]

Regarding the observed[13] crystallographic transition in solid He^3 at pressures of the order of 100 atm, our calculations do not seem to be successful.

It should be pointed out that any contribution coming from exchange energy would leave all the conclusions of this paper unchanged, except, possibly, the results about the relative stability of a bcc and close-packed lattices, in the event that these two lattices turn out to have completely different nuclear magnetic properties. A magnetic transition has been predicted[3] at about the same pressure, and the question of whether or not a change in crystallographic phase accompanies such magnetic transition has not yet been investigated.

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[14] *Note added in proof.* R. D. Etters has extended the present calculations to include terms up to $n=5$, i.e., up to α^{10} in Eq. (5). The convergence of the results is very good, and all the results in the present paper remain valid. In particular the hcp lattice is still more stable with respect to the bcc lattice.