

TABLE V. Results.

Volume (cm ³ /mole)	$\langle V \rangle$ (K)	$\langle T \rangle$ (K)	E_0 (K)	Pressure (atm $\times 10^3$)	β (σ^{-2})	κ (σ^{-1})
23.30	-150.5	65.5	-85.0		7	1.19
18.52	-188.0	126.0	-62.0	1.06	30	1.14
13.99	-149.0	243.5	94.5	6.12	67	1.12
12.35	-25.5	297.5	272.0	11.95	80	1.11
11.11	159.0	353.5	512.5	21.69	95	1.10
9.26			1306	60.1	150	1.12
7.72			3120	147.7	300	1.10
6.17			8290	454.9	375	1.10
5.56			12 280	726.0	500	1.12
5.14			17 000	998.0	650	1.12

it is in principal possible to determine and solve the coupled differential equations for the optional form of φ and f which minimize the energy. This is possible because the dynamics of only a limited number of particles are involved. Another valuable feature is that the exchange energy can be calculated in a simple direct fashion. Work on this problem is in progress.

APPENDIX

To evaluate $G(\vec{r}_\lambda, \vec{r}_\kappa)$ for a particular value of \vec{r}_λ and \vec{r}_κ , there are a product of three-dimen-

sional integrals to solve, i.e.,

$$G(\vec{r}_\lambda, \vec{r}_\kappa) \sim \prod_{i,j,l} M_i(\vec{r}_\lambda) M_j(\vec{r}_\kappa) N_l(\vec{r}_\lambda, \vec{r}_\kappa), \quad (17)$$

where N_i, M_i are defined by Eqs. (13) and (14). The products extend over all different nearest neighbors to particles (λ, κ). Let the integrand of $M_i(\vec{r}_\lambda)$ be $I(\vec{r}_\lambda, \vec{r}_i, \vec{R}_i)$ and of $N_i(\vec{r}_\lambda, \vec{r}_\kappa)$, $H(\vec{r}_\lambda, \vec{r}_\kappa, \vec{r}_i, \vec{R}_i)$. A Monte Carlo integration routine is used to evaluate these integrals, in which case they are expressed as sums:

$$G(\vec{r}_\lambda, \vec{r}_\kappa) \sim \prod_{i,j,l} \left(N^{-1} \sum_{n=1}^N I_n(\vec{r}_\lambda, \vec{r}_{in}, \vec{R}_i) \right)_i \left(N^{-1} \sum_{n=1}^N I_n(\vec{r}_\kappa, \vec{r}_{jn}, \vec{R}_j) \right)_j \left(N^{-1} \sum_{n=1}^N H_n(\vec{r}_\lambda, \vec{r}_\kappa, \vec{r}_{ln}, \vec{R}_l) \right)_l. \quad (18)$$

In a bcc lattice structure and with (λ, κ) nearest neighbors, there are 14 such three-dimensional integrals (sums). The index n on the set of vectors $\Pi_{i,j,l} \{ \vec{r}_{in}, \vec{r}_{jn}, \vec{r}_{ln} \}$ specifies a particular value for these 14 vectors, selected at random. Each three-dimensional integral in Eq. (18) is evaluated by summing the N values of its integrand, obtained using the N randomly selected vectors $\{ \vec{r}_{in} \}$, and then dividing by N . It is important to note that the integral $M_i(\vec{r}_\lambda)$ with integrand $I(\vec{r}_\lambda, \vec{r}_i, \vec{R}_i)$ and $M_j(\vec{r}_\lambda)$ with integrand $I(\vec{r}_\lambda, \vec{r}_j, \vec{R}_j)$, $i \neq j$, are independent of one another with respect to the vari-

ables \vec{r}_i and \vec{r}_j . Clearly, every integral in $G(\vec{r}_\lambda, \vec{r}_\kappa)$ is independent of one another in the set of variables $\Pi_{i,j,l} \{ \vec{r}_i, \vec{r}_j, \vec{r}_l \}$. This means that the same randomly selected vector, \vec{a}_n , which is used to evaluate one integrand at one point, may also be used to evaluate the integrands in all the sums of Eq. (18).

Hence, instead of selecting 3×14 different random values to define the vectors in the set $\Pi_{i,j,l} \{ \vec{r}_{in}, \vec{r}_{jn}, \vec{r}_{ln} \}$, at one point in phase space, a single vector \vec{a}_n can be used to evaluate the integrand in each of the 14 sums. This, of course,

TABLE VI. Product of correlation functions approximation. Energy calculated from the dynamic-field approximation incorporating pair correlations between particles (λ, κ) and their first; first and second; or first, second, and third shells of nearest neighbors.

Number of $f(r_{ij})$ products in calculation of $G(\vec{r}_\lambda, \vec{r}_\kappa)$	$\langle V \rangle$ (K)	$\langle T \rangle$ (K)	$\langle E_0 \rangle$ (K)
1st-nearest neighbors	-24.10	20.40	-3.70
1st- and 2nd-nearest neighbors	-25.17	19.95	-5.22
1st-, 2nd-, and 3rd-nearest neighbors	-25.10	19.95	-5.15

TABLES VII. Energy contribution from different nearest-neighbor shells in lattice sum.

Volume (cm ³ /mole)	Nearest-neighbor shell	Contribution to $\langle V \rangle$ (K)		Contribution to $\langle T \rangle$ (K)		Contribution to E_0 (K)	
		Dynamic field	Rigid lattice	Dynamic field	Rigid lattice	Dynamic field	Rigid lattice
21.60	1st	-14.95		12.50		-2.45	
	2nd	-6.64		2.38		-4.26	
	3rd-10th	-5.33		0.97		-4.36	
	11th-38th	-0.39	-0.39	0.03	0.03	-0.36	-0.36
				6.25	$= 3\hbar^2\beta/4m$	+6.25	
	Total	-27.31		22.13		-5.18	
10.25	1st	+8.77		42.45		51.22	
	2nd	-11.45		8.92		-2.53	
	3rd	-8.19		1.84		-6.35	
	4th	-5.52	-5.69	1.03	1.00	-4.49	-4.69
	5th-10th	-4.93	-4.96	0.70	0.70	-4.23	-4.26
	11th-38th	-1.74	-1.74	0.15	0.15	-1.59	-1.59
				27.80	$= 3\hbar^2\beta/4m$	+27.80	
	Total	-23.06		82.89		59.83	

simplifies the evaluation considerably. $G(\vec{r}_\lambda, \vec{r}_\kappa)$ is then substituted into Eq. (8) and the resulting six-dimensional integral is solved to obtain the energy.

As an experiment, it was decided to constrain the motion of the atoms comprising the molecular field in such a way that they all move in concert

about (λ, κ) as a single entity. That is, the displacement vectors of all nearest-neighbor molecular-field atoms are taken to be the same, $(\vec{y}_n = \vec{r}_{in} - \vec{R}_i, i = 1, 2, \dots, 14)$, in each configuration used in evaluating $G(\vec{r}_\lambda, \vec{r}_\kappa)$. The \vec{y}_n are selected randomly to generate other configurations. Then, Eq. (18) becomes

$$G(\vec{r}_\lambda, \vec{r}_\kappa) \sim N^{-1} \sum_{n=1}^N \left(\prod_{i,j,l} I_{ni}(\vec{r}_\lambda, \vec{y}_n, \vec{R}_i) I_{nj}(\vec{r}_\kappa, \vec{y}_n, \vec{R}_j) H_{nl}(\vec{r}_\lambda, \vec{r}_\kappa, \vec{y}_n, \vec{R}_l) \right). \quad (19)$$

The value of the energy, obtained with $G(\vec{r}_\lambda, \vec{r}_\kappa)$ calculated in this fashion, agrees to within 1% of the exact numerical evaluation. Within the statistical error associated with the Monte Carlo

integration routine, the results of these two different methods of calculation agree completely. This conclusion was fortified by comparing results of the two methods at several different volumes for ³He and ⁴He. As a result, the calculation of $G(\vec{r}_\lambda, \vec{r}_\kappa)$, as expressed by Eq. (19), requires the solution of only one three-dimensional integral rather than 14 such integrals. The total energy then results from the evaluation of a nine-dimensional integral. The considerable simplification of algebraic analysis is obvious.

Although we do not fully understand all the implications of this result, it does seem apparent that the dynamical behavior of an arbitrary pair (λ, κ) is insensitive to the relative orientations of the molecular-field atoms with respect to one another but instead depends only on their individual orientations with respect to (λ, κ) . In practice the evaluation of Eq. (8) utilized the following procedure. All of the equations were first rewritten for the computer program in terms of the vector displacement of each molecule from its equilibrium lattice site. That is, the following vectors were introduced:

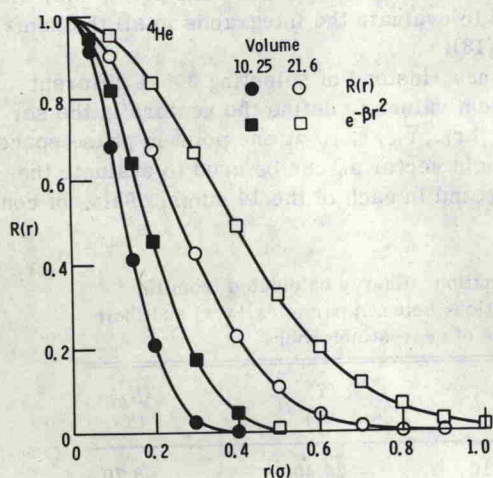


FIG. 15. Comparison of $R(r)$ and $e^{-\beta r^2}$ for solid ⁴He at two different volumes.