Monte Carlo calculation of the Feynman-Cohen excitation spectrum for helium*

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A Monte Carlo method is used to calculate the excitation spectrum of He II. The variational method and the trial wave function of Feynman and Cohen (FC) are used. No approximations, such as the Kirkwood superposition approximation, or estimates are employed. Important terms in the FC calculation are found to be in error by as much as 10–20% but the final answer, $\Delta = 11.2$ K, at the equilibrium density, is hardly different from the FC value $\Delta = 11.5$ K. Results of calculations for densities up to 1.2 times the equilibrium density (i.e., the freezing density) are also presented; we find that the FC wave function does not lead to the expected pressure dependence of Δ. Some modifications to the usual Monte Carlo methods, necessary for this calculation, are discussed.

I. INTRODUCTION

The careful and ingenious variational calculation of Feynman and Cohen[1] (FC) of the excitation spectrum of HeII gave the first (and perhaps only) detailed insight into the structure of the roton and illuminated the role of the He-He interaction in the properties of the energy spectrum. Some questions were raised by their work, however, and remain. How good was their estimate of the errors involved in the Kirkwood superposition[2] approximation? How about the neglect of oscillating integrands and other analytic approximations? Why does the FC spectrum not seem to approach the Feynman phonon[3] spectrum for $k \to 0$? What is the effect of using an "up-to-date" structure factor in the calculation? Is the FC method able to reproduce the behavior of the roton energy under pressure? And finally, how good is the FC wave function in the first place? The present work is an attempt to answer these questions.

In Sec. II we review the FC theory and explain how the Monte Carlo method[4] is applied. Tail corrections are very important in this calculation and must be handled carefully to obtain sensible results; this aspect of the problem is discussed in detail. Section III presents the results of the calculation and a comparison with FC. In the Appendixes we comment on the "sparse-averaging" Monte Carlo technique used here and on a simple lattice-sum technique.

II. CALCULATING THE SPECTRUM

A. Theory of Feynman and Cohen

FC write for a trial wave function

$$\psi(\vec{k}) = \phi \sum_i e^{i\vec{k}\cdot\vec{r}_i} \exp\left(i \sum_{j \neq i} g(\vec{r}_{ji})\right), \tag{1}$$

where

$$g(\vec{r}) = A\vec{k}\cdot\vec{r}/r^3, \tag{2}$$

and ϕ is the wave function of the ground state. The function $\psi(\vec{k})$ describes an excitation of wave vector $\vec{k}$; since $\psi(\vec{k})$ is an eigenfunction of momentum (with eigenvalue $\hbar\vec{k}$) the expression

$$E(k) = \int \psi^\dagger H \psi \Big/ \int \psi^\dagger \psi \tag{3}$$

provides a variationally correct estimate of the energy for each $\vec{k}$. Variation of the parameter A in (2) leads to a still better estimate of $E(k)$. We can imagine Eq. (1) as describing a motion consisting of a representative atom moving through the system with wave vector $\vec{k}$ and a flow ("backflow") around that atom. The backflow has the velocity potential $g(\vec{r})$, which has the form of the ordinary dipolar flow around an object moving through an incompressible fluid.

In order to simplify the calculations FC expanded the exponential in (1) and calculated instead with the trial function

$$\psi(\vec{k}) = \phi \sum_i e^{i\vec{k}\cdot\vec{r}_i}\left(1 + i\sum_{j\neq i} g(\vec{r}_{ji})\right), \tag{4}$$

which does not substantially change the physical content of ψ, so long as the $\sum g$ is not too large.

The Hamiltonian H has the standard form

$$H = \sum_i \left(-\frac{\hbar^2}{2m}\nabla_i^2\right) + \tfrac{1}{2}\sum_{i\neq j} V(r_{ij}), \tag{5}$$

and we have used

$$V(r) = 4\epsilon\left[(\sigma/r)^{12} - (\sigma/r)^6\right], \tag{6}$$

with $\sigma = 2.556$ Å and $\epsilon/k_B = 10.22$ K. FC found that when (4) and (2) are substituted in (3) an expression of the form

$$\frac{E(k)}{N} = \frac{\hbar^2 k^2}{2mS(k)} \frac{\left[1 + A(I_1 + I_2) + A^2(k^2 I_3 + I_4 + I_5 + kI_6 + I_7)\right]}{1 + AkI_9/I_8 + A^2k^2 I_{10}/I_8} \tag{7}$$

results, where $S(k)$ is the structure factor for the ground state and $I_1, I_2, \ldots, I_{10}$ are integrals involving g, ∇g, and two-, three-, and four-point correlation functions. The dependence on A is exhibited explicitly.

B. Reformulation of the problem

The evaluation of the three- and four-point averages by Monte Carlo averaging is very costly, especially since the integrands are complicated and often highly oscillatory because of factors of $e^{i\vec{k}\cdot\vec{r}}$ which appear. It is possible, however, to rewrite the Feynman integrals as N-point averages (where N is the number of particles in the Monte Carlo system and $N \gtrsim 50$). There is only *one* N-tuplet for a given configuration versus roughly $N^3/6$ triplets or $N^4/24$ quadruplets. The snag of course is that the quantity to be averaged is still more complicated, in our case generally involving a double summation as well as g, ∇g, etc. The labor of calculating in this way is thus comparable to that involved in calculating a two-point average, however, so we still gain via the reformulation.

Here, in detail, is what we mean. Substituting (4) and (2) in (3) and expressing the results in terms of ground-state configuration averages (denoted by angular brackets) we find

$$I_1 = -2\left\langle \sum_l H_z^{(l)} \right\rangle \Big/ N, \tag{8a}$$

$$I_2 = 2\left\langle \sum_l \mathrm{Re}F_z^{(l)} \right\rangle \Big/ N, \tag{8b}$$

$$I_3 = \left\langle \sum_l G^{(l)2} \right\rangle \Big/ N, \tag{8c}$$

$$I_4 = \left\langle \sum_l |\vec{\mathbf{H}}^{(l)}|^2 \right\rangle \Big/ N, \tag{8d}$$

$$I_5 = \left\langle \sum_l |\vec{\mathbf{F}}^{(l)}|^2 \right\rangle \Big/ N, \tag{8e}$$

$$I_6 = 2\left\langle \sum_l G^{(l)}\,\mathrm{Im}F_z^{(l)} \right\rangle \Big/ N, \tag{8f}$$

$$I_7 = -2\left\langle \sum_l \vec{\mathbf{H}}^{(l)} \cdot \mathrm{Re}\vec{\mathbf{F}}^{(l)} \right\rangle \Big/ N, \tag{8g}$$

$$I_8 = \langle |S|^2 \rangle / N, \tag{8h}$$

$$I_9 = 2\langle (\mathrm{Im}\,S)(\mathrm{Re}T) - (\mathrm{Re}\,S)(\mathrm{Im}T) \rangle / N, \tag{8i}$$

$$I_{10} = \langle |T|^2 \rangle / N, \tag{8j}$$

where we define

$$G^{(l)} = \sum_{j\neq l} g_1(\vec{r}_{jl}), \tag{9a}$$

$$\vec{\mathbf{H}}^{(l)} = \sum_{j\neq l} \nabla_l\, g_1(\vec{r}_{jl}), \tag{9b}$$

$$E^{(l)} = \sum_{j\neq l} e^{i\vec{k}\cdot\vec{r}_{jl}}\, g_1(\vec{r}_{jl}), \tag{9c}$$

$$\vec{\mathbf{F}}^{(l)} = \sum_{j\neq l} e^{i\vec{k}\cdot\vec{r}_{jl}}\, \nabla_l\, g_1(\vec{r}_{jl}), \tag{9d}$$

and

$$S = \sum_i e^{i\vec{k}\cdot\vec{r}_i}, \tag{10a}$$

$$T = \sum_i e^{i\vec{k}\cdot\vec{r}_i}\, G^{(i)}, \tag{10b}$$

all summations going from 1 to N, $\hat{k} = \hat{z}$, and

$$g_1(\vec{r}) = (Ak)^{-1} g(\vec{r}) = (\hat{k}\cdot\hat{r})/r^2. \tag{11}$$

Thus each FC integral involves only a double summation for each configuration of N particles, except for $I_8 = S(k)$, which requires only a single sum. The simplification we have achieved is of the same sort that enables efficient calculation of elastic constants by Monte Carlo techniques.[5]

Because the terms to be averaged are quite complicated it is inconvenient, and unnecessarily expensive, to compute using the standard "block-averaging" technique in which the terms are recalculated each time a particle is moved, or a move rejected. Instead we calculate contributions to the averages much less frequently, typically once every four passes through the N particles. Little information is lost in this way since configurations sampled more frequently would be less independent. This "sparse-averaging" technique,[6] which has been employed previously[7] for the calculation of three-point averages, is discussed further in Appendix A.

C. Tail corrections

The last question to be faced is the problem of tail corrections. Because the computing time per configuration increases as N^2, only relatively small ($N=50$ to 80) systems were considered. (This is large enough to give accurate values for the parameters of the ground state and also, we expected, for the excited states.) Even for three-point averages, however, the problem of evaluating tail corrections is complicated by the contributions of triplets forming "thin" triangles where, say, $r_{13} \gg \sigma$ but $r_{12} \approx \sigma$. For N-point averages the situation is still more complicated. Worse, the factors g and ∇g decay very slowly with distance so the tail corrections are quite important.

Our idea to overcome this problem is as follows. The Monte Carlo configurations are generated in a box with periodic boundary conditions; we can, of course, also regard the configurations as infinite, but periodic. This is what we do, except that we do *not* regard the flow superposed on the ground state as periodic. Thus when we consider

$$\psi(\vec{k}) = \phi \sum_i e^{i\vec{k}\cdot\vec{r}_i}\left(1 + i\sum_{j\neq i} g(\vec{r}_{ji})\right),$$

we mean for the summations to go over *every* particle in the infinite periodic system. If $\vec{k}$ is chosen as a vector of the reciprocal lattice of the lattice of Monte Carlo boxes, then the first summation becomes trivial:

$$\sum_{\text{all } i} \to N_B \sum_{i \text{ in one box}}, \tag{12}$$

where N_B is the number of boxes (temporarily regarded as finite). The second summation, however, receives a different contribution from each box:

$$\sum_{j\neq i} g(\vec{r}_{ji}) \to \sum_{\substack{j\neq i \\ j \text{ in one box}}} \sum_{\text{images of } j} g(\vec{r}_{ji}), \tag{13}$$

in which performing the infinite sum is reduced to performing a lattice sum of the form

$$\sum_\lambda \frac{\cos\theta_{\vec{R}-\vec{r}_\lambda}}{|\vec{R}-\vec{r}_\lambda|^2},$$

where $\vec{r}_\lambda$ is a lattice vector indexed by λ. The summation over images of i does not appear in (13) but it is identically zero. A simple but efficient method of evaluating this and another lattice sum we required is discussed in Appendix B.

We have found a way of averaging over configurations with a large (infinite) number of particles, but of course the question arises whether the class of periodic configurations is an adequate sample. Recall, however, that the physics we are trying to include is the contributions of "thin triangles" (and similarly deformed higher-order polygons). This contribution is sensitive to the correlation between the vertices of the short side, but much less so to a correlation which gives a weak bias to the direction and length of the long sides. The latter is the false correlation we have introduced by periodically extending the system and we are therefore motivated to neglect it.

Now use the above approach to transform the I's, and redefine $G^{(1)}$, $\vec{H}^{(1)}$, etc. according to (13). Consider I_i, $i=1,7$. The $\sum_l$ generates a factor N_B which is canceled by the factor N_B by which the number of particles in the system is increased. Hence

$$I_i \to I_i, \quad i=1,7. \tag{14}$$

Furthermore, provided $\vec{k}$ is a vector of the reciprocal lattice, we have

$$S \to N_B S,$$

$$T \to N_B T,$$

so that

$$I_i \to N_B I_i, \quad i=8,10 \tag{15}$$

again redefining the $\sum_j$ in S and T according to (13). Hence the N_B's cancel out of Eq. (7) and N_B can be regarded as infinite.

The calculations were done in two stages. First ground-state configurations were produced by a Monte Carlo[4] program and checked by comparison of the ground-state properties with the molecular-dynamics calculations of Schiff and Verlet.[8] Configurations of 50, 64, and 80 particles were generated, although the bulk of the running was done with $N=50$ and $N=64$. The configurations were then analyzed as described above. Reciprocal-lattice vectors pointing along the coordinate axes were used and the results for different $\vec{k}$ but equal k were averaged together. Because there are ten separate integrals and because moderately complex lattice sums had to be evaluated for each pair in a configuration, the calculations were fairly lengthy. At least 20 minutes of computing time on a CDC 6600 computer (150 50-particle configurations or 100 64-particle configurations) is required to obtain adequate statistical precision and at least two runs with different N are necessary in order to obtain a dense enough set of reciprocal-lattice vectors. Representative results are shown in Fig. 1, where I_2, I_5, and I_6 are plotted as a function of k for the equilibrium density $\rho_0 = 0.02185/\text{Å}^3$. There is no detectable N dependence (indicating that our configurations are large enough, and that our method of incorporating the tail corrections is working according to expectations). These

results, which will be discussed in Sec. III, are quite consistent with those obtained by FC.

In Fig. 2 are plotted results for I_9. These are of special interest because it was found necessary in this case (and for I_{10}) to abandon the lattice-sum method.[9] A clue to the reason for the catastrophe is found if T [Eq. (9f)] is rewritten

$$T = \sum_{ij} e^{i\vec{k}\cdot\vec{r}_i} g(\vec{r}_{ji}) = \sum_{ij} e^{i\vec{k}\cdot\vec{r}_j} g(\vec{r}_{ij}) = -\sum_i e^{i\vec{k}\cdot\vec{r}_i} \sum_{j\neq i} e^{i\vec{k}\cdot\vec{r}_{ji}} g(\vec{r}_{ji}) \quad (16)$$

or

$$T = -\sum_i e^{i\vec{k}\cdot\vec{r}_i} E^{(i)} . \quad (17)$$

The second sum in (16), $E^{(i)}$, is the villain. In a nonperiodic configuration the contribution from particles in a shell at $r >> \sigma$ is the order of the angular average of $e^{i\vec{k}\cdot\vec{r}}[(\cos\theta)/r^2]r^2\,dr$, i.e., shells at $r=\infty$ contribute equally with nearby shells. In the lattice sum of g's, however, the periodic structure leads to a more convergent situation where the contribution of successive shells decreases with r.

Equation (16) also provides the seed of the solution that we adopted, which was to evaluate T in the form (17), and carry out the $\sum_{j\neq i}$ only for r_{ji} up to some cutoff radius r_0 (within the Monte Carlo box, i.e., $r_0 < \frac{1}{2}a$, where a is the box side). The sum $E^{(i)}$ was then corrected by adding

$$\rho \int_{r_0}^{\infty} e^{i\vec{k}\cdot\vec{r}} g_1(\vec{r})\, d\vec{r} .$$

If r_0 is chosen to be $\frac{1}{2}a$ exactly then this correction is precisely zero (since we use $k = 2\pi n/a$, $n = 1, 2, \ldots$). Results of calculating I_9 in this way with $N = 50$, 64, and 80 and $\rho = \rho_0$ are shown in Fig. 2 as triangles, circles, and squares, respectively. Also shown are the results of FC, which fall within the statistical uncertainties in our results. The objection to the lattice-sum method applies only to I_9 and I_{10} and, so far as we can tell, there are no other pitfalls lurking in the method. The internal consistency of the results (for different N's) and the agreement with the analytic but approximate work of FC bolster this belief.

A final point is worth mentioning. When evaluating I_1 FC introduce a convergence factor $e^{-\epsilon r}$ in $g(\vec{r})$ in order to get rid of an unwanted term. This physically motivated modification of the trial function was also found to be necessary in the present work. The net effect of the substitution (after ϵ is allowed to approach zero) is to add $-\frac{4}{3}\pi\rho$ to each $H_z^{(i)}$. The reason for the difficulty is that I_1 is essentially the integrated momentum density. It is well known from the theory of classical fluids[10] that such integrals are only conditionally convergent. The introduction of a convergence factor and a density profile $p(r)$ which vanishes near a surface makes the classical integral well defined and equal to the impulse.

III. RESULTS AND DISCUSSION

A. Energy spectrum

The final excitation energy is determined by minimizing (7) with respect to A using the values of I_i determined in the Monte Carlo calculation. In Fig. 3 we plot the quantity E_2/E_1 of FC, which is the ratio of the variational excitation spectrum

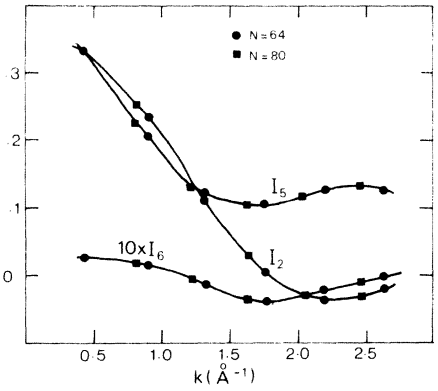

FIG. 1. FC integrals I_2, I_5, and I_6 (in Angstrom units) for the equilibrium density, as a function of wave number. Results of runs with 64 and 80 particles are shown.

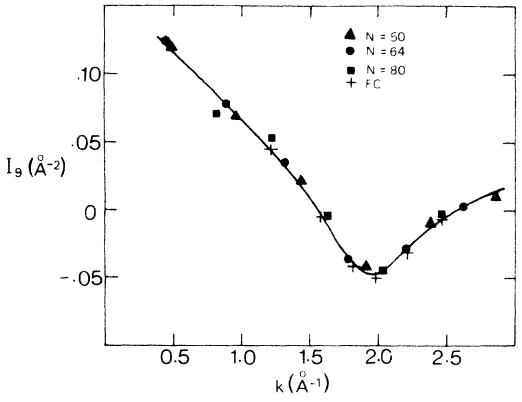

FIG. 2. FC integral I_9, evaluated using Eq. (17), as a function of wave number. Results of runs with 50, 64, and 80 particles are shown. The original calculation of FC is given by the plus symbols.

just determined to the spectrum[3]

$$E_1(k) = \hbar^2 k^2 / 2mS(k). \tag{18}$$

Equation (18) is the "Feynman spectrum" resulting from the trial function

$$\phi \sum_i e^{i\vec{k}\cdot\vec{r}_i}. \tag{19}$$

Results for a number of runs at $\rho = \rho_0$ are shown, together with the values determined by FC. Also shown on the same graph is the optimum value of the variational parameter A.

Noteworthy is the fact that E_2/E_1 approaches unity and A zero for $k \to 0$; this simply reflects the fact that the simple Feynman wave function (19) is exact in this limit. These features are not exhibited by the calculations of FC, however. One should not be surprised at this as one of the approximations in FC depends on the neglect of integrands oscillating from factors of $e^{i\vec{k}\cdot\vec{r}}$, an approximation which fails for small k. We see that trouble sets in for $k \lesssim 1.8$ Å. FC were fortunate indeed as this is just the location of the roton minimum.

In Fig. 4 we plot the actual energy spectrum for three densities, $\rho = \rho_0$, $1.1\rho_0$, and $1.2\rho_0$, which is near the solidification density at $T = 0$. We also show for comparison the neutron scattering data of Yarnell *et al.*[11] The roton parameters we find for $\rho = \rho_0$ are $\Delta = 11.2 \pm 0.5$ K and $k_0 = 1.75 \pm 0.05$ Å^{-1}, compared with $\Delta = 11.5 \pm 0.5$ K and $k_0 = 1.85$ Å^{-1} obtained by FC. The closeness of the agreement is actually somewhat fortuitous, as we discuss below.

The results at higher densities are a little bit surprising. Experimentally[12] the roton gap decreases by about 20% as the density increases to $\rho \approx 1.2\rho_0$. Such a change would be readily resolved in this calculation, but instead we see that Δ comes out independent of pressure within our uncertainty. It is true that the roton minimum is almost twice as deep at $\rho = 1.2\rho_0$ as at $\rho = \rho_0$ and this may be a remnant of the expected behavior. The deepening of the minimum is, however, due mostly to the sharpening of the first peak in $S(k)$. It does not seem, therefore, that the FC wave function is as good as has generally been believed. The error in the wave function, which is one order lower than the error in the energy, must be substantial at the freezing density, where Δ is about 50% higher than experiment. One advantage of the Monte Carlo method is that different and more complex trial functions can be used without generating insurmountable analytical difficulties. Introduction of one additional free parameter would be economically quite feasible, especially if the search were confined to the vicinity of the minimum at k_0. Such calculations should be undertaken.

There may also be a slight shift of k_0 to higher wave number with density, which would be consistent with the 10% shift observed experimentally. The values of the roton effective mass μ at the three densities were found to be approximately $0.17m$, $0.17m$, and $0.13m$, which can be compared with the observed[12] $0.16m$, $0.15m$, and $0.13m$. The behavior of μ reflects the deepening

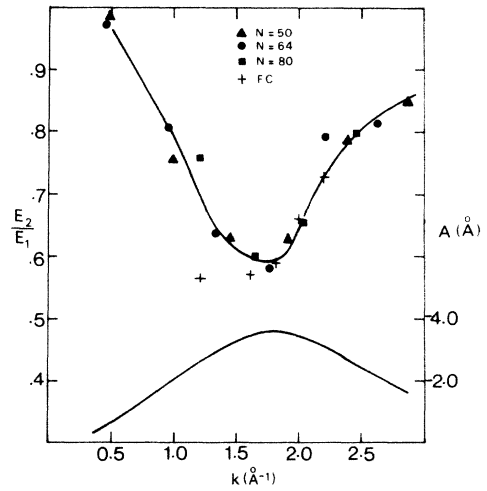

FIG. 3. Upper curve: The ratio E_2/E_1 of the FC spectrum to the Feynman spectrum. The original calculation of FC is given by the plus symbols. Results of runs with 50, 64, and 80 particles are shown. Lower curve: The optimum value of the variational parameter A.

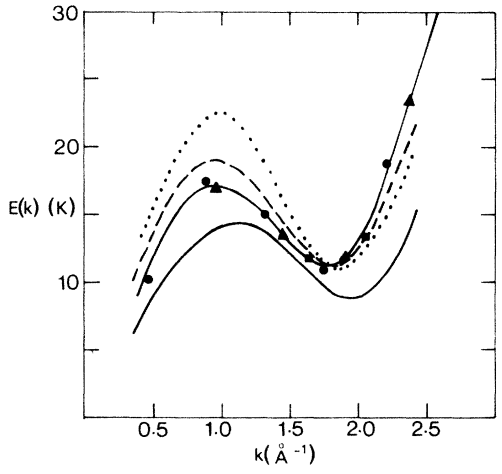

FIG. 4. The FC spectrum, as determined in this work, for three densities: solid line, $\rho = \rho_0$; dashed line, $\rho = 1.1\rho_0$; dots, $\rho = 1.2\rho_0$. The raw computer calculations are shown only for $\rho = \rho_0$. The lower solid curve is the experimental dispersion curve from Ref. 11.

of the roton minimum discussed above.

One curious feature of the results is the closeness of the variational and experimental curves for $k \approx 1.5$ Å. This probably reflects an inadequacy in the representation of the ground state, however, rather than excellence of the trial wave function. In particular, the results depend sensitively on the value of $S(k)$ in this region. We have used the Monte Carlo/molecular-dynamics results for $S(k)$ throughout rather than an experimental $S(k)$. One reason is simply for consistency and the other is that there has been a significant drift in experimental $S(k)$'s over the years.[13] It is interesting to note, however, that the experimental $S(k)$ is in fact slightly smaller in this region than our $S(k)$, which would lead to a larger $E(k)$.

B. FC integrals

The conclusions presented in this section apply to all densities examined although the numbers quoted will refer to $\rho = \rho_0$.

There are two main sources of error in FC which are avoided in the present calculation. The first is the use of the Kirkwood superposition principle and the second is the neglect of terms in various integrals on the basis that oscillating factors of the form $e^{i\vec{k}\cdot\vec{r}}$ render their contributions small, or the assumption that $g_1(\vec{r})$ is slowly varying compared to the correlation functions.

In addition the two calculations can be expected to differ because the ground-state ϕ is different, i.e., the $p(r)$ and $S(k)$ used by FC are not the same as those implied by the Jastrow wave function we have used. As remarked above the excitation spectrum is sensitive to the details of $S(k)$, particularly in the region around $k = 1$ to 1.5 Å^{-1}, where $S(k)$ is changing rapidly. This dependence of the FC spectrum on the ground state has been investigated in detail by Burke *et al.*[14]

The validity of the Kirkwood superposition principle in systems of comparable density (argon at liquid densities) has been investigated by Krumhansl and Wang.[15] Their results are consistent with the FC analytical estimates, which show the approximation to be quite good when used in the I_i's. In fact, the FC estimate of the error introduced by the Kirkwood principle is the order of our own numerical uncertainty so we can do little to improve the estimates of FC.

On the other hand, we have found that some significant errors are introduced by approximations [Eqs. (40) and (41) in FC] based on the assumption that $g_1(r)$ is slowly varying in the range $2 \lesssim r \lesssim 4$ Å. For example, I_6 is estimated by FC to vanish to a precision of 0.001 Å^{-6}; we find (Fig. 2) that I_6, an oscillating function of k, is -0.003 Å^{-6} near the roton minimum. And the estimate $I_7 \approx \frac{4}{3}\pi\rho I_2$ [Eq. (58) in FC] is in error by 0.002 to 0.004 Å^{-6} in the vicinity of the roton minimum. (See Fig. 5.) FC approximate I_5 and I_{10} by neglecting terms containing the oscillatory factor $e^{i\vec{k}\cdot\vec{r}}$, which clearly is a poor approximation for $k \to 0$. But even for $k \approx 2$ Å^{-1} the approximation $I_{10} \approx I_3$ fails by about 10%. I_5 is a constant, according to FC; Fig. 1 shows this is only a rough approximation, although by chance $I_5(k)$ is fairly flat in the vicinity of k_0.

Each of the errors discussed in the previous paragraph typically lead to an error of 5% or so in $E(k)$ or E_2/E_1, and differences in $S(k)$ and $g(r)$ could easily account for another 5 to 10%. A net error of 20% or more would not have been unexpected. That our result $\Delta = 11.2$ K is within 0.3 K of FC is therefore a surprise.

The Monte Carlo averages for the normalization integrals I_8, I_9, and I_{10} are very noisy and limit the precision of the calculation. The noisiest of these is $I_8 = S(k)$. Fortunately, however, I_8, involving only a single sum, is an order of magnitude cheaper to calculate than the other I's. Hence in the results presented here we have used values of $S(k)$ taken from much more extended Monte Carlo runs. The only effect of using the accurate $S(k)$'s is to reduce the scatter of the results by about a factor of 2. The central values do not seem to be affected.

IV. CONCLUSIONS

We have been able to carry out a complete and consistent Monte Carlo calculation of the FC in-

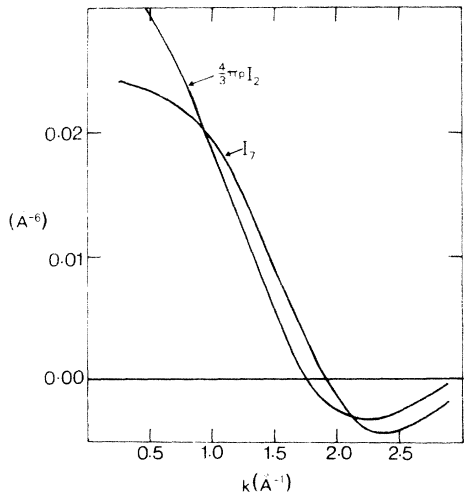

FIG. 5. FC integrals I_2 and I_7, as a function of wave number, as determined in this work.

tegrals, without recourse to approximations other than the Jastrow approximation to the ground state. Our results differ in detail, at points substantially, from FC. The roton parameters, however, are in substantial, albeit somewhat fortuitous, agreement with FC.

Calculations at elevated densities did not show the expected decrease of Δ with density, raising a question as to the excellence of the FC wave function. The Monte Carlo approach allows, however, the possibility of treating more realistic wave functions.

We plan to extend these calculations to two dimensions in the hope of gaining insight into the properties of rotonlike states in films and restricted geometries where large van der Waals forces restrict the motion of the helium atoms.

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APPENDIX A: SPARSE AVERAGING

The complex nature of the averages we evaluate in this work makes the sparse averaging technique described in Sec. II B very useful. This method, suggested by Woods,[6] and used by Murphy *et al.*[7] to evaluate three- and four-point averages, consists of averaging over a relatively few configurations selected from the totality of configurations generated by the Monte Carlo program. If the sampling interval is sufficiently small very little statistical information is lost; the larger the interval, of course, the lower the computing costs.

We made a number of runs for liquid helium employing the usual "block-averaging" system and also sparse averaging with an interval of $4N$ (four passes through the N particles). The results for averages of r^{-6}, r^{-12}, and r^{-7} agreed to within statistical errors. Furthermore the statistical deviations were essentially equal for the two methods.

The interval $4N$, which implies that each particle has been moved an average of about two times, seems about optimum for simple averages like $\langle r^n \rangle$. This implies a saving (presuming no loss of information) of about a factor of 2 in the time taken to calculate the averages. Intervals of $6N$ and $8N$ were used in the present work for two reasons: (i) Even for an interval of $8N$ it still took substantially longer to evaluate the averages than to generate the configurations. (ii) For an interval of $4N$ weak correlations between successive configurations were detected in some of the I_i.

APPENDIX B: LATTICE SUMS

The most general and elegant method for doing lattice sums that we know of is the method described by Nijboer and de Wette[16] which involves splitting the sum into a highly convergent part and a part which is Fourier transformed to make it convergent also.

For our purposes their method suffers on two counts. First, it involves two sums, and also special functions which are inconvenient. Second, for one of the lattice sums we need their method does not converge. Consequently we used a much more naive, but, for our purposes, equally effective method.

We have to evaluate lattice sums of the type

$$A = \sum_{\lambda} f(\vec{r}_{\lambda} - \vec{R}), \tag{B1}$$

where $\vec{r}_{\lambda}$ are lattice vectors indexed with λ. We write this

$$A = A^{(\mathrm{in})} + A^{(\mathrm{out})}, \tag{B2}$$

where in $A^{(\mathrm{in})}$ the summation goes over the lattice vectors in a (small) cube centered at the origin and $A^{(\mathrm{out})}$ includes all the other terms.

Now expand

$$A^{(\mathrm{out})} = A^{(\mathrm{out})}(\vec{0}) - \vec{R}\cdot\nabla A^{(\mathrm{out})}(\vec{0}) + (\text{higher-order terms}). \tag{B3}$$

Because of the cubic symmetry, for the case $f(\vec{r}) = (\cos\theta)/r^2$ the first nonzero term in (B3) is

$$-\tfrac{1}{6}\vec{R}\vec{R}\vec{R}:\nabla\nabla\nabla A^{(\mathrm{out})}(0) = -\tfrac{1}{6}\vec{R}\vec{R}\vec{R}:\sum_{\lambda}^{(\mathrm{out})}\nabla\nabla\nabla f(\vec{r}_{\lambda}). \tag{B4}$$

Performing the indicated operations and using the cubic symmetry one finds

$$A^{(\mathrm{out})} \approx c[\tfrac{1}{3}z^3 - \tfrac{1}{2}(x^2+y^2)z], \tag{B5}$$

where

$$c = \sum_{\lambda}^{(\mathrm{out})} \tfrac{1}{2}(105 z_{\lambda}^4 - 21 r_{\lambda}^4) r_{\lambda}^{-9} \tag{B6}$$

and

$$\vec{R} = (x, y, z), \quad \vec{r}_{\lambda} = (x_{\lambda}, y_{\lambda}, z_{\lambda}).$$

Equation (B6) can be evaluated once and for all by the method of Nijboer and de Wette or by brute force. The answer, taking the sum in $A^{(\mathrm{in})}$ over the nine lattice vectors nearest the origin, is

$$c = 1.406. \tag{B7}$$

We also need the components (ζ, η, ξ) of ∇A and we similarly find

$$\zeta^{(\mathrm{out})} = -c[\, z^2 - \tfrac{1}{2}(x^2+y^2)]\,,$$
$$\eta^{(\mathrm{out})} = cyz\,, \tag{B8}$$
$$\xi^{(\mathrm{out})} = cxz\,.$$

We found that so long as $\vec{R}$ is referred to the nearest lattice point that (B5), (B7), and (B8) give A and ∇A accurate to about 0.1%, which was adequate for our purposes. If more accuracy is desired, more λ's can be included in $A^{(\mathrm{in})}$ but because the convergence goes like a power it eventually becomes advantageous to switch to a method like that of Nijboer and de Wette where the convergence is exponential.

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