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Excitation Spectrum for a Bose Gas with Repulsive Core and Attractive Well

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The correct qualitative features of the helium II elementary excitation spectrum are derived microscopically for a realistic interparticle potential using a form of pair Hamiltonian. The strong repulsive core is included by using reaction matrix elements in the Hamiltonian, and the attractive well is successfully included by assuming a generalized Bose-Einstein condensation. The pair Hamiltonian is diagonalized by the thermodynamically equivalent Hamiltonian method of Wentzel. Numerical solution of the equations yields spectra with phonon and roton regions. Since the energies in the spectrum are too high when the Yntema-Schneider potential is used, another potential is constructed which still fits the second-virial-coefficient data and gives better results. Spectra calculated for a series of attractive well strengths show the effect of weaker wells.

I. INTRODUCTION

The attempts which have been made to derive the fundamental excitation spectrum of superfluid helium have met with success and with difficulties, depending on the level of the approach. On the successful side are the phenomenological theories with empirically adjusted parameters such as those of Landau[1] and of Feynman.[2] On the less successful side are the microscopic theories which attempt to derive the properties of liquid helium II from the interatomic forces of helium atoms. No microscopic theory has been able to predict the energy spectrum for a realistic potential. Prior to the present work, not even the qualitative features of the spectrum (the phonon-like part and the roton minimum) have been successfully derived from an interatomic potential including both a strong repulsive core and an attractive well.

The spectrum has been measured experimentally by neutron scattering.[3,4] A chief aim of the many-body problem for helium is to derive this spectrum from the theoretically or experimentally determined interatomic forces of helium atoms, without further input from experiments. This work derives the spectrum from a realistic interparticle potential by combining three methods. First, a generalized or "smeared" Bose-Einstein condensation is assumed because the scattering length of the interparticle potential is negative. Second, a modified Brueckner reaction matrix is introduced to handle the strong repulsive core of the helium potential. Third, the "thermodynamically equivalent Hamiltonian" (TEH) method of Wentzel[5,6] is used to include all forward, exchange, and pair scattering interaction terms.

II. THE IMPERFECT BOSE GAS

The microscopic problem of the imperfect Bose gas has been considered by numerous authors.[5–16] The starting point is the second quantized Hamiltonian for a system of interacting bosons:

$$H=\sum_k (\hbar^2k^2/2m)a_k^\dagger a_k + \tfrac{1}{2}\sum_{k_1k_2k_3k_4} \langle k_1k_2|V|k_3k_4\rangle a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}\,, \qquad (1)$$

where $a_k^\dagger$ and a_k are the creation and destruction operators for a plane-wave state with propagation vector $\vec{k}$, the interaction potential $v(r)$ is a spherically symmetric function of the distance r between two atoms, and appears here in matrix elements with respect to free-particle two-body states, e.g., $\langle \vec{k}_1\vec{k}_2|V|\vec{k}_3\vec{k}_4\rangle$. Summation indices are to be understood to be vectors. The full Hamiltonian (1) has not been diagonalized. The Hamiltonian to be used here is a truncated one, the "pair Hamiltonian" of Girardeau and Arnowitt.[14] All interaction terms are neglected except those known as forward scattering, exchange scattering, and pair scattering. These three types of terms are shown in Fig. 1. The truncated Hamiltonian, which we shall call the pair Hamiltonian H_p, is

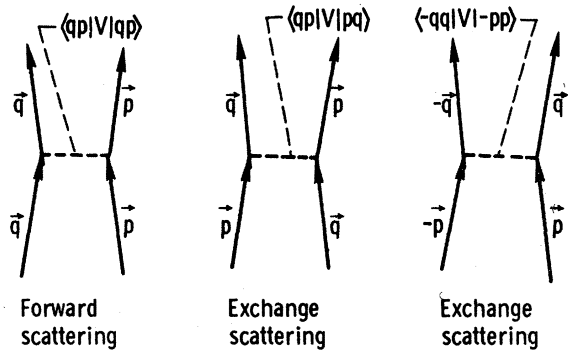

FIG. 1. Interaction terms retained in the pair Hamiltonian. Solid lines represent particles with wave numbers as labeled. Dotted line represents the interaction and is labeled by the appropriate matrix element.

$$\begin{aligned} H_p &= \sum_p (\hbar^2 p^2/2m) a_p{}^\dagger a_p \\ &+ \sum_{qp} \langle qp|V|qp\rangle a_q{}^\dagger a_p{}^\dagger a_q a_p \\ &+ \frac{1}{2} \sum_{\substack{qp \\ q\neq\pm p}} \langle qp|V|pq\rangle a_q{}^\dagger a_p{}^\dagger a_p a_q \\ &+ \frac{1}{2} \sum_{\substack{qp \\ q\neq p}} \langle -qq|V|-pp\rangle a_{-q}{}^\dagger a_q{}^\dagger a_{-p} a_p \,. \end{aligned} \tag{2}$$

Here we do not introduce the Fourier transform $\hat{v}(k)$ of the interaction potential because the theory to follow does not depend solely on the momentum transfer k. The restrictions on the sums are necessary to prevent duplication of terms.

Even the simplified Hamiltonian (2) has not been diagonalized. If two additional simplifications are made, diagonalization can be achieved. These are: (1) keeping only those interaction terms containing at least two creation or annihilation operators with subscript zero, (2) approximate both $a_0{}^\dagger$ and a_0 by N. If the potential is repulsive, i.e., $\hat{v}(0) > 0$, the resulting Bogoliubov Hamiltonian can be diagonalized. The second simplification, known as the Bogoliubov approximation, is justified for weak interactions near absolute zero because nearly all particles are expected to be in the zero-momentum state. The Bogoliubov Hamiltonian can be diagonalized by the Bogoliubov transformation, which will be used later. A phonon spectrum for low momenta occurs in this approximation and a free-particle spectrum at high momenta. In the intermediate range of momenta the spectrum has a region connecting the linear and quadratic sections. For an appropriate repulsive potential this region could have the general shape of the roton region of the liquid-helium spectrum. The model thus has two features resembling liquid helium: the low-momentum phonon spectrum and at least a hint of a roton region.

Girardeau and Arnowitt[14] used a variational method to consider the entire pair Hamiltonian of Eq. (2) without making the Bogoliubov approximation. Wentzel[5] and Luban[6] studied this Hamiltonian allowing thermal excitation and found a simpler diagonalizable Hamiltonian which gives the same thermodynamics as that of Eq. (2). Results of all three of these studies show an energy gap in the low-momentum excitation spectrum. That is,

$$E(0) = 0, \quad \text{but} \lim_{k\to 0} E(k) \neq 0 \,.$$

These results are for weak interparticle potentials with $\hat{v}(0) > 0$ and the assumption that Bose-Einstein condensation takes place with particles "condensing" into the zero-momentum state. The spectrum of this pair Hamiltonian model, which includes more terms than the Bogoliubov Hamiltonian, is, nevertheless, further from that of helium II.

There are two important differences between the interparticle potential used in the above studies and the actual helium potential. First, the helium potential is strongly repulsive at small distances. Second, the scattering length for helium is negative. (In fact, the scattering length is so negative that the atoms can almost form a two-body bound state.) For a potential with a singular repulsive core, as in helium, the sign of the scattering length plays the role that the sign of $\hat{v}(0)$ plays in a weak potential, roughly speaking. Thus one may expect a system of atoms with negative scattering length to correspond more nearly to a system with $\hat{v}(0) < 0$ than to one with $\hat{v}(0) > 0$. The repulsive core and the negative scattering length each require changes from the methods used by the authors mentioned in the previous paragraph.

III. METHODS

Three main methods will now be described, which in combination allow a potential with a singular repulsive core and an attractive well to be studied using the pair Hamiltonian. To deal with potentials with negative scattering length (like helium), a generalized or "smeared" Bose-Einstein condensation is assumed. To avoid the infinite matrix elements of the repulsive core, a type of reaction matrix is used in place of the potential. Finally, to obtain a diagonalized form from the pair Hamiltonian, the Wentzel method of the thermodynamically equivalent Hamiltonian is used. These three methods are discussed in the following sections.

A. Generalized Bose-Einstein Condensation

Consider first the effect of having a potential with $\hat{v}(0) < 0$. Girardeau[15] has given arguments to show that; for weak attractive potentials, the lowest energy state is not one in which the zero-momentum state contains a finite fraction of the particles (simple Bose-Einstein condensation). It is, rather, one in which a larger number of distinct low-momentum states contain a finite fraction of the particles but any single state contains only a negligibly small fraction. One assumes that in this generalized condensation all states with momentum less than a cutoff momentum p_0 have zero energy. A finite fraction of the particles occupy the group of states, but no single state, not even the $p = 0$ state, contains a finite fraction. The group of states containing the condensed particles draws arbitrarily close to zero momentum and bears a deceptive resemblance to simple condensation. It is the fact that no *single* state is macroscopically occupied (that is, contains a finite fraction of the total particles) that distinguishes the two types of condensation.

In Ref. 6 the descriptive statements about generalized condensation are formulated as follows. As the thermodynamic limit is taken, that is, $N \to \infty$ with N/Ω constant,

$$\begin{gathered} p_0 = O(\Omega^{-x}), \quad (x > 0) \\ \langle a_p{}^\dagger a_p\rangle = O(\Omega^{x(p)}), \quad \text{for } |p| < p_0, \\ \text{and } 0 < x(p) = O(1) < 1 \,, \\ \text{and } \sum_{|p|<p_0} \langle a_p{}^\dagger a_p\rangle = O(\Omega) \,. \end{gathered} \tag{3}$$

The results of three studies support the assumption of a smeared condensation. Girardeau demonstrates by variational means that smearing gives a lower energy for weakly attractive systems than does a simple condensation. Sawada and Vasudevan[17] have shown in a simplified model with negative scattering length, that the states into which the particles condense should be a combination of zero- and nonzero-momentum states. This combination of states may be viewed as a smeared condensation. Additional incentive to investigate the smeared type of condensation is provided by the work of Luban (Appendix E of Ref. 6). He showed that in the pair Hamiltonian model with a hard-core pseudopotential and weak attractive interactions, a smeared condensation leads to a phononlike spectrum for low-momentum excitations rather than to the energy gap predicted by simple condensation. The modifications to be made below to treat strong potentials do not change the character of these low-momentum excitations if the scattering length is negative, but give a more correct treatment of the hard-core part of the potential.

B. The Reaction Matrix

To treat an interparticle potential with a strong repulsive core, the pair Hamiltonian is inadequate as it stands. The matrix elements of the interaction potential that appear in Eq. (2) are arbitrarily large for arbitrarily strong cores. However, one can still make progress by summing enough terms in a many-body perturbation series of the exact Hamiltonian to obtain a finite result. Some of the terms that must be summed are not contained in a perturbation series derived from Eq. (2), but these can be introduced by a rather simple modification of the Hamiltonian. The method used here to effect this presumming is similar to that of Brueckner and Sawada.[9] The matrix elements of the interparticle potential operator are replaced by the elements of a type of reaction matrix. Since the reaction matrix K is defined by

$$K = V + VGK, \qquad (4)$$

where V is the exact two-body potential operator and G is a Green's function operator, it has an expansion of the form

$$K = V + VGV + VGVGV + \cdots .$$

The use of matrix elements of K in place of matrix elements of V (which is the first term in the expansion of K) brings many more interaction terms into the Hamiltonian without complicating its form.

The arguments for replacement of V by K and the selection of the operator G are made in Appendices A and B by considering the many-body perturbation expansion of the free energy. The perturbation expansion of the free energy based on the pair Hamiltonian containing K's instead of V's is more nearly like the expansion of the free energy based on a complete (nontruncated) Hamiltonian. The operator G must be appropriately chosen, however. The argument in Appendix A shows that $G = -1/H_0$ can be used, where H_0 is the kinetic-energy operator.

Matrix elements of K with respect to two-body plane-wave states are needed in the truncated Hamiltonian. To reduce the calculation of the matrix elements to manageable proportions, the matrix elements of K with respect to two-body states are approximated by elements with respect to one-body "center-of-mass" states. Details of this center-of-mass approximation, and the types of matrix elements needed are given in Appendix B. The important results from the Appendix are:

(1) Matrix elements $\langle \vec{k}\,\vec{p}\,|V|\,\vec{q}\,\vec{r}\rangle$ in the Hamiltonian are replaced by the corresponding reaction matrix elements $\langle \vec{k}\,\vec{p}\,|K|\,\vec{q}\,\vec{r}\rangle$.

(2) The two-body elements $\langle \vec{k}\,\vec{p}\,|K|\,\vec{q}\,\vec{r}\rangle$ are approximated by the one-body center-of-mass elements $\langle \tfrac{1}{2}(\vec{k}-\vec{p})|K|\tfrac{1}{2}(\vec{q}-\vec{r})\rangle$. The integral equation $K = V + VGK$ for these one-body elements is decomposed into a similar equation for each partial wave by expanding all elements of the matrices in spherical harmonics. The integral equation for each partial wave can be solved numerically. Only even partial waves are needed, and three of these give sufficient accuracy in the energy spectrum from zero momentum to just past the roton minimum.

C. The Thermodynamically Equivalent Hamiltonian

The modification of the truncated Hamiltonian of Eq. (2) to allow treatment of strongly repulsive cores has not changed its basic form. It is still of the type which can be treated by the thermodynamically equivalent Hamiltonian (TEH) method of Wentzel.[5,6] In the first part of this section the meaning of "thermodynamically equivalent" is discussed, and especially the question of how this method can be applied in the present work where the use of the reaction matrix has been justified only in the limit as temperature $T \to 0$.

The essence of Wentzel's method is that a simpler Hamiltonian can be found which can be exactly diagonalized by the Bogoliubov transformation but which gives the same partition function as (2) in the limit as $\Omega \to \infty$ (the thermodynamic limit). Two systems with the same partition function have exactly the same thermodynamics, but in general, this does not guarantee microscopic similarity. The microscopic similarity is a central point of this work, however, in which we attempt to find the energy spectrum of elementary excitations (normal modes) in a dense Bose gas resembling helium. The relation, if any, between the spectrum of excitations found by diagonalizing the thermodynamically equivalent Hamiltonian and the experimentally determined spectrum of excitations[3,4] for liquid helium must be examined.

The grand partition function of a general interacting system is

$$Q(\beta,\mu) = \sum_{\substack{\text{all distin-}\\\text{guishable}\\\text{states}}} \exp[-\beta(E_{\text{state}} - \mu N)] ,$$

where N is the number of particles in the state. If one could diagonalize the system Hamiltonian (2) so it could be written

$$H = \sum_k E_k \alpha_k^{\dagger} \alpha_k ,$$

where $a_k{}^\dagger$ creates $|\vec{k}\rangle$, a state with quantum numbers $\vec{k}$, then the partition function would be

$$Q(\beta, \mu) = \sum_{\{n_k\}} \exp[-\beta \textstyle\sum_k (E_k - \mu) n_k]$$

$$\equiv \sum_{\{n_k\}} \exp[-\beta \textstyle\sum_k \epsilon_k n_k], \qquad (5)$$

where the sum over $\{n_k\}$ indicates a sum over all possible sets of occupation numbers n_k. The energies ϵ_k in this last expression are temperature independent numbers. Wentzel's method diagonalizes the truncated Hamiltonian (3) in the sense that

$$Q(\beta, \mu) = \sum_{\{n_k\}} \exp[-\beta \textstyle\sum_k \epsilon_k(\beta) n_k]. \qquad (6)$$

Here, as in Eq. (5), the summation runs over all sets of occupation numbers n_k. The partition function of Eq. (6) is constructed to be equal to that of Eq. (5) for any β, but in general $\epsilon_k(\beta)$ bears no simple relation to ϵ_k of Eq. (5). If, however, for a range of temperature from zero to some finite temperature T_f, the quantities μ and $\epsilon_k(\beta)$ are independent of temperature, then one expects that

$$\epsilon_k(\beta) = \epsilon_k, \quad \text{for } T < T_f .$$

It is found that the $\epsilon_k(\beta)$ are temperature independent near $T = 0$ because the integral equations that determine the $\epsilon_k(\beta)$ are not sensitive to temperature near $T = 0$. The physical reason for this is that the lowest energy excitations are phonon-like, that is, their energies are proportional to momentum. This type of excitation spectrum is much more rigid against thermal excitation than, for example, a quadratic free-particle spectrum. In the former case many fewer states have energies of the order of kT than in the latter case. This rigidity against excitations causes the number of excited particles to be relatively constant near zero temperature. This, in turn, leads to the insensitivity of the excitation spectrum and all thermal expectation values to temperature as $T \to 0$. Thus the phonon-like spectrum leads to the temperature independence of $\epsilon_k(\beta)$ as $\beta \to \infty$ ($T \to 0$) and hence to the assertion that the $\epsilon_k(\beta \to \infty)$ found by Wentzel's method is the same as the ϵ_k normal mode spectrum.

IV. INTEGRAL EQUATIONS FOR THE SPECTRUM

Consider again the pair Hamiltonian, replacing the V-matrix elements with the corresponding K-matrix elements.

$$H_P = \sum_k \left(\frac{\hbar^2 k^2}{2m} - \mu - \frac{1}{2} K_{kkkk}\right) a_k{}^\dagger a_k + \frac{1}{2} \sum_{\substack{qp \\ q \neq p}} K_{qpqp} a_q{}^\dagger a_q a_p{}^\dagger a_p + \frac{1}{2} \sum_{\substack{pq \\ p \neq \pm q}} K_{pqpq} a_p{}^\dagger a_q{}^\dagger a_q a_p$$

$$+ \frac{1}{2} \sum_{\substack{pq \\ p \neq q}} K_{-qq-pp} a_{-q}{}^\dagger a_q{}^\dagger a_{-p} a_p , \qquad (7)$$

where $K_{pqrs} = \langle pq | K | rs \rangle$.

(Note that $\sum_{pq} K_{qpqp} a_q{}^\dagger a_p{}^\dagger a_q a_p = \sum_{pq} K_{qpqp} a_q{}^\dagger a_q a_p{}^\dagger a_p - \sum_k K_{kkkk} a_k{}^\dagger a_k$.)

The form (7) can be treated by the TEH method.[5,6] As in Luban's version[6] of Wentzel's method, μ, the chemical potential, has been inserted in H_P to facilitate using the grand ensemble. This is soon eliminated from the equations. To find the TEH, first define new operators B_k, $B_k{}^\dagger$, C_k, and $C_k{}^\dagger$:

$$a_k{}^\dagger a_k \equiv B_k + \xi_k, \quad a_{-k} a_k \equiv C_k + \eta_k ,$$

where the values of the real c numbers ξ_k and η_k will be chosen to eliminate some terms from the new equivalent Hamiltonian. Note that $B_k{}^\dagger = B_k$ $K_{qpqp} = K_{pqpq}$, and $K_{qppq} = K_{pqqp}$. (The reaction matrix element is symmetric with respect to interchange of the first and second pairs of indices.) Using these facts and manipulating the dummy indices yields

$$H_P = \textstyle\sum_k (\hbar^2 k^2/2m - \mu - \frac{1}{2} K_{kkkk}) a_k{}^\dagger a_k + \frac{1}{2} \sum_{pq} K_{qpqp} (B_p{}^\dagger B_q + 2\xi_p a_q{}^\dagger a_q - \xi_p \xi_q)$$

$$+ \frac{1}{2} \sum_{\substack{pq \\ p \neq \pm q}} K_{qppq} (B_q{}^\dagger B_p - 2\xi_p a_q{}^\dagger a_q + \xi_p \xi_q) + \frac{1}{2} \sum_{\substack{pq \\ p \neq q}} K_{-qq-pp} [C_q{}^\dagger C_p + \eta_p (a_q{}^\dagger a_{-q}{}^\dagger + a_q a_{-q}) - \eta_q \eta_p] .$$

Now collect the terms into two groups, putting those containing B, $B^\dagger$, C, and $C^\dagger$ into

$$H_1 = \frac{1}{2}\sum_{qp} K_{qpqp} B_p{}^\dagger B_q + \frac{1}{2}\sum_{\substack{pq\\ p\neq\pm q}} K_{qppq} B_q{}^\dagger B_p + \frac{1}{2}\sum_{\substack{pq\\ p\neq q}} K_{-qq-pp} C_q{}^\dagger C_p .$$

All the other terms are put into

$$H_{\mathrm{TE}} = U + \sum\nolimits_k (\hbar^2 k^2/2m - \mu - \tfrac{1}{2}K_{kkkk}) a_k{}^\dagger a_k + \sum\nolimits_{qp} K_{qpqp} \xi_p a_q{}^\dagger a_q$$

$$+ \sum_{\substack{qp\\ q\neq\pm p}} K_{qppq} \xi_p a_q{}^\dagger a_q + \frac{1}{2}\sum_{\substack{qp\\ q\neq p}} K_{-qq-pp} \eta_p (a_q{}^\dagger a_{-q}{}^\dagger + a_q a_{-q}),$$

where

$$U = -\frac{1}{2}\sum_{qp} K_{qpqp} \xi_p \xi_q - \frac{1}{2}\sum_{\substack{pq\\ p\neq\pm q}} K_{qppq} \xi_p \xi_q - \frac{1}{2}\sum_{\substack{qp\\ q\neq p}} K_{-qq-pp} \eta_p \eta_q ,$$

which is a c number. Let

$$f_k = \frac{\hbar^2 k^2}{2m} - \mu - \frac{1}{2}K_{kkkk} + \sum_p K_{kpkp} \xi_p + \sum_{p\neq\pm k} K_{kppk} \xi_p, \quad h_k = \sum_{p\neq k} K_{-kk-pp} \eta_p . \tag{8}$$

Then $H_{\mathrm{TE}} = U + \sum_k f_k a_k{}^\dagger a_k + \frac{1}{2}\sum_k h_k (a_k{}^\dagger a_{-k}{}^\dagger + a_k a_{-k})$. (9)

According to the TEH method, H_{TE} will lead to the same thermodynamic properties as H_P if ξ_p and η_p are chosen as $\xi_p = \langle a_p{}^\dagger a_p \rangle$ and $\eta_p = \langle a_p{}^\dagger a_{-p}{}^\dagger \rangle = \langle a_{-p} a_p \rangle$, where the bracket denotes average over a grand ensemble. This result remains valid for the Hamiltonian which has resulted from replacement of V-matrix elements by K-matrix elements.

We now use the Bogoliubov transformation to diagonalize Eq. (9). Let

$$a_k{}^\dagger = u_k \alpha_k + v_k \alpha_k{}^\dagger, \quad \text{and} \quad a_k = u_k \alpha_k{}^\dagger + v_k \alpha_k .$$

We also require that

$$f_k u_k v_k + \tfrac{1}{2} h_k (u_k{}^2 + v_k{}^2) = 0, \quad u_k{}^2 = f_k/(2\epsilon_k) + 1, \quad v_k{}^2 = h_k/(2\epsilon_k) - 1,$$

and $u_k v_k = -h_k/(2\epsilon_k)$, where $\epsilon_k = (f_k{}^2 - h_k{}^2)^{1/2}$. (10)

With these conditions on u_k and v_k the TEH is diagonalized as follows:

$$H_{\mathrm{TE}} = U_o + \sum\nolimits_k \epsilon_k \alpha_k{}^\dagger \alpha_k, \quad \text{where} \quad U_o = U + \sum\nolimits_k (\epsilon_k - f_k)/2 . \tag{11}$$

The Bogoliubov transformation is not valid for any $\vec{k}$ for which $\epsilon_k = 0$. In a "smeared" condensation there is a group of states with $\epsilon_k = 0$, but these states are grouped arbitrarily close to $k = 0$ in the limit of infinite system volume. Since all the equations are to be solved only in the limit of infinite volume, the Bogoliubov transformation can be performed for all states not in the condensate, i.e., that have finite momenta. The generalized or smeared Bose-Einstein condensate exists in states with $\epsilon = 0$, and it is not necessary to perform any transformation to find the energy of these states. The number of particles in these states is the difference between the number in excited states and the total number.

In Eq. (8) the limit as k approaches zero gives [denoting $\lim\limits_{k\to 0} f(k)$ by $f(0)$ and $\lim\limits_{k\to 0} h(k)$ by $h(0)$]

$$\text{(a)} \quad f(0) = -\mu - K_{0000} + \sum\nolimits_p K_{0p0p} \xi_p + \sum\nolimits_p K_{0pp0} \xi_p, \quad \text{(b)} \quad h(0) = \sum\nolimits_p K_{00-pp} \eta_p . \tag{12}$$

Because $\epsilon(0) = [f^2(0) - h^2(0)]^{1/2} = 0$ for BE condensation, we must have $f(0) = \pm h(0)$. Paralleling Luban[6] we choose $f(0) = -h(0)$. Then μ can be eliminated from the equations using Eq. (12):

$$-\mu = \tfrac{1}{2}K_{0000} - K_{0000}\left(\sum_{p<p_0} \xi_p + \sum_{\substack{p<p_0\\ p\neq 0}} (\xi_p + \eta_p)\right) - \sum_{p>p_0} K_{0p0p}\xi_p - \sum_{p>p_0} K_{0pp0}\xi_p - \sum_{p>p_0} K_{00-pp}\eta_p .$$

Equations (8) become

$$f_k=\frac{\hbar^2k^2}{2m}+\sum_{p<p_0}\xi_p(K_{k0k0}+K_{k00k}-K_{0000})-K_{0000}\sum_{\substack{p<p_0\\p\neq0}}(\xi_p+\eta_p)$$
$$+\sum_{p>p_0}(K_{pkpk}+K_{pkkp}-K_{p0p0}-K_{p00p})\xi_p-\sum_{p>p_0}K_{00p-p}\eta_p,$$

$$h_k=\sum_{p<p_0}K_{k-k00}\eta_p+\sum_{\substack{p>p_0\\p\neq k}}K_{k-kp-p}\eta_p\ ,$$

where terms with $p<p_0$ are separated from the sums, and continuity of the K-matrix elements near zero momenta with respect to any of the indices is used. Two terms, $\frac{1}{2}K_{0000}$ and $-\frac{1}{2}K_{kkkk}$, have been dropped from f_k because they cancel in the center-of-mass approximation (see Appendix B). It was shown by Luban[6] that in the thermodynamic limit as $p\rightarrow0$, $\eta_p\rightarrow\xi_p+\frac{1}{2}$. Then, since $\xi_p=\langle a_p{}^\dagger a_p\rangle$, the sums over $p<p_0$ of ξ_p and η_p are merely the ensemble averages of the number of particles in the smeared condensate. If this number is N_0, and the sums are replaced by integrals by using $\sum_p\rightarrow(\Omega/8\pi^3)\int d^3p$, then

$$f_k=\hbar^2k^2/2m+N_0(K_{k0k0}+K_{k00k}-3K_{0000})+[\Omega/(2\pi)^3]\int[(K_{pkpk}+K_{pkkp}-K_{p0p0}-K_{p00p})\xi_p-K_{00p-p}\eta_p]d^3p\,,$$

$$h_k=N_0K_{k-k00}+[\Omega/(2\pi)^3\int K_{k-kp-p}\eta_p d^3p\ .$$

Note that in the integral form it is permissible to ignore the restrictions $\vec{p}\neq\vec{k}$, $\vec{p}\neq\pm\vec{k}$, and $p>p_0$ and to carry out the integrals throughout $\vec{p}$ space. The first two restrictions do not affect the integration since the excluded discrete states, $\vec{p}=\vec{k}$ or $\vec{p}=\pm\vec{k}$, make negligible contributions. In the thermodynamic limit, p_0 is assumed to approach 0, and the interval of integration that would be excluded by the last restriction makes a negligible contribution.

From Ref. (6)

$$\xi_k=\tfrac{1}{2}[(f_k/\epsilon_k)\coth(\tfrac{1}{2}\beta\epsilon_k)-1];\quad \eta_k=-\tfrac{1}{2}(h_k/\epsilon_k)\coth(\tfrac{1}{2}\beta\epsilon_k)\,.$$

The one remaining relation[18] needed is

$$N=\sum_k\langle a_k{}^\dagger a_k\rangle=\sum_k\xi_k,\quad\text{or}\quad N_0=N-[\Omega/(2\pi)^3]\int\xi_k d^3k\ .$$

These equations constitute a set of nonlinear coupled integral equations. Once the necessary elements of the reaction matrix K are calculated, the equations may be solved numerically for $\epsilon(k)$, the quasiparticle energy spectrum, and for N_0/N, the fraction of particles (not quasiparticles) in the zero-momentum state.

It is convenient for numerical solution (and for simplicity of form) to put the integral equations in dimensionless form. This can be done by making the following definitions:

$$x\equiv ka,\quad y\equiv pa,\quad \gamma\equiv\frac{r}{a};\quad F(x)\equiv\frac{2ma^2}{\hbar^2}f_k,\quad H(x)\equiv\frac{2ma^2}{\hbar^2}h_k,\quad E(x)\equiv\frac{2ma^2}{\hbar^2}\epsilon_k\ ;$$

$$P\equiv\frac{N}{\Omega}a^3,\quad P_0\equiv\frac{N_0}{\Omega}a^3,\quad B\equiv\frac{\hbar^2}{2ma^2}\beta;\quad \mathcal{K}_{pqrs}\equiv\frac{\Omega m}{4\pi\hbar^2a}K_{pqrs},\quad \mathcal{V}(\gamma)\equiv\frac{ma^2}{\hbar^2}v(r)\ ;$$

where a is a reference dimension, taken to be 2.3 Å, the approximate core size, in this work. In these dimensionless quantities the equations are

$$F(x)=x^2+8\pi P_0(\mathcal{K}_{x0x0}+\mathcal{K}_{x00x}-3\mathcal{K}_{0000})$$
$$+(1/\pi^2)\int d^3y\,\xi_y(\mathcal{K}_{xyxy}+\mathcal{K}_{xyyx}-\mathcal{K}_{y0y0})-\mathcal{K}_{y00y}-(4/\pi)\int_0^\infty y^2dy\ \mathcal{K}_{00y-y}\eta_y\,, \tag{13a}$$

$$H(x)=8\pi P_0\mathcal{K}_{x-x00}+(4/\pi)\int_0^\infty y^2dy\ \mathcal{K}_{x-xy-y}\eta_y\,, \tag{13b}$$

$$E(x)=[F^2(x)-H^2(x)]^{1/2},\ \text{(13c)};\qquad P_0=P-(2\pi^2)^{-1}\int_0^\infty\xi_y y^2dy\ . \tag{13d}$$

As discussed in Appendix B, a general element $K_{\vec{x}\vec{y}\vec{z}\vec{u}}$ of the reaction matrix is approximated in this work by the one particle, center-of-mass reaction matrix element $K_{\frac{1}{2}(\vec{x}-\vec{y}),\frac{1}{2}(\vec{z}-\vec{u})}$. Hence, $K_{\vec{x}0\vec{x}0}$ is replaced by $K_{\frac{1}{2}\vec{x},\frac{1}{2}\vec{x}}$, for example. The equations for the one-particle reaction matrix elements, analyzed in partial waves, are

$$\langle\vec{k}|\mathcal{K}|\vec{p}\rangle=\sum_l(2l+1)P_l(\hat{k}\cdot\hat{p})\langle k|\mathcal{K}|p\rangle_l, \tag{14a}$$

where $\langle k|\mathcal{K}|p\rangle_l=\langle k|\mathfrak{v}|p\rangle_l-(2/\pi)\int_0^\infty d(qa)\langle k|\mathfrak{v}|q\rangle_l\langle q|\mathcal{K}|p\rangle_l$, (14b)

and $\langle k|\mathfrak{v}|q\rangle_l\equiv\int_0^\infty r^2\mathfrak{v}(r)j_l(kar)j_l(qar)dr$. (14c)

Equations (13) are coupled and nonlinear but can be solved by relatively simple numerical methods on a computer. The same basic method is used as for solving the reaction matrix integral equation. Although the equations for F, H, and E are coupled and nonlinear, their solution is less demanding of machine computing time and memory storage than the solution of the reaction matrix equations, Eq. (14). One reason is that $F, H,$ and E are only one dimensional arrays as compared to the two dimensional $\mathcal{K}_{xy}$ and require two orders of magnitude less storage. Secondly, the integrands in the F, H, and E equations vanish much more rapidly with large momentum and the numerical integration may be stopped sooner.

The method of solution is to start with a reasonable guess for the functions $F(ka)$, $H(ka)$, and $E(ka)$ and $P_0=P$ and to insert these quantities in the right-hand members of Eqs. (13). The new values for the functions calculated by doing the integrals were then averaged with the original guesses, the result being used as the next approximation. With a reasonable initial guess this iterative method converged to within a fraction of 1% in about 10 iterations. The reason for averaging new values with old was to prevent oscillations around the actual solution.

Because all the integrands decrease very rapidly after the momentum or roton minimum is passed, it is necessary to carry the integration only to $p/\hbar\approx 4\,\text{Å}^{-1}(4\times10^{10}\,\text{m}^{-1})$. (The roton minimum is observed experimentally at $p/\hbar=1.8\,\text{Å}^{-1}$.)

V. THE INTERPARTICLE POTENTIAL

To solve the integral equations numerically, one must choose a specific potential function $v(r)$. The results presented in the next section will show great sensitivity to the strength of the potential well. Unfortunately, the well region has not been determined accurately by either experiment or theory. Consequently two potentials are presented in this section. They both fit the measured virial coefficients. One is an accepted potential; the other is constructed simply to illustrate the effect of a weaker attractive well.

Probably the best known expressions for the helium potential are the Slater-Kirkwood potential[19]

$$v(r)=(770e^{-4.6r}-1.49r^{-6})\times10^{-12}\text{erg}, \tag{15}$$

and the Yntema-Schneider potential[20]

$$v(r)=(1200e^{-4.72r}-1.24r^{-6}-1.89r^{-8})\times10^{-12}\text{erg},\quad (r\text{ in Å}) \tag{16}$$

The former was derived on theoretical grounds. The attractive tail is calculated from second-order perturbation theory for the van der Waals interaction of two neutral atoms. The form of the repulsive core, due to Slater[21] is a first approximation to the overlap energy of two atoms which are close together. The attractive part dominates for large interparticle separation and the repulsive part for very small separation. The potential for intermediate separations, in particular in the vicinity of the minimum of the potential well, is not determined with any great accuracy, but in fact is the result of adding the repulsive and attractive terms together in the range of intermediate separation.

The Yntema-Schneider (YS) potential was derived from experimental measurements of the second virial coefficient between 273 and 1473°K.[22] The form $ae^{-br}-cr^{-6}-dr^{-8}$ was assumed. The value for c was taken from a theoretical derivation of London[23] and the value of d from Margenau,[24] who calculated it to correspond to the London value of c. The values of a and b were then chosen to give a reasonable fit to the experimentally determined virial coefficients.[25–27] This was done by calculating the second virial coefficient classically from

$$B(T)=2\pi n_0\int_0^\infty(1-e^{-v(r)/kT})r^2dr, \tag{17}$$

using various values of a and b to see what combination produced the best agreement between the calculated and experimental $B(T)$. Figures 2 and 3 show $B(T)$ calculated from Eq. (17) using $v(r)$ from Eq. (16) and also show experimental data.[22,38] The Slater-Kirkwood potential gives values of $B(T)$ that are up to 8% too low in the range 273 to 1473°K. It will not be used further here.

Virial coefficients for helium at high temperatures (>500°K) are very insensitive to the attractive part of the potential. Even at lower temperatures (down to approximately 80°K) the shape and depth of the well cannot be accurately determined by a virial-coefficient fit. Thus the attractive well is not accurately determined by the fit of Yntema-Schneider. In Eq. (16), just as in Eq. (15), the values of potential in the region of the well result from extrapolation of the limiting forms for larger and smaller r.

The well cannot be determined accurately by

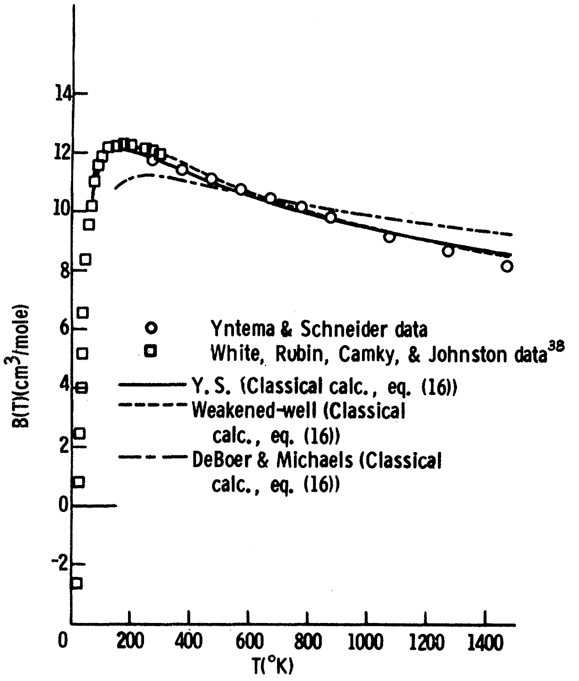

FIG. 2. Second virial coefficient for helium.

matching virial coefficients using the classical formula.[17] At temperatures where $B(T)$ is sensitive to the well shape and depth, a quantum-mechanical calculation of $B(T)$ must be made. Figure 3 shows an example of the inadequacy of the classical formula. It contains $B(T)$ for a six-twelve potential[28] as calculated from Eq. (17) and quantum-mechanical calculations taken from Ref. (29). [The six-twelve potential used for the example does not fit the high-temperature coefficients very well. For that reason it is used here only to contrast classical and quantum results for $B(T)$.] The quantum-mechanical calculation of $B(T)$ is much more difficult and lengthy than the classical, and this apparently has prevented a quantum-mechanical determination of the potential well. It is unfortunately the case that neither virial-coefficient fits nor other methods have yet determined the attractive well accurately.[30]

In spite of the inadequacy of the classical formula (17), another potential has been constructed which fits the measured virial coefficients as well as the YS potential does. This new potential has a weaker well than that of YS and a different core shape. It is introduced here simply to show that another potential can give a classical fit to $B(T)$ and yet yield (in the next section) an energy spectrum in better agreement with experiment than that from the YS potential. The new potential will be designated as the "weakened-well" potential and is shown in Fig. 4. The classical $B(T)$ calculations from it are shown in Figs. 2 and 3.

Two more potentials are used in the next section to further illustrate the effects of a shallower attractive well. These two potentials are identical with the YS potential for $v(r) > 0$ but for $v(r) < 0$ are equal to $\alpha v_{\mathrm{YS}}(r)$, where α is chosen as 0.6 for one potential and 0.8 for the other.

A total of four potentials will be used in the next

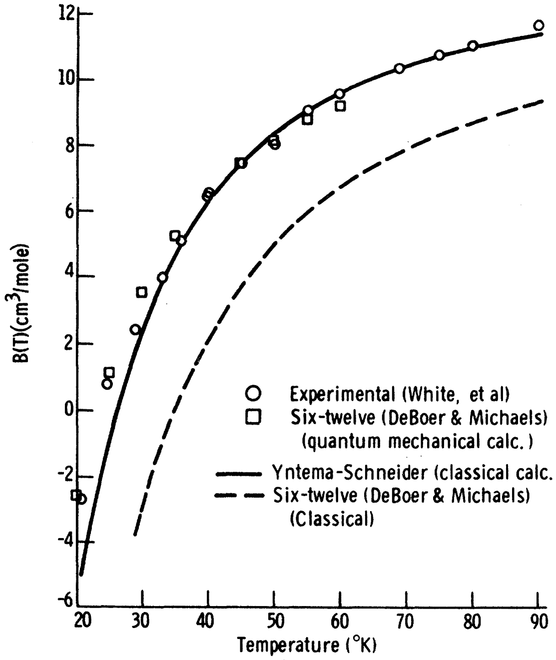

FIG. 3. Second virial coefficient for various potentials.

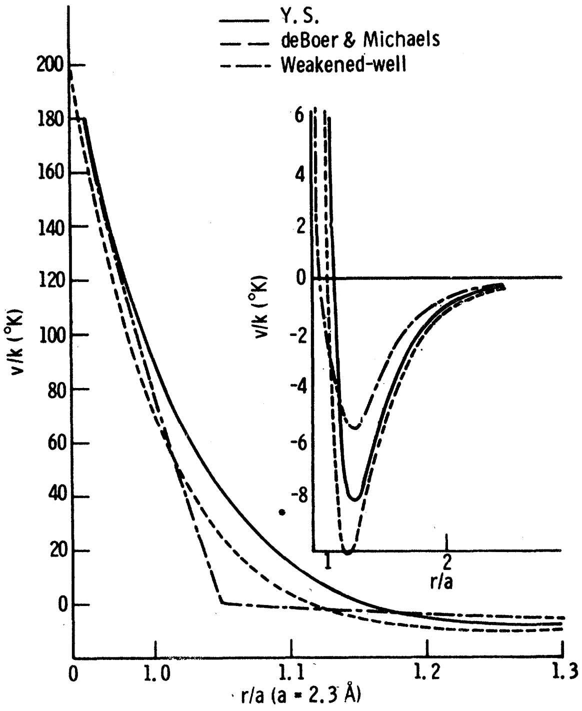

FIG. 4. Comparison of potentials.

section. Two of these, the YS potential and the weakened well potential, give good fits of the classically calculated virial coefficients to the experimental ones. The other two potentials with uniformly reduced wells are simply artificial potentials used to show the effects of gradually reducing the attractive well.

VI. CALCULATED SPECTRA

The integral equations (13) have been solved numerically for four potentials: the YS potential, the weakened-well potential of Fig. 4, and the two potentials derived from the YS by reducing the well by factors of 0.6 and 0.8. The resulting spectra are presented in this section beginning with the spectrum from the YS potential. The qualitative features of that spectrum will be seen to be correct. The energies of all excitations will be seen to be high, however, and simple arguments will indicate that shallower wells should give better results. The spectrum corresponding to the weakened-well potential (which was shown to fit virial-coefficient measurements) will be seen to be much better but still too high in energy. Lastly, the results for the uniformly reduced wells of 0.8 and 0.6 of YS values are given.

The partial-wave components of the reaction matrix were calculated from Eq. (14) as the first step in finding the spectrum. The YS potential produced the diagonal elements of the first three even-numbered waves shown in Fig. 5. These partial waves were summed through $l = 4$ according to Eq. (14), and then the integral equations (13) were solved for the energy spectrum. Figure 6 gives the result. Curves obtained using only one or two partial waves in the reaction matrix are also shown. A comparison of the calculated spectrum with the experimentally measured one shows the energy scale of the present results to be nearly an order of magnitude too high.

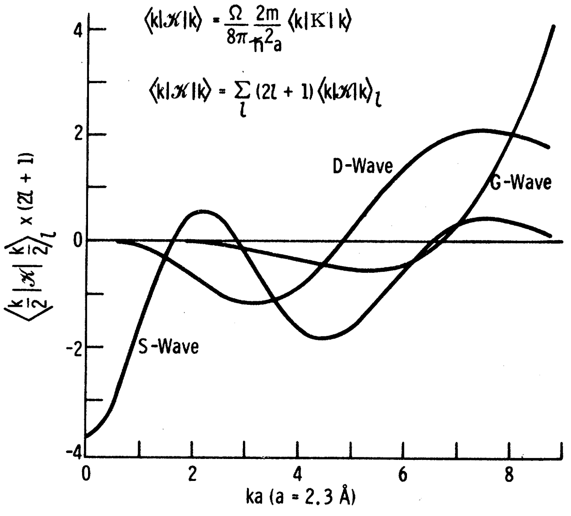

FIG. 5. Partial-wave contributions to diagonal elements of reaction matrix. (Yntema-Schneider potential.)

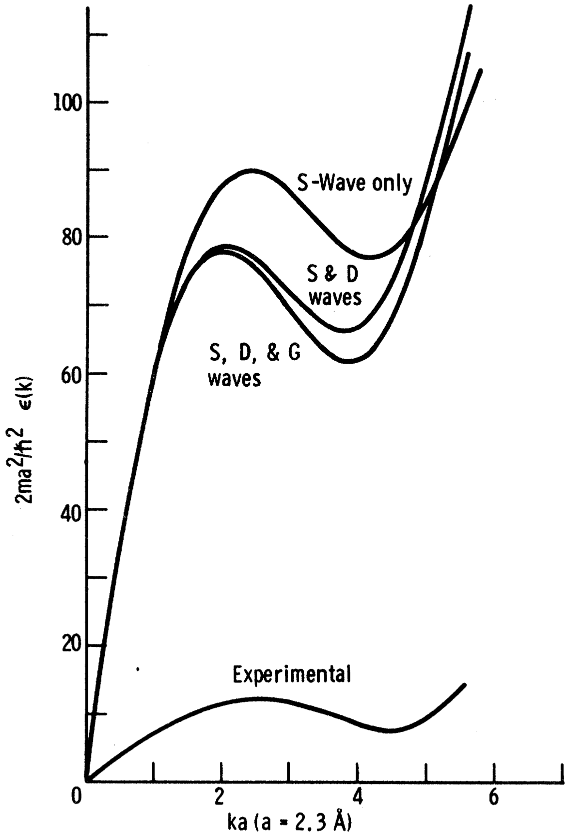

FIG. 6. Energy spectrum for Yntema-Schneider potential.

The disparity in scale tends to obscure the important similarities: the phonon-like low-momentum excitations and the roton minimum. The momenta at which the roton minimum and the relative maximum occur are approximately the same as those of the experimental spectrum. Previous attempts to include both singular core and attractive well have failed to reproduce even these qualitative features. Brueckner's treatment[9] of the hard core gave a qualitatively good spectrum, and as noted in a previous section gave semiquantitative agreement with the experimental spectrum for an appropriate choice of a parameter in the theory. But best agreement was achieved for a nonphysical value of the parameter that implied that the number of particles in excited states exceeded the total number of particles. The attempt by Parry and ter Haar to use Brueckner's method and to include an attractive well led to the loss of even the qualitative features of the helium II spectrum. In the context of these previous results, the qualitative features of the present spectrum – phonons at low momentum and the roton minimum – are gratifying.

The speed c of ordinary sound (first sound) is equal to the initial slope of the energy versus momentum curve. The value of c from the YS potential is 2300 m/sec, to be compared with the actual value of 240 m/sec (extrapolated to $T = 0$).

It is easy to see what causes the integral equations for E versus ka to give such high energies. It is primarily the influence of $\mathcal{K}_{00}$ in the equations for $F(x)$ and $H(x)$. $\mathcal{K}_{00}$ is a rather large negative number for the YS potential because that potential is nearly attractive enough to produce a zero-energy bound state. A potential that is just strong enough to have a zero-energy bound state will have a scattering length of $-\infty$, and the value of $\mathcal{K}_{00}$ will also be $-\infty$. For large negative $\mathcal{K}_{00}$ the integrals in Eq. (13) may be neglected and the equations become approximately

$$F(x) = x^2 + 8\pi P_0(2\mathcal{K}_{\frac{1}{2}x,\frac{1}{2}x} - 3\mathcal{K}_{00}),$$

$$H(x) = 8\pi P_0 \mathcal{K}_{0x},$$

$$E(x) = [F^2(x) - H^2(x)]^{1/2}.$$

Near $x = 0$, $\mathcal{K}_{\frac{1}{2}x,\frac{1}{2}x}$ and $\mathcal{K}_{0x}$ have the expansions:

$$\mathcal{K}_{\frac{1}{2}x,\frac{1}{2}x} = \mathcal{K}_{00} + dx^2, \quad \mathcal{K}_{0x} = \mathcal{K}_{00} + bx^2 .$$

Hence

$$E(ka) \to [-128\pi^2 P_0^2(2d+b)\mathcal{K}_{00}]^{1/2} ka, \qquad \text{for small } ka.$$

The initial slope of the spectrum is thus approximately proportional to $-\mathcal{K}_{00}^{1/2}$. But an examination of Fig. 7 shows that the value of d increases rapidly as $\mathcal{K}_{00}$ decreases. (The same is true for b.) Thus the initial slope of the spectrum is very roughly proportional to $-\mathcal{K}_{00}$, for large negative $\mathcal{K}_{00}$.

Figure 7 shows the extreme sensitivity of $\mathcal{K}_{00}$ to the strength of the attractive well. The curves in that figure correspond to the potentials of Fig. 8. These potentials are identical in the core region but have potential wells of three different strengths.

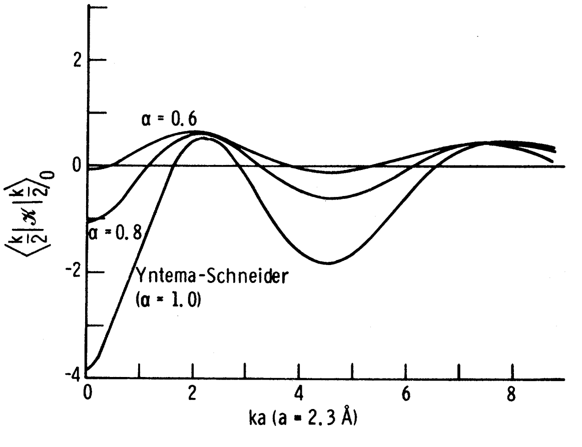

FIG. 7. Dependence of diagonal elements of K matrix on well depth (S wave only). Well-strength parameter α is defined in Fig. 8.

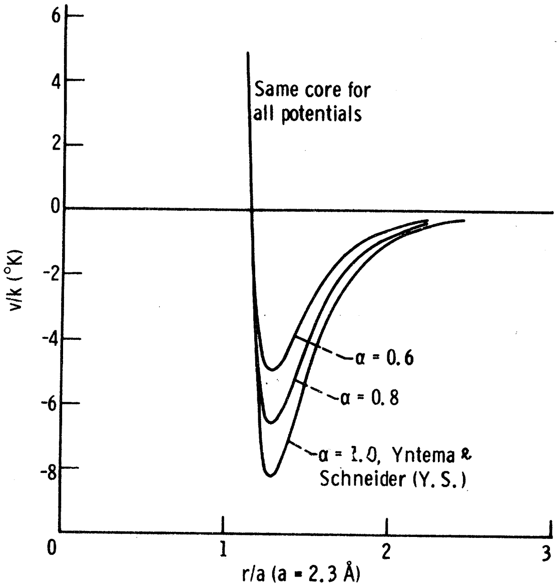

FIG. 8. Potentials with uniformly reduced wells. Potentials are identical for $v(r) > 0$. For $v(r) < 0$ the potentials obey $v(r) = \alpha v_{\mathrm{YS}}(r)$.

The two potentials with reduced well strength were obtained from the YS potential by multiplying all negative values of $v(r)$ by a parameter α, having values of 0.8 and 0.6. The reduction of well strength to 60% of the YS strength reduces $\mathcal{K}_{00}$ to about $\frac{1}{40}$ of the value it has for the YS potential as shown in Fig. 7. This strong sensitivity of $\mathcal{K}_{00}$ to well strength is what prompted the construction of the weakened-well potential of Fig. 4. This potential was designed to have a much smaller $\mathcal{K}_{00}$ than that of YS, and yet to fit the measured second virial coefficients just as well.

The weakened-well potential gives much better results than the YS potential. Figure 9 shows the first three even partial waves of the diagonal elements of the reaction matrix. Comparison with

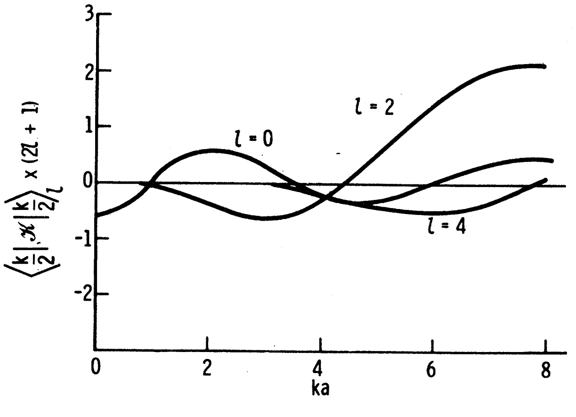

FIG. 9. Diagonal elements of reaction matrix for weakened-well potential.

Fig. 5 shows that $\mathcal{K}_{00}$ is reduced to $\frac{1}{6}$ of the YS value. The consequent improvement in the energy scale of the spectrum is evident in Fig. 10.

The improvement in energy is significant but short of what is needed to agree with experiment. Comparing the spectrum with that of the YS potential, one notes a shift toward lower momentum of the roton minimum and of the relative maximum. The minimum is much less pronounced. The fraction of particles in the condensed group of states is 90%, slightly down from the 93% result for the YS potential.

There is some possibility that effects not taken into account might lead to an effective weakening of the potential well. For example, the Hamiltonian upon which this work is based includes only two-body interaction terms. It is recognized that nonadditive three- and many-body interactions[31,32] exist in liquids because of the composite nature of the atoms. That is, because atoms are not simple particles but instead have internal structure, and because the interparticle force is a result of a modification (polarization) of that structure, the force between a pair of atoms is not independent of the presence of other atoms in the vicinity. At low densities this is unimportant. But at liquid-helium density the effects may not be negligible. Inclusion of many-body interactions in the Hamiltonian[33] is out of the question in the present theory, but it might be possible to include the many-particle effects approximately by modifying the two-particle potential to make it an effective two-particle potential appropriate for the observed liquid density.

Whether the presence of the other particles weakens or strengthens the van der Waals attraction between two particles is not at all obvious.

An approximate microscopic treatment of this problem,[32] yields a very small weakening of the attraction. Macroscopic methods taking frequency dependence of the dielectric constant into account[34] have not been applied to this specific problem. In any case, because many-body forces or some other phenomenon might effectively weaken the attractive well, it is desirable to calculate spectra for a series of wells of varying strength. Such an approach serves to uncover trends in the spectra and to further show the sensitivity to well strength.

The potentials of Fig. 8 form a series of three such potentials, related by the single parameter, α. The calculated energy spectra can be compared in Fig. 11. The results show that as α decreases, the energy scale of the spectrum improves and can even fall partially below the observed spectrum. A marked shift toward lower momentum occurs, however, which was noted to a lesser degree in Fig. 10. The cause of this shift is not known.

VII. DISCUSSION

A. Relation to Previous Work

To place the above results in the proper context,

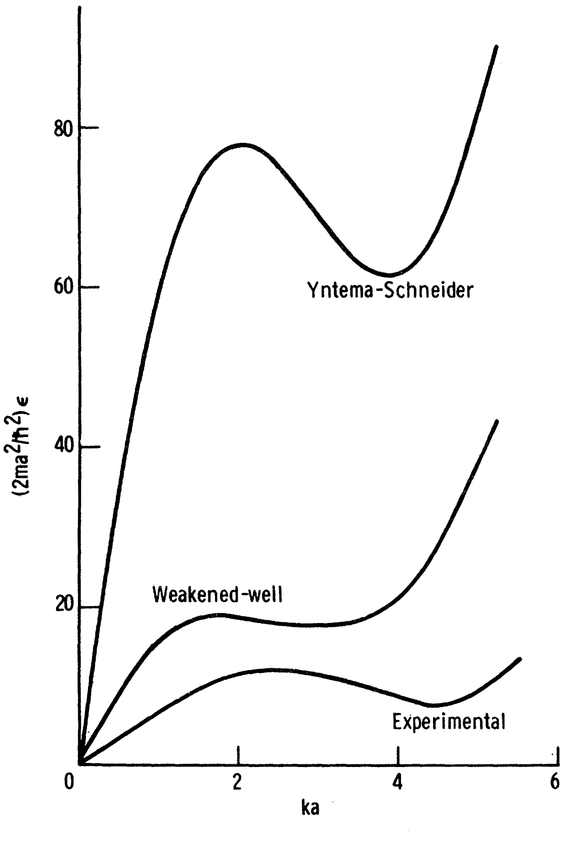

FIG. 10. Comparison of spectra from YS and weakened-well potentials with experimental spectrum.

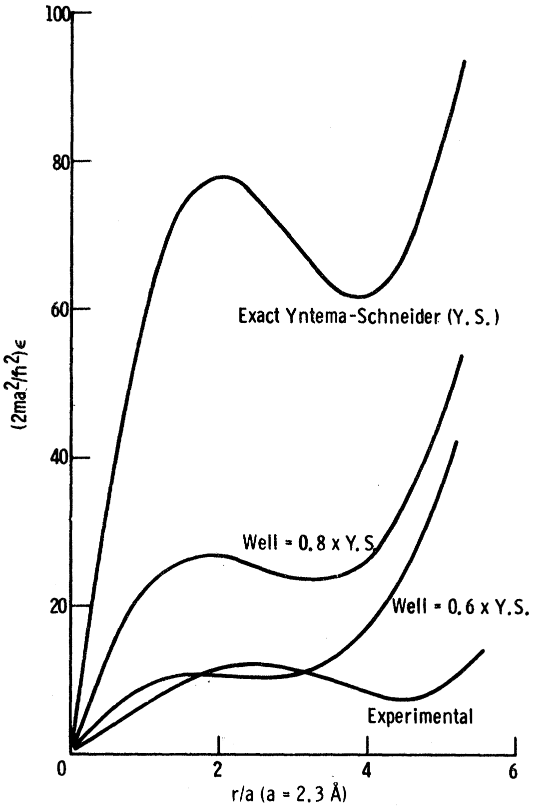

FIG. 11. Spectra for uniformly reduced wells.

the following comparisons of the present methods and results are made with other work.

Most of the microscopic theories have been forced to deal with truncated Hamiltonians. Of these theories several are valid only for weak potentials. Bogoliubov[7] first obtained a phonon-like low-momentum spectrum for weak repulsive interactions near absolute zero. His Hamiltonian contained forward, exchange, and pair scattering terms, but was diagonalized only by approximating some of the operators by *c* numbers. Wentzel[5] and Luban[6] found an energy gap at low momenta using the pair Hamiltonian. The actual helium II spectrum, of course, has no such gap. Using the idea of Girardeau[15] that, for an attractive interaction, condensation should occur into many states instead of into just one, Luban showed that the spectrum is phononlike at low momentum for an appropriate attractive potential with pair scattering in the Hamiltonian. Hence the present work has assumed a generalized condensation and has included pair-to-pair scattering. The spectrum obtained herein has a phononlike low-momentum region as observed in liquid helium.

The above mentioned works by other authors were based on weak potentials. Brueckner and Sawada[9] used the reaction matrix method of handling strong potentials, but included only forward and exchange scattering and one special type of pair scattering in their Hamiltonian. For hard spheres with no attractive well, they found a phononlike low-momentum spectrum. This is similar to Wentzel's result for repulsive but weak potentials. The Brueckner and Sawada spectrum had a roton minimum which approximated the experimental one for an appropriate choice of a parameter in their theory. But this parameter was proportional to the density of condensed (zero-momentum) particles, and thus was not really arbitrary. In fact the value of the parameter giving the best spectrum leads to the contradiction that the density of excited particles is 2.7 times the total density. Parry and ter Haar[11] used approximately the same method but consistently handled the density of condensed particles. However, their attempt to include an attractive well in the potential was unsuccessful. All qualitative similarity to the experimental spectrum was lost, including the phononlike part.

The present work uses a reaction matrix to handle the strong repulsion. It differs from the Brueckner and Sawada reaction matrix, however, in that only kinetic energy is included in the propagator G. The additional terms included in the unperturbed Hamiltonian by Brueckner and Sawada and by Parry and ter Haar are not necessary with net attractive forces. The successful inclusion of the attractive potential in this work is due to the inclusion of pair interaction terms and to the assumption of generalized condensation.

Parmenter(7) has shown that a simple Bose condensate may mediate an attractive interaction (much as phonons do in superconductivity). For some interparticle potentials this effect might make a simple condensation energetically more favorable than a smeared condensation. One might interpret this as casting doubt on the advisability of assuming a smeared condensation in the present work. However, inclusion of the strong repulsion takes the problem outside the scope of the analysis of Ref. 7, which presumed the potential had finite matrix elements with $\hat{v}(0) > 0$. The present work uses K rather than V because of the strong repulsive core, and K_{00} [which takes the place of $\hat{v}(0)$] is less than zero.

The most significant result is that the two important qualitative features of the helium potential – strong repulsion, but net attraction – have been treated with methods that were able to produce the two important qualitative features of the excitation spectrum – phonons and rotons.

B. Discussion of Approximations

As in all other attempts to derive the energy spectrum, simplifications and approximations have been made to make the problem tractable. The methods of this work have produced an energy spectrum of correct qualitative character from a microscopic theory using realistic potentials with both singular core and attractive well. It is appropriate to review the simplifications, approximations, and omissions since they may be responsible for the lack of quantitative agreement with experiment. Unfortunately the most important cause of error has not been identified because of the complexity of the integral equations.

The first simplification was to restrict the second quantized Hamiltonian to two-body interaction terms. Three-body, four-body, and more-body operators have been omitted, but they should be included for an exact treatment of helium.

It has been shown in the last section that a weakening of the attractive part of the potential by about 40% gives approximately the correct speed of sound. Perhaps the interaction of two helium atoms could be modified to this degree by the presence of several near neighbors (speaking microscopically) or (speaking phonomenologically) the presence of the dielectric medium composed of the other atoms. One treatment of many-body forces[32] gives only a 1% effect; however, it may not be accurate for liquid-helium densities.

The second simplification was to truncate the Hamiltonian. Only forward-scattering, exchange-scattering, and pair-scattering terms were retained. Ways of handling more terms than these are not known. Actually the use of K in place of V does, in effect, include more terms, but the form of the Hamiltonian is unchanged.

To allow the inclusion of a singular repulsive core in the potential, the V matrix elements were replaced by reaction matrix elements. This, in effect, sums enough terms of the many-body perturbation series to give finite matrix elements in the interaction part of the Hamiltonian. But it is shown in Appendix A that the perturbation series for the free energy derived from the "Hamiltonian" with K contains some duplicated terms. The extra terms needed to treat singular cores therefore come at the price of including some terms twice. This was recognized by previous authors[9,11] but neglected on the basis of cancelling errors for ground and excited states. But one cannot say that the elementary excitation spectrum would be unaffected. The duplication of terms in the perturbation series for the free energy means the partition function would also be in error since $F = -kT\ln Z$.

The justification for putting K into the Hamiltonian was valid only near absolute zero. This is, however, simply a limit on the allowed temperature rather than an approximation. If the method is used for higher temperatures, then an approximation is thereby made.

The Wentzel method of thermodynamically equivalent Hamiltonian is not an approximate method in itself. The equivalent Hamiltonian has exactly the same partition function as the Hamiltonian from which it was derived and thus the same thermodynamics. It has been argued in an earlier section that the spectrum of elementary excitations is also the same if it turns out to be temperature independent.

The last approximation made was to replace the two-body reaction matrix elements with their approximately equal one-body central-force counterparts. There is no reason, in principle, why this must be done. However, the solution of the integral equation for the one-body K matrix was barely practical. The numerical solution of the integral equation for a two-body K matrix, which would be a function of four variables instead of two, would be impossible without completely different techniques.

The assumed generalized or "smeared" Bose-Einstein condensation is probably not an approximation. It has been shown[15,17] to be a consequence of a predominantly attractive interaction, which permits the system to lower its energy by spreading out the condensate over many zero-energy degenerate states of different momenta.

ACKNOWLEDGMENT

The authors wish to thank Dr. John R. Reitz for suggestions which led to the analysis of this problem.

APPENDIX A. USE OF K INSTEAD OF V

Consider the cumulant expansion of the free energy F.[35,36] Let the exact nontruncated Hamiltonian be split into the unperturbed part H_0 (kinetic energy) and the perturbation H' (interaction terms) $H = H_0 + H'$. Then

$$\beta(F - F_0) = \sum_{n=1}^{\infty} \frac{1}{n!} M_n ,$$

where F_0 is the unperturbed free energy, and

$$M_1 \equiv \int_0^\beta \langle H'(\lambda)\rangle\, d\lambda , \quad M_2 \equiv \int_0^\beta d\lambda \int_0^\lambda d\lambda' [\langle H'(\lambda) H'(\lambda')\rangle - \langle H'(\lambda)\rangle \langle H'(\lambda')\rangle] ,$$

$$M_3 \equiv \int_0^\beta d\lambda \int_0^\lambda d\lambda' \int_0^{\lambda'} d\lambda'' [\langle H'(\lambda) H'(\lambda') H'(\lambda'')\rangle - 3\langle H'(\lambda) H'(\lambda')\rangle \langle H'(\lambda'')\rangle + 2\langle H'(\lambda)\rangle \langle H'(\lambda')\rangle \langle H'(\lambda'')\rangle], \quad \text{etc.}$$

The bracket means the thermodynamic expectation value

$$\langle \mathcal{O}\rangle \equiv \mathrm{tr}(\mathcal{O}\, e^{-\beta H_0}) / \mathrm{tr} e^{-\beta H_0} .$$

$H'(\lambda)$ is a temperature analog of the interaction picture of an operator:

$$H'(\lambda) \equiv e^{\lambda H_0} H' e^{-\lambda H_0} .$$

The operator H' for a complete (nontruncated) second-quantized Hamiltonian including only two-body interactions is

$$H' = \frac{1}{2} \sum_{k_1 k_2 k_3 k_4} \langle k_1 k_2 | V | k_3 k_4 \rangle a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \tag{A1}$$

as in Eq. (1). The $a_k^\dagger$ and a_k, respectively create and annihilate plane-wave states. Summation indices are understood to be vectors.

Since the expectation values $\langle \mathcal{O}\rangle$ are exceedingly complicated for finite β, we consider only the limit of zero temperature ($\beta \to \infty$). The excitation spectrum, which is the primary result of this work, is thus valid only near $T = 0$. The use here of the thermodynamically equivalent Hamiltonian method of Wentzel is justified, and in fact the meaning of "excitation spectrum" is definite, only if the spectrum is temperature independent for a range of temperature near $T = 0$.

At an arbitrary temperature

$$\langle \mathcal{O}\rangle = \sum_{\{n_i\}} \langle n_0, n_1, n_2, \ldots | \mathcal{O}\, e^{-\beta H_0} | n_0, n_1, n_2, \ldots \rangle \Big/ \sum_{\{n_i\}} \langle n_0, n_1, n_2, \ldots | e^{-\beta H_0} | n_0, n_1, n_2, \ldots \rangle ,$$

where the sum over $\{n_i\}$ indicates a sum over all possible sets of n_0, n_1, n_2, $n_3, \ldots$, and $i = 0, 1, 2, \ldots$ indicate various free-particle states, that is, eigenstates of H_0, the kinetic energy. The zero subscript here indicates the zero-momentum state. As $T \to 0$ and hence $\beta \to \infty$ the factor $\exp(-\beta H_0)$ in the numerator causes all other terms to become negligible compared to the ground-state term, $n_0 = N$ and $n_i = 0$ for $i \neq 0$. Thus

$$\lim_{T\to 0} \langle \mathcal{O} \rangle = \lim_{\beta\to\infty} \langle \mathcal{O} \rangle = \langle N, 0, 0, \ldots | \mathcal{O} | N, 0, 0, \ldots \rangle / \langle N, 0, 0, \ldots | 1 | N, 0, 0, \ldots \rangle = \langle 0 | \mathcal{O} | 0 \rangle ,$$

where $|0\rangle \equiv |N, 0, 0, \ldots\rangle$ denotes the ground state of a system of noninteracting bosons, which is all particles in the zero-momentum state.

The first few cumulants can now be evaluated in the zero-temperature limit.

$$M_1 \sim \beta \lim_{\beta\to\infty} \frac{1}{\beta} \int_0^\beta \langle H'(\lambda) \rangle \, d\lambda = \beta \lim_{\beta\to\infty} \frac{1}{\beta} \int_0^\beta d\lambda \langle 0 | H'(\lambda) | 0 \rangle$$

$$= \beta \lim_{\beta\to\infty} \frac{1}{2\beta} \sum_{k_1 k_2 k_3 k_4} \int_0^\beta d\lambda \langle 0 | \exp[\lambda(\omega_{k_1} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4})] a_{k_1}{}^\dagger a_{k_2}{}^\dagger a_{k_3} a_{k_4} | 0 \rangle \langle k_1 k_2 | V | k_3 k_4 \rangle .$$

Here ω_{k_i} is the kinetic energy of a particle with wave number k_i. But

$$\langle 0 | a_{k_1}{}^\dagger a_{k_2}{}^\dagger a_{k_3} a_{k_4} | 0 \rangle = 0, \quad \text{except for } k_1 = k_2 = k_3 = k_4 = 0 .$$

Further $\omega_0 = 0$, and $\langle 0 | a_0{}^\dagger a_0{}^\dagger a_0 a_0 | 0 \rangle = N_0{}^2 - N_0 \approx N^2$ for large N. Then

$$M_1 \sim \tfrac{1}{2} \beta \rho N \hat{v}(0) , \tag{A2}$$

where $\hat{v}(0) \equiv \Omega \langle 00 | V | 00 \rangle$.

The second cumulant becomes, as $\beta \to \infty$,

$$\lim_{\beta\to\infty} \frac{1}{\beta} M_2 = - \lim_{\beta\to\infty} \frac{1}{4\beta} \int_0^\beta d\lambda \int_0^\lambda d\lambda' \Bigg(\sum_{k_1 k_2 k_3 k_4} \langle 00 | V | k_1 k_2 \rangle \langle k_3 k_4 | V | 00 \rangle$$
$$\times \exp[-\lambda(\omega_{k_1} + \omega_{k_2}) + \lambda'(\omega_{k_3} + \omega_{k_4})] \langle 0 | a_0{}^\dagger a_0{}^\dagger a_{k_1} a_{k_2} a_{k_3}{}^\dagger a_{k_4}{}^\dagger a_0 a_0 | 0 \rangle - \hat{v}^2(0) \langle 0 | a_0{}^\dagger a_0{}^\dagger a_0 a_0 | 0 \rangle^2 \Bigg) .$$

Only those elements of the V matrix which conserve total momentum give nonzero contributions, so that we have

$$\lim_{\beta\to\infty} \frac{1}{\beta} M_2 = - \lim_{\beta\to\infty} \frac{1}{4\beta} \int_0^\beta d\lambda \int_0^\lambda d\lambda' \Bigg(2 \sum_{k\neq 0} \frac{\hat{v}^2(k)}{\Omega^2} \exp(-2\lambda\omega_k + 2\lambda'\omega_k)$$
$$\times \langle 0 | a_0{}^\dagger a_0{}^\dagger a_{-k} a_k a_{-k}{}^\dagger a_k{}^\dagger a_0 a_0 | 0 \rangle + \frac{\hat{v}^2(0)}{\Omega^2} \langle 0 | a_0{}^\dagger a_0{}^\dagger a_0 a_0 a_0{}^\dagger a_0{}^\dagger a_0 a_0 | 0 \rangle - \frac{\hat{v}^2(0)}{\Omega^2} N^2 (N-1)^2 \Bigg)$$
$$= - \lim_{\beta\to\infty} \frac{1}{4\beta} \int_0^\beta d\lambda \int_0^\lambda d\lambda' \Bigg(\frac{2}{\Omega^2} \sum_{k\neq 0} \hat{v}^2(k) \exp[(\lambda' - \lambda)\hbar^2 k^2/m] N(N-1) \Bigg)$$

$$= - \frac{\rho N}{2\Omega} \lim_{\beta\to\infty} \sum_{k\neq 0} \frac{m \hat{v}^2(k)}{\hbar^2 k^2} \left(1 + \frac{\exp(-\beta\hbar^2 k^2/m) - 1}{\beta\hbar^2 k^2/m} \right) = - \frac{\rho N}{2} \frac{1}{2\pi^2} \frac{m}{\hbar^2} \int_0^\infty \hat{v}^2(k) dk . \tag{A3}$$

In a similar manner M_3 may be evaluated for $\beta \to \infty$. The result is

$$\lim_{\beta\to\infty} \frac{1}{\beta} M_3 = \frac{\rho N}{8} \frac{1}{(2\pi)^6} \frac{m^2}{\hbar^4} \int d^3k_1 \int d^3k_2 \frac{\hat{v}(k_1)\hat{v}(k_2)\hat{v}(|k_1 - k_2|)}{k_1{}^2 k_2{}^2} + \frac{\rho^2 N}{8} \frac{1}{(2\pi)^3} \frac{m^2}{\hbar^4} \hat{v}(0) \int d^3k \frac{\hat{v}^2(k)}{k^4} . \tag{A4}$$

The above first three terms in the expansion of the free energy of a nontruncated Hamiltonian are sufficient to indicate what type of reaction matrix may be used in the truncated Hamiltonian H_P to introduce more terms into the expansion.

Consider first the series expansion of a general element of the reaction matrix with respect to two-particle (noninteracting) plane-wave states:

$$\langle k_1 k_2 | K | k_3 k_4 \rangle = \langle k_1 k_2 | (V + VGV + VGVGV + \cdots) | k_3 k_4 \rangle$$
$$= \langle k_1 k_2 | V | k_3 k_4 \rangle + \sum_{k_5 k_6 k_7 k_8} \langle k_1 k_2 | V | k_5 k_6 \rangle \langle k_5 k_6 | G | k_7 k_8 \rangle \langle k_7 k_8 | V | k_3 k_4 \rangle$$
$$+ \sum_{\substack{k_5 k_6 k_7 k_8 \\ k_9 k_{10} k_{11} k_{12}}} \langle k_1 k_2 | V | k_5 k_6 \rangle \langle k_5 k_6 | G | k_7 k_8 \rangle \langle k_7 k_8 | V | k_9 k_{10} \rangle \langle k_9 k_{10} | G | k_{11} k_{12} \rangle \langle k_{11} k_{12} | V | k_3 k_4 \rangle + \cdots . \tag{A5}$$

Many of the above terms vanish because V has nonzero elements only between momentum-conserving states.

If the free energy is now expanded in a perturbation series with K's instead of V's in the interaction term of H_P, the series will contain in first order many terms which previously appeared in higher order. Each higher order of the series with K in the truncated Hamiltonian has terms which the series with V had only in higher orders or not at all. One therefore hopes that the series based on K (in the truncated Hamiltonian) more nearly resembles the exact perturbation series based on a nontruncated Hamiltonian. This can be achieved if G is chosen so that its matrix elements contain the same energy denominators as those which appear in the exact perturbation series. The first cumulant containing K in place of V will now be examined to show what G must be. It will be seen that zero-energy propagators should be used.

Clearly, the first term in the expansion (A5), which is simply the potential itself, will make the same contribution to the free energy as the potential would have made. Consider, however, the second-order terms of (A5)

$$\sum_{k_5 k_6 k_7 k_8} \langle k_1 k_2 | V | k_5 k_6 \rangle \langle k_5 k_6 | G | k_7 k_8 \rangle \langle k_7 k_8 | V | k_3 k_4 \rangle ,$$

and their contribution to M_1. Note first that only $k_1 = k_2 = k_3 = k_4 = 0$ make any contribution at all to M_1. Since momentum-nonconserving elements of V vanish, only terms with $k_5 = k_6$ and $k_7 = k_8$ appear. Further, when G is defined using H_0 as the kinetic energy alone, only terms with $k_5 = k_7$ will be nonzero. Hence the second-order terms in (A5) give in M_1 as $\beta \to \infty$

$$\tfrac{1}{2}\beta N^2 \sum_k \langle 00 | V | k - k \rangle \langle k - k | G | k - k \rangle \langle k - k | V | 00 \rangle = -\frac{\beta \rho N}{2} \frac{1}{2\pi^2} \int_0^\infty \frac{k^2 \hat{v}^2(k) dk}{-E + \hbar^2 k^2 / m} . \tag{A6}$$

This term has the same form as the second-order terms in the perturbation series based on V if E is set equal to zero. The resulting "zero-energy propagator" contains the same energy denominators which arise in M_2 upon integrating with respect to λ' [see algebra leading to (A3) above]. In a similar way the third-order terms in (A5) produce terms in M_1 with the right type of energy denominators if E is always set equal to zero. This value for E was also used by Brueckner and Sawada.[9]

A Green's function is not uniquely specified until the manner of handling the singularities is given. That the principal value should be used is due to the fact that the integrals [such as (A6)] which arise from the expansion of K in terms of V actually come from sums over intermediate states. We desire these sums to be like those that occur in the semi-invariants M_i. The sums occurring there appeared first as the sums in the interaction parts of the Hamiltonian (A1). There, $\vec{k}_1$, $\vec{k}_2$, $\vec{k}_3$, and $\vec{k}_4$ are the allowed wave vectors of plane waves. As the thermodynamic limit is taken, the equally spaced allowed values of the x, y, and z components of any $\vec{k}_i$ become more and more closely spaced. The sum over the states [see Eq. (A5), second term] therefore approaches the principal value of the integral (by the definition of the latter).

As previously noted,[9,11] the use of a reaction matrix is seen to cause a duplication of some terms in the perturbation expansion. The first-order term of (A5), which is simply the potential, produces the result (A3) in M_2/β, that is, $-(\rho N/4\pi^2\hbar^2)\int_0^\infty m\hat{v}^2(k)dk$. But the very same contribution is produced by the second-order terms of (A5) in M_1/β as shown in Eq. (A6). Similar duplications occur in higher order, though not every term is duplicated. According to Parry and ter Haar,[14] it can be shown that if the linked-cluster expansion is valid, the same error occurs in the energy of an excited state as in the ground-state energy. We therefore expect the total energy of the system to be incorrectly given by this model, but that if thermal excitation is allowed, the difference between the excited and ground-state energies will not contain the error.

APPENDIX B. CALCULATION OF REACTION MATRIX ELEMENTS

Center of Mass Approximation

The equations for the quantities f, h, and ϵ involve the following types of elements of the reaction matrix:

$$\langle \vec{p} - \vec{p} | K | \vec{p} - \vec{p} \rangle , \quad \langle \vec{p} - \vec{p} | K | - \vec{p}\vec{p} \rangle , \quad \langle \vec{k}\vec{p} | K | \vec{k}\vec{p} \rangle , \quad \langle \vec{k}\vec{p} | K | \vec{p}\vec{k} \rangle . \tag{B1}$$

The required elements include those in which k and p may be zero. To reduce the calculation to manageable size in terms of machine memory storage and computing time, we make a center-of-mass approximation. It reduces the above matrix elements to matrix elements of a one-particle K operator with respect to one-particle states.

The K matrix needed is defined by the integral equation

$$K = V + VGK = V + VGV + VGVGV + \cdots ,$$

where V is the interparticle potential. G has been chosen to be a zero-energy Green's function, $G = -1/H_0$, where H_0 is the unperturbed Hamiltonian, taken to be simply the kinetic energy.

The elements of K with respect to two-body free-particle states which are required are $\langle \vec{k}_1\vec{k}_2|K|\vec{k}_3\vec{k}_4\rangle$, where $|\vec{k}_3\vec{k}_4\rangle$ is a state with the wave function $\Omega^{-1}\exp(i\vec{k}_3\cdot\vec{r}_1)\exp(i\vec{k}_4\cdot\vec{r}_2)$. A general element of the K matrix then satisfies

$$\langle \vec{k}_1\vec{k}_2|K|\vec{k}_3\vec{k}_4\rangle = \langle \vec{k}_1\vec{k}_2|V|\vec{k}_3\vec{k}_4\rangle + \sum_{\vec{k}_5\vec{k}_6\vec{k}_7\vec{k}_8} \langle \vec{k}_1\vec{k}_2|V|\vec{k}_5\vec{k}_6\rangle \langle \vec{k}_5\vec{k}_6|K|\vec{k}_7\vec{k}_8\rangle \langle \vec{k}_7\vec{k}_8|V|\vec{k}_3\vec{k}_4\rangle \, .$$

Since the operator G is diagonal with respect to free-particle eigenfunctions, we have

$$\langle \vec{k}_5\vec{k}_6|G|\vec{k}_7\vec{k}_8\rangle = -\delta_{\vec{k}_5\vec{k}_7}\delta_{\vec{k}_6\vec{k}_8}/H_0 = -\delta_{\vec{k}_5\vec{k}_7}\delta_{\vec{k}_6\vec{k}_8}/[\hbar^2(k_5^2+k_6^2)/2m] \, . \tag{B2}$$

Hence $\langle \vec{k}_1\vec{k}_2|K|\vec{k}_3\vec{k}_4\rangle = \langle \vec{k}_1\vec{k}_2|V|\vec{k}_3\vec{k}_4\rangle - \sum_{\vec{k}_5\vec{k}_6} \langle \vec{k}_1\vec{k}_2|V|\vec{k}_5\vec{k}_6\rangle \frac{2m/\hbar^2}{k_5^2+k_6^2} \langle \vec{k}_5\vec{k}_6|K|\vec{k}_3\vec{k}_4\rangle$.

The central potential $v(r)$ has the one-body matrix elements

$$\langle \tfrac{1}{2}(\vec{k}_1-\vec{k}_2)|V|\tfrac{1}{2}(\vec{k}_3-\vec{k}_4)\rangle = \frac{1}{\Omega}\int d^3r\, e^{i(\vec{k}_1-\vec{k}_3)\cdot\vec{r}}\, v(r), \quad (\text{for } \vec{k}_1+\vec{k}_2=\vec{k}_3+\vec{k}_4),$$

after integration over the center of mass coordinate. This is the same as $\langle \vec{k}_1\vec{k}_2|V|\vec{k}_3\vec{k}_4\rangle$. The matrix elements of G, however, do not simply reduce to one-body elements. Let the definition of the center-of-mass one-body G be $G \equiv -1/H_0 = -m/\hbar^2k^2$, where m occurs rather than $2m$ because the reduced mass is $m/2$. Matrix elements are taken with respect to single-particle plane-wave states. Then

$$\langle \tfrac{1}{2}(\vec{k}_1-\vec{k}_2)|G|\tfrac{1}{2}(\vec{k}_3-\vec{k}_4)\rangle = -\delta_{(\vec{k}_1-\vec{k}_2),(\vec{k}_3-\vec{k}_4)}/[\hbar^2(k_1-k_2)^2/4m] = -\delta_{(\vec{k}_1-\vec{k}_2),(\vec{k}_3-\vec{k}_4)}/[\hbar^2(k_1^2+k_2^2-2\vec{k}_1\cdot\vec{k}_2)/4m] \, .$$

This quantity approaches the form of the two-body element (B2) above if $\vec{k}_1 \approx -\vec{k}_2$. It equals the two-body element for a pair excitation, where $\vec{k}_1$ and $\vec{k}_2$ are equal and opposite momenta, produced, for example, by pair-to-pair scattering from the condensate. For $\vec{k}_1$ and $\vec{k}_2$ such that the total momentum is not negligible compared to the relative momentum, the approximation is poorer. The exact effect of using this approximation is certainly not known for the present application.[37] Parry and ter Haar[11] made some approximate calculations to estimate errors, and drew the qualitative conclusion that the error would be small.

The matrix elements (B1) thus reduce (to the accuracy of the center-of-mass approximation) as follows:

$$\langle \vec{p}-\vec{p}|K|\vec{p}-\vec{p}\rangle \to \langle \vec{p}|K|\vec{p}\rangle \equiv K_{\vec{p}\vec{p}} \, ,$$
$$\langle \vec{p}-\vec{p}|K|-\vec{p}\vec{p}\rangle \to \langle \vec{p}|K|-\vec{p}\rangle \equiv K_{\vec{p}-\vec{p}} \, ,$$
$$\langle \vec{k}\vec{p}|K|\vec{k}\vec{p}\rangle \to \langle \tfrac{1}{2}(\vec{k}-\vec{p})|K|\tfrac{1}{2}(\vec{k}-\vec{p})\rangle \equiv K_{\frac{1}{2}(k-p),\frac{1}{2}(k-p)} \, ,$$
$$\langle \vec{k}\vec{p}|K|\vec{p}\vec{k}\rangle \to \langle \tfrac{1}{2}(\vec{k}-\vec{p})|K|\tfrac{1}{2}(\vec{p}-\vec{k})\rangle \equiv K_{\frac{1}{2}(k-p),\frac{1}{2}(p-k)} \, .$$

Special Elements

There are no special problems in calculating the first two of the above elements. The elements $K_{\frac{1}{2}(\vec{k}-\vec{p}),\pm\frac{1}{2}(\vec{k}-\vec{p})}$ are really of the simple form $K_{\vec{q}\pm\vec{q}}$, where $\vec{q}=\frac{1}{2}(\vec{k}-\vec{p})$. In the integral equations derived in the text, the elements appear in an integral of the form

$$[\Omega/(2\pi)^3]\int d^3p\, K_{\frac{1}{2}(\vec{k}-\vec{p}),\pm\frac{1}{2}(\vec{k}-\vec{p})}\xi(p) \, .$$

Note that $q=(k^2+p^2-2kp\mu)^{1/2}$ from the law of cosines, where μ is the cosine of the angle between $\vec{k}$ and $\vec{p}$. Let the polar axis of the $\vec{p}$ space be parallel to $\vec{k}$, and denote $K_{\frac{1}{2}(\vec{k}-\vec{p}),\pm\frac{1}{2}(\vec{k}-\vec{p})}$ by $K_\pm(q)$. Then

$$[\Omega/(2\pi)^3]\int d^3p\, K_{\frac{1}{2}(\vec{k}-\vec{p}),\pm\frac{1}{2}(\vec{k}-\vec{p})}\xi(p) = (\Omega/4\pi^2)\int_0^\infty p^2dp\,\xi(p)\int_{-1}^{1} d\mu\, K_\pm(\tfrac{1}{2}(k^2+p^2-2kp\mu)^{1/2})$$
$$= (\Omega/4\pi^2k)\int_0^\infty p\,dp\,\xi(p)[Q_\pm(\tfrac{1}{2}(k+p)) - Q_\pm(\tfrac{1}{2}|k-p|)]$$

where $Q_\pm(z) \equiv \int_0^z z' K_\pm(z')dz'$.

Partial-Wave Decomposition of Reaction Matrix

The general one-body reaction matrix element $\langle \vec{k}|K|\vec{p}\rangle$ can be decomposed into partial-wave components, each of which obeys a simple integral equation. The decomposition, which simplifies the numerical calculation is

$$\langle \vec{k}|\mathcal{K}|\vec{p}\rangle = \sum_l (2l+1)\langle k|\mathcal{K}|p\rangle_l P_l(\hat{k}\cdot\hat{p}),$$

where $\hat{k}$ and $\hat{p}$ are unit vectors parallel to $\vec{k}$ and $\vec{p}$, respectively, $P_l(n)$ is a Legendre polynomial, and

$$\langle k|\mathcal{K}|p\rangle_l \equiv \tfrac{1}{2}\int_{-1}^{1}\langle \vec{k}|\mathcal{K}|\vec{p}\rangle P_l(\hat{k}\cdot\hat{p})d(\hat{k}\cdot\hat{p}).$$

The partial waves are solutions of

$$\langle k|\mathcal{K}|p\rangle_l = \langle k|\mathcal{V}|p\rangle_l - (2/\pi)\int_0^\infty d(qa)\langle k|\mathcal{V}|q\rangle_l \langle q|\mathcal{K}|p\rangle_l \,, \tag{B3}$$

where $\langle k|\mathcal{V}|q\rangle_l \equiv \int_0^\infty \gamma^2 \mathcal{V}(\gamma) j_l(ka\gamma) j_l(qa\gamma)d\gamma \,, \quad \mathcal{V}(\gamma) \equiv (ma^2/\hbar^2)V(r),$ (B4)

and $j_l(x)$ is a spherical Bessel function.

Equation (B3) can be solved rather simply with a computer for any potential for which $\langle k|\mathcal{V}|p\rangle_l$ exists. The simplest method of solution is "guess and iterate". The partial wave components $\langle k|\mathcal{V}|p\rangle_l$ are first calculated, and then they and the first guess for $\langle k|\mathcal{K}|p\rangle_l$ are substituted into the right-hand side of Eq. (B3). The resulting left-hand side could serve as the next approximation to $\langle k|\mathcal{K}|p\rangle_l$, but averaging that value with the original guess before starting a new iteration helps reduce or prevent oscillations about the final answer. The situation is rather analogous to underdamping, overdamping, or critical damping in a mechanical oscillator. The relative weighting of the old and new values of the elements $\langle k|\mathcal{K}|p\rangle_l$ determine the damping characteristics. Where the elements $\langle k|\mathcal{K}|p\rangle_l$ are large, a large relative weight must be given to the nth approximation in comparison to the $(n+1)$th in order to prevent overshooting and oscillating about the solution,

For a hard core or any singular repulsive core that increases faster than $1/r$, $\langle k|\mathcal{V}|p\rangle_0$ (S wave) does not exist, and higher partial waves may also be divergent. However, $\langle k|\mathcal{K}|p\rangle_l$ does exist for such potentials for any l if it is considered to be the limit of the class of solutions of Eq. (B3) as a finite repulsive core is made progressively stronger. In fact, this is the way the integral equation was solved numerically. A modestly strong repulsive core was first introduced, and the strength was increased until further increases had negligible effect on the resulting reaction matrix elements. Figure 6 shows the Yntema-Schneider potential with the core cut off at $\mathcal{V}$ equal to 300 and 400. These energies correspond to V/k of 684 and 912°K. Values of the diagonal elements, $\langle p|\mathcal{K}|p\rangle_0$ (the S-wave component), of the reaction matrix differed by less than 1% for these two cutoffs. Further increase of the cutoff has a still smaller effect on the elements. The higher partial waves are less sensitive to the core details because of the angular-momentum barrier.

The matrix elements of $\mathcal{V}$ and $\mathcal{K}$ are square arrays of numbers. Storing these arrays (for small enough increments and large enough ranges in ka for good accuracy) and doing the required numerical operations in a reasonable time on the computer was a problem. For a given potential (such as YS) about 5 minutes of computing time was needed to calculate the K matrix. Perhaps a more efficient method exists for solving the integral equation for K, although the iterative method is undoubtedly the most straighforward.

The number of partial waves to be calculated is small for two reasons. First, one sees from

$$\langle \vec{k}|\mathcal{K}|\vec{p}\rangle = \sum_l (2l+1)P_l(\hat{k}\cdot\hat{p})\langle k|K|p\rangle_l \,,$$

that if $(\langle \vec{k}|\mathcal{K}|\vec{p}\rangle + \langle \vec{k}|\mathcal{K}|-\vec{p}\rangle)$ occurs, the odd partial wave terms will cancel because $\langle k|\mathcal{K}|p\rangle_l$ depends only on the magnitude of $\vec{k}$ and $\vec{p}$ whereas $P_l(\vec{k}\cdot\vec{p}) = \pm P_l(-\vec{k}\cdot\vec{p})$, depending on whether l is even (upper sign) or odd (lower sign). In our equations it is fortunate that only even-numbered waves are required. Second, if either $\vec{k}$ or $\vec{p}$ is zero, then $\langle k|\mathcal{K}|p\rangle_l = 0$ for $l \neq 0$, so only the S wave need be calculated.

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