Critical analysis of the hard-sphere model for superfluid ^{4}He. I.

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The basic goal of this paper is to present the theory which stands at the basis of the calculations of the ^{4}He excitation spectrum reported by Wong and Huang. The exact N-particle hard-sphere pseudopotential is constructed through the method of non-local-field operators developed earlier. Keeping only the two-body interaction terms, this pseudopotential replaces the exact two-particle boundary conditions which is demonstrated here and thus has been proposed as a model potential for actual helium-helium interaction in the liquid state. A pair state of the Bogoliubov type is used to calculate the ground-state energy of such a system. An expansion-parameter scheme is presented which drastically simplifies the mathematics involved and justifies previous approximations employed by one of the authors. The expansion describes the dilute case by assuming a large portion of the particles in the zero-momentum state and the dense case by assuming only a negligible portion of the particles in the Bose-Einstein state.

I. INTRODUCTION

The analysis of a quantum-mechanical system of many particles with hard-sphere interactions is important in many physical models such as, for example, liquid ^{3}He and ^{4}He or nuclear matter. Such systems exhibit very strong and short-range repulsive forces which closely resemble those of hard spheres. Attractive forces can be treated simultaneously with the hard-sphere formalism or can be handled if they are sufficiently weak by ordinary perturbation theory. These are some of the reasons why the hard-sphere problem has received considerable attention for more than a decade.[1-14] In order to deal with this problem it is desirable to replace the N-particle hard-sphere boundary conditions by an equivalent Hamiltonian, the "pseudo-Hamiltonian," so that we can treat this problem in the usual second-quantization manner. However, most treatments either are valid only for the S-wave component or they are not actually nonpenetrable. Although there exist two approaches which give the exact solution for the two-particle problem, they are hard to apply in the N-particle case. One of them requires a subsidiary condition,[9] and the other leads to a non-Hermitian pseudopotential.[13] These difficulties have perhaps limited all former pseudopotential treatments to only dilute systems. In this paper we utilize an exact method developed earlier,[3,14] a presentation of which as far as needed, is given in Sec. II. This method is equivalent to that of Ref. 13 for the two-particle problem, but the generalization to the N-particle problem leads to a Hermitian pseudopotential in our case. Section III contains the treatment of the two-particle system using this formalism.

In Sec. IV, we begin the analysis of the N-body pseudo-Hamiltonian, which we reduce to an approximate form maintaining the pair-particle boundary conditions only. This approximate pseudo-Hamiltonian, which we call the *two-body potential Hamiltonian*, would be exact for two particles but is only an approximation for more than two particles in the case for which the approximation becomes strictly accurate only in dilute systems. Nevertheless, the two-body potential Hamiltonian is analytically tractable, and has therefore been adopted here as a model.[1,2] Our Hamiltonian is shown here to be Hermitian, a property not retained in previous work employing similar approximate pseudo-Hamiltonians. The problem of "Hermiticity" is discussed in detail, and some discrepancies in previous work are resolved.

In Sec. V, we investigate strictly analytically the possibility of lowering the energy of a Hartree-Fock ground state due to formation of opposite momenta pairs.

The analysis of the two-body potential Hamiltonian is continued in Sec. VI, where we extract from it for further analysis a set of terms which we call the *pair Hamiltonian* H_p. Sections VI–VIII contain justification for discarding the terms by which the pair Hamiltonian differs from the two-body potential Hamiltonian. We have taken special care in treating the zero-momentum components correctly, using the Bolsterli transformation for this purpose. After obtaining the pair Hamiltonian, we rewrite it in a new representation, the basis of which is obtained from the old one by a Bogoliubov transformation. The new basis states, we call them *interacting states*, are formally given in

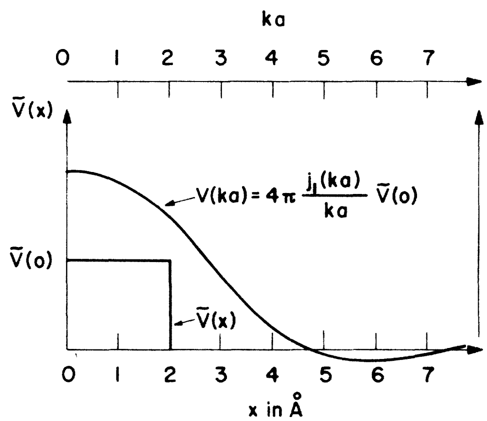

FIG. 1. Plot of $\tilde{V}(x)$ and its Fourier transform $V(ka)$. $\tilde{V}(x)$ and $V(ka)$ are in arbitrary units. x and a are in Å and k is in $Å^{-1}$.

Sec. VI. In Sec. VII we develop the expansion parameter scheme and in Sec. VIII we discuss the concept of "off-diagonal long-range ordering" (ODLRO) in detail. The onset of such an order is typical for the occurance of a new thermodynamic phase; in our case superfluid He.

The new interacting states contain undetermined functions which will be chosen to minimize the ground-state energy. This variational problem is set up in Sec. IX, where the integral equations for the Bogoliubov functional are derived and the equations for the excitation spectrum are set up. These equations are simpler than those derived earlier by one of the authors,[1] because of the new expansion-parameter scheme for estimating the importance of the various terms in the two-body potential Hamiltonian. The actual solution of these equations for the Bogoliubov functional has been obtained numerically by Wong and Huang.[1]

We emphasize that this is a microscopic theory containing only the hard-sphere radius as a parameter, which can be chosen to agree with other experimental data than the excitation spectrum.

In Sec. X, we show that the Bogoliubov transformation and the minimization of the ground-state energy of H_p is equivalent to an exact calculation of the ground-state energy of H_p.

The remainder of this section will be devoted to a simple discussion of the finite-momentum condensate in dense systems. This forms the basis for the estimation scheme which we use later to identify negligible terms in the two-body potential Hamiltonian. The discussion also provides physical insight into the hard-sphere model. In their numerical computation Wong and Huang simulated dilute and dense systems, considering the diameter a of a hard sphere as a parameter, and found that the ratio $N_0/N \equiv 1-\gamma \equiv \beta$, representing the numbers of particles in zero-momentum states divided by the total number of particles in the system, remains much less than 10% down to densities only half of that of realistic liquid-helium densities. For $a = 2.17$ Å, corresponding to actual liquid-^{4}He density, they found $\beta = 0$ within machine accuracy. This result is not too astonishing. In the dilute system the particles hardly interact because of their relatively large mutual spatial separation. The system therefore can be pictured as an ideal Bose gas. On the other hand, in a hard-sphere system of liquid-helium density, a lower bond of 92% on the depletion factor is verified experimentally and theoretically.[15,16]

This small value of β suggests that this has to be the appropriate smallness parameter in a perturbational treatment of the dense case. Hence, results or conclusions drawn from methods that depend on the smallness of γ cannot be expected to be valid in superfluid ^{4}He.

The fact that in a dense system, where supposedly the repulsive forces between the molecules play an important role, the particles do not condense in the zero-momentum state anymore, but rather accumulate at some finite momentum, might not be unexpected from the following plausibility consideration. Let us consider a finite repulsive potential as shown in Fig. 1. We shall calculate the energy expectation value of the Hamiltonian

$$H=\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2V} \sum_{\vec{p},\vec{q},\vec{k}} V(\vec{k}) a^\dagger_{\vec{p}} a^\dagger_{\vec{q}} a_{\vec{q}+\vec{k}} a_{\vec{p}-\vec{k}}$$

($a^\dagger_{\vec{k}}$ and $a_{\vec{k}}$ are plane-wave Bose operators) for two hypothetical variational states. The states are $|N, 0\rangle$, where all the particles are in the zero-momentum state, and $|\frac{1}{2}N, \pm\frac{1}{2}\vec{k}\rangle$, where all the particles are in pair states with momenta of magnitude $\cong \frac{1}{2}k$. The expectation values for the energies are given by

$$E_1 = \langle 0, N|H|N, 0\rangle = 0 + \frac{N(N-1)}{2V} V(0)$$

$$= \frac{4\pi}{3} \frac{N(N-1)}{2V} \tilde{V}(0),$$

$$E_2 = \langle \pm\tfrac{1}{2}\vec{k}, \tfrac{1}{2}N|H|\tfrac{1}{2}N, \pm\tfrac{1}{2}\vec{k}\rangle$$

$$= N\frac{\hbar^2(\frac{1}{2}k)^2}{2m} + \alpha \frac{N^2}{2V} V(ka),$$

where α is a constant between 1 and $1/N$. Choosing $\tilde{V}(0)$ big enough and $k = k_0$, we shall have a situation where $E_2 < E_1$ due to the fact that $V(k_0 a) = 4\pi[j_1(k_0 a)/k_0 a]\tilde{V}(0) < 0$. According to the variational principle the second state is therefore closer to the true eigenstate of H than the first one. Choosing $a \cong 2$ Å (compare Fig. 1) this second state exhibits a condensation in momentum space at a momentum lying between the peak and dip value of the experimental excitation curve. This kind of condensate is qualitatively close to the one resulting from the more elaborate computation performed in Ref. 1.

II. N-PARTICLE PSEUDO-HAMILTONIAN

Field operators representing particles with impenetrable cores can not satisfy the usual commutation rules. Although the common derivation of the second quantization formalism cannot be applied to nonintegrable potentials such as hard spheres exhibit, Siegert[14] has shown that we can define nonlocal field operators $\psi(\vec{x})$ and $\psi^\dagger(\vec{x})$ by a matrix representation which exhibits them explicitly as transformations of functions of N position vectors into functions of $N-1$ and $N+1$ position vectors, respectively. The assumption of impenetrable cores is introduced in this definition by taking the matrix elements which lead to prohibited configurations of position vectors equal to zero. A configuration of the position vectors that contains at least one pair of vectors whose difference is less or equal a—the hard-core diameter—is called prohibited.

Siegert defines a field operator $\psi(\vec{x},t)$ in the Heisenberg representation as the matrix whose only nonvanishing elements are

$$\langle \vec{x}_1', \vec{x}_2', \ldots, \vec{x}_{N-1}' | \psi(\vec{x},t) | \vec{x}_1'', \vec{x}_2'', \ldots, \vec{x}_N'' \rangle = N^{1/2} \int K_{N-1}^\dagger(\vec{x}_1, \ldots, \vec{x}_{N-1}, \vec{x}_1', \ldots, \vec{x}_{N-1}', t) \times K_N(\vec{x}_1, \ldots, \vec{x}_{N-1}, \vec{x}; \vec{x}_1'', \ldots, \vec{x}_N'', t) \times \prod_{j=1}^{N-1} d^3x_j \quad \text{for } N>1 \tag{1}$$

and

$$\langle 0 | \psi(\vec{x},t) | \vec{x}_1'' \rangle = K_1(\vec{x}; \vec{x}_1'', t), \tag{2}$$

where $\langle 0|$ denotes the vacuum, and

$$K_n(\vec{x}_1, \ldots, \vec{x}_N; \vec{x}_1'', \ldots, \vec{x}_N'', t) = (1/\sqrt{N!}) \langle 0 | \psi(\vec{x}_1, t) \cdots | \vec{x}_1'', \ldots, \vec{x}_N'' \rangle \tag{3}$$

is the symmetrized propagator for the N-particle Schrödinger equation. Note that K_n vanishes for prohibited configurations. In the case of time-independent interaction this can be transformed to the Schrödinger picture

$$\langle \nu_{N-1} | \psi(\vec{x}) | \nu_N \rangle = N^{-1/2} \int \prod_{i=1}^{N-1} d^3x_i \, \phi_{N-1}^*(q_{N-1}; \nu_{N-1}) \, \phi_N(q_{N-1}, \vec{x}; \nu_N), \tag{4}$$

where $|\nu_N\rangle$ is an eigenstate of the N-particle Schrödinger equation and

$$q_N \equiv \vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N \tag{5}$$

represents the position vectors. Equations (1)–(3) define the nonlocal operators in terms of their matrix elements. Wong[3] has shown that the field operators themselves, and not simply their matrix elements, can be defined in terms of the free-field operators $\psi_0(\vec{x})$ and $\psi_0^\dagger(\vec{x})$. For the sake of completeness and later convenience, we shall rewrite his definitions here:

$$\psi(\vec{x}) \equiv P(\vec{x})\psi_0(\vec{x}), \quad \psi^\dagger(\vec{x}) \equiv \psi_0^\dagger(\vec{x})P(\vec{x}), \tag{6}$$

where $P(\vec{x})$ is a projection operator defined as follows:

$$P(\vec{x}) \equiv \sum_{N=0}^{\infty} \int \prod_{i=0}^{N} C(\vec{x}, q_N) P_N(q_N) \, d^3x_i, \tag{7}$$

and $C(\vec{x}, q_N)$ is a step function,

$$\begin{aligned} C(\vec{x}, q_N) &= C(\vec{x}, \vec{x}_1) \cdots C(\vec{x}, \vec{x}_N) C(\vec{x}_1, \vec{x}_2) \cdots \\ &\quad \times C(\vec{x}_1, \vec{x}_N) \cdots C(\vec{x}_{N-1}, \vec{x}_N), \\ C(\vec{x}_i, \vec{x}_j) &\equiv \begin{cases} 1 & \text{for } |\vec{x}_i - \vec{x}_j| > a, \\ 0 & \text{for } |\vec{x}_i - \vec{x}_j| \le a, \end{cases} \\ P_N(q_N) &\equiv (N!)^{-1} \prod_{i=0}^{N} \psi_0^\dagger(\vec{x}_i) |0\rangle\langle 0| \prod_{j=0}^{N} \psi_0(\vec{x}_j), \end{aligned} \tag{8}$$

with the formal definition

$$P_0(q_0) \equiv |0\rangle\langle 0|.$$

It has been shown[3,11] that $P(\vec{x})$ can also be written

$$P(\vec{x}) \equiv P + \Lambda(\vec{x}), \tag{9}$$

where

$$P \equiv \sum_{N=0}^{\infty} \int \prod_{i=0}^{N} d^3x_i \, C(q_N) P_N(q_N) \tag{10}$$

and

$$\Lambda(\vec{x}) \equiv \sum_{l=1}^{M} \frac{(-1)^l}{l!} \int_{S_{\vec{x}}} \cdots \int \prod_{i=1}^{l} \psi^\dagger(\vec{x}_i) \prod_{j=1}^{l} \psi(\vec{x}_j) \, d^3x_j, \tag{11}$$

where $M=13$ is the maximum number of particles of diameter $a+\epsilon$ $(\epsilon \to 0^+)$ one can pack into a sphere of diameter $3a$. $S_{\vec{x}}$ is the volume bounded by the surface $|\vec{x} - \vec{x}_i| = \lim_{\epsilon=0^+} a+\epsilon$. As shown by Siegert[12] the meaning of $\Lambda(x)$ simply is

$$-\Lambda(\vec{x}) = N_1(S_{\vec{x}}) - N_2(S_{\vec{x}}) + \cdots (-1)^{M+1} N_M(S_{\vec{x}}), \tag{12}$$

where $N_1(S_{\vec{x}})$ can be interpreted as number of particles in the domain $S_{\vec{x}}$, $N_2(S_{\vec{x}})$ as number of pairs, $N_3(S_{\vec{x}})$ as number of triplets, etc. A particle is "in" $S_{\vec{x}}$ when it is in $S_{\vec{x}}$.

We shall show that in the two-body potential approximation P in Eq. (9) may be replaced by the identity operator. First, however, let us investigate the right-hand side of Eq. (9) to clarify its physical meaning. First we rewrite Eqs. (10) and (11) in a more explicit form

$$P=|0\rangle\langle 0| + \int \psi_0^\dagger(\vec{x})|0\rangle\langle 0|\psi_0(\vec{x})\,d^3x + \frac{1}{2!}\int C(\vec{x}_1,\vec{x}_2)\psi_0^\dagger(\vec{x}_1)\psi_0^\dagger(\vec{x}_2)|0\rangle \times\langle 0|\psi_0(\vec{x}_1)\psi_0(\vec{x}_2)\,d^3x_1\,d^3x_2+\cdots, \quad (13)$$

$$\Lambda(\vec{x})=-\int_{S_{\vec{x}}}\psi^\dagger(\vec{x}')\psi(\vec{x}')\,d^3x' + \frac{1}{2!}\int_{S_{\vec{x}}}\psi^\dagger(\vec{x}')\psi^\dagger(\vec{y}')\psi(\vec{y}')\psi(\vec{x}')\,d^3x'\,d^3y' - \cdots + \cdots \text{ (up to 26 operators)}. \quad (14)$$

The maximum number of hard-sphere particles of diameter a that can be packed in an imaginary sphere $K_{3a}(\vec{x})$ of diameter $3a$ is 13. To investigate the functional behavior of P and $\Lambda(\vec{x})$ we consider diagonal-matrix elements in the coordinate representation. For example, having P between hypothetical states with more than 13 particles inside $K_{3a}(\vec{x}), P$ acts like a zero operator, because that term in Eq. (13) that contains the matching projection operator leads, due to the presence of $C(\vec{x}_1\cdots\vec{x}_{12},\vec{x}_{14}\cdots)$ to a vanishing integrand in the domain under consideration. For the same reason P still acts as a zero operator in the case of 13 or less particles inside $K_{3a}(\vec{x})$ if at least two of the extra particles overlap. However, if the hypothetical states contain 13 or less nonoverlapping extra particles inside $K_{3a}(\vec{x})$, then P acts like an identity operator. On the other hand, from definitions (6), (7), and (8), or more explicitly, from the "commutation relations" (17), it follows that $\Lambda(\vec{x})$ leads to zero diagonal matrix elements if the states involved contain more than 13 extra particles in $K_{3a}(\vec{x})$. The matrix element is also zero for states having 13 or fewer extra particles of which at least two overlap inside $K_{3a}(\vec{x})$. What is going to happen when 1, 2, 3, etc., extra particles approach the hypothetical particle sitting at $\vec{x}$ in a nonoverlapping and nontouching manner.

As long as the particles are outside $K_{3a}(\vec{x})$, $P(\vec{x})\equiv \underline{1}$ which is trivial. Therefore let us look at them only when they are inside $K_{3a}(\vec{x})$.

One particle approaching leads to $P=1$, $\Lambda(\vec{x}) =-1\to P(\vec{x})=0$. Two particles approaching leads to $P=1$, $\Lambda(\vec{x})=-2+1\to P(\vec{x})=0$. Thirteen particles approaching leads to $P=1$, $\Lambda(\vec{x})=-\binom{13}{1}+\cdots-\binom{13}{13} \to P(\vec{x})=0$. From the above considerations we can learn two things.

(i) We see that in an expansion of $P(\vec{x})$ in powers of $\psi_0(\vec{x})$ and $\psi_0^\dagger(\vec{x})$ including only two-body interaction, P can be replaced by $\underline{1}$ because the incoming particle can never overlap with itself. However, as soon as we include high powers of the field operators, P is not the identity anymore.

(ii) From the correct functional behavior of $P(\vec{x})$ defined in Eqs. (9)–(11) we conclude that it is the same as the one defined via Eqs. (7) and (8). A mathematical proof of this statement can be found in Refs. 3 and 11.

The new commutation rules imposed on the nonlocal field operators due to the hard-core assumption are[14]

$$[\psi(\vec{x}),\psi(\vec{x}')]=[\psi^\dagger(\vec{x}),\psi^\dagger(\vec{x}')]=0, \quad \forall\,\vec{x},\vec{x}', \quad (15)$$

$$[\psi(\vec{x}),\psi^\dagger(\vec{x}')]=0, \quad \forall\,|\vec{x}-\vec{x}'|>a, \quad (16)$$

$$\psi(\vec{x})\psi(\vec{x}')=\psi^\dagger(\vec{x})\psi^\dagger(\vec{x}')=0, \quad \forall\,|\vec{x}-\vec{x}'|\le a, \quad (17)$$

$$\psi(\vec{x})\psi^\dagger(\vec{x}')=\delta(\vec{x}-\vec{x}')P(\vec{x}), \quad \forall\,|\vec{x}-\vec{x}'|\le a. \quad (18)$$

For further properties of these nonlocal field operators we refer the reader to Siegert *et al.*,[11] where they also have shown that in terms of the nonlocal field operators the many-body pseudo-Hamiltonian with periodic boundary conditions has the form

$$H=-\int d^3x\,\psi^\dagger(\vec{x})\nabla_x^2\,\psi(\vec{x}). \quad (19)$$

In Eq. (19) we have set $\hbar=2m=1$. We shall use these units throughout this work. Using the commutation relations and the algebraic identities mentioned above, Eq. (19) can be written[3] in the following exact form:

$$H=-\int d^3x\,\psi_0^\dagger(\vec{x})\nabla_{\vec{x}}^2 P(\vec{x})\psi_0(\vec{x})+\lim_{\epsilon=0^+}\frac{1}{f(a)} \times\int d^3x'\,d^3x\,\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\delta(r-a) \times\left(\frac{\partial}{\partial r}f(r)P(\vec{x})P(\vec{x}')\psi_0(\vec{x}')\psi_0(\vec{x})\right)_{r=a+\epsilon}, \quad (20)$$

where $f(r)$ is an arbitrary function of r that is analytic at $r=a$.

Our next step is to show that in the two-particle case Eq. (20) leads to the exact solution of the two-particle hard-sphere boundary problem. Calculating the scattering length for vanishing scattering energies in the Born approximation (S scattering) and comparing it with the radius of a hard sphere we shall be able to determine $f(r)$ in a unique fashion.

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Expressing Eq. (20) in the energy-matrix representation and using the identity

$$\sqrt{2!}\,\phi_{\nu_2}(r)=\langle 0|\psi(\vec{x})\psi(\vec{y})|\nu_2\rangle, \quad (21)$$

we find

$$E_{\nu 2}=\langle\nu_2|H|\nu_2\rangle=-2\sum_{\nu_1\nu_1'}\int\phi^*_{\nu_2}(\vec{x},\vec{q})\nabla^2_{\vec{x}}\phi_{\nu_1}(\vec{q})\langle\nu_1|P(\vec{x})|\nu_1'\rangle\phi^*_{\nu_1'}(\vec{q}')\phi_{\nu_2}(\vec{q},\vec{x})\,d^3q\,d^3q'\,d^3x$$
$$+\lim_{\epsilon=0^+}\frac{2}{f(a)}\int d^3x\,d^3x'\,\phi^*_{\nu_2}(\vec{x},\vec{x}')\delta(r-a)\frac{\partial}{\partial r}[f(r)\phi_{\nu_2}(\vec{x},\vec{x}')]_{r=a+\epsilon}\,. \tag{22}$$

The matrix element $\langle\nu_1|P(\vec{x})|\nu_1'\rangle$ is given with Eqs. (9) and (11) by

$$\langle\nu_1|P(\vec{x})|\nu_1'\rangle=\langle\nu_1|1-\int_{S_{\vec{x}}}\psi_0^\dagger(\vec{y})\psi_0(\vec{y})\,d^3y|\nu_1'\rangle=\delta_{\nu_1\nu_1'}-\int_{S_{\vec{x}}}d^3y\,\phi^*_{\nu_1}(\vec{y})\phi_{\nu_1'}(\vec{y})\,. \tag{23}$$

From Eqs. (22) and (23) we obtain

$$E_{\nu_2}=-2\int\phi^*_{\nu_2}(\vec{x},\vec{q})\nabla^2_{\vec{x}}\phi_{\nu_2}(\vec{x},\vec{q})\,d^3q\,d^3x+2\sum_{\nu_1}\int\phi^*_{\nu_2}(\vec{x},\vec{q})\nabla^2_{\vec{x}}\phi_{\nu_1}(\vec{q})\int_{S_{\vec{x}}}d^3y\,\phi^*_{\nu_1}(\vec{y})\phi_{\nu_2}(\vec{y},\vec{x})\,d^3q\,d^3x$$
$$+\lim_{\epsilon=0^+}\frac{2}{f(a)}\int d^3y\,d^3x\,\phi^*_{\nu_2}(\vec{x},\vec{y})\delta(r-a)\frac{\partial}{\partial r}[f(r)\phi_{\nu_2}(\vec{x},\vec{y})]_{r=a+\epsilon}\,. \tag{24}$$

Equation (24) leads to the following Schrödinger equation in Cartesian coordinates:

$$E_{\nu_2}\phi_{\nu_2}(\vec{x},\vec{y})=-(\nabla^2_{\vec{x}}+\nabla^2_{\vec{y}})\phi_{\nu_2}(\vec{x},\vec{y})+\sum_{\nu_1}\left(\nabla^2_{\vec{x}}\phi_{\nu_1}(\vec{y})\int_{S_{\vec{x}}}d^3q\,\phi^*_{\nu_1}(\vec{q})\phi_{\nu_2}(\vec{q},\vec{x})\right)$$
$$+\sum_{\nu_1}\left(\nabla^2_{\vec{y}}\phi_{\nu_1}(\vec{x})\int_{S_{\vec{y}}}d^3q\,\phi^*_{\nu_1}(\vec{q})\phi_{\nu_2}(\vec{q},\vec{y})\right)+\lim_{\epsilon=0^+}\frac{2}{f(a)}\delta(r-a)\left(\frac{\partial}{\partial r}f(r)\phi_{\nu_2}(\vec{x},\vec{y})\right)_{r=a+\epsilon}\,. \tag{25}$$

The summation over ν_1 leads to terms like

$$\nabla^2_{\vec{x}}\int_{S_{\vec{x}}}\delta(\vec{y}-\vec{q})\phi_{\nu_2}(\vec{q},\vec{x})\,d^3q=\lim_{\epsilon=0^+}\nabla^2_{\vec{x}}\theta(|\vec{y}-\vec{x}|-a-\epsilon)\phi_{\nu_2}(\vec{y},\vec{x})\,, \tag{26}$$

where $\theta(|\vec{x}-\vec{y}|-a-\epsilon')\equiv 1\,\forall\,|\vec{y}-\vec{x}|\leq a+\epsilon'$, and $\epsilon>\epsilon'>0$ and zero otherwise. Going to spherical coordinates, Eq. (25) together with Eq. (26) leads to

$$\tfrac{1}{2}E_{\nu_2}\phi_{\nu_2}(\vec{r})=-\nabla^2_{\vec{r}}\phi_{\nu_2}(\vec{r})+\nabla^2_{\vec{r}}\theta(r-a-\epsilon')\phi_{\nu_2}(\vec{r})+\frac{1}{f(a)}\delta(r-a)\left(\frac{\partial}{\partial r}f(r)\phi_{\nu_2}(\vec{r})\right)_{r=a+\epsilon}\,, \tag{27}$$

with the boundary conditions $\phi_{\nu_2}(0)=\phi_{\nu_2}(\infty)=0$ and $\frac{1}{2}E_{\nu_2}=k^2$, where $\vec{k}$ is the momentum of one particle in the center-of-mass system (center-of-mass motion is assumed to be zero). In order to transform the second term on the right-hand side of Eq. (27) into a well-defined form we ought to go back to an expression analogous to the one of Eq. (24):

$$\int\phi^*_{\nu_2}(\vec{r})\nabla^2_{\vec{r}}[\theta(r-a-\epsilon')\phi_{\nu_2}(\vec{r})]\,d^3r=\int\nabla_{\vec{r}}\phi^*_{\nu_2}(\vec{r})[\nabla_{\vec{r}}\theta(r-a-\epsilon')\phi_{\nu_2}(\vec{r})]\,d^3r-\int[\nabla_{\vec{r}}\phi^*_{\nu_2}(\vec{r})][\nabla_{\vec{r}}\theta(r-a-\epsilon')\phi_{\nu_2}(\vec{r})]\,d^3r\,. \tag{28}$$

The first term on the right-hand side of Eq. (28) can be transformed into a surface integral and contributes zero. With the second term we go through the same procedure again and finally find

$$\int\phi^*_{\nu_2}(\vec{r})\nabla^2_{\vec{r}}[\theta(r-a-\epsilon')\phi_{\nu_2}(\vec{r})]\,d^3r=\int[\nabla^2_{\vec{r}}\phi^*_{\nu_2}(\vec{r})]\theta(r-a-\epsilon')\phi_{\nu_2}(\vec{r})\,d^3r\,. \tag{29}$$

On the other hand taking only the radial Schrödinger equation of Eq. (27),

$$\frac{\partial^2U_l(r)}{\partial r^2}+\left(\tfrac{1}{2}E_{\nu_2}-\frac{l(l+1)}{r^2}\right)U_l(r)=\frac{1}{f(a)}\delta(r-a)\left(\frac{\partial}{\partial r}f(r)U_l(r)\right)_{r=a+\epsilon'}+\frac{\partial^2}{\partial r^2}[\theta(r-a-\epsilon')U_l(r)]-\frac{l(l+1)}{r^2}[\theta(r-a-\epsilon')U_l(r)]\,, \tag{30}$$

and integrating both sides of Eq. (30) twice from $a-\epsilon$ to $a+\epsilon$, we find, from the first and second integration,

$$\lim_{\epsilon=0^+}\frac{\partial}{\partial r}U_l(r)\bigg|_{r=a-\epsilon}=0\,,\qquad \lim_{\epsilon=0^+}U_l(a+\epsilon)=0\,,\quad\epsilon>\epsilon'>0\,, \tag{31}$$

where $U_l(r)$ is defined via

$$\phi_{\nu_2}(\vec{r}) = \sum_{l,m} A_{lm} \frac{U_l(r)}{r} Y_{lm}(\theta, \xi) . \tag{32}$$

The restrictions imposed on $U_l(r)$ by Eqs. (30), (31), and (32) together with the boundary conditions lead to

$$\begin{aligned} &U_l(r) = 0, \quad r \leq a , \\ &U_l(r) = kr\,[n_l(ka) j_l(kr) - j_l(ka) n_l(kr)], \quad r > a . \end{aligned} \tag{33}$$

Hence we know that all the allowed solutions of Eq. (27) can be chosen without restriction of generality to have a real radial part. Now coming back to Eq. (29) we argue the following way: Since $U_l(r)$ can be chosen real and since Y^*_{lm} and Y_{lm} lead to the same eigenvalue under the operation $\nabla^2_{\vec{r}}$ we can write the second term on the right-hand side of Eq. (29) as

$$\int \phi^*_{\nu_2}(\vec{r}) \theta(r - a - \epsilon) \nabla^2_{\vec{r}} \phi_{\nu_2}(\vec{r})\, d^3 r . \tag{34}$$

This last step is peculiar to the two-body problem. Now we can turn back to the Schrödinger equation and finally arrive at

$$\tfrac{1}{2} E_{\nu_2} \phi_{\nu_2}(\vec{r}) = -\nabla^2_{\vec{r}} \phi_{\nu_2}(\vec{r}) + \lim_{\epsilon=0^+} \left[\theta(r - a - \epsilon) \nabla^2_{\vec{r}} \phi_{\nu_2}(\vec{r}) + \frac{1}{f(a)} \delta(r-a) \times \left(\frac{\partial}{\partial(r)} f(r) \phi_{\nu_2}(\vec{r}) \right)_{r=a+\epsilon} \right] . \tag{35}$$

It is obvious that Eq. (35) has to lead to the correct solution for two particles with hard-sphere interaction. For $r > a$ we have the free-particle equation. For $r \leq a$ the right-hand side of Eq. (35) is zero; therefore, $\phi_{\nu_2}(\vec{r}) = 0$. When we cross the boundary, the last term in Eq. (35) will compensate the infinity due to the discontinuity of the slope at $r = a$. It is important to realize that Eq. (35) cannot simply be generalized to N particles by casting it into second quantization as Luban[13] did. He ended up with a non-Hermitian Hamiltonian and arrived at the conclusion that the non-Hermiticity of the pseudo-Hamiltonian is an inherent property of the hard-sphere boundary problem. This is not true because Eq. (27) is Hermitian as we shall show in Sec. IV. The non-Hermiticity was introduced by utilizing a particular property of the solution of Eq. (27) while going from Eq. (29) to Eq. (34). In case of more than two particles the mutual angular dependence is no longer trivial and therefore the steps from Eq. (29) to Eq. (34) cannot be performed anymore!

In order finally to determine the function $f(r)$ we shall consider the scattering length $A(0)$ in the Born approximation for the limit of vanishing scattering energy[17]

$$A(0) = \lim_{k=0^+} -\frac{1}{4\pi} \int e^{-i\vec{k}_x \cdot \vec{r}} d^3 r \times \left(\theta(r-a) \nabla^2_{\vec{r}} + \frac{1}{f(a)} \delta(r-a) \frac{\partial}{\partial r} f(r) \right) e^{i\vec{k}\cdot\vec{r}} , \tag{36}$$

where $|\vec{k}_x| = |\vec{k}|$ for elastic scattering. Integrating Eq. (36) leads to

$$A(0) = \lim_{k=0^+} -\frac{1}{f(a)} \left.\frac{\partial f(r)}{\partial r}\right|_{r=a} j_0(ka) a^2 + k j_1(ka) a^2 + O(k^2) . \tag{37}$$

For hard spheres, $-A(0)$ has to be equal to a since the total scattering cross section $\sigma(0) \equiv 4\pi A^2(0)$ is four times the classical scattering cross section. Hence, we conclude that

$$f(r) = r . \tag{38}$$

In principle, any choice of $f(r)$ would lead to the same result in the limit of an exact solution of the two-body problem as we have seen in Eq. (35). However, as soon as we have a partial wave expansion up to a finite l in mind then the form of $f(r)$ is crucial in order to guarantee the correct scattering amplitude in the zero-energy case. Matching $f(r)$ with the Born approximation guarantees a fast convergence. In the many-particle case, we can no longer solve the problem exactly. Thus considering only a finite number of terms in the integral equation to be solved, we restrict ourselves implicitly to a finite number of partial waves. Assuming that the Born approximation still leads to a fastly converging series in this case, is our whole motivation for choosing $f(r) = r$.

IV. TWO-BODY POTENTIAL HAMILTONIAN

Combining Eqs. (20) and (38) we can write the exact N-particle pseudo-Hamiltonian leading to the correct Born zero-energy scattering cross section in the two-particle case as

$$H = -\int d^3 x\, \psi_0^\dagger(\vec{x}) \nabla^2_{\vec{x}} P(\vec{x}) \psi_0(\vec{x}) + \lim_{\epsilon=0^+} \frac{1}{a} \int d^3 x'\, d^3 x\, \psi_0^\dagger(\vec{x}) \psi_0^\dagger(\vec{x}') \delta(r-a) \times \left(\frac{\partial}{\partial r} r P(\vec{x}) P(\vec{x}') \psi_0(\vec{x}) \psi_0(\vec{x}') \right)_{r=a+\epsilon} . \tag{39}$$

In the two-body potential approximation we replace $P(\vec{x})P(\vec{x}')$ by unity in the second term and

$$P(\vec{x}) = \underline{1} - \int_{S_{\vec{x}} = \lim_{\epsilon=0^+} (\vec{x}-\vec{x}') < a+\epsilon} \psi_0^\dagger(\vec{x}') \psi_0(\vec{x}')\, d^3 x' \tag{40}$$

in the first term of Eq. (39) as discussed in Sec. II. Transforming Eq. (39) in automatically well-defined form (see Appendix A) we obtain the two-body potential Hamiltonian in the following form:

$$H=-\int d^3x\,\psi_0^\dagger(\vec{x})\nabla_{\vec{x}}^2\psi_0(\vec{x})+\lim_{\epsilon=0^+}\Big[-\int_{|\vec{x}-\vec{x}'|\leq a_{\vec{x}}\epsilon} d^3x\,d^3x'\,[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\nabla_{\vec{x}}\psi_0(\vec{x}')\psi_0(\vec{x})]$$
$$+\int d^3x'\,d^3x\,\delta(r-a)\left(\frac{\partial}{\partial r}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\right)_{r=a+\epsilon}\psi_0(\vec{x}')\psi_0(\vec{x}')$$
$$+\frac{1}{a}\int d^3x'\,d^3x\,\delta(r-a)\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\left(\frac{\partial}{\partial r}r\psi_0(\vec{x}')\psi_0(\vec{x})\right)_{r=a+\epsilon}\Big], \quad (41)$$

where the first term on the right-hand side of Eq. (41) represents the kinetic energy, the second and third ones originate from the volume exclusion, and the last one is due to the discontinuity of the slope of the wave function at $r=a$. In the two-particle case, Eq. (41) is exact and leads us to Eq. (25) after similar steps as performed in Eq. (21) to Eq. (24). It is also obvious that Eq. (41) is Hermitian. Therefore, Eqs. (25) and (27) are Hermitian, which was actually the last missing link in the discussion of the two-body problem of Sec. III. The exact description of the meaning of the approximations made in Eq. (41) for the N-particle case shall be our next goal. In the two-body potential approximation of Eq. (41) we have taken into account the exact exclusion of terms that correspond to the physical situation shown in Fig. 2, types I and II. Configurations of type I and II result from the volume exclusion. The discontinuity of the slope at the surface also leads to terms like II. Configurations III, IV, and their generalization to more than three particles are also taken into account but will be overestimated because the overlap E is ignored. The correction to this overestimation would be provided by contributions from a genuine three-body potential. Configurations representing the contributions from a genuine three-body potential are shown in Fig. 3 and their origin is pointed out in Appendix B. In Appendix B we also give a rough estimate of the upper bound of these three-body potential contributions to our two-body potential Hamiltonian equation (41). In Fig. 3, terms like I, II, III, IV are the result of the "volume-exclusion term" in Eq. (39). I and II are taken into account exactly, in a three-body potential approach but III and IV again, would have to be corrected by higher-order potentials. Configurations like V and VI result from the "surface-matching term" in Eq. (39), where V is exact and VI would have to be subject to higher-order correction. A sufficiently accurate method of estimating an upper bound of the genuine three-body potential contribution to the Hamiltonian in the case of hard spheres cannot be given because it means in the first place that we can solve the two-body potential approximation exactly which is virtually impossible. In the dilute case the situation is much simpler. The two-body potential approximation definitely becomes good even in the rigorous N-particle hard-sphere model. Since the contributions from the genuine three, four-body, etc., potentials are proportional to ρ^2, ρ^3, etc. Because of its analytical tractability and its validity in the low-density limit, we propose the two-body potential Hamiltonian equation (41) as a trial Hamiltonian to represent the actual liquid-helium state. The ultimate test for such a trial Hamiltonian has to be the experiment: calculation of the pair-corre-

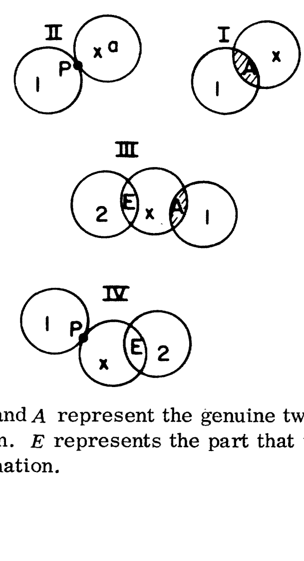

FIG. 2. P and A represent the genuine two-body boundary condition. E represents the part that is ignored in this approximation.

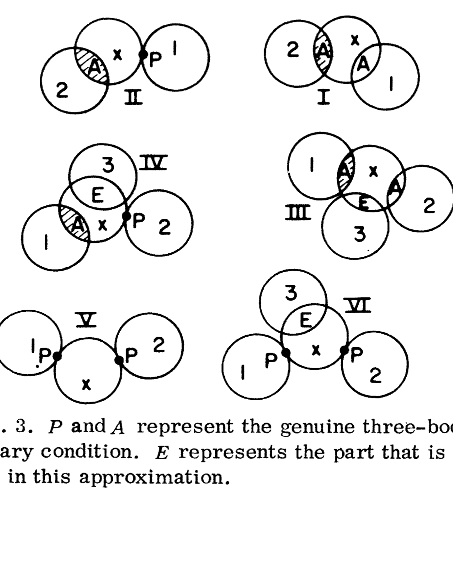

FIG. 3. P and A represent the genuine three-body boundary condition. E represents the part that is ignored in this approximation.

lation function, excitation energy, etc.

Let us write the Fourier transform of the two-body potential Hamiltonian. Using the plane-wave expansions

$$\psi_0(\vec{x}) = V^{-1/2}\sum_{\vec{k}} a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}, \qquad \psi_0^\dagger(\vec{x}) = V^{-1/2}\sum_{\vec{k}} a_{\vec{k}}^\dagger e^{-i\vec{k}\cdot\vec{x}}, \tag{42}$$

we can transform the trial Hamiltonian Eq. (42) (see Appendix C) into momentum representation where it becomes

$$H = \sum_{\vec{k}} k^2 a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{4\pi a}{V}\sum_{\vec{p},\vec{q},\vec{k}} V(\vec{k},\vec{p})\, a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}+\vec{k}} a_{\vec{q}-\vec{k}}, \tag{43}$$

$$V(\vec{k},\vec{p}) = \cos(ka)_+ - a\,\frac{\vec{p}(\vec{p}+\vec{k})}{k}\, j_1(ka)_-, \tag{44}$$

where the $\pm$ subscripts mean that we actually should write $a\pm\epsilon$ with $\epsilon\to 0^+$ in order to ensure that the derivatives on the wave function are taken at the proper place. The first term in Eq. (44) has its origin in the volume exclusion and the surface matching, the second one originates from volume exclusion only. The unusual form of the Fourier transform of the potential in the second term of Eq. (44) is a direct consequence of the impenetrability of the hard sphere described by the second term on the right-hand side of Eq. (41). In the case of weak interaction ($\equiv$ integrable potential) the Fourier transform only depends on the momentum exchange and never on the momentum of the incident particle. But we also know that in the case of a hard sphere, simulated by a δ function pseudopotential alone, there exists for each angular momentum component of the incoming wave function an infinite countable set of "leak-in" solutions depending on the scattering energy.[8] It is therefore to be expected that the exact exclusion of leak-in solutions leads to a Fourier transform that also depends on the momentum of the incident particle.

V. INSTABILITY OF THE HARTREE-FOCK GROUND STATE

In their work on hard sphere interaction Wong and Huang[1] obtained a numerical solution for the ground state of a hard-sphere system of liquid-He density. In that letter they reported the absence of a zero-momentum condensate by simply using the pair-approximated part of the two-body Hamiltonian. The question therefore must be raised as to why such a numerical conclusion is in principle possible, contrary to the usual belief that Bose-Einstein condensation is essential in a model for superfluidity. This problem will be discussed here more rigorously than has been done in Sec. I. To study this problem we start with the Hamiltonian given in Eq. (43).

Using the pair-approximated part only, the form of which is easily derived via Eqs. (62) and (65) presented in Sec. VI, we obtain

$$\begin{aligned} H_p = {}& \frac{4\pi a}{V} N^2 + \frac{4\pi a}{V}\sum_{\vec{k}}{}' \left[\left(\frac{4\pi a}{V}\right)^{-1} k^2 - 2N + NV(0,0) + NV(\vec{k},0) + NV(0,\vec{k}) + NV(-\vec{k},\vec{k})\right] a_{\vec{k}}^\dagger a_{\vec{k}} \\ & + \frac{4\pi a}{V}\left(\sum_{\vec{k},\vec{q}}{}'' [1 - V(-\vec{k},\vec{k}) - V(\vec{k},0) - V(0,0)] + \sum_{\vec{k},\vec{q};\,\vec{k}\neq\vec{q}}{}' V(\vec{k}-\vec{q},\vec{q})\right) a_{\vec{k}}^\dagger a_{\vec{k}} a_{\vec{q}}^\dagger a_{\vec{q}} \\ & + \frac{4\pi a}{V}\sum_{\vec{p},\vec{k};\,\vec{p}\neq-\vec{k};\,\vec{k}\neq-2\vec{p}}{}' V(\vec{k},\vec{p})\, a_{\vec{p}}^\dagger a_{-\vec{p}}^\dagger a_{\vec{p}+\vec{k}} a_{-\vec{p}-\vec{k}} + \frac{4\pi a}{V}\sum_{\vec{k}}{}' V(\vec{k},-\vec{k})_0^\dagger a_0^\dagger a_{\vec{k}} a_{-\vec{k}} + V(\vec{k},-\vec{k})\, a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger a_0 a_0 , \end{aligned} \tag{45}$$

where $V(\vec{k},\vec{q})$ is defined in Eq. (44).

To study the instability of the normal Hartree-Fock ground state against the formation of opposite momenta pairs, let us first define what we mean by a "normal" state of an interacting Bose system. A normal state is a state such that it is physical to associate an equation of motion of a single particle to a single excitation out of the noninteracting ground state and the concept of effective mass of this single particle is both physical and measurable. Mathematically therefore, the normal state is a state of the system, for which the number operator in momentum representation is a good quantum number. In fact a normal N-particle state of an interacting system is usually approximated by some eigenstate of the Hartree-Fock Hamiltonian associated with the original problem. Such a general state can be written simply as

$$|\phi_0^N\rangle = \prod_{\vec{k}} |n_{\vec{k}}\rangle = \prod_{\vec{k}} \frac{1}{(n_{\vec{k}}!)^{1/2}} (a_{\vec{k}}^\dagger)^{n_{\vec{k}}} |0\rangle, \tag{46}$$

where $|0\rangle$ is the vacuum and $|\phi_0^N\rangle$ satisfies

$$a_{\vec{k}}^\dagger a_{\vec{k}} |\phi_0^N\rangle = n_{\vec{k}} |\phi_0^N\rangle, \tag{47}$$

$$N=\sum_{\vec{k}=0}^{\infty} n_{\vec{k}} . \quad (48)$$

Now the Hartree-Fock ground state is therefore obtained by minimizing $\langle\phi_0^N|H_p|\phi_0^N\rangle$ with respect to $\{n_{\vec{k}}\}$, which leads to an integral equation for $n_{\vec{k}}$ (see Appendix D):

$$\xi(k)+\sum_{\vec{q}}[W_{\text{HF}}(\vec{k},\vec{q})+W_{\text{HF}}(\vec{q},\vec{k})]n_{\vec{q}}=0 , \quad (49)$$

where

$$\xi(k)=k^2(1-\tfrac{4}{3}\pi a^3\rho)+8\pi a\rho\cos(ka)_+ , \quad (50)$$

$$W_{\text{HF}}(\vec{k},\vec{q})=(4\pi a/V)[V(\vec{k}-\vec{q},\vec{q})-2\cos(ka)_+] . \quad (51)$$

Terms that vanish in the thermodynamic limit are neglected.

To study the energy required to form extra opposite momenta pairs out of the Hartree-Fock ground state we construct the state

$$|\psi\rangle=\sum_{\vec{p}}A(\vec{p})a_{\vec{p}}^\dagger a_{-\vec{p}}^\dagger|\phi_0^N\rangle , \quad (52)$$

with the normalization condition

$$1=2\sum_{\vec{k}}{}'A^2(\vec{k})(n_{\vec{k}}+1)^2+A^2(0)(n_0+1)(n_0+2) . \quad (53)$$

The energy increase per particle due to pair formation is given by

$$\Delta E=(N+2)^{-1}\langle\psi|H_p|\psi\rangle-N^{-1}\langle\phi_0^N|H_p|\phi_0^N\rangle , \quad (54)$$

and in the thermodynamic limit we obtain (see Appendix D)

$$\Delta E=\frac{16\pi a}{NV}\bigg(\sum_{\vec{p},\vec{q}}{}'V(\vec{q}-\vec{p},\vec{p})A(\vec{p})A(\vec{q})(n_{\vec{p}}+1)^2(n_{\vec{q}}+1)^2 +\sum_{\vec{k}}{}'A(\vec{k})(n_{\vec{k}}+1)^2A(0) \times(n_0+1)(n_0+2)\cos(ka)_+\bigg) . \quad (55)$$

Expression (55) can formally be simplified with the definitions

$$\hat{D}=\frac{1}{V}\sum_{\vec{k}}{}'\cos(ka)_+A(\vec{k})(n_{\vec{k}}+1) ,$$
$$\hat{E}_0=\frac{1}{V}\sum_{\vec{k}}{}'j_0(ka)_+A(\vec{k})(n_{\vec{k}}+1) , \quad (56)$$
$$\hat{E}'_{2l}=\frac{1}{V}\sum_{\vec{k}}{}'j_{2l}(ka)_-A(\vec{k})(n_{\vec{k}}+1) ,$$

and one arrives at

$$\Delta E=16\pi a\bigg(N^{-1}\hat{D}A(0)(n_0+1)(n_0+2)+2\rho^{-1}\hat{E}_0\hat{D} -\rho^{-1}\hat{E}_0^2-\rho^{-1}\sum_{l=1}^{\infty}(4l+1)\hat{E}'^2_{2l}\bigg) . \quad (57)$$

If the pair state also satisfies the Lieb boundary condition, then we have

$$\lim_{r=a+\epsilon}\langle\phi_0^N|\psi_0(\vec{r})\psi_0(0)|\psi\rangle=0 . \quad (58)$$

Decomposing the local-field operators $\psi_0(\vec{r})$, $\psi_0^\dagger(\vec{r})$ in their Fourier components, Eq. (58) leads to

$$A(0)(n_0+1)(n_0+2)+2V\hat{E}_0=0 . \quad (59)$$

From Eqs. (57) and (59) we learn that the energy per particle decreases under the formation of opposite momenta pairs out of the Hartree-Fock ground state. Therefore, the Hartree-Fock ground state is unstable against formation of opposite momenta pairs. It is important to point out that the Hartree-Fock ground state constructed here might not satisfy the boundary condition

$$\lim_{r=a+\epsilon}\langle\phi_0^{N-2}|\psi_0(\vec{r})\psi_0(0)|\phi_0^N\rangle=0 . \quad (60)$$

This constraint in fact cannot be imposed unless the nonpair terms in the Hamiltonian are included in solving for the wave function ($|\phi_0^N\rangle$ is an exact solution of a pair Hamiltonian, whereas $|\psi\rangle$ is not). For the same reasons the pair-correlation function does not vanish inside the core if only the pair-approximated two-body pseudo-Hamiltonian H_p is included in the variational calculation of the ground state since H_p does not exactly replace the hard-core interaction.

Our conclusion—formation of opposite momenta pairs lowers the ground-state energy per particle—does not depend on whether there is any single-particle Bose-Einstein condensate in the opposite momenta pair states we have constructed. In fact the existence of a residual amount of Bose-Einstein condensate in the superfluid ground state where opposite momenta pairs are important must only depend on the density of our hard-sphere system.

It must be pointed out here that the variational set $\{|\psi\rangle\}$ [Eq. (52)] is not contained in the variational set $\{|\psi_0'\rangle\}$ discussed in Sec. VI and employed in the numerical computation in Ref. 1. But both variational sets are based on the formation of opposite momenta pairs which enhances our confidence in the numerical results obtained with $\{|\psi_0'\rangle\}$ where such an analytical statement cannot be obtained.

VI. PAIR APPROXIMATION

As mentioned in Sec. I, the outcome of any physical quantity calculated from the Hamiltonian

(43) will depend sensitively on the density of the system and therefore also on the amount of zero-momentum condensate which in turn governs the method of solution. Our initial guess of how to solve the problem has to be in accord with the results. Therefore we have to pay special attention to the treatment of the zero-momentum component in H. We regroup H in the following way:

$$H = H_p + H_t + H , \tag{61}$$

$$\begin{aligned} H_p = {} & \sum_{\vec{k}}{}' k^2 a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{4\pi a}{V} \hat{N}_0(\hat{N}_0 - 1) + \frac{4\pi a}{V} \sum_{\vec{k}}{}' [V(\vec{k},0) a_0^\dagger a_0^\dagger a_{\vec{k}} a_{-\vec{k}} + V(\vec{k},-\vec{k}) a_{-\vec{k}}^\dagger a_{\vec{k}}^\dagger a_0 a_0] \\ & + \frac{4\pi a}{V} \sum_{\vec{k}}{}' [V(\vec{k},-\vec{k}) a_{-\vec{k}}^\dagger a_{-\vec{k}} a_0^\dagger a_0 V(\vec{k},0) a_0^\dagger a_0 a_{\vec{k}}^\dagger a_{\vec{k}}] + \frac{4\pi a}{V} \sum_{\vec{p}}{}' [V(0,0) a_{\vec{p}}^\dagger a_{\vec{p}} a_0^\dagger a_0 + V(0,\vec{p}) a_{\vec{p}}^\dagger a_{\vec{p}} a_0^\dagger a_0] \\ & + \frac{4\pi a}{V} \sum_{\vec{p},\vec{k},\vec{p}\neq -\vec{k}\neq 2\vec{p}}{}' V(\vec{k},\vec{p}) a_{\vec{p}}^\dagger a_{-\vec{p}}^\dagger a_{\vec{p}+\vec{k}} a_{-\vec{p}-\vec{k}} + \frac{4\pi a}{V} \sum_{\vec{p},\vec{q}}{}' V(0,\vec{p}) a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}} a_{\vec{q}} + \frac{4\pi a}{V} \sum_{\vec{p},\vec{q},\vec{p}\neq\vec{q}}{}' V(\vec{q}-\vec{p},\vec{p}) a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{q}} a_{\vec{p}} , \end{aligned} \tag{62}$$

$$\begin{aligned} H_t = {} & \frac{4\pi a}{V} \sum_{\vec{p},\vec{q},\vec{p}+\vec{q}\neq 0}{}' V(\vec{q},\vec{p}) a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}+\vec{q}} a_0 + \frac{4\pi a}{V} \sum_{\vec{p},\vec{q},\vec{p}+\vec{q}\neq 0}{}' V(-\vec{p},\vec{p}) a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_0 a_{\vec{q}+\vec{p}} \\ & + \frac{4\pi a}{V} \sum_{\vec{q},\vec{k},\vec{q}-\vec{k}\neq 0}{}' V(\vec{k},0) a_0^\dagger a_{\vec{q}}^\dagger a_{\vec{k}} a_{\vec{q}-\vec{k}} + \frac{4\pi a}{V} \sum_{\vec{p},\vec{k},\vec{q}+\vec{k}\neq 0,\vec{p}+\vec{k}\neq 0}{}' V(\vec{k},\vec{p}) a_{\vec{p}}^\dagger a_0^\dagger a_{\vec{p}+\vec{k}} a_{-\vec{k}} , \end{aligned} \tag{63}$$

$$H_r = \frac{4\pi a}{V} \sum_{\vec{p},\vec{q},\vec{k},\vec{p}+\vec{k}\neq 0,\vec{q}-\vec{k}\neq 0,\vec{p}+\vec{q}\neq 0,\vec{p}+\vec{k}\neq\vec{q}}{}' V(\vec{k},\vec{p}) a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}+\vec{k}} a_{\vec{q}-\vec{k}} , \tag{64}$$

where the prime on the sum means that none of the summation variables reaches zero. Using the definition

$$\hat{N}_0 \equiv N - \sum_{\vec{k}}{}' a_{\vec{k}}^\dagger a_{\vec{k}} , \tag{65}$$

where N is the total number of particles, the definition (44) for $V(\vec{k},\vec{p})$ and introducing the ordering parameters $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ to keep track of the different terms we obtain

$$\begin{aligned} H_p = {} & \frac{4\pi a}{V} N(N-1) + \sum_{\vec{k}}{}' k^2 a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{8\pi a}{V} \sum_{\vec{k}}{}' \lambda_1 \hat{N}_0 \cos(ka)_+ a_{\vec{k}}^\dagger a_{\vec{k}} \\ & + \frac{4\pi a}{V} \sum_{\vec{k}}{}' \lambda_2 \cos(ka)_+ a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger a_0 a_0 + (\text{c.c.}) - \frac{4\pi a}{V}(N-1) \sum_{\vec{p}}{}' \left(\frac{a^2 p^2}{3}\right) a_{\vec{p}}^\dagger a_{\vec{p}} \\ & + \frac{4\pi a}{V} \sum_{\vec{p},\vec{q}}{}' \lambda_3 \left(\cos(|\vec{q}-\vec{p}|a)_+ - j_1(|\vec{q}-\vec{p}|a)_- \frac{\vec{p}\cdot\vec{q}a}{|\vec{q}-\vec{p}|}\right) a_{\vec{p}}^\dagger a_{\vec{p}} a_{\vec{q}}^\dagger a_{\vec{q}} \\ & + \frac{4\pi a}{V} \sum_{\vec{p},\vec{q}}{}' \lambda_4 \left(\cos(|\vec{q}-\vec{p}|a)_+ - j_1(|\vec{q}-\vec{p}|a)_- \frac{\vec{p}\cdot\vec{q}a}{|\vec{q}-\vec{p}|}\right) a_{\vec{p}}^\dagger a_{-\vec{p}}^\dagger a_{\vec{q}} a_{-\vec{q}} . \end{aligned} \tag{66}$$

In Eq. (66) we restrict our attention to the pair Hamiltonian H_p only. The reasons for this choice are pointed out here in short, and some of them will be discussed in depth later on in the same sequence as they are listed here.

(i) H_p leads to a true upper bound of the ground-state energy of H.

(ii) In the dense case we think it is reasonable, based on experimental[15] and theoretical[16] data, to assume that the zero-momentum condensate is small compared to the total number of particles, such that we can expand our Hamiltonian in powers of $\beta = N_0/N$. It will be shown later that $\beta \to 0$ implies $\lambda_1 = \lambda_2 = 0$. This simplifies the analysis of H_p greatly, and also implies that H_t is negligible. It will be shown that H_t contributes to H only to order $\beta^{1/2}$.

(iii) H_p leads to a condensation in momentum space around the roton branch of the excitation spectrum and seems to exhibit in this sense the repulsive property of the pseudopotential in analogy to the finite repulsive potential illustrated in Sec. I. It also gives rise to an off-diagonal long-range order[18] (ODLRO) of the reduced density matrix in the coordinate representation. The onset of such an order is typical for the occurrence of a new thermodynamic phase, in our case superfluid He.

(iv) The numerical calculation based on H_p reproduces some features of the experimentally measured excitation spectrum.

In addition to these reasons for selecting the H_p terms, we note that in the thermodynamic limit the ground-state energy of H_p can be calculated exactly.

The disadvantages of choosing H_p to be the leading term are the following ones: (a) H_r contributes to the Hamiltonian H to order β^0, and therefore is an important term in a perturbational correction. (b) The pair Hamiltonian gives rise to an incorrect pair-correlation function for distances closer than the hard-sphere diameter. (This problem will be discussed more sincerely in a second paper.) It should be emphasized that this does not necessarily mean that our two-body potential approximation (41) has failed to reproduce the correct pair-correlation function. It is in our opinion rather the pair approximation that fails. This belief has been substantiated by calculations of the roton-roton scattering frequency due to H_r.[19]

Before discussing in detail some of the points just mentioned, we describe the origin of the different terms in Eq. (66) and then proceed with the analytical treatment of H_p as far as possible. The origin of the terms on the right-hand side of Eq. (66) is as follows:

The first term is obtained from splitting up the zero-momentum operators $\hat{N}_0(\hat{N}_0 - 1)$ according to Eq. (65). The nonzero momentum operators $a_{\vec{k}}^\dagger a_{\vec{k}}$ have been absorbed by terms originated from surface matching and volume exclusion (≡s.v. terms) on one hand, described in the discussion of Eqs. (41) and (44), and on the other hand by the correction to the kinetic energy which constitutes the fifth term in Eq. (66).

The second term is obtained from the kinetic energy.

The fifth term is obtained from the decomposition of the zero-momentum operators mentioned, and by the volume-exclusion term (≡v. term).

The sixth and seventh terms represent the Hartree-Fock- and BCS-like terms. The j_1 contribution comes from v. terms, the cos contribution form v.s. terms. The cos terms have also been considered by Girardeau[20] using a pseudo-Hamiltonian proposed by Lieb.[9] If we compare the kinetic energy correction due to the fifth term with the one of Ref. 13, we find a difference of a factor of 2. This difference from Ref. 13 arises from the non-Hermiticity of the Hamiltonian used in that paper, which led to both improper mathematics and misleading results.

Our next step consists of rewriting Hamiltonian (66) in a particle-number invariant form. This can be accomplished by making use of a Bolsterli transformation[21] given by

$$b_{\vec{k}} = a_0^\dagger(\hat{N}_0 + 1)^{-1/2} a_{\vec{k}} ,\qquad b_{\vec{k}}^\dagger = a_{\vec{k}}^\dagger(\hat{N}_0 + 1)^{-1/2} a_0 , \tag{67}$$

where $\hat{N}_0$ has to be further replaced by

$$\hat{N}_0 = N - {\sum_{\vec{k}}}' b_{\vec{k}}^\dagger b_{\vec{k}} . \tag{68}$$

Definitions (65) and (68) of $\hat{N}_0$ are equivalent as can be seen from the properties of the operators $b_{\vec{k}}^\dagger$ and $b_{\vec{k}}$. For further properties of these operators we refer the reader to Kromminga and Bolsterli.[21]

In b-operator representation, (66) becomes

$$\begin{aligned} H_p = {} & 4\pi a\rho(N-1) + {\sum_{\vec{k}}}' k^2 b_{\vec{k}}^\dagger b_{\vec{k}} + 8\pi a\rho\lambda_1 {\sum_{\vec{k}}}' \cos(ka)_+ b_{\vec{k}}^\dagger b_{\vec{k}} - \frac{8\pi a}{V}\lambda_1 {\sum_{\vec{k},\vec{q}}}' \cos(ka)_+ b_{\vec{k}}^\dagger b_{\vec{k}} b_{\vec{q}}^\dagger b_{\vec{q}} \\ & + \frac{4\pi a}{V}\lambda_2 {\sum_{\vec{k}}}' \cos(ka)_+ \Big\{ b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger \Big[\Big(N - {\sum_{\vec{q}}}' b_{\vec{q}}^\dagger b_{\vec{q}}\Big)\Big(N - {\sum_{\vec{q}}}' b_{\vec{q}}^\dagger b_{\vec{q}} - 1\Big)\Big]^{1/2} \\ & \qquad + \Big[\Big(N - {\sum_{\vec{q}}}' b_{\vec{q}}^\dagger b_{\vec{q}}\Big)\Big(N - {\sum_{\vec{q}}}' b_{\vec{q}}^\dagger b_{\vec{q}} - 1\Big)\Big]^{1/2} b_{-\vec{k}} b_{\vec{k}} \Big\} \\ & - \frac{4\pi a}{3V}\lambda_3 {\sum_{\vec{k}}}' (a^2k^2)_- b_{\vec{k}}^\dagger b_{\vec{k}} + \frac{4\pi a}{V} {\sum_{\vec{p},\vec{q}}}' V(\vec{q}-\vec{p},\vec{p})(\lambda_3 b_{\vec{p}}^\dagger b_{\vec{p}} b_{\vec{q}}^\dagger b_{\vec{q}} + \lambda_4 b_{\vec{p}}^\dagger b_{-\vec{p}}^\dagger b_{\vec{q}} b_{-\vec{q}}) . \end{aligned} \tag{69}$$

The zero-momentum component has disappeared in this notation but is taken care of exactly in the definition of b. The square-root expressions can be approximated by $N - \sum_{\vec{k}}' b_{\vec{k}}^\dagger b_{\vec{k}}$. This is obviously a good approximation if $N_0 \gg 1$ and a very bad one if $N_0 \approx 1$. However if $N_0 \to 0$ the contribution of the whole term $\lambda_2 \sum_{\vec{k}}' \cdots$ in Eq. (69) goes to zero anyway, as we shall point out later. Therefore, any error in this term does not matter for $N_0 \to 0$. Thus we find, neglecting terms of order ρ/V,

$$H_p = 4\pi a\rho N + \sum_{\vec{k}}{}' \left[\left(1 - \frac{4\pi a^3}{3V}N\right)k^2 + \lambda_1 8\pi a\rho\cos(ka)_+\right] b_{\vec{k}}^\dagger b_{\vec{k}} + \lambda_2 4\pi a\rho \sum_{\vec{k}}{}' \cos(ka)_+ (b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger + b_{\vec{k}} b_{-\vec{k}})$$
$$- \lambda_2 \frac{4\pi a}{V} \sum_{\vec{k},\vec{q}}{}' \cos(ka)_+ (b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger b_{\vec{q}}^\dagger b_{\vec{q}} + b_{\vec{q}}^\dagger b_{\vec{q}} b_{\vec{k}} b_{-\vec{k}}) + \frac{4\pi a}{V} \sum_{\vec{k},\vec{q}}{}' [\lambda_3 V(\vec{q} - \vec{k}, \vec{k}) - 2\lambda_1 \cos(ka)_+] b_{\vec{k}}^\dagger b_{\vec{k}} b_{\vec{q}}^\dagger b_{\vec{q}}$$
$$+ \frac{4\pi a}{V}\lambda_4 \sum_{\vec{k},\vec{q}}{}' V(\vec{q} - \vec{k}, \vec{k}) b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger b_{\vec{q}} b_{-\vec{q}} . \tag{70}$$

Wong and Huang have minimized the ground state energy of the full pair Hamiltonian H_p with respect to a normalized set of variational ground states

$$|\psi_0'\rangle = \prod_{\vec{k}>0}^{\infty} (1 - U_{\vec{k}}^2)^{1/2} e^{-U_k b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger} |\psi_0\rangle ,$$
$$\beta_{\vec{k}} |\psi_0'\rangle = 0, \quad \forall \vec{k} \neq 0 , \tag{71}$$

which we shall call "interacting" ground states induced by the Bogoliubov transformation

$$\beta_{\vec{k}} = (1 - U_{\vec{k}}^2)^{-1/2} (b_{\vec{k}} + U_{\vec{k}} b_{-\vec{k}}^\dagger) ,$$
$$\beta_{\vec{k}}^\dagger = (1 - U_{\vec{k}}^2)^{-1/2} (b_{\vec{k}}^\dagger + U_{\vec{k}} b_{-\vec{k}}) . \tag{72}$$

$|\psi_0\rangle$ represents the so called "noninteracting" ground state and is given by

$$|\psi_0\rangle = (1/\sqrt{N!})(a_0^\dagger)^N |0\rangle ,$$
$$b_{\vec{k}} |\psi_0\rangle = 0, \quad \forall \vec{k} \neq 0 , \tag{73}$$

where $|0\rangle$ is the vacuum state.

The product over all $\vec{k}>0$ extends only over an "open semisphere" in k space, such that if $\vec{k}$ is inside, $-\vec{k}$ is outside. $\vec{k}=0$ is excluded also. The exact eigenstate of H_p has to have the general form

$$|\psi_0^g\rangle \sim \Big(1 + \sum_{\vec{k}}{}' a_1(\vec{k}) b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger + \sum_{\vec{k},\vec{q}}{}'' a_2(\vec{k},\vec{q}) b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger b_{\vec{q}}^\dagger b_{-\vec{q}}^\dagger + \sum_{\vec{k},\vec{q},\vec{p}}{}''' a_3(\vec{k},\vec{q},\vec{p}) \cdots + \sum_{\vec{k}_1,\ldots,\vec{k}_{N/2}}{}''^{\cdots\prime} a_{N/2}(\vec{k}_1, \vec{k}_2, \ldots, \vec{k}_{N/2}) \cdots \Big) |\psi_0\rangle . \tag{74}$$

From expanding Eq. (71),

$$|\psi_0'\rangle \sim \Big(1 + \sum_{\vec{k}}{}' - U_k b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger + \sum_{\vec{k},\vec{q}}{}'' U_k U_q b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger b_{\vec{q}}^\dagger b_{-\vec{q}}^\dagger + \cdots \Big) |\psi_0\rangle , \tag{75}$$

it is obvious that the Bogoliubov states form a subset of $\{|\psi_0^g\rangle\}$. Thus the variation with respect to U_k leads to a true upper bound of H_p, and since $\langle\psi_0^g|H_t + H_r|\psi_0^g\rangle = 0$, the true upper bound of H_p is also a true upper bound of H.

VII. EXPANSION PARAMETERS

Taking the result that in superfluid helium $N_0/N \leq 0.08$ as a physical guide,[15,16] we have to expand H_p in powers of $\beta = N_0/N$. To do so we go back to Eq. (66) and inspect the interacting ground-state expectation value resulting from the right-hand side of Eq. (66) in terms of order of magnitude and powers of N_0/N:

$$(1/N)\langle\psi_0'|H_p|\psi_0'\rangle \sim 1 + (1-\beta) + \lambda_1\beta(1-\beta) + \lambda_2\beta(1-\beta) + \lambda_3(1-\beta)^2 + \lambda_4(1-\beta)^2 . \tag{76}$$

Here we have combined the two kinetic-energy contributions of Eq. (66) into one term. The idea is, that for $\beta \ll 1$, we neglect the terms denoted by λ_1 and λ_2 initially, solve for the remaining terms of H_p, and include λ_1 and λ_2 at the very end in the form of a perturbational treatment if necessary. For the sake of completeness let us inspect the dilute case. There we know that $\gamma = (N - N_0)/N \ll 1$. Hence we obtain

$$(1/N)\langle\psi_0'|H_p|\psi_0'\rangle \sim 1 + \gamma + \lambda_1\gamma(1-\gamma) + \lambda_2\gamma(1-\gamma) + \lambda_3\gamma^2 + \lambda_4\gamma^2 . \tag{77}$$

Besides the constant 1, the leading term here is γ. Therefore, neglecting λ_3 and λ_4 we end up with the Bogoliubov pair Hamiltonian. For intermediately dense cases we cannot draw any conclusion from these expansion schemes and one would have to go through the minimization of the full pair Hamiltonian H_p as has been done in Ref. 1.

The contribution of $\Delta \equiv H_r + H_t$ in terms of above expansion parameters occurs in second order

$$\langle\psi_0'|\Delta|\psi_0'\rangle = \sum_{\phi} \frac{\langle\psi_0'|\Delta|\phi\rangle\langle\phi|\Delta|\psi_0'\rangle}{E_{\psi_0'} - E_\phi} , \tag{78}$$

where ϕ now also includes nonpair terms. For our purposes we only have to consider the numerator. H_r and H_t can be treated separately. Using the relations between $a_{\vec{k}}$ and $\beta_{\vec{k}}$, Eqs. (67) and (72), we find for H_r [Eq. (69)] in the dense case:

$$(1/N)\langle H_r\rangle \sim (1-\beta)^2 \tag{79}$$

and for H_t [Eq. (63)] in the dense case:

$$(1/N)\langle H_t\rangle \sim \beta^{1/2}(1-\beta)^{1/2} . \tag{80}$$

Expression (79) indicates that in the dense case H_r might play an important role. We shall come back to this statement later.

VIII. OFF-DIAGONAL LONG-RANGE ORDERING

Now we also can investigate the ODLRO of our system by inspecting the reduced-density matrix ρ_2 in the coordinate representation $\langle \vec{x}', \vec{y}' | \rho_2 | \vec{x}, \vec{y} \rangle$ (Ref. 18) defined by

$$\begin{aligned}\langle \vec{x}', \vec{y}' | \rho_2 | \vec{x}, \vec{y} \rangle &= \langle \psi_0^\dagger(\vec{x}) \psi_0^\dagger(\vec{y}) \psi_0(\vec{x}') \psi_0(\vec{y}') \rangle \\ &= \frac{1}{V^2} \sum_{\vec{p},\vec{q},\vec{p}',\vec{q}'} \exp(-i\vec{p}\cdot\vec{x} - i\vec{q}\cdot\vec{y} + i\vec{p}'\cdot\vec{x}' + i\vec{q}'\cdot\vec{y}') \\ &\quad \times \langle a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}'} a_{\vec{q}'} \rangle = T_F \langle a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}'} a_{\vec{q}'} \rangle . \end{aligned} \tag{81}$$

The brackets mean thermodynamic average and $\psi_0^\dagger$, ψ_0 are the free-field operators. We can have different types of ODLRO in ρ_2, namely, if in the neighborhood of

$$\left.\begin{aligned} \alpha:\ & \vec{x}' = \vec{x} \text{ and } \vec{y}' = \vec{y} \\ \text{or } & \vec{x}' = \vec{y} \text{ and } \vec{y}' = \vec{x} \end{aligned}\right\} \ V\vec{x} \text{ and } \vec{y}, \tag{82}$$

$$\beta:\ \vec{x}' = \vec{y}' \text{ and } \vec{x} = \vec{y} \ \ (\text{but } |\vec{x}' - \vec{x}| \text{ may be } \infty),$$

the matrix element $\langle \vec{x}', \vec{y}' | \rho_2 | \vec{x}, \vec{y} \rangle$ in either case α or β yields

$$\langle \vec{x}', \vec{y}' | \rho_2 | \vec{x}, \vec{y} \rangle \sim \tilde{\alpha} N^2 | V^2 , \tag{83}$$

where $\tilde{\alpha}$ is a constant of order unity. First we shall look at the Hartree-Fock (HF) terms in Eq. (81) considering only $\vec{p} = \vec{p}'$, $\vec{q} = \vec{q}'$ ($\vec{p} = \vec{q}'$, $\vec{q} = \vec{p}'$ would lead to the same result with switched roles of α and β), and obtain for $T \cong 0$,

$$\begin{aligned}\langle \vec{x}', \vec{y}' | \rho_2 | \vec{x}, \vec{y} \rangle_{\text{HF}} &= \frac{1}{V^2} \sum_{\vec{p},\vec{q}}{}'' \exp[-i\vec{p}\cdot(\vec{x} - \vec{x}') - i\vec{q}\cdot(\vec{y} - \vec{y}')] \\ &\quad \times \langle a_{\vec{p}}^\dagger a_{\vec{q}}^\dagger a_{\vec{p}} a_{\vec{q}} \rangle . \end{aligned} \tag{84}$$

Applying condition α and keeping in mind $N_0 = 0$, we find

$$\alpha:\ \langle \vec{x}, \vec{y} | \rho_2 | \vec{x}, \vec{y} \rangle_{\text{HF}} = \frac{1}{V^2} \left(\sum_{\vec{q}}{}' \rho_{\vec{q}} \right)^2 = \rho^2 , \tag{85}$$

which represents a HF contribution to the pair-correlation function. Equation (85) just expresses a constant probability of finding a particle at a point knowing that there is one at another point, and therefore cannot be called ODLRO. Applying condition β we find

$$\beta:\ \langle \vec{x}, \vec{x} | \rho_2 | \vec{y}, \vec{y} \rangle_{\text{HF}} = \frac{1}{V^2} \left(\sum_{\vec{q}}{}' \rho_q e^{i\vec{q}\cdot(\vec{x} - \vec{y})} \right)^2 . \tag{86}$$

This is essentially the Green's function representing the probability that two particles at position $\vec{y}$ with any initial momenta $\vec{k}_1$ and $\vec{k}_2$ get annihilated while two other particles with the same momenta get created at a different position $\vec{x}$. Even if we assume that $p^2 \rho_p$ is highly peaked around the location of the roton dip p_0 such that we can approximate Eq. (86) by

$$\langle \vec{x}, \vec{x} | \rho_2 | \vec{y}, \vec{y} \rangle_{\text{HF}} \cong (\tilde{\alpha}^2 N^2 / V^2) j_0^2(p_0 |\vec{x} - \vec{y}|) , \tag{87}$$

we do not have off-diagonal long-range ordering for $|\vec{x} - \vec{y}| \to \infty$.

Investigating the BCS-like terms in Eq. (81) by considering $\vec{p} = -\vec{q}$ and $\vec{p}' = \vec{q}'$, we find

$$\begin{aligned}\langle \vec{x}', \vec{y}' | \rho_2 | \vec{x}, \vec{y} \rangle_{\text{BCS}} &= \frac{1}{V} \sum_{\vec{p},\vec{q}}{}'' \exp[i\vec{p}\cdot(\vec{x} - \vec{y}) + i\vec{q}\cdot(\vec{x}' - \vec{y}')] \\ &\quad \times \langle a_{\vec{p}}^\dagger a_{-\vec{p}}^\dagger a_{\vec{q}} a_{-\vec{q}} \rangle . \end{aligned} \tag{88}$$

With α this leads to

$$\alpha:\ \langle \vec{x}, \vec{y} | \rho_2 | \vec{x}, \vec{y} \rangle_{\text{BCS}} = \frac{1}{V^2} \left(\sum_{\vec{p}}{}'' e^{i\vec{p}\cdot(\vec{x} - \vec{y})} \frac{U_p}{1 - U_p^2} \right)^2 , \tag{89}$$

representing the BCS contribution to the pair-correlation function going to zero for $|\vec{x} - \vec{y}| \to \infty$. In the case of β, we again find an expression of the Green's-function type

$$\beta:\ \langle \vec{x}, \vec{x} | \rho_2 | \vec{y}, \vec{y} \rangle_{\text{BCS}} = \frac{1}{V^2} \left(\sum_{\vec{p}}{}'' \frac{U_p}{1 - U_p^2} \right)^2 = \frac{\tilde{\alpha} N^2}{V^2} , \tag{90}$$

which represents a true ODLRO for $T \cong 0$, where the statistical average has been replaced by the ground-state expectation value. Since

$$\begin{aligned}\langle \vec{x} | \rho_1 | \vec{y} \rangle &\equiv \langle \psi_0^\dagger(\vec{x}) \psi_0(\vec{y}) \rangle \\ &= \frac{1}{V} \sum_{\vec{p},\vec{q}} \langle e^{-i\vec{p}\cdot\vec{x} + i\vec{q}\cdot\vec{x}'} a_{\vec{p}}^\dagger a_{\vec{q}} \rangle \\ &= \sum_{\vec{p}} \frac{U_p^2}{1 - U_p^2} e^{i\vec{p}\cdot(\vec{x} - \vec{x}')} \end{aligned} \tag{91}$$

goes to zero for $|\vec{x} - \vec{x}'| \to \infty$, the lowest-order ODLRO is provided by the BCS-like terms of H_p.

These results are of course ultimately all implied by our choice of wave functions participating in the variational principle, which is the same as choosing the Bogoliubov transformation for the diagonalization of H_p. In principle this does not exclude the possibility that H_t and H_r could also lead to ODLRO of the same order in a more elaborate diagonalization procedure. The purpose of this demonstration is only to show that the Bogoliubov transformation gives not only a good fit to the experimentally measured energy spectrum but also provides ODLRO which is characteristic of any superfluid.[18] In this approximation (choice of a Bogoliubov transformation for partial diagnoalization) H_r and H_t can only provide ODLRO of higher order in terms of perturbational treatment.

IX. VARIATIONAL GROUND-STATE AND EXCITATION ENERGY IN THE DENSE CASE

Although the total number of particles in H_p of Eq. (70) is conserved, the number of zero-momentum states is not. For the dense case we shall have to set $\lambda_1 = \lambda_2 = 0$. As soon as we do this the number of zero-momentum states is kept constant, namely, zero. Thus the total number of particles is not conserved anymore. That can also be seen directly from Eq. (70). Because, once $\lambda_1 = \lambda_2 = 0$, the $\beta_{\vec{k}}$ operators can all be replaced by $a_{\vec{k}}$ operators which do not conserve particle number. To ensure the conservation of particle number in any case we apply the usual transformation

$$H_p' = H_p - \mu(\hat{N}_0 + \hat{N}'), \tag{92}$$

where μ is the chemical potential per particle. N_0 and N' are the number of particles in the zero- and non-zero-momentum states, respectively, and H_p represents the pair Hamiltonian equation (70). Minimizing $\langle\psi_0'|H_p'|\psi_0'\rangle = E_0'$ with respect to N leads to

$$\frac{\partial E_0'}{\partial N} = \frac{\partial E_0'}{\partial N_0}\bigg|_{N'=\text{const}} = \frac{\partial E_0}{\partial N_0}\bigg|_{N'=\text{const}} - \mu = 0, \tag{93}$$

where $\langle\psi_0'|H_p|\psi_0'\rangle \equiv E$. The ground state $|\psi_0'\rangle$ is the same for H_p and H_p' plus the subsidiary condition $\partial E_0' | \partial N_0|_{N'=\text{const}} = 0$. The minimization procedure will not only change the form of H_p, it also changes the ground state $|\psi_0'\rangle$ by varying the function U_k. Since the norm of $|\psi_0'\rangle$ does not depend on the form of U_k [see Eq. (71)], we can write Eq. (93),

$$\frac{\partial E_0}{\partial N_0}\bigg|_{N'=\text{const}} = \langle\psi_0'|\frac{\partial}{\partial N_0}H_p|\psi_0'\rangle = \mu. \tag{94}$$

μ has been computed in the Appendix E 1 and is given by

$$\mu = (4/\pi a^2)(F - D), \tag{95}$$

where

$$F = \sum_{l=0}^{\infty} (-1)^l (4l+1) B_{2l}, \tag{96}$$

$$D = \sum_{l=0}^{\infty} (-1)^l (4l+1) E_{2l}, \tag{97}$$

$$B_{2l} = \int_0^\infty x^2 j_{2l}(\vec{x}) \frac{U^2(x)}{1 - U^2(x)} d^3x, \tag{98}$$

$$E_{2l} = \int_0^\infty x^2 j_{2l}[x(1+\epsilon)] \frac{U(x)}{1 - U^2(x)} d^3x, \quad \epsilon \to 0^+, \tag{99}$$

$$\overline{E}_{2l} = \int_0^\infty x^2 j_{2l}[x(1-\epsilon)] \frac{U^2(x)}{1 - U^2(x)} d^3x, \quad \epsilon \to 0^+. \tag{100}$$

For the sake of completeness and later convenience [see Eq. (107)] we have also given the definition of the quantity $\overline{E}_{2l}$.

The next step is to determine the Bogoliubov functional $U(x)$. In the dense case the assumption $\beta = 0 \to \lambda_1 = \lambda_2 = 0$ makes the leading term of H_p' [Eq. (92)] to be of the form [see Eq. (70)]

$$H_p' = 4\pi a\rho N + \sum_{\vec{k}}{}' \left[(1 - \tfrac{4}{3}\pi a^3\rho)k^2 - \mu\right] b_{\vec{k}}^\dagger b_{\vec{k}} + \frac{4\pi a}{V}\lambda_3 \sum_{\vec{q},\vec{k}}{}' V(\vec{q}-\vec{k},\vec{k}) b_{\vec{k}}^\dagger b_{\vec{k}} b_{\vec{q}}^\dagger b_{\vec{q}} + \frac{4\pi a}{V}\lambda_4 \sum_{\vec{q},\vec{k}}{}' V(\vec{q}-\vec{k},\vec{k}) b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger b_{\vec{q}} b_{-\vec{q}}. \tag{101}$$

We keep in mind that

$$H_p' = H_p(\beta = 0) - \mu \sum_{\vec{k}}{}' b_{\vec{k}}^\dagger b_{\vec{k}}. \tag{102}$$

Here μ guarantees the conservation of particle number. Assumption $\lambda_1 = \lambda_2 = 0$ is self-consistent if the wave function resulting from H_p' leads to $\langle\psi_0'|\sum_{\vec{k}}' a_{\vec{k}}^\dagger a_{\vec{k}}|\psi_0'\rangle \cong N$. Minimization of the ground-state energy of Eq. (101) is performed in Appendix E 2 and leads to the condition

$$\tfrac{1}{2}(1 + U_k^2) S_1(k) + U_k S_2(k) = 0, \tag{103}$$

where

$$S_1(k) = 2a^2 \frac{4\pi a}{V}\lambda_4 \sum_{\vec{q}}{}' V(\vec{q}-\vec{k},\vec{k}) \frac{U_q}{1 - U_q^2}, \tag{104}$$

$$S_2(k) = a^2\left[\left(1 - \frac{4\pi a^3}{3}\rho\right)k^2 + 2\lambda_3 \frac{4\pi a}{V} \times \sum_{\vec{q}}{}' V(\vec{q}-\vec{k},\vec{k}) \frac{U_q^2}{1 - U_q^2} - \mu\right], \tag{105}$$

with the excitation energy given by

$$E(k) = (1/a^2)[S_2^2(k) - S_1^2(k)]^{1/2}. \tag{106}$$

In Appendix E 3 we utilize the separability of $V(\vec{q}-\vec{k},\vec{k})$ and arrive at expressions for S_1 and S_2 that allow in principle an exact solution of the integral equation (103). S_1 and S_2 turn out to be

$$S_1(k) = \frac{4}{\pi}\Big(j_0(ka)D + \cos kaE_0 - j_0(ka)E_0 - \sum_{l=1}^{\infty}(4l+1)j_{2l}(ka)\bar{E}_{2l}\Big), \qquad (107)$$

$$S_2(k) = \Big(1 - \frac{4\pi}{3}a^3\rho\Big)(ka)^2 + \frac{4}{\pi}\Big(-\frac{a^2\pi}{4}\mu + j_0(ka)F + \cos(ka)B_0 - \sum_{l=0}(4l+1)j_{2l}(ka)B_{2l}\Big). \qquad (108)$$

It should be noted that the expansion of $S_1(k)$ and $S_2(k)$ in terms of $j_{2l}(ka)$'s has nothing to do with an angular-momentum expansion. The form of this expansion is simply a mathematical consequence of the particular form of our separable pseudopotential.

Comparing Eqs. (107) and (108) with the expressions by Wong and Huang,[1] S_1 and S_2 are exactly the same provided $N_0 = 0$ as they actually should be if the concept of expansion parameters is correct. Since N_0 is reported to be zero in Ref. 1 for the dense case under consideration, our approximation $\lambda_1 = \lambda_2 = 0$ is self-consistently correct and a perturbational treatment of the terms associated with λ_1 and λ_2 can therefore be omitted. Furthermore, the numerical calculation also showed that $\bar{E}_{2l} = E_{2l}$ consistent with the absence of the zero-momentum condensate, which is shown in Appendix E 4. Therefore, one can ignore the difference between $\bar{E}_{2l}$ and E_{2l} in a numerical computation. The fact that $\bar{E}_{2l} = E_{2l}$ in the dense case implies that not only the wave function, but also its first derivative is continuous across the boundary of the hard core.

It is easy to see from Eqs. (103), (107), and (108) as pointed out in Appendix E 4, that U_k goes to zero for increasing k at least as fast as k^{-3}. The density of single particles ρ_k has a $1/k$ singularity at the origin which is counterbalanced by the phase space factor k^2. At $k \cong 2\,\text{Å}^{-1}$ corresponding to the location of the roton dip, ρ_k has a maximum, and drops to zero at least as fast as k^{-6} for k large (see Fig. 4). Therefore, one is inclined to believe that the significant contribution to any integral involving a functional dependence on the single particle density stems from the region near the roton minimum. In this sense the roton momentum resembles very much the Fermi momentum in a superconductor.

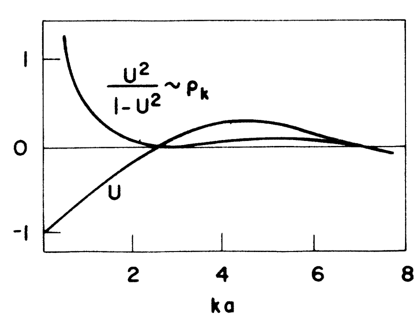

FIG. 4. Single-particle density and Bogoliubov transformation parameter computed from data of Ref. 1.

X. DISCUSSION OF THE GROUND-STATE ENERGY OF H_p

Since Eqs. (70) and (101) lead to the same solution for the ground and low excitational states in the dense case, we shall therefore base all our further discussions on Eq. (101) which allows us a simple interpretation of its terms and is also much easier to manipulate than Eq. (70). H_p' in Eq. (101) consists of a kinetic-energy term including the correction due to volume-exclusion effect plus a chemical potential μ. λ_3 designates the Hartree-Fock term and λ_4 the BCS term. We neglect λ_4 for the moment and replace

$$\sum_{\vec{k},\vec{q}}{}' \lambda_3 V(\vec{q}-\vec{k},\vec{k})b_{\vec{k}}^\dagger b_{\vec{k}} b_{\vec{q}}^\dagger b_{\vec{q}} \qquad (109)$$

in the sense of a Hartree-Fock approximation by

$$2\sum_{\vec{k},\vec{q}}{}' \lambda_3 V(\vec{q}-\vec{k},\vec{k})b_{\vec{k}}^\dagger b_{\vec{k}}\langle\psi_0'|b_{\vec{q}}^\dagger b_{\vec{q}}|\psi_0'\rangle - \sum_{\vec{k},\vec{q}}{}' \frac{U_k^2 U_q^2 V(\vec{q}-\vec{k},\vec{k})}{(1-U_k^2)(1-U_q^2)}. \qquad (110)$$

The factor 2 follows from the invariance of Eq. (110) with respect to exchanging $\vec{q}$ with $\vec{k}$ and vice versa [see Eq. (44)]. The subtraction of the sum $\sum'$ comes from the fact that the ground-state contribution has been overcounted in the HF approximation. Hence we find for the Hamiltonian equation (101),

$$H_p' = 4\pi a\rho N + \sum_{\vec{k}}{}' \frac{S_2(k)}{a^2} b_{\vec{k}}^\dagger b_{\vec{k}} - \frac{4\pi a}{V}\sum{}' \frac{U_k^2 U_q^2 V(\vec{q}-\vec{k},\vec{k})}{(1-U_k^2)(1-U_q^2)}. \qquad (111)$$

Adding the λ_4 term and minimizing with respect to U_k leads to exactly the same results as given in Eqs. (103)–(106). Therefore, Eq. (101) can be expressed equivalently [see also definition of $S_2(k)$ in Eq. (105)] as

$$H_p' = 4\pi a\rho N + \frac{1}{2}\sum_{\vec{k}}{}' \left(\alpha k^2 - \mu - \frac{S_2(k)}{a^2}\right)\frac{U_k^2}{1-U_k^2} + \sum_{\vec{k}}{}' \frac{S_2(k)}{a^2} b_{\vec{k}}^\dagger b_{\vec{k}} + \frac{4\pi a}{V}\lambda_4 \sum_{\vec{k},\vec{q}}{}' V(\vec{q}-\vec{k},\vec{k}) b_{\vec{k}}^\dagger b_{-\vec{k}}^\dagger b_{\vec{q}} b_{-\vec{q}}. \tag{112}$$

Now we shall show that the Bogoliubov transformation equation (72) and the minimization of the ground state is equivalent to an exact calculation of the ground-state energy of H_p in the thermodynamic limit. In order to verify our statement, we simply have to combine Eqs. (72) and (112), regroup the Hamiltonian, and find (see Appendix E1)

$$H_p' = H_0 + H_1, \quad H_0 = C + \sum_{\vec{k}}{}' H_{\vec{k}},$$

$$C = 4\pi a\rho N + \sum_{\vec{k}}{}' \frac{S_2(k)U_k^2}{a^2(1-U_k^2)} + \sum_{\vec{k}}{}' \frac{S_1(k)U_k}{a^2(1-U_k^2)} - \frac{4\pi a}{V}\sum_{\vec{k},\vec{q}}{}'' \frac{U_k^2 U_q^2}{(1-U_k^2)(1-U_q^2)} V(\vec{q}-\vec{k},\vec{k})$$

$$- \frac{4\pi a}{V}\sum_{\vec{k},\vec{q}}{}'' \frac{U_k U_q}{(1-U_k^2)(1-U_q^2)} V(\vec{q}-\vec{k},\vec{k}),$$

$$H_{\vec{k}} = \frac{\beta_{\vec{k}}^\dagger \beta_{\vec{k}}}{1-U_k}\left(\frac{S_2(k)}{a^2}(1+U_k^2) + 2\lambda_4 U_k \frac{S_1(k)}{a^2}\right) - \frac{\beta_{\vec{k}}^\dagger \beta_{-\vec{k}} + \beta_{\vec{k}}\beta_{-\vec{k}}}{1-U_k^2}\left(\frac{S_2(k)}{a^2}U_k + (1-U_k^2)\frac{\lambda_4}{2}\frac{S_1(k)}{a^2}\right), \tag{113}$$

$$H_1 = \frac{4\pi a}{V}\lambda_4 \sum_{\vec{k},\vec{q}}{}' \frac{V(\vec{q}-\vec{k},\vec{k})}{(1-U_k^2)(1-U_q^2)} \left(B_{\vec{k}}^\dagger B_{\vec{q}} - \beta_{-\vec{k}}\beta_{-\vec{k}}^\dagger \beta_{\vec{q}}\beta_{\vec{q}}^\dagger U_k U_q\right),$$

$$B_{\vec{k}}^\dagger = \beta_{\vec{k}}^\dagger \beta_{-\vec{k}}^\dagger - U_k(\beta_{\vec{k}}^\dagger \beta_{\vec{k}} + \beta_{-\vec{k}}\beta_{-\vec{k}}^\dagger) + U_k^2 \beta_{-\vec{k}}\beta_{\vec{k}}, \qquad B_{\vec{k}} = (B_{\vec{k}}^\dagger)^\dagger.$$

The contribution of H_1 in all orders of perturbation to C is obviously $1/V$ smaller and can be neglected. [The same conclusion is valid even if we do not restrict ourselves to the HF approximation in Eq. (110).]

In order to obtain the expressions of Ref. 1 in the case where $N' \neq N$ (intermediate or dilute case) we replace S_1 and S_2 in C and $H_{\vec{k}}$ by their more general form given in Appendix E 2 and keep in mind that C in Eq. (113) represents $E_0' - \mu N'$ with

$$\mu = -2\sum_{\vec{q}}{}' V_2(\vec{q},\vec{k}) \frac{U_q(U_q - 1)}{1-U_q^2} < 0.$$

H_1 also will include more terms but they will still be proportional to $1/V$ and therefore will not contribute to the ground-state energy.

The decomposition equation (113) reveals the meaning of the minimization procedure performed in Appendix E 2. Condition (103) just guarantees that $H_{\vec{k}}$ leads immediately to $E(k)$ given in Eq. (106).

XI. REMARKS

We have checked Wong and Huang's results with respect to the expression [see Appendix E 1, Eq. (E 1.13)]

$$\sum_{\vec{k}}{}' \frac{(ka)^2 U_k^2}{1-U_k^2} = 6N, \quad \text{if } N_0 = 0, \tag{114}$$

which had not been investigated in their work.[1] The disagreement was beyond machine accuracy. This implies that $N_0 = 0$ was actually not a self-consistent result and the λ_1 and λ_2 terms should be included at least in the form of a perturbational calculation.

These computational inaccuracies originate from the slow convergence of the integrands of E_{2l} in $S_1(k)$ which had been overlooked in previous numerical computations. This deficiency can be overcome by considering the asymptotic part of E_{2l} separately. The discussion of which will be included in a second paper.

We have also investigated the influence of an attractive tail to the hard-sphere potential and found that for reasonable choices of attractive square-well potentials a modified version of Eq. (114) holds; meaning that in this case $N_0 = 0$ is a self-consistent result. This extension of the hard-sphere potential including an attractive tail with numerical results for the various cases will also be presented in a second paper, where we shall also analyze the problem of the pair-correlation function based on the hard-sphere model.

APPENDIX A

Here we shall truncate the N-particle pseudo-Hamiltonian with the help of the two-body potential approximation, and cast it into a form that is easy to be Fourier transformed. We start with the exact N-particle pseudo-Hamiltonian (39). Considering only the first term in H, we use partial integration twice and find, throwing out the surface integrations,

$$\int d^3x\, \psi_0^\dagger(\vec{x})\nabla_{\vec{x}}^2 P(\vec{x})\psi_0(\vec{x}) = \int d^3x\, [\nabla_{\vec{x}}^2 \psi_0^\dagger(\vec{x})] P(\vec{x})\psi_0(\vec{x}). \tag{A1}$$

Utilizing the two-body potential approximation in Eq. (40) we obtain

$$\int d^3x\, \psi_0^\dagger(\vec{x})\nabla_{\vec{x}}^2 P(\vec{x})\psi_0(\vec{x}) = \int d^3x\, \psi_0^\dagger(\vec{x})\nabla_{\vec{x}}^2\psi_0(\vec{x}) - \int d^3x[\nabla_{\vec{x}}^2\psi_0^\dagger(\vec{x})]\int_{S_{\vec{x}}} d'^3x\, \psi_0^\dagger(\vec{x}')\psi_0(\vec{x}')\psi_0(\vec{x}). \tag{A2}$$

The second term of Eq. (A2) we shall transform further. Using partial integration again we arrive at

$$\int_{|\vec{x}-\vec{x}'|<\lim_{\epsilon=+0}a+\epsilon} d^3x\, d'^3x[\nabla_{\vec{x}}^2\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')]\,\psi_0(\vec{x}')\psi_0(\vec{x}) = \int_{|\vec{x}-\vec{x}'|\le\lim_{\epsilon=0^+}a+\epsilon} d^3x\, d'^3x\nabla_{\vec{x}}\{[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\psi_0(\vec{x}')\psi_0(\vec{x})]\}$$
$$- \int_{|\vec{x}-\vec{x}'|\le\lim_{\epsilon=0^+}a+\epsilon} d^3x\, d'^3x[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\nabla_{\vec{x}}\psi_0(\vec{x}')\psi_0(\vec{x})]. \tag{A3}$$

The first term on the right-hand side of (A3) leads to

$$\int d^3x'\int_{S_{\vec{x}}} d\sigma_{\vec{x}}\frac{\vec{x}-\vec{x}'}{a}[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\psi_0(\vec{x}')\psi_0(\vec{x})] = \frac{1}{2}\int d^3x'\int_{S_{\vec{x}'}} d\sigma_{\vec{x}}\frac{\vec{x}-\vec{x}'}{a}\cdot[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\psi_0(\vec{x}')\psi_0(\vec{x})]$$
$$+\frac{1}{2}\int d^3x\int_{S_{\vec{x}}} d\sigma_{\vec{x}'}\frac{\vec{x}'-\vec{x}}{a}\cdot[\nabla_{\vec{x}'}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\psi_0(\vec{x}')\psi_0(\vec{x})]. \tag{A4}$$

The last step follows from the fact that we can replace $\nabla_{\vec{x}}^2$ by $\nabla_{\vec{x}'}^2$ on the left-hand side of Eq. (A3) without changing anything. The two surface integrals on the right-hand side of Eq. (A4) can be transformed into volume integrals by inserting $\delta(r-a-\epsilon)$. Utilizing

$$\frac{\vec{x}-\vec{x}'}{r}(\nabla_{\vec{x}}-\nabla_{\vec{x}'}) = 2\frac{\partial}{\partial r} \quad \text{for } \vec{x}+\vec{x}'=\text{const}, \tag{A5}$$

we find

$$\int d^3x'\int_{S_{\vec{x}'}} d\sigma_{\vec{x}}[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\psi_0(\vec{x}')\psi_0(\vec{x}')]$$
$$=\lim_{\epsilon=0^+}\int d^3x'd^3x\,\delta(r-a-\epsilon)$$
$$\times\left(\frac{\partial}{\partial r}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\right)\psi_0(\vec{x}')\psi_0(\vec{x}), \tag{A6}$$

and collecting all the terms produces Eq. (41).

APPENDIX B

Here we shall investigate the kind of "physical terms" that had been neglected by only including a two-body potential in the approximation of the exact N-particle pseudo-Hamiltonian (39). We shall also estimate the contribution of genuine three-body terms in the approximation of Eq. (39). The approximation of Eq. (39) is based on expanding the projection operator $P(\vec{x})$ in powers of free-field operators. $P(\vec{x})$ is given by

$$P(\vec{x}) = P + \Lambda(\vec{x}). \tag{B1}$$

The first term in Eq. (39) denotes the volume-exclusion term and the second denotes the surface-matching term. The term we want to expand in Eq. (39) is

$$\Lambda(\vec{x}) = -\int_{S_{\vec{x}}}\psi^\dagger(\vec{x}')\,\psi(\vec{x}')d^3x'$$
$$+\frac{1}{2}\int\psi^\dagger(\vec{x}')\psi^\dagger(\vec{y})\,\psi(\vec{x}')\,\psi(\vec{y})\,d^3x'\,d^3y\cdots \tag{B2}$$

(expansion of P would lead to additional terms similar to the ones we are going to discuss).

Since we are only interested up to three-body contributions in Eq. (39), $\Lambda(\vec{x})$ becomes

$$\Lambda(\vec{x}) = -\int_{S_{\vec{x}}}\psi_0^\dagger(\vec{x}')\,\psi_0(\vec{x}')\,d^3x'$$
$$+\int_{S_{\vec{x}}}\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})\psi_0(\vec{y})\,d^3y\,\psi_0(\vec{x}')\,d^3x'$$
$$+\frac{1}{2!}\int_{S_{\vec{x}}}\psi_0^\dagger(\vec{x}')\,\psi_0^\dagger(\vec{y})\,\psi_0(\vec{x}')\,\psi_0(\vec{y})\,d^3x'\,d^3y. \tag{B3}$$

Thus the three-body contribution to the volume exclusion term in Eq. (39) is

$$\Delta H_{\text{vol}} = \lim_{\epsilon=0^+}\Big(-\int d^3x[\nabla_{\vec{x}}^2\psi_0^\dagger(\vec{x})]\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})\,\psi_0(\vec{y})\,\psi_0(\vec{x})\,\psi_0(\vec{x}')\,\Theta(|\vec{x}-\vec{x}'|-a-\epsilon)\,\Theta(|\vec{x}'-\vec{y}|-a-\epsilon)\,d^3y\,d^3x'$$
$$-\frac{1}{2!}\int d^3x[\nabla_{\vec{x}}^2\psi_0^\dagger(\vec{x})]\psi_0^\dagger(\vec{x}')\,\psi_0^\dagger(\vec{y})\,\psi_0(\vec{x}')\,\psi_0(\vec{y})\,\psi_0(\vec{x})\,\Theta(|\vec{x}-\vec{x}'|-a-\epsilon')\,\Theta(|\vec{x}-\vec{y}|-a-\epsilon')\,d^3x'\,d^3y\Big), \tag{B4}$$

with $\epsilon \geq \epsilon' \geq 0$, where we have applied the same steps as in Eq. (A2) and the Θ-function is defined by

$$\Theta(\vec{x}) = \begin{cases} 1 & \text{for } x \leq 0, \\ 0 & \text{for } x > 0. \end{cases} \tag{B5}$$

Without changing the result we can replace $[\nabla^2_{\vec{x}} \psi_0^\dagger(\vec{x})]$ by $[\nabla^2_{\vec{y}} \psi_0^\dagger(\vec{y})]$ in the first term of Eq. (B4) and rename $\vec{x}$ by $\vec{x}'$ and $\vec{x}'$ by $\vec{x}$ in the second one. Hence, we obtain

$$\Delta H_{\text{vol}} = \lim_{\epsilon=0^+} \Big(-\frac{1}{2} \int d^3x\, d^3x'\, d^3y\, \Theta(|\vec{x}' - \vec{x}| - a - \epsilon')\Theta(|\vec{x}' - \vec{y}| - a - \epsilon') \times [(\nabla^2_{\vec{x}} + \nabla^2_{\vec{x}'} + \nabla^2_{\vec{y}})\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})]\psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x})\Big). \tag{B6}$$

Applying the Gauss theorem in analogy with Eqs. (A4), (A5), etc., we find, with $\alpha \equiv \vec{x}, \vec{x}', \vec{y}$,

$$\begin{aligned}\Delta H_{\text{vol}} = \lim_{\epsilon=0^+} \Big[\frac{1}{2} \int d^3x\, d^3x'\, d^3y \Big\{ &\Theta(|\vec{x}' - \vec{x}| - a + \epsilon)\Theta(|\vec{x}' - \vec{y}| - a + \epsilon) \sum_\alpha [\nabla_\alpha \psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})][\nabla_\alpha \psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x})] \\ &- \frac{\vec{x} - \vec{x}'}{a}\delta(|\vec{x} - \vec{x}'| - a - \epsilon)\Theta(|\vec{y} - \vec{x}'| - a - \epsilon')[\nabla_{\vec{x}} \psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})]\psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x}) \\ &- \frac{\vec{y} - \vec{x}'}{a}\delta(|\vec{y} - \vec{x}'| - a - \epsilon)\Theta(|\vec{x} - \vec{x}'| - a - \epsilon')[\nabla_{\vec{y}} \psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})]\psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x}) \\ &- \Big(\frac{\vec{x}' - \vec{x}}{a}\delta(|\vec{x} - \vec{x}'| - a - \epsilon)\Theta(|\vec{y} - \vec{x}'| - a - \epsilon') + \frac{\vec{x}' - \vec{y}}{a}\delta(|\vec{y} - \vec{x}'| - a - \epsilon) \\ &\times \Theta(|\vec{x} - \vec{y}| - a - \epsilon')\Big)[\nabla_{\vec{x}'} \psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})]\psi_0(\vec{y})\psi_0(\vec{x}')\psi(\vec{x})\Big\}\Big]; \end{aligned} \tag{B7}$$

utilizing Eq. (A6), Eq. (B7) can be transformed into

$$\begin{aligned}\Delta H_{\text{vol}} = \lim_{\epsilon=0^+} \Big\{ &\frac{1}{2} \int d^3x\, d^3x'\, d^3y \Big(\Theta(|\vec{x}' - \vec{x}| - a + \epsilon)\Theta(|\vec{x}' - \vec{y}| - a + \epsilon) \sum_\alpha [\nabla_\alpha \psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})][\nabla_\alpha \psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x})]\Big) \\ &- \int d^3x\, d^3x'\, d^3y \Big[\delta(|\vec{x} - \vec{x}'| - a - \epsilon)\Theta(|\vec{y} - \vec{x}| - a - \epsilon')\Big(\frac{\partial}{\partial|\vec{x} - \vec{x}'|}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\Big)\psi_0^\dagger(\vec{y}) + \delta(|\vec{y} - \vec{x}'| - a - \epsilon) \\ &\times \Theta(|\vec{x} - \vec{x}'| - a - \epsilon)\psi_0^\dagger(\vec{x})\Big(\frac{\partial}{\partial|\vec{x}' - \vec{y}|}\psi_0(\vec{x}')\psi_0(\vec{y})\Big)\Big]\psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x})\Big\}. \end{aligned} \tag{B8}$$

Comparing with Eq. (41), the different terms in Eq. (B8) have to be interpreted as follows:

The first terms containing two Θ functions and zero δ functions in product form represent Fig. 3, I and III. The second terms containing one Θ function and one δ function in product form represent Fig. 3, II and IV.

Now concentrating on the three-body contribution to the surface-matching term in Eq. (39), we obtain

$$\Delta H_{\text{surf}} = -\lim_{\epsilon=0^+} \frac{1}{a} \int d^3x\, d^3x'\, \psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\delta(|\vec{x} - \vec{x}'| - a - \epsilon)\Big(1 + a\frac{\partial}{\partial|\vec{x} - \vec{x}'|}\Big) \times \{[\Theta(|\vec{y} - \vec{x}| - a - \epsilon')]\psi_0^\dagger(\vec{y})\psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x})\}d^3y; \tag{B9}$$

performing the $\partial/\partial|\vec{x} - \vec{x}'|$ operation on the Θ functions in Eq. (B9) leads to a δ function with a strength σ bound by $-1 \leq \sigma \leq 1$. Therefore an upper bound to Eq. (B9) is

$$\begin{aligned}\Delta H_{\text{surf}} < \Big| -\lim_{\epsilon=0^+} \frac{1}{a} \int d^3x\, d^3x'\, d^3y\, &\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})\psi_0(\vec{y})\delta(|\vec{x} - \vec{x}'| - a - \epsilon) \\ &\times\Big([\Theta(|\vec{y} - \vec{x}| - a - \epsilon') + \Theta(|\vec{y} - \vec{x}'| - a - \epsilon')]\frac{\partial}{\partial|\vec{x} - \vec{x}'|}[|\vec{x} - \vec{x}'|\psi_0(\vec{x}')\psi_0(\vec{x})] \\ &+ [\delta(|\vec{y} - \vec{x}| - a - \epsilon) + \delta(|\vec{y} - \vec{x}'| - a - \epsilon)]\psi_0(\vec{x}')\psi_0(\vec{x})\Big)\Big|. \end{aligned} \tag{B10}$$

Again comparing with Eq. (A9), the different terms in Eq. (B10) have to be interpreted as follows:

The first terms containing one δ function and one Θ function in product form represent Fig. 3, II and IV. The second terms containing two δ functions and zero Θ functions in product form represent Fig. 3, V and VI. As far as an order-of-magnitude estimate of the different terms in Eqs. (B8) and (B10) is concerned we restrict ourselves to pick one term for demonstration purposes. We compare, for example, the two terms given by Figs. 2, I and 3, I. The expression for the former is [see Eq. (41)]

$$-\lim_{\epsilon=0^+}\int d^3x\, d^3x'\,\Theta(|\vec{x}-\vec{x}'|-a+\epsilon)\times[\nabla_{\vec{x}}\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')][\nabla_{\vec{x}}\psi_0(\vec{x})\psi_0(\vec{x}')]\,. \tag{B11}$$

The expression for the latter is [see Eq. (B8)]

$$\frac{1}{2}\lim_{\epsilon=0^+}\int d^3x\, d^3x'\, d^3y\,\Theta(|\vec{x}-\vec{x}'|-a+\epsilon')\times\Theta(|\vec{x}'-\vec{y}|-a-\epsilon')\times\sum_\alpha[\nabla_\alpha\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0^\dagger(\vec{y})]\times[\nabla_\alpha\psi_0(\vec{y})\psi_0(\vec{x}')\psi_0(\vec{x})]\,. \tag{B12}$$

Taking the expectation values of Eqs. (B11) and (B12) with respect to the hard-sphere ground state we obtain

$$\sim-\langle\phi_0|\frac{1}{V}\int\sum_{\vec{k}_1,\vec{k}_2}\vec{k}_1\cdot\vec{k}_2 e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{x}}a^\dagger_{\vec{k}_1}a_{\vec{k}_2}\sum_\phi|\phi\rangle\times\langle\phi|\Theta(|\vec{x}-\vec{x}'|-a)\rho(\vec{x}')|\phi_0\rangle\, d^3x\, d^3x' \tag{B13}$$

and

$$\sim+\tfrac{3}{2}\langle\phi_0|\frac{1}{V}\int\sum_{\vec{k}_1,\vec{k}_2}\vec{k}_1\cdot\vec{k}_2 e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{x}}a^\dagger_{\vec{k}_1}a_{\vec{k}_2}\sum_\phi|\phi\rangle\times\langle\phi|\Theta(|\vec{x}'-\vec{x}|-a)\Theta(|\vec{x}'-\vec{y}|-a)\times\rho(\vec{x})\rho(\vec{y})\,d^3x\,d^3y\,d^3x'|\phi_0\rangle\;, \tag{B14}$$

respectively, where $\rho(\vec{x})$ is the particle-density operator. Making the crude approximation that $\rho(\vec{x})$ is a constant, the relevant terms to be compared are

$$\rho(\tfrac{4}{3}\pi)a^3, \tag{B15}$$

from Eq. (B13), and

$$\tfrac{3}{2}\rho^2(\tfrac{4}{3}\pi a^3)^2, \tag{B16}$$

from Eq. (B14).

In the dilute case $\rho(\frac{4}{3}\pi)a^3\ll 1$, which means that the three-body potential contributions can be neglected. At realistic liquid-^{4}He densities however, we have $\frac{3}{2}\rho(\frac{4}{3}\pi)a^3\cong 1.2$. This would mean that three-body contributions cannot be neglected. But of course Eq. (B16) is an overestimation of Eq. (B14) as can be seen by remembering that the coordinates $\vec{x}$ and $\vec{y}$ in Eq. (B14) should always be farther apart from each other than the diameter a if $|\phi_0\rangle$ is to represent a hard-sphere state. Hence, the integration of the Θ functions over d^3x and d^3y will lead to a value that is about $\frac{1}{2}$ of what we found in Eq. (B16). Thus, in the dense case, we are led to compare the quotient

$$\rho(\tfrac{4}{3}\pi)a^3/[\tfrac{3}{2}\rho^2(\tfrac{4}{3}\pi a^3)^2\tfrac{1}{2}]\cong 0.6\,. \tag{B17}$$

We have to remember that Eq. (B17) constitutes only a very rough estimate [$\rho(\vec{x})=$const], but at least the result indicates the possibility that higher-order potentials can be neglected. A better way to test this is to check the accuracy with which the two-body Hamiltonian reproduces physically measurable entities. This of course, cannot be considered an ultimate test either, because many additional approximations are needed to calculate physically measurable entities.

APPENDIX C

In order to Fourier transform Eq. (41), we combine the last two terms in Eq. (41) to

$$\lim_{\epsilon=0^+}\left(\int d^3x\, d'^3x\,\delta(r-a-\epsilon)\frac{\partial}{\partial r}[\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0(\vec{x}')\psi_0(\vec{x})]+\frac{1}{a}\int d^3x\, d'^3x\,\delta(r-a-\epsilon)\psi_0^\dagger(\vec{x})\psi_0^\dagger(\vec{x}')\psi_0(\vec{x}')\psi_0(\vec{x})\right), \tag{C1}$$

with

$$\vec{r}\equiv\vec{x}-\vec{x}',\quad 2\vec{R}\equiv\vec{x}+\vec{x}',\quad \vec{x}=\vec{R}+\tfrac{1}{2}\vec{r},\quad \vec{x}'=\vec{R}-\tfrac{1}{2}\vec{r}, \tag{C2}$$

and Eq. (42), we obtain

$$= \frac{1}{V^2} \lim_{\epsilon = 0^+} \int d^3R d^3r \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} \delta(r - a - \epsilon)\left(\frac{\partial}{\partial r} + \frac{1}{a}\right) e^{-i\vec{k}_1 \cdot (\vec{R} + \vec{r}/2)} e^{-i\vec{k}_2 \cdot (\vec{R} - \vec{r}/2)} e^{i\vec{k}_3 \cdot (\vec{R} - \vec{r}/2)} e^{i\vec{k}_4 \cdot (\vec{R} + \vec{r}/2)} a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_4} \tag{C3}$$

$$= \frac{1}{V^2} \lim_{\epsilon = 0^+} \Big[\int d^3R\, d^3r \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} \delta(r - a - \epsilon) \left(-\frac{i}{2} \cos\Theta(|\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4|) + \frac{1}{a}\right) e^{-i(\vec{r}/2)\cdot(\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4)} \times e^{-i\vec{R}\cdot(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4)} a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_4} \Big], \tag{C4}$$

where Θ is the angle between $\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4$ and $\vec{r}$. The term $1/a$ in large parentheses leads to

$$\lim_{\epsilon = 0^+} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} \frac{1}{Va} \int d^3r\, \delta(r - a - \epsilon) e^{i\vec{r}\cdot(\vec{k}_2 - \vec{k}_3)} a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_1 + \vec{k}_2 - \vec{k}_3} \tag{C5}$$

$$= \lim_{\epsilon = 0^+} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} \frac{4\pi}{Va} \int r^2 dr\, \delta(r - a - \epsilon) j_0(r|\vec{k}_2 - \vec{k}_3|) a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_1 + \vec{k}_2 - \vec{k}_3} \tag{C6}$$

$$\frac{4\pi a}{V} \lim_{\epsilon = 0^+} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} j_0(aq)_{+\epsilon}\, a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_2 - \vec{q}} a_{\vec{k}_1 + \vec{q}}\ . \tag{C7}$$

The term $-i/2 \cos\Theta |\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4|$ leads, ignoring the a operators for the moment, to

$$-\frac{2i\pi}{V} \lim_{\epsilon = 0^+} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \int r^2 dr\, \delta(r - a - \epsilon) \cos\Theta_{\vec{q},\vec{r}}\, q \times e^{-irq\cos\Theta_{\vec{q},\vec{r}}}\, d\cos\Theta_{\vec{q},\vec{r}}\ . \tag{C8}$$

The angular integral is given by

$$\int_{-1}^{1} d\cos\Theta\, e^{-irq\cos\Theta} = 2i\left(\frac{\cos qr}{qr} - \frac{j_0(qr)}{qr}\right), \tag{C9}$$

thus, inserted in Eq. (C8), we find

$$\frac{4\pi a}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} [\cos(qa)_{+\epsilon} - j_0(qa)_{+\epsilon}]\, a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_2 - \vec{q}} a_{\vec{k}_1 + \vec{q}}\ . \tag{C10}$$

Equations (C7) and (C10) finally lead to

$$\frac{4\pi a}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \cos(qa)_{+\epsilon} a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_2 - \vec{q}} a_{\vec{k}_1 + \vec{q}}\ . \tag{C11}$$

Now the Fourier transform of the first term in Eq. (41),

$$-\int d^3x \int_{|\vec{x} - \vec{x}| \le \lim_{\epsilon = 0^+} a - \epsilon} [\nabla_{\vec{x}} \psi_0^\dagger(\vec{x}) \psi_0^\dagger(\vec{x}')] \times [\nabla_{\vec{x}} \psi_0(\vec{x}') \psi_0(\vec{x})]\, d'^3x\,,$$

becomes

$$-\frac{1}{V^2} \lim_{\epsilon = 0^+} \int d^3x\, d^3r\, \Theta(r - a + \epsilon) \times \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} (-i\vec{k}_1)(i\vec{k}_4) e^{-\vec{k}_1 \cdot \vec{x}} e^{-i\vec{k}_2 \cdot (\vec{x} - \vec{r})} \times e^{i\vec{k}_3 \cdot (\vec{x} - \vec{r})} e^{i\vec{k}_4 \cdot \vec{x}} (a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_4})\,, \tag{C12}$$

with the help of

$$\int_0^a d^3x\, e^{i\vec{k}\cdot\vec{x}} = \frac{4\pi a^2}{k} j_1(ka)\,, \tag{C13}$$

the r integration gives us

$$-\frac{4\pi a^2}{V^2} \int d^3x \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} \frac{\vec{k}_1 \cdot \vec{k}_4}{|\vec{k}_2 - \vec{k}_4|} j_1(a|\vec{k}_2 - \vec{k}_3|)_{-\epsilon} \times e^{-i\vec{x}\cdot(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4)} \times a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_4}\,, \tag{C14}$$

which finally equals

$$-\frac{4\pi a^2}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \frac{\vec{k}_1 \cdot (\vec{k}_1 + \vec{q})}{q} j_1(qa)_{-\epsilon}\, a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_2 - \vec{q}} a_{k_1 + \vec{q}}\ . \tag{C15}$$

The kinetic energy term in Eq. (41) is trivial and therefore we obtain the Fourier transform of the two body potential Hamiltonian

$$H = \sum_{\vec{k}} k^2 a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{4\pi a}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \left(\cos(qa)_{+\epsilon} - \frac{a\vec{k}_1 \cdot (\vec{k}_1 + \vec{q})}{q} j_1(qa)_{-\epsilon}\right) \times a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_2 - \vec{q}} a_{\vec{k}_1 + \vec{q}}\ . \tag{C16}$$

It is interesting to remark that in the more general case of choosing $f(r) = r^n$, the $\cos(qa)_{+\epsilon}$ term in Eq. (C16) has to be replaced [see Eq. (41)] by

$$\cos(qa)_{+\epsilon} + (n - 1) j_0(qa)_{+\epsilon}\ . \tag{C17}$$

APPENDIX D

Here we shall calculate the lowering of the ground-state energy of a Hartree-Fock ground-state under the formation of opposite-momenta pairs.

From Eq. (45) and defining

$$\xi(\vec{k}) = k^2(1-\tfrac{4}{3}\pi a^3\rho) + 8\pi a\rho\cos(ka)_+ \tag{D1}$$

and

$$W_{HF}(\vec{k},\vec{q}) = (4\pi a/V)[V(\vec{k}-\vec{q},\vec{q}) - 2\cos(ka)_+], \tag{D2}$$

one obtains

$$H = \frac{4\pi a}{V}N^2 + \sum_{\vec{t}}{}' \xi(k)a^\dagger_{\vec{k}}a_{\vec{k}} + \sum_{\vec{k},\vec{q}}{}'' W_{HF}(\vec{k},\vec{q})a^\dagger_{\vec{k}}a_{\vec{k}}a^\dagger_{\vec{q}}a_{\vec{q}} + \frac{4\pi a}{V}\sum_{\vec{q},\vec{p}}{}'' V(\vec{q}-\vec{p},\vec{p})a^\dagger_{\vec{p}}a^\dagger_{-\vec{p}}a_{\vec{q}}a_{-\vec{q}} + \frac{4\pi a}{V}\sum_{\vec{k}}{}' \cos(ka)(a^\dagger_0 a^\dagger_0 a_{\vec{k}}a_{-\vec{k}} + a^\dagger_{\vec{k}}a^\dagger_{-\vec{k}}a_0 a_0). \tag{D3}$$

The terms $\vec{q}=\vec{p}$ in Eq. (D3) and $\vec{k}=\vec{q}$ in Eq. (45) should be excluded, but their contribution is negligible. A normalized N-particle Hartree-Fock eigenstate is given by

$$|\phi_0^N\rangle = \prod_{\vec{k}}(n_{\vec{k}}!)^{-1/2}(a^\dagger_{\vec{k}})^{n_{\vec{k}}}|0\rangle, \qquad \sum_{\vec{k}=0}^{\infty} n_{\vec{k}} = N. \tag{D4}$$

Minimizing $\langle\phi_0^N|H_p|\phi_0^N\rangle$ with respect to $\{n_{\vec{k}}\}$ leads to

$$\xi(k) + \sum_{\vec{q}}{}' [W_{HF}(\vec{k},\vec{q}) + W_{HF}(\vec{q},\vec{k})]n_{\vec{q}} = 0. \tag{D5}$$

We define the augmented HF state by

$$|\psi\rangle = \sum_{\vec{p}} A(\vec{p})a^\dagger_{\vec{p}}a^\dagger_{-\vec{p}}|\phi_0^N\rangle. \tag{D6}$$

Its normalization leads to

$$1 = \langle\psi|\psi\rangle = \langle\phi_0^N|\sum_{\vec{p}\,\vec{q}} A^*(\vec{p})a_{\vec{p}}a_{-\vec{p}} \times A(\vec{q})a^\dagger_{\vec{q}}a^\dagger_{-\vec{q}}|\phi_0^N\rangle \tag{D7}$$

with $A^*(\vec{q}) = A(\vec{q})$ and assuming $\hat{n}_{\vec{k}}|\phi_0^N\rangle = \hat{n}_{-\vec{k}}|\phi_0^N\rangle$, Eq. (D7) becomes

$$1 = 2\sum_{\vec{k}}{}' A^2(\vec{k})(n_{\vec{k}}+1)^2 + A^2(0)(n_0+1)(n_0+2). \tag{D8}$$

The expressions to be calculated are given below. First:

$$\langle\psi|\sum_{\vec{k}}{}' \xi(\vec{k})a^\dagger_{\vec{k}}a_{\vec{k}}|\psi\rangle = 2\sum_{\vec{t}}{}' A^2(\vec{t})(n_{\vec{t}}+1)^2\sum_{\vec{k}}{}'(n_{\vec{k}}+\delta_{\vec{k},\pm\vec{t}})\xi(k) + A^2(0)(n_0+1)(n_0+2)\sum_{\vec{k}}{}'(n_{\vec{k}}+2\delta_{\vec{k},0})\xi(\vec{k})$$
$$= 4\sum_{\vec{t}}{}' A^2(\vec{t})(n_{\vec{t}}+1)^2\xi(t) + \left(2\sum_{\vec{t}}{}' A^2(\vec{t})(n_{\vec{t}}+1)^2 + A^2(0)(n_0+1)(n_0+2)\right)\sum_{\vec{k}}{}' n_{\vec{k}}\xi(k), \tag{D9}$$

with Eq. (D8) we finally obtain

$$\langle\psi|\sum_{\vec{k}}{}' \xi(\vec{k})a^\dagger_{\vec{k}}a_{\vec{k}}|\psi\rangle = \sum_{\vec{k}}{}' [4A^2(\vec{k})(n_{\vec{k}}+1)^2 + n_{\vec{k}}]\xi(k). \tag{D10}$$

Second:

$$\langle\psi|\sum_{\vec{k},\vec{q}}{}'' W_{HF}(\vec{k},\vec{q})a^\dagger_{\vec{k}}a_{\vec{k}}a^\dagger_{\vec{q}}a_{\vec{q}}|\psi\rangle = 2\sum_{\vec{t}}{}' A^2(\vec{t})(n_{\vec{t}}+1)^2\sum_{\vec{p},\vec{q}}{}'' W_{HF}(\vec{p},\vec{q})(n_{\vec{p}}+\delta_{\vec{p},\pm\vec{t}})(n_{\vec{q}}+\delta_{\vec{q},\pm\vec{t}})$$
$$+ A^2(0)(n_0+1)(n_0+2)\sum_{\vec{p},\vec{q}}{}'' W_{HF}(\vec{p},\vec{q})(n_{\vec{p}}+2\delta_{\vec{p},0})(n_{\vec{p}}+2\delta_{\vec{q},0}). \tag{D11}$$

Using Eq. (D8), we obtain

$$= \sum_{\vec{p},\vec{q}}{}'' W_{HF}(\vec{p},\vec{q})n_{\vec{p}}n_{\vec{q}} + 4\sum_{\vec{p},\vec{q}}{}'' [W_{HF}(\vec{p},\vec{q}) + W_{HF}(\vec{q},\vec{p})]A^2(\vec{p}) \times(n_{\vec{p}}+1)^2 n_{\vec{q}} + 4\sum_{\vec{t},\vec{p}}{}' [W_{HF}(\vec{t},\vec{t}) + W_{HF}(\vec{t}-\vec{t})]A^2(\vec{p})(n_{\vec{p}}+1)^2, \tag{D12}$$

where the last term $\sum'_{\vec{t}}$ in Eq. (D12) is of order N smaller than the first two terms and therefore negligible.

Third:

$$\langle\psi|\sum_{\vec{p},\vec{q};\,\vec{p}\neq\pm\vec{q}}{}'' \frac{4\pi a}{V} V(\vec{q}-\vec{p},\vec{p}) a^\dagger_{\vec{p}} a^\dagger_{-\vec{p}} a_{\vec{q}} a_{-\vec{q}} |\psi\rangle = 4\sum_{\vec{p},\vec{q}} \frac{4\pi a}{V} V(\vec{q}-\vec{p},\vec{p}) A(\vec{p}) A(\vec{q}) (n_p+1)^2 (n_q+1)^2$$

$$-4\sum_{\vec{p}}{}' A^2(\vec{p})(n_{\vec{p}}+1)^2[V(0,\vec{p})+V(-2\vec{p},\vec{p})] \ . \qquad \text{(D13)}$$

The last term $\sum_{\vec{p}}'$ in Eq. (D13) is of order N times smaller than the rest and therefore negligible. Fourth:

$$\langle\psi|\sum_{\vec{k}}{}' \frac{4\pi a}{V}[V(\vec{k},0)a^\dagger_0 a^\dagger_0 a_{\vec{k}} a_{-\vec{k}} + V(\vec{k},-\vec{k}) a^\dagger_{\vec{k}} a^\dagger_{-\vec{k}} a_0 a_0]|\psi\rangle$$

$$= 2\frac{4\pi a}{V}\sum_{\vec{k}}{}' A(\vec{k})(n_{\vec{k}}+1)^2 A(0)(n_0+1)(n_0+2)[V(\vec{k},0)+V(\vec{k},-\vec{k})] \ . \qquad \text{(D14)}$$

Collecting all the terms of order N we obtain

$$\langle\psi|H|\psi\rangle - \langle\phi_0^N|H|\phi_0^N\rangle = 4\sum_{\vec{k}}{}' A^2(\vec{k})(n_{\vec{k}}+1)^2\xi(k) + 4\sum_{p,q}{}''[W_{HF}(\vec{p},\vec{q})+W_{HF}(\vec{q},\vec{p})]A^2(\vec{p})(n_{\vec{p}}+1)^2 n_q$$

$$\times 4\frac{4\pi a}{V}\sum_{\vec{p},\vec{q}}{}'' V(\vec{q}-\vec{p},\vec{p}) A_{\vec{p}} A_{\vec{q}} (n_{\vec{p}}+1)^2 (n_{\vec{q}}+1)\, 4\frac{4\pi a}{V}$$

$$\times \sum_{\vec{k}}{}' A(\vec{k})(n_{\vec{k}}+1)^2 A(0)(n_0+1)(n_0+2)\cos(ka) \ .$$

With Eq. (D5), Eq. (D15) leads to

$$\Delta E = \frac{16\pi a}{NV}\left(\sum_{\vec{p},\vec{q}}{}'' V(\vec{q}-\vec{p},\vec{p})A(\vec{p})A(\vec{q})(n_{\vec{p}}+1)^2(n_{\vec{q}}+1)^2 + \sum_{\vec{k}}{}' A(\vec{k})(n_{\vec{k}}+1)^2 A(0)(n_0+1)(n_0+2)\cos(ka)_+\right) \ . \qquad \text{(D16)}$$

From Appendix E3, Eqs. (E3.5)–(E3.22) we know that if

$$f(k) = \sum_{\vec{q}}{}' V(\vec{q}-\vec{k},\vec{k}) g(qa)_- \ ,$$

where $g(qa)$ does not depend on the direction of $\vec{q}$ and converges faster than q^{-3}, can be written

$$f(qa) = 4\pi a\Big(\hat{D} j_0(ka)_+ + \hat{E}_0\cos(ka)_+ - \hat{E}_0 j_0(ka)_+ - \sum_{l=1}(4l+1)\hat{E}_{2l} j_{2l}(ka)_-\Big), \qquad \text{(D17)}$$

$$\hat{D} = \frac{1}{V}\sum_{\vec{k}}{}' \cos(ka)_+ g(ka) \ ,$$

$$\hat{E} = \frac{1}{V}\sum_{\vec{k}}{}' j_0(ka)_+ g(ka), \qquad \text{(D18)}$$

$$\hat{E}' = \frac{1}{V}\sum_{\vec{k}}{}' j_{2l}(ka)_- g(ka).$$

Choosing $g(ka) = A(\vec{k})(n_k+1)$, Eq. (D16) becomes, after one integration,

$$\Delta E = \frac{16\pi a}{N}\sum_{\vec{p}}{}' A(\vec{p})(n_{\vec{p}}+1)^2 \times\Big(\hat{D} j_0(pa)_+ + \hat{E}_0\cos(pa)_+ - \hat{E}_0 j_0(pa)_+ - \sum_{l=1}{}'(4l+1)\hat{E}'_{2l} j_{2l}(pa)_- + A(0)(n_0+1)(n_0+2)\cos(pa)_+\Big), \qquad \text{(D19)}$$

and a second integration leads to

$$\Delta E = 16\pi a\Big(\hat{D}(n_0+1)(n_0+2)A(0)/N + 2\delta^{-1}\hat{E}_0\hat{D} - \hat{E}^2\rho^{-1} \times\sum_{l=1}^{\infty}(4l+1)\hat{E}'^2_{2l}\Big). \qquad \text{(D20)}$$

APPENDIX E1

In order to calculate the chemical potential μ in the general case $N_0 \neq 0$ we have to evaluate the expression

$$\langle\psi_0'|\frac{\partial}{\partial N_0}H_p|\psi_0'\rangle \ \text{ with } \lambda_1=\lambda_2=\lambda_3=\lambda_4=1 \ . \qquad \text{(E1.1)}$$

We write H_p, neglecting terms of order $1/N$, the following way:

$$H_p = 4\pi a(\rho_0+\rho')^2 V - \sum_{\vec{k}}{}'\left[\left(1-\frac{4\pi a^3}{3}(\rho_0+\rho')\right)k^2 + 8\pi a(\rho_0+\rho')\cos(ka)_+\right] b^\dagger_{\vec{k}} b_{\vec{k}} + 4\pi a(\rho_0+\rho')$$
$$\times \sum_{\vec{k}}{}' \cos(ka_+)(b_{\vec{k}}b_{-\vec{k}} + b^\dagger_{\vec{k}}b^\dagger_{-\vec{k}}) - \frac{4\pi a}{V}\sum_{\vec{k},\vec{q}}{}'' \cos(ka)_+ (b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} b^\dagger_{\vec{q}} b_{\vec{q}} + b^\dagger_{\vec{q}} b_{\vec{q}} b_{\vec{k}} b_{-\vec{k}})$$
$$+\frac{8\pi a}{V}\sum_{\vec{k},\vec{q}}{}''\left(-\cos(ka)_+ + \tfrac{1}{2}\cos(|\vec{q}-\vec{k}|a) + \frac{1}{2}\frac{\vec{k}\cdot\vec{q}a}{|\vec{q}-\vec{k}|} j_1(|\vec{q}-\vec{k}|a)\right) b^\dagger_{\vec{k}} b_{\vec{k}} b^\dagger_{\vec{q}} b_{\vec{q}}$$
$$+\frac{4\pi a}{V}\sum_{\vec{k},\vec{q}}{}''\left(\cos(|\vec{q}-\vec{k}|) - \frac{\vec{k}\cdot\vec{q}a}{|\vec{q}-\vec{k}|} j_1(|\vec{q}-\vec{k}|a)\right) b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} b_{\vec{q}} b_{-\vec{q}} \ . \quad \text{(E1.2)}$$

$\partial H_p/\partial N_0$ is then given by

$$\frac{\partial H}{\partial N_0} = \frac{1}{V}\frac{\partial H}{\partial \rho_0} = 8\pi a\rho - \frac{4\pi a}{3V}\sum_{\vec{k}}{}'(ka)^2 b^\dagger_{\vec{k}} b_{\vec{k}} + \frac{8\pi a}{V}\sum_{\vec{k}}{}' \cos(ka)_+ b^\dagger_{\vec{k}} b_{\vec{k}} + \frac{4\pi a}{V}\sum_{\vec{k}}{}' \cos(ka)_+ (b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} + b_{\vec{k}} b_{-\vec{k}}) \ . \quad \text{(E1.3)}$$

Keeping in mind that we shall form the matrix element of Eq. (E1.3) with the interacting ground state $|\psi_0'\rangle$ we can replace

$$b^\dagger_{\vec{q}} b_{\vec{q}} \text{ by } [U_q^2/(1-U_q^2)]\beta_{-\vec{k}}\beta^\dagger_{-\vec{k}} \quad \text{(E1.4)}$$

and

$$b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} + b_{\vec{k}} b_{-\vec{k}} \text{ by } -[2U_k/(1-U_k^2)]\beta_{-\vec{k}}\beta^\dagger_{-\vec{k}} \ . \quad \text{(E1.5)}$$

Together with the identities

$$\cos(ka) = \sum_l (-1)^l (4l+1) j_{2l}(ka) \quad \text{(E1.6)}$$

and the definitions

$$\sum_{\vec{k}}{}' j_{2l}(ka)_+ \frac{U_k}{1-U_k^2} = \frac{V}{(2\pi)^3}\frac{4\pi}{a^3}E_{2l} \ , \quad \text{(E1.7)}$$

$$\sum_{\vec{k}}{}' j_{2l}(ka)\frac{U_k^2}{1-U_k^2} = \frac{V}{(2\pi)^3}\frac{4\pi}{a^3}B_{2l} \ , \quad \text{(E1.8)}$$

$\mu = \langle\psi_0'|\partial H_p/\partial N_0|\psi_0'\rangle$ equals

$$\mu = \frac{8\pi a}{V}\left(N - \frac{1}{6}\sum_{\vec{k}}{}'\frac{(ak)^2 U_k^2}{1-U_k^2}\right) + \frac{8\pi a}{V}\sum_{l=0}^{\infty}(-1)^l(4l+1)$$
$$\times\frac{V}{(2\pi)^3}\frac{4\pi}{a^3}B_{2l} - \frac{4\pi a}{V}\sum_{l=0}^{\infty}(-1)^l(4l+1)\frac{2V}{(2\pi)^3}\frac{4\pi}{a^3}E_{2l} \ . \quad \text{(E1.9)}$$

Further, defining

$$F \equiv \sum_{l=0}^{\infty}(-1)^l(4l+1)B_{2l} \ , \quad \text{(E1.10)}$$

$$D \equiv \sum_{l=0}^{\infty}(-1)^l(4l+1)E_{2l} \ , \quad \text{(E1.11)}$$

we obtain

$$\mu = \frac{8\pi a}{V}\left(N - \frac{1}{6}\sum_{\vec{k}}{}'\frac{(ka)^2 U_k^2}{1-U_k^2}\right) + \frac{4\pi}{(a\pi)^2}(F-D) \ . \quad \text{(E1.12)}$$

In the case of $N_0=0$ we know that the first bracket has to be zero in order that Eqs. (E1.12) and (95) are the same. This gives a relation to be used in calculating the ground-state energy in case of $N_0 = 0$,

$$\sum_{\vec{k}}{}'\frac{(ka)^2 U_k^2}{1-U_k^2} = 6N \quad (\text{only for } N_0 = 0) \quad \text{(E1.13)}$$

and ultimately

$$\mu = (4/\pi a^2)(F-D) \quad (\text{only for } N_0 = 0) \ . \quad \text{(E1.14)}$$

APPENDIX E2

In order to minimize the ground-state energy of H_p [Eq. (70)], which is given by

$$H_p = 4\pi a\rho(N-1) + \sum_{\vec{k}}{}' V_0(\vec{k}) b^\dagger_{\vec{k}} b_{\vec{k}}$$
$$+ \sum_{\vec{k}}{}' V_1(\vec{k})(b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} - b_{\vec{k}} b_{-\vec{k}})$$
$$+ \sum_{\vec{k},\vec{q}}{}'' V_2(\vec{k},\vec{q})(b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} b^\dagger_{\vec{q}} b_{\vec{q}} + b^\dagger_{\vec{q}} b_{\vec{q}} b_{\vec{k}} b_{-\vec{k}})$$
$$+ \sum_{\vec{k},\vec{q}}{}'' V_3(\vec{k},\vec{q}) b^\dagger_{\vec{k}} b_{\vec{k}} b^\dagger_{\vec{q}} b_{\vec{q}} + \sum_{\vec{k},\vec{q}}{}'' V_4(\vec{k},\vec{q}) b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} b_{\vec{q}} b_{-\vec{q}} \ , \quad \text{(E2.1)}$$

where

$$V_0(\vec{k}) = (1 - \tfrac{4}{3}\pi a^3 - \rho)k^2 + \lambda_1 8\pi a\rho\cos(ka) \ , \quad \sim\text{order } 1 \ ,$$
$$V_1(\vec{k}) = \lambda_2 4\pi a\rho\cos(ka)_+ \ , \quad \sim\text{order } 1 \ ,$$
$$V_2(\vec{k},\vec{q}) = -\lambda_2(4\pi a/V)\cos(ka)_+ \ , \quad \sim\text{order } 1/N \ ,$$
$$V_3(\vec{k},\vec{q}) = (4\pi a/V)[-\lambda_1 2\cos(ka)_+ + \lambda_3 V(\vec{q}-\vec{k},\vec{k})] \ , \quad \sim\text{order } 1/N \ ,$$
$$V_4(\vec{k},\vec{q}) = (4\pi a/V)\lambda_4 V(\vec{q}-\vec{k},\vec{k}) \ , \quad \sim\text{order } 1/N \ , \quad \text{(E2.2)}$$

with respect to the functional U_k we have to cast Eq. (E2.1) from the $b_{\vec{k}}$ to the $\beta_{\vec{k}}$ coordinates. Only terms of the form $\sum_{\vec{k}}\beta_{\vec{k}}\beta^\dagger_{\vec{k}}$ or $(1/V)\sum\beta_{\vec{k}}\beta^\dagger_{\vec{k}}\beta_{\vec{q}}\beta^\dagger_{\vec{q}}$ contribute in the right order to the ground-state energy. Thus the expression to be minimized is

$$H_{\text{ground}} = \sum_{\vec{k}}{}' \frac{V_0(\vec{k})}{1-U_k^2} U_k^2 + \sum_{\vec{k}}{}' \frac{V_1(\vec{k})}{1-U_k^2} (-2U_k) \sum_{\vec{k},\vec{q}}{}'' \frac{\beta_{-\vec{k}}\beta^{\dagger}_{-\vec{k}}\beta_{-\vec{q}}\beta^{\dagger}_{-\vec{q}}}{(1-U_k^2)(1-U_q^2)} [-2U_k U_q^2 V_2(\vec{k},\vec{q}) + U_k^2 U_q^2 V_3(\vec{k},\vec{q})]$$
$$\times \sum_{\vec{k},\vec{q}}{}'' \frac{V_4(\vec{k},\vec{q})}{(1-U_k^2)(1-U_q^2)} U_k U_q \beta_{-\vec{k}}\beta^{\dagger}_{-\vec{k}}\beta_{\vec{q}}\beta^{\dagger}_{\vec{q}} + 4\pi a\rho N . \qquad \text{(E2.3)}$$

Taking the matrix element

$$\langle \psi_0'\{U_k\} | H_{\text{ground}} | \psi_0'\{U_k\}\rangle , \qquad \text{(E2.4)}$$

and setting its variation w.r.t. $\{U_k\}$ equal to zero, we obtain

$$0 = 2V_0(\vec{k})\left(\frac{U_k}{1-U_k^2} + \frac{U_k^3}{(1-U_k^2)^2}\right) - 2V_1(\vec{k})\left(\frac{1}{1-U_k^2} + \frac{2U_k^2}{(1-U_k^2)^2}\right) - 2\sum_{\vec{q}}{}' V_2(\vec{k},\vec{q})\left(\frac{U_q^2}{(1-U_k^2)(1-U_q^2)} + \frac{2U_k^2 U_q^2}{(1-U_k^2)(1-U_q^2)}\right)$$
$$- 2\sum_{\vec{q}}{}' V_2(\vec{q},\vec{k})\left(\frac{2U_q U_k}{(1-U_k^2)(1-U_q^2)} + \frac{2U_q U_k^3}{(1-U_q^2)(1-U_k^2)^2}\right)$$
$$+ \sum_{\vec{q}}{}' [V_3(\vec{k},\vec{q}) + V_3(\vec{q},\vec{k})]\left(\frac{2U_k U_q^2}{(1-U_q^2)(1-U_k^2)} + \frac{2U_k^3 U_q^2}{(1-U_q^2)(1-U_k^2)^2}\right)$$
$$+ 2\sum_{\vec{q}}{}' V_4(\vec{k},\vec{q})\left(\frac{U_q}{(1-U_q^2)(1-U_k^2)} + \frac{2U_k^2 U_q}{(1-U_q^2)(1-U_k^2)^2}\right) . \qquad \text{(E2.5)}$$

Multiplying Eq. (E2.5) with $\frac{1}{2}a^2(1-U_k^2)^2$ and using the definitions

$$S_1(k) \equiv 2a^2\left(-V_1(\vec{k}) - \sum_{\vec{q}}{}' V_2(\vec{k},\vec{q})\frac{U_q^2}{1-U_q^2} + \sum_{\vec{q}}{}' V_4(\vec{k},\vec{q})\frac{U_q}{1-U_q^2}\right) , \qquad \text{(E2.6)}$$

$$S_2(k) \equiv a^2\left(V_0(\vec{k}) + \sum_{\vec{q}}{}' [V_3(\vec{k},\vec{q}) + V_3(\vec{q},\vec{k})]\frac{U_q^2}{1-U_q^2} - 2\sum_{\vec{q}}{}' V_2(\vec{q},\vec{k})\frac{U_q}{1-U_q^2}\right) ; \qquad \text{(E2.7)}$$

we arrive at the integral equation

$$\tfrac{1}{2}(1+U_k^2)S_1(\vec{k}) + U_k S_2(\vec{k}) = 0 . \qquad \text{(E2.8)}$$

Collecting now all the terms proportional to $\beta^{\dagger}_{\vec{k}}\beta_{\vec{k}}$ which represent the new excitations we obtain

$$H_{\text{ex}} = \sum_{\vec{k}}{}' E_{\vec{k}}\beta^{\dagger}_{\vec{k}}\beta_{\vec{k}} = \sum_{\vec{k}}{}' \left[V_0(\vec{k})\frac{1+U_k^2}{1-U_k^2} - 4V_1(\vec{k})\frac{U_k}{1-U_k^2} - 2\frac{1+U_k^2}{1-U_k^2}\left(\sum_{\vec{q}}{}' V_2(\vec{q},\vec{k})\frac{U_q}{1-U_q^2}\right)\right.$$
$$- 4\frac{U_k}{1-U_k^2}\left(\sum_{\vec{q}}{}' V_2(\vec{k},\vec{q})\frac{U_q^2}{1-U_q^2}\right) + \frac{1+U_k^2}{1-U_k^2}\left(\sum_{\vec{q}}{}' [V_3(\vec{k},\vec{q}) + V_3(\vec{q},\vec{k})]\frac{U_q^2}{1-U_q^2}\right)$$
$$\left. + 2\frac{U_k}{1-U_k^2}\left(\sum_{\vec{q}}{}' [V_4(\vec{k},\vec{q}) + V_4(-\vec{k},\vec{q})]\frac{U_q}{1-U_q^2}\right)\right]\beta^{\dagger}_{\vec{k}}\beta_{\vec{k}} . \qquad \text{(E2.9)}$$

E_k can be written

$$E(\vec{k}) = \frac{1}{a^2}\left(S_2(k)\frac{1+U_k^2}{1-U_k^2} + 2S_1(k)\frac{U_k}{1-U_k^2}\right) ; \qquad \text{(E2.10)}$$

from Eq. (E2.8), we have

$$U_k = \frac{S_2(k) - [S_2^2(k) - S_1^2(k)]^{1/2}}{-S_1(k)} . \qquad \text{(E2.11)}$$

Equations (E2.10) and (E2.11) lead to

$$E_k = (1/a^2)[S_2^2(k) - S_1^2(k)]^{1/2} . \qquad \text{(E2.12)}$$

We should keep in mind that so far we have not yet restricted ourselves to $\lambda_1 = \lambda_2 = 0$. Thus if we set $\lambda_1 = \lambda_2 = 0$ we know that in case of $N_0 = 0$, the excitation spectrum has to remain unchanged, i.e., $S_2^2 - S_1^2$ does not change. Inspecting Eqs. (E2.6) and (E2.7), we see that S_1 does not change if λ_1 and λ_2 are set equal to zero assuming that $\sum_{\vec{k}} U_k^2/(1-U_k^2) = N$. Under the same conditions S_2 in Eq. (E2.7) can be written

$$S_2(k) = a^2\left((1 - \tfrac{4}{3}\pi a^3\rho_-)k^2 + 2\lambda_3\frac{4\pi a}{V}\right.$$
$$\left. \times \sum_{\vec{q}} V(\vec{q}-\vec{k},\vec{k})\frac{U_q^2}{1-U_q^2} - \mu\right) , \qquad \text{(E2.13)}$$

where we have defined the chemical potential

$$\mu=-2\sum_{\vec{q}}\frac{V_2(\vec{q},\vec{k})U_q(U_q-1)}{1-U_q^2} \qquad \text{(E2.14)}$$

in such a way that Eqs. (E2.13) and (E2.7) lead to the same numerical values Vk. We should keep in mind that the determination of μ in this way is only correct if $N_0=0$!

APPENDIX E3

For the calculation of $S_1(k)$ and $S_2(k)$ in the dense case, i.e., $\lambda_1=\lambda_2=0$ we recall the following definitions[22]:

$$P_n^m(z)=(1-z^2)^{m/2}\frac{d^m}{dz^m}P_n(z),$$

$$\frac{d^m}{dz^m}P_n=T_{n-m}^m, \qquad \text{(E3.1)}$$

$$T_l^0=P_l^0=P_l,\quad P_0^0=T_0^0=T_0'=1,$$

where the $P_n(z)$ are the Legendre polynomials,

$$j_1(|\vec{k}-\vec{q}|a)=\frac{|\vec{k}-\vec{q}|}{a\vec{k}\cdot\vec{q}}\sum_{l=0}^{\infty}(2l+3)T_l'(\cos\theta)j_l(ka)j_l(qa), \qquad \text{(E3.2)}$$

$$\cos(|\vec{k}-\vec{q}|a)=\sum_{l=0}^{\infty}(2l+1)T_l^0(\cos\theta)j_l(ka)j_l(qa)-\frac{|\vec{k}-\vec{q}|^2}{kq}\sum_{l=0}^{\infty}(2l+3)T_l'(\cos\theta)\times j_{l+1}(ka)j_{l+1}(qa), \qquad \text{(E3.3)}$$

we also recall

$$\int_{-1}^{1}T_l^1\,dz=\int_{-1}^{1}\frac{d}{dz}P_{l+1}\,dz=P_{l+1}\Big|_{-1}^{1}=\begin{cases}2 & \text{for } l \text{ even},\\ 0 & \text{for } l \text{ odd},\end{cases}$$

$$\int_{-1}^{1}P_1T_l^1\,dz=\int_{-1}^{1}P_1\frac{d}{dz}P_{l+1}\,dz=P_1P_{l+1}\Big|_{-1}^{1}-\Big|_{-1}^{1}P_{l+1}\,dz=\begin{cases}2 & \text{for } l \text{ odd},\\ 0 & \text{for } l \text{ even},\end{cases} \qquad \text{(E3.4)}$$

from Eqs. (104) and (105) we see that we only need to calculate $S_1(k)$. Hence we write

$$-\frac{S_1(k)}{2a^2}=-\sum_{\vec{q}}{}'\,V_4(\vec{q}-\vec{k},\vec{k})\frac{U_q}{1-U_q^2}$$

$$=-\frac{4\pi a}{V}\sum_{\vec{q}}{}'\left(\cos(|\vec{q}-\vec{k}|a)_+-j_1(|\vec{q}-\vec{k}|a)_-\frac{\vec{k}\cdot\vec{q}a}{|\vec{q}-\vec{k}|}\right)\frac{U_q}{1-U_q^2}$$

$$=\frac{4\pi a}{V}\sum_{\vec{q}}{}'\frac{U_q}{1-U_q^2}\left(\frac{|\vec{k}-\vec{q}|^2}{kq}\sum_{l=0}^{\infty}(2l+3)T_l'(\cos\theta)j_{l+1}(ka)_+j_{l+1}(qa)_+-\sum_{l=0}^{\infty}(2l+1)T_l^0(\cos\theta)j_l(ka)_+j_l(qa)_+\right.$$

$$\left.+\frac{\vec{k}\cdot\vec{q}}{kq}\sum_{l=0}^{\infty}(2l+3)T_l'(\cos\theta)j_{l+1}(ka)_-j_{l+1}(qa)_-\right), \qquad \text{(E3.5)}$$

$$-\frac{S_1(k)}{2a^2}=\frac{4\pi a}{V}\left(-j_0(ka)_+\sum_{\vec{q}}{}'j_0(qa)_+\frac{U_q}{1-U_q^2}+k\sum_{l=0}^{\infty}(2l+3)j_{l+1}(ka)_+\sum_{\vec{q}}{}'\frac{1}{q}j_{l+1}(qa)_+\frac{U_q}{1-U_q^2}T_l'\right.$$

$$+\frac{1}{k}\sum_{l=0}^{\infty}(2l+3)j_{l+1}(ka)_+\sum_{\vec{q}}{}'qj_{l+1}(qa)_+\frac{U_q}{1-U_q^2}T_l'-2\sum_{l=0}^{\infty}(2l+3)j_{l+1}(ka)_+\sum_{\vec{q}}{}'j_{l+1}(qa)_+T_l'P_1\frac{U_q}{1-U_q^2}$$

$$\left.+\sum_{l=0}^{\infty}(2l+3)j_{l+1}(ka)_-\sum_{\vec{q}}{}'j_{l+1}(qa)_-T_l'P_1\frac{U_q}{1-U_q^2}\right). \qquad \text{(E3.6)}$$

Using Eq. (E3.4), we obtain

$$-\frac{S_1(k)}{2a^2}=\frac{4\pi a}{V}\left(-j_0(ka)_+\sum_{\vec{q}}{}'j_0(qa)_+\frac{U_q}{1-U_q^2}+ak\sum_{l=0}^{\infty}(4l+3)j_{2l+1}(ka)_+\sum_{\vec{q}}{}'\frac{1}{qa}j_{2l+1}(qa)_+\frac{U_q}{1-U_q^2}\right.$$

$$+\frac{1}{ak}\sum_{l=0}^{\infty}(4l+3)j_{2l+1}(ka)_+\sum_{\vec{q}}{}'qaj_{2l+1}(qa)_+\frac{U_q}{1-U_q^2}-2\sum_{l=0}^{\infty}(4l+5)j_{2l+2}(ka)_+\sum_{\vec{q}}{}'j_{2l+2}(qa)_+\frac{U_q}{1-U_q^2}$$

$$\left.+\sum_{l=0}^{\infty}(4l+5)j_{2l+2}(ka)_-\sum_{\vec{q}}{}'j_{2l+2}(ka)\frac{U_q}{1-U_q^2}\right). \qquad \text{(E3.7)}$$

Using the relations[22]

$$j_{n-1}(z)+j_{n+1}(z)=\frac{2n+1}{z}j_n(z),\quad zj_{n+1}(z)=(2n+1)j_n(z)-zj_{n-1}(z),\quad \frac{1}{z}j_{n+1}(z)=\frac{1}{2n+3}j_{n+2}(z)+\frac{1}{2n+3}j_n(z), \tag{E3.8}$$

we find

$$-\frac{S_1(k)}{2a^2}=\frac{4\pi a}{V}\Big(-j_0(ka)_+\sum_{\vec q}j_0(qa)_+\frac{U_q}{1-U_q^2}+ak\sum_{=0}^{\infty}j_{2l+1}(ka)_+\sum_{\vec q}[j_{2l+2}(qa)_++j_{2l}(qa)_+]\frac{U_q}{1-U_q^2}$$
$$+\sum_{l=0}^{\infty}[j_{2l+2}(ka)_++j_{2l}(ka)_+]\sum_{\vec q}qaj_{2l+1}(qa)_+\frac{U_q}{1-U_q^2}-2\sum_{l=0}^{\infty}(4l+5)j_{2l+2}(ka)_+\sum_{\vec q}j_{2l+2}(qa)_+\frac{U_q}{1-U_q^2}$$
$$+\sum_{l=0}^{\infty}(4l+5)j_{2l+2}(ka)_-\sum_{\vec q}j_{2l+2}(qa)_-\frac{U_q}{1-U_q^2}\Big), \tag{E3.9}$$

with

$$\sum_{l=0}^{\infty}j_{2l+1}(ka)[j_{2l+2}(qa)+j_{2l}(qa)] \tag{E3.10}$$

and $l\to l+1$,

$$\sum_{l=1}^{\infty}j_{2l-1}(ka)[j_{2l}(qa)+j_{2l-2}(qa)], \tag{E3.11}$$

we can combine Eqs. (3.10) and (3.11) to

$$=\sum_{l=1}^{\infty}j_{2l-1}(ka)j_{2l}(qa)+\sum_{l=1}^{\infty}j_{2l+1}(ka)j_{2l}(qa)+j_1(ka)j_0(qa)=j_1(ka)j_0(qa)+\sum_{l=1}^{\infty}j_{2l}(qa)[j_{2l-1}(ka)+j_{2l+1}(ka)]$$
$$=j_1(ka)j_0(qa)+\sum_{l=1}^{\infty}j_{2l}(qa)(4l+1)\frac{j_{2l}(ka)}{ka}, \tag{E3.12}$$

thus

$$ak\sum_{l=0}^{\infty}j_{2l+1}(ka)_+\sum_{\vec q}[j_{2l+2}(qa)_++j_{2l}(qa)_+]\frac{U_q}{1-U_q^2}=\sum_{l=1}(4l+1)j_{2l}(ka)_+\sum_{\vec q}j_{2l}(qa)_+\frac{U_q}{1-U_q^2}$$
$$+[j_0(ka)_+-\cos(ka)_+]\sum_{\vec q}j_0(qa)_+\frac{U_q}{1-U_q^2}, \tag{E3.13}$$

and therefore

$$-\frac{S_1(k)}{2a^2}=\frac{4\pi a}{V}\Big(-j_0(ka)_+\sum_{\vec q}j_0(qa)_+\frac{U_q}{1-U_q^2}+\sum_{l=1}^{\infty}(4l+1)j_{2l}(ka)_+\sum_{\vec q}j_{2l}(qa)_+\frac{U}{1-U_q^2}$$
$$+[j_0(ka)_+-\cos(ka)_+]\sum_{\vec q}j_0(qa)_+\frac{U}{1-U_q^2}+\sum_{l=1}^{\infty}(4l+1)j_{2l}(ka)_+\sum_{\vec q}j_{2l}(qa)_+\frac{U_q}{1-U_q^2}$$
$$+j_0(ka)_+\sum_{\vec q}[j_0(ka)_+-\cos(ka)_+]\frac{U_q}{1-U_q^2}-2\sum_{l=0}(4l+5)j_{2l+2}(ka)_+\sum_{\vec q}j_{2l+2}(qa)_+\frac{U_q}{1-U_q^2}$$
$$+\sum_{l=0}(4l+5)j_{2l+2}(ka)_-\sum_{\vec q}j_{2l+2}(qa)_-\frac{U_q}{1-U_q^2}\Big), \tag{E3.14}$$

with the definition

$$\frac{4\pi a}{V}\sum_{\vec q}\equiv\frac{2}{\pi a^2}\int_0^{\infty}x^2dx, \tag{E3.15}$$

and the abbreviations

$$\bar E_{2l}\equiv\int_0^{\infty}x^2j_{2l}(x)_-\frac{U(x)}{1-U^2(x)}dx,\qquad E_{2l}\equiv\int_0^{\infty}x^2j_{2l}(x)_+\frac{U(x)}{1-U^2(x)}dx \tag{E3.16}$$

where $(x)_\pm\equiv q(a\pm\epsilon)$ and $\epsilon\to0^+$ and

$$S_1(k)=\frac{4}{\pi}\Big([\cos(ka)_+-j_0(ka)_+]E_0+j_0(ka)\sum_{l=0}^{\infty}(-1)^l(4l+1)E_{2l}-\sum_{l=1}^{\infty}(4l+1)j_{2l}(ka)\bar E_{2l}\Big), \tag{E3.17}$$

$$\cos(kr) \equiv \sum_{l=0} (-1)^l (4l+1) j_{2l}(kr)\,, \qquad \text{(E3.18)}$$

and with

$$D \equiv \sum_{l=0}^{\infty} (-1)^l (4l+1) E_{2l}\,, \qquad \text{(E3.19)}$$

we finally obtain

$$S_1(k) = \frac{4}{\pi}\Big(D j_0(ka)_+ + E_0 \cos(ka)_+ - E_0 j_0(ka)_+ - \sum_{l=1} (4l+1)\bar{E}_{2l} j_{2l}(ka)_- \Big)\,; \qquad \text{(E3.20)}$$

for the calculation of $S_2(k)$ we have to define the quantities

$$B_{2l} = \int_0^\infty x^2 j_{2l}(x) \frac{U^2(x)}{1-U^2(x)}\, dx\,, \qquad \text{(E3.21)}$$

$$F = \sum_{l=0}^{\infty} (-1)^l (4l+1) B_{2l}\,. \qquad \text{(E3.22)}$$

Here we do not have to distinguish between $a \pm \epsilon$ anymore because the integrand of B_{2l} converges fast enough. Thus we obtain

$$S_2(k) = (1 - \tfrac{4}{3}\pi a^3 \rho)(ak)^2 + \frac{4}{\pi}\Big(-\mu' + F j_0(ka) + B_0 \cos(ka) - \sum_{l=0}^{\infty} (4l+1) j_{2l} B_{2l} \Big)\,, \qquad \text{(E3.23)}$$

where

$$\mu \equiv (4/\pi a^2)(F - D) \equiv (4/\pi a^2)\mu' \qquad \text{(E3.24)}$$

represents the chemical potential.

APPENDIX E4

In case of an exact solution the condition

$$\lim_{r=a} \langle \psi_{0\,N}' | \psi_0(r)\psi_0(0) | \psi_{0\,N+2}' \rangle = 0 \qquad \text{(E4.1)}$$

has to be satisfied. Fourier transforming the local-field operators, and applying Bogoliubov transformation to the resulting plane-wave operators, we end up with the leading contribution

$$\rho - \frac{1}{V}\sum_{\vec{k}}{}' \frac{U_k^2}{1-U_k^2} - \frac{1}{2\pi^2 a^3} \times \int_0^\infty j_0(x) x^2 \frac{U(x)}{1-U^2(x)}\, dx = 0\,. \qquad \text{(E4.2)}$$

Equation (4.2) is satisfied for any liquid-He density which also means for any zero-momentum condensate, in agreement with the numerical calculations performed by Wong and Huang.[1] In the dense case, however, the calculation has shown that the first two terms in Eq. (4.2) cancel each other ($N_0 = 0$). The last term in Eq. (4.2), therefore, equals zero, which means $E_{2l} = 0$ for $l = 0$. Looking at the definitions of E_{2l} and $\bar{E}_{2l}$ we see that the expressions

$$E_{2l} = \lim_{\epsilon=0^+} \int_0^\infty dx\, x^2 j_{2l}[x(1+\epsilon)] \frac{U(x)}{1-U^2(x)} \qquad \text{(E4.3)}$$

and

$$\bar{E}_{2l} = \lim_{\epsilon=0^+} \int_0^\infty dx\, x^2 j_{2l}[x(1-\epsilon)] \frac{U(x)}{1-U^2(x)} \qquad \text{(E4.4)}$$

have to be compared with each other. If we look at the asymptotic limit of the integrands using

$$j_{2l}(x) \to (-1)^l \sin(x) | x\,, \qquad \text{(E4.5)}$$

$$\frac{U(x)}{1-U^2(x)} \to -\frac{1}{2}\frac{4}{\pi}\frac{\cos(x)E_0}{(1-\frac{4}{3}\pi a^3\rho)x^2}\,, \qquad \text{(E4.6)}$$

we obtain in the case of E_{2l},

$$(-1)^l \frac{-2/\pi E_0}{1-\frac{4}{3}\pi a^3 \rho} \int_0^\infty dx \frac{\sin(x)\cos x(1-\epsilon)}{x}$$

$$= (-1)^l \frac{-2/\pi E_0}{1-\frac{4}{3}\pi a^3\rho}\left(\frac{1}{2}\int_0^\infty \frac{\sin x(2-\epsilon)}{x(2-\epsilon)}\, dx(2-\epsilon) + \frac{1}{2}\int_0^\infty \frac{\sin(\epsilon x)}{\epsilon x}\, d\epsilon x \right)$$

$$= (-1)^l \frac{-2/\pi E_0}{1-\frac{4}{3}\pi a^3\rho}\frac{\pi}{2} \qquad \text{(E4.7)}$$

in the case of $\bar{E}_{2l}$ we have to replace ϵ by $-\epsilon$ and clearly obtain zero. Hence

$$\bar{E}_{2l} - E_{2l} = (-1)^l E_0/(1 - \tfrac{4}{3}\pi a^3 \rho) \qquad \text{(E4.8)}$$

is proportional to E_0 which equals zero in the case of no zero-momentum condensate. The fact that $E_0 = 0$ also implies that

$$\lim_{k=\infty} |S_1(k)| \leq (\text{const}) k^{-1} \qquad \text{(E4.9)}$$

together with

$$\lim_{k=\infty} S_2(k) \sim k^2\,, \qquad \text{(E4.10)}$$

it leads to

$$\lim_{k=\infty} |U_k| \leq (\text{const}) k^{-3}\,. \qquad \text{(E4.11)}$$

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