Deduction of the two-particle potential function of liquid-^{4}He system from scattering data

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In treating a many-body system, the concept of correlation has been used by various authors to calculate the interacting ground state. In particular, in the Wong-Fung theory, the interacting ground state is expressed in terms of the correlation operators and the noninteracting ground state. Including pair (u_2) and three-particle (u_3) correlations, the wave function can be written as explicit algebraic functions of u_2 and u_3 and the noninteracting wave function [K. W. Wong *et al.*, Phys. Rev. A. **22**, 1272 (1980)]. On the other hand, the authors of the present paper have recently developed a U-matrix theory [Phys. Rev. A **27**, 1760 (1983)] to study general quantum-mechanical problems. For a time-independent problem, we can use this theory to find an analytic solution for the interacting wave function in terms of the potential functions of the system. A bridge between the correlation functions and the potential functions is built by identifying the interacting wave functions of the stated two theories to be the same quantity. Using the above idea, we are able to express the two-particle potential function v_2 as a simple function of the pair correlation u_2 and a "switching integral" I, which determines how the interaction Hamiltonian is switched on, to the lowest order of approximation. Instead of using a model for u_2, we obtain the explicit form of u_2 through the neutron scattering data of Henshaw and the concept of radial distribution function g_2. It is interesting to note that this u_2 is not divergent at any point and is Fourier transformable. Then we proceed to deduce the resulting two-particle potential function. The deduced two-particle potential is shown to be similar in form to the Lenard-Jones potential, with the same depth, a smaller hard-core radius, and a softer core.

I. INTRODUCTION

The same authors have developed a new method of solving general quantum-mechanical problems based on the previous basic U-matrix formalism.[1] The essential ideas and steps of this new approach are: (i) We treat the Schrödinger equation as an operator equation so that the noncommutability properties of all operators involved are taken into consideration. (ii) Previously, the U matrix was written down as a multiple integral of the interaction Hamiltonian, controlled by a proper time sequence. We have been able to express the U matrix as one dominant term plus an infinite series. (iii) We treat every problem as a time-dependent one to begin with. The interaction Hamiltonian is assumed to be switched on "suddenly" or "gradually" in time for every problem. The particular nature of the switch-on process is described by a switching function S_w. (iv) We define a time-independent problem as one for which the total Hamiltonian remains constant in time after the switch-on process is completed. For the process where the agency of interaction has very high speeds (like the exchange of photons in electromagnetic interaction), we may use the sudden switching model to turn on the interaction. We have discovered that for this type of problem, the U matrix is exact, given only by the dominant term stated in (ii). (v) For a more general problem where the Hamiltonian is still a function of time after the switch-on process is completed, we have shown that we can solve for the wave function approximately, in general. However, for a class of Hamiltonians which satisfy certain operator conditions, our solution for the U matrix and hence the wave function is still exact. In this paper, based on our approach and the Wong-Fung theory of many-body problems[2–4] we are able to build a bridge between the concepts of correlation and interaction, at least to the lowest order of approximation, which have been treated practically as two somewhat "independent" entities in the past.

For the past two decades, the correlated-basis-function (CBF) method[5–8] is developed to describe the state of a many-body system using correlation functions. For example, the pair correlation describes how the particles correlate themselves in space due to two-particle interaction. Combining the CBF method and the canonical transformation approach, Wong and Fung[2–4] have proposed a method with which the exact ground-state wave function including interaction is expressible in terms of the noninteracting ground-state wave function $|\phi_0\rangle$ by operating a function of the correlation operators $\hat{Q}_2,\hat{Q}_3,\ldots$ on $|\phi_0\rangle$. After the stated operation, the interacting wave function is expressible in principle as an algebraic function of the multiparticle correlation functions $u_2,u_3,u_4,\ldots$. In practice, using the Wong-Fung theory, one can express the three-particle correlation function u_3 in terms of the pair correlation u_2 explicitly to a high degree of accuracy.[4] Now the pair correlation function $u_2(r_{12})$ is simply related to the radial distribution function $g_2(r_{12}=|\vec{r}_1-\vec{r}_2|)$ which describes the probability of finding one particle in position $\vec{r}_1$ if another particle is in position $\vec{r}_2$. Since $g_2(r_{12})$ is related to the liquid-structure function $S(\vec{k})$, where $\vec{k}$ is the momentum, and $S(\vec{k})$ is deducible from experimental result,[9–12] one can start from experimental

evidence and deduce quantities like the momentum distribution function using the Wong-Fung theory, including effects of pair and three-particle correlations.[13] However, whenever the Hamiltonian begins to be involved, as in the calculation of ground-state energy and excitation spectrum, a model potential function has to be employed. In the study of liquid helium both the spherical shell model[14–16] and the Lennard-Jones potential[17] have been used to calculate the ground-state energy. Thus the correlation function and the potential function are treated as two unrelated (in the explicit sense) functions. We would emphasize that for a neutral system where long-range Coulomb interaction can be neglected, it is precisely the characteristics of the potential around each particle which determine what state a multiparticle system would settle in at the end of the transient interaction period. The above statement is particularly true for a dense system like the liquid-helium system. Thus the wave function given by the Wong-Fung theory describes the "end result" of interaction.

The main aim of this paper is to establish an explicit relationship between the correlation function and the interaction potential function. As a concrete example we apply our concept and theory to study a liquid-helium system at very low temperatures. It is interesting to note that, starting from experimental data on the liquid-structure function, we *deduce* a two-particle potential which is very close to the Lennard-Jones potential in form, but with a softer core and a smaller core radius—this result is not at all surprising if we understand the meaning of correlation and interaction as briefly sketched above. In our deduction we need to use the uncertainty principle and a certain model to specify the "characteristic interaction length" due to phonons interaction. At this point we can only claim that we have roughly obtained the two-particle potential, due to unknown information of the switching process. Our result, however, seems to be consistent with the experimental measurement of the phonon speed in a liquid-helium system.

II. SERIES EXPANSION OF THE MANY-BODY POTENTIAL OPERATOR

In order to avoid repetition, we omit the formalism and foundations of the U-matrix theory developed in Ref. 1, but list only relevant results, using the same symbols, which have not been stated. Readers are asked to treat this paper as a continuation after Sec. IV of Ref. 1. To simplify notation we add "I" in front of an equation to indicate that it is the equation of Ref. 1.

Consider a general interacting N-body system. We assume that the interaction potential operator $\hat{v}(t)$ [in (I2.2)] is expressible in the additive form

$$\hat{v}(t)=\sum_{n=2}^{N}\hat{v}_n(t)\ , \tag{2.1}$$

where $\hat{v}_n(t)$ denotes the n-particle interaction operator.

If $\hat{\psi}^*(\vec{x}_i(t))$ and $\hat{\psi}(\vec{x}_i(t))$ represent, respectively, the creation and annihilation field operator for a particle in position $\vec{x}_i$, we may write the interaction potential operator $\hat{v}_n(t)$ in the following form:

$$\hat{v}_2(t)=\frac{1}{2!}\sum_{i<j}\int\hat{\psi}^*[\vec{x}_i(t)]\hat{\psi}^*[\vec{x}_j(t)]v_2(\,|\,\vec{x}_i-\vec{x}_j\,|\,;t)\hat{\psi}[\vec{x}_j(t)]\hat{\psi}[\vec{x}_i(t)]d^3x_i\,d^3x_j\ ,$$

$$\hat{v}_3(t)=\frac{1}{3!}\sum_{i<j<k}\int\hat{\psi}^*[\vec{x}_i(t)]\hat{\psi}^*[\vec{x}_j(t)]\hat{\psi}^*[\vec{x}_k(t)]v_3(\vec{x}_i,\vec{x}_j,\vec{x}_k;t)\hat{\psi}[\vec{x}_k(t)]\hat{\psi}[\vec{x}_j(t)]\hat{\psi}[\vec{x}_i(t)]d^3x_i\,d^3x_j\,d^3x_k\ , \tag{2.2}$$

$$\cdots\ ,$$

$$\hat{v}_n(t)=\frac{1}{n!}\sum_{i_1<i_2<i_3\cdots<i_n}\int\hat{\psi}^*[\vec{x}_{i_1}(t)]\hat{\psi}^*[\vec{x}_{i_2}(t)]\hat{\psi}^*[\vec{x}_{i_n}(t)]v_n(\vec{x}_{i_1},\vec{x}_{i_2},\ldots,\vec{x}_{i_n};t)\hat{\psi}[\vec{x}_{i_n}(t)]$$

$$\times\hat{\psi}[\vec{x}_{i_{n-1}}(t)]\hat{\psi}[\vec{x}_{i_2}(t)]\hat{\psi}[\vec{x}_{i_1}(t)]d^3x_{i_1}\,d^3x_{i_2}d^3x_{i_n}\ ,$$

where $v_2(\,|\,\vec{x}_1-\vec{x}_2\,|\,;t),v_3(\vec{x}_1,\vec{x}_2,\vec{x}_3;t),\ldots,v_n(\vec{x}_{i_1},\vec{x}_{i_2},\ldots,\vec{x}_{i_n};t)$ are the two-body, three-body, ..., and n-body interaction potential functions, respectively. In (2.2) the spin index has been omitted for simplicity. Note that even though the general form of $\hat{v}_n(t)$ is similar to that of the correlation operator $\hat{Q}_n$ in the Wong-Fung theory,[2–4] they are, in general, different and arise from explicitly different mathematical sources; in fact, it is the purpose of this paper to find an explicit relationship between them. Now in a many-body system, the termination operators in the U-matrix theory become [see (I3.3)]

$$\hat{\Gamma}_1(t)=\left[\hat{H}_0,\sum_{n=2}^{N}\hat{v}_n(t)\right]=\sum_{n=2}^{N}\hat{\Gamma}_1(n,t)\ ,$$

$$\hat{\Gamma}_2(t)=[\hat{H}_0,\hat{\Gamma}_1(t)]=\sum_{n=2}^{N}\hat{\Gamma}_2(n,t)\ , \tag{2.3}$$

$$\cdots\ ,$$

$$\hat{\Gamma}_r(t)=\sum_{n=2}^{N}\hat{\Gamma}_r(n,t)\ ,$$

where

$$\hat{\Gamma}_r(n,t)=[\hat{H}_0,[\hat{H}_0,\ldots,[\hat{H}_0,\hat{v}_n(t)]]\cdots] , \tag{2.4}$$

with $[\hat{H}_0,[\hat{H}_0,\ldots,[\hat{H}_0$ representing an r-fold nesting of the commutators, so that in view of (2.3), (I2.7) and (I3.2) appear as

$$\hat{V}(t)=\sum_{n=2}^{N}\left[\hat{v}_n(t)+\sum_{i=1}^{\infty}\frac{(it/\hbar)^r}{r!}\hat{\Gamma}_r(n,t)\right] . \tag{2.5}$$

Substituting (2.2) into (I2.7) and comparing the result with (2.11), we arrive at

$$\begin{aligned}\hat{V}_n(t)&=e^{i\hat{H}_0t/\hbar}\hat{v}_n(t)e^{-i\hat{H}_0t/\hbar}\\&=\hat{v}_n(t)+\sum_{r=1}^{\infty}\frac{(it/\hbar)^r}{r!}\hat{\Gamma}_r(n,t) .\end{aligned} \tag{2.6}$$

The expressions derived in this section will be used later in calculating the wave function.

III. RELATING THE WONG-FUNG CORRELATION OPERATOR $\hat{Q}_n$ TO THE INTERACTION HAMILTONIAN OPERATOR $\hat{V}_n(0)$

A. Interacting ground state obtained via the U-matrix theory

We first introduce the transformation operator

$$\hat{T}_{H_0}(\cdots)\equiv e^{i\hat{H}_0t/\hbar}(\cdots)e^{-i\hat{H}_0t/\hbar} . \tag{3.1}$$

It is easy to see that from (I2.9) and (I2.7) the Schrödinger equation in the interaction picture becomes

$$i\hbar\frac{\partial\Psi(t)}{\partial t}=S_w(t)[\hat{T}_{H_0}\hat{v}(t)]\Psi(t) , \tag{3.2}$$

where

$$\Psi(t)=e^{i\hat{H}_0t/\hbar}\Phi(t) \tag{3.3}$$

in which $\Phi(t)$ is the time-dependent wave function of the system in the Schrödinger picture and $\Psi(t)$ is obviously the wave function in the interaction picture.

We have already found[1] the solution to (3.2),

$$\Psi(t)=\hat{U}(t,t_0)\Psi(t_0) , \tag{3.4}$$

where

$$\hat{U}(t,t_0)=\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}S_w(t')[\hat{T}_{H_0}\hat{v}(t')]dt'\right]+\hat{\Delta}(t,t_0) \tag{3.5}$$

and

$$\hat{\Delta}(t,t_0)=\sum_{n=2}\frac{1}{n!}\sum_{r=0}^{n-2}(r+1)![\hat{U}_1(t,t_0)]^{n-(r+2)}\hat{B}_r(t,t_0) , \tag{3.6}$$

while

$$\hat{B}_r(t,t_0)=\sum_{j=0}^{r}\left[-\frac{i}{\hbar}\right]^j\int_{t_0}^{t}dt_1\,\hat{H}_1(t_1)\int_{t_0}^{t_1}dt_2\,\hat{H}_1(t_2)\times\cdots\times\int_{t_0}^{t_j}dt_{j+1}\,\hat{A}(t_{j+1},t_0)\hat{U}_{r-j}(t_{j+1},t_0) \tag{3.7}$$

and

$$\begin{aligned}\hat{A}(t_{j+1},t_0)=&\left[\int_{t_0}^{t_{j+1}}dt_{j+2}\hat{H}_1(t_{j+2})\right]\hat{H}_1(t_{j+1})\\&-\hat{H}_1(t_{j+1})\int_{t_0}^{t_{j+1}}\hat{H}_1(t_{j+2})dt_{j+2} ,\end{aligned} \tag{3.8}$$

with

$$\hat{H}_1(t)=S_w(t)e^{i\hat{H}_0t/\hbar}\hat{v}(t)e^{-i\hat{H}_0t/\hbar} \tag{3.9}$$

and

$$\hat{U}_n(t,t_0)=-\frac{i}{\hbar}\int_{t_0}^{t}dt'\,\hat{H}_1(t')\hat{U}_{n-1}(t',t_0)$$

with $\hat{U}_0(t',t_0)\equiv 1$. Then the explicit form of the wave function $\Phi(t)$ in the Schrödinger picture is, using the explicit expressions of $\hat{\Gamma}_r$ which have been given previously,

$$\begin{aligned}\Phi(t)&=e^{-i\hat{H}_0t/\hbar}\Psi(t)\\&=e^{-i\hat{H}_0t/\hbar}\left[\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}S_w(t')\hat{T}_{H_0}\hat{v}(t')dt'\right]+\hat{\Delta}(t,t_0)\right]e^{i\hat{H}_0t_0/\hbar}\Phi(t_0)\\&=e^{-i\hat{H}_0t/\hbar}\left[\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}\hat{g}_n(t,t_0)\right]+\hat{\Delta}(t,t_0)\right]e^{i\hat{H}_0t_0/\hbar}\Phi(t_0) ,\end{aligned} \tag{3.10}$$

while

$$\hat{g}_n(t,t_0)\equiv\int_{t_0}^{t}S_w(t')\left[\hat{v}_n(t')+\sum_{r=1}^{\infty}\frac{(it'/\hbar)^r}{r!}\hat{\Gamma}_r(n,t')\right]dt' . \tag{3.11}$$

We now express (3.10) as

$$\Phi(t)=e^{-i\hat{H}_0t/\hbar}\left[\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}\hat{g}_n(t,t_0)\right]+\hat{\Delta}(t,t_0)\right]e^{i\hat{H}_0t/\hbar}e^{-i\hat{H}_0(t-t_0)/\hbar}\Phi(t_0) \tag{3.12}$$

and we write the term involving $\hat{\Delta}(t,t_0)$ as

$$e^{-i\hat{H}_0 t/\hbar}\hat{\Delta}(t,t_0)e^{i\hat{H}_0 t/\hbar}e^{-i\hat{H}_0(t-t_0)/\hbar}\Phi(t_0)=\sum_{s=0}^{\infty}\frac{(-it/\hbar)^s}{s!}\hat{\mathscr{D}}_s(t,t_0)e^{-i\hat{H}_0(t-t_0)/\hbar}\Phi(t_0)\ , \tag{3.13}$$

where

$$\hat{\mathscr{D}}_s(t,t_0)=[\hat{H}_0,\hat{\Delta}(t,t_0)]_s\ . \tag{3.14}$$

If E_0 is the eigenvalue of $\hat{H}_0$, we can substitute (3.13) and (3.14) into (3.12), giving

$$\Phi(t)=e^{-iE_0(t-t_0)/\hbar}\left[\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}e^{-i\hat{H}_0 t/\hbar}\hat{g}_n(t,t_0)e^{i\hat{H}_0 t/\hbar}\right]+\sum_{s=0}^{\infty}\frac{(-it/\hbar)^s}{s!}\hat{\mathscr{D}}_s(t,t_0)\right]\Phi(t_0)\ , \tag{3.15a}$$

making use of the fact that

$$e^{-i\hat{H}_0 t/\hbar}\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}\hat{g}_n(t,t_0)\right]e^{i\hat{H}_0 t/\hbar}=\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}e^{-i\hat{H}_0 t/\hbar}\hat{g}_n(t,t_0)e^{i\hat{H}_0 t/\hbar}\right]\ . \tag{3.15b}$$

Now, we treat the He^4 system as a time-independent system, so we need only to know the solution of the Schrödinger equation up to the time $t=0$. So the wave function is

$$\Phi(0)=e^{-iE_0 b/\hbar}\left[\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}\hat{g}_n(0,-b)\right]+\hat{\Delta}(0,-b)\right]\Phi(-b) \tag{3.16}$$

when the perturbative Hamiltonian is suddenly turned on. Then

$$\Phi(0)=e^{-iE_0 b/\hbar}\left[\exp\left[-\frac{i}{\hbar}\sum_{n=2}^{N}\hat{g}_n(0,-b)\right]\right]\Phi(-b) \tag{3.17a}$$

is the *exact* form of the wave function of the system, since $\hat{\Delta}(0,-b)=0$.

When the switching process is not exactly sudden, as in the case of a liquid-helium system where interaction is due to exchange of phonons, $\hat{\Delta}(0,-b)$ in (3.16) is not equal to zero. However, for a weak perturbing Hamiltonian operator $\hat{v}(t)$ in the Schrödinger picture, the contribution $\hat{\Delta}(0,-b)$ to $\hat{U}(0,-b)$ is very small, and we can take the wave function to be

$$\Phi(0)\simeq e^{-iE_0 b/\hbar}\left[\exp\left[-\frac{i}{\hbar}\sum_{n=2}\hat{g}_n(0,-b)\right]\right]\Phi(-b)\ . \tag{3.17b}$$

Based on definition (3.11), we obtain using the mean value theorem

$$\hat{g}_n(0,-b)=\left[\int_{-\xi}^{0}S_w(t)dt\right]\times\left[\hat{v}_n(0)+\sum_{r=1}^{\infty}\frac{\left[\frac{i}{\hbar}0\right]}{r!}\hat{\Gamma}_r(n,0)\right]$$

$$=\hat{v}_n(0)\int_{-\xi}^{0}S_w(t)dt\ , \tag{3.18}$$

where ξ is a positive number satisfying $0<\xi<b$.

B. Relation between WF correlation operator $\hat{Q}_n$ and interaction operator $\hat{V}_n(0)$

We now turn to joining our U-matrix theory to the Wong-Fung theory. The first postulate of the WF theory states that the interacting ground state of the many-boson system is obtainable from the noninteracting ground state $|\phi_0\rangle$ via the operation of exp $(\hat{Q})$:

$$|\Phi_0\rangle=Ae^{\hat{Q}}|\phi_0\rangle\ , \tag{3.19}$$

where $\hat{Q}$ is the total n-particle correlation operator, expressible in the additive form

$$\hat{Q}=\hat{Q}_2+\hat{Q}_3+\cdots+\hat{Q}_N=\sum_{n=2}^{N}\hat{Q}_n \tag{3.20}$$

and

$$\hat{Q}_2=\frac{1}{2!}\sum_{i<j}\int u_2(r_{ij}=|\vec{x}_i-\vec{x}_j|)\hat{\psi}^*(\vec{x}_i)\hat{\psi}^*(\vec{x}_j)\times\hat{\psi}(\vec{x}_j)\hat{\psi}(\vec{x}_i)d^3x_i\,d^3x_j\ . \tag{3.21}$$

Similar expressions can be written for $\hat{Q}_3,\hat{Q}_4,\ldots$, where u_2 is the two-particle correlation function in the coordinate space. Obviously, $\hat{\psi}^*$ and $\hat{\psi}$ are, respectively, the usual creation and destruction free-boson field operators.

In a many-body system the particles distribute spacewise and momentumwise in a certain way, as we observe. The main cause of such a distribution is due to the behavior of each particle in the presence of the potential field and other fields (such as the long-range order electromagnetic field). In an electrically neutral, dense system like liquid helium, we expect the influence of the potential field of the particles on one another controls how the system would distribute in the way stated. In the presence of the fields due to other particles, the particles arrange themselves until a steady state is reached. In the language of the correlated-basis-function method, the wave func-

tion of a many-body problem is described or obtainable from the knowledge of the correlation function, of all orders in general. The "interacting wave function" of the CBF method is a description of the system after the steady state is reached. On the other hand, using the U-matrix formalism, the interacting potentials of various orders are turned on by a switching process. If this switching process bears a close resemblance to the transient behavior of the particles in their distributing towards the steady state, then the interacting wave functions of the Wong-Fung theory and the Lam-Fung theory are two definite, identical quantities. Under such a condition we can identify (3.17b) with (3.19), namely,

$$\Phi(0)\equiv|\Phi_0\rangle\ ,$$
$$\Phi(-b)\equiv|\phi_0\rangle\ . \tag{3.22}$$

We would emphasize again that although (3.21) is similar in form to (2.2), $\hat{v}_2$ (etc.) cannot be directly taken to be identical to $\hat{Q}_2$ (etc.). The weighting function in $\hat{v}_2$ is $v_2(r_{ij};t)$ which is one term of the perturbative Hamiltonian, while the weighting function in $\hat{Q}_2$ in $u_2(r_{ij}=|\vec{x}_i-\vec{x}_j|)$ is a two-particle correlation function—it measures indirectly the probability of finding one particle in $\vec{x}_j$ while the other is in $\vec{x}_i$. Combining (3.17b) and (3.19), we arrive at the following identifications:

$$A=e^{-iE_0b/\hbar}\ , \tag{3.23}$$

$$\hat{Q}=\sum_{n=2}^{N}\hat{Q}_n=-\frac{i}{\hbar}\sum_{n=2}^{N}\hat{g}_n(0,-b)\ . \tag{3.24}$$

Substituting (3.18) back into (3.24),

$$\hat{Q}_n=-\frac{i}{\hbar}\hat{g}_n(0,-b)=-\frac{i}{\hbar}\hat{v}_n(0)\int_{-\xi}^{0}S_w(t)dt\ . \tag{3.25}$$

Comparing (3.21) and (3.25), we obtain right away

$$u_2(r_{ij})=-\frac{i}{\hbar}\left[\int_{-\xi}^{0}S_w(t)dt\right]v_2(r_{ij};0)\ . \tag{3.26}$$

Similar expressions can be established between the higher-order relevant functions.

IV. BRIDGE BETWEEN THE PAIR-CORRELATION FUNCTION AND THE TWO-PARTICLE POTENTIAL FUNCTION OF A LIQUID-HELIUM SYSTEM

Based on x-ray and neutron scattering experiments[9–12,18] we can obtain a rather accurate plot of the liquid-structure function $S_2(k)$ in momentum space. In this investigation, we base our study on the neutron scattering experiment of Henshaw.[12] As the incident beam is very narrow and the scattered beam has a rather definite direction, we can take that the scattering process results mainly from two-particle interaction. In other words, to the lowest order of approximation, we assume that what was measured was the two-particle liquid-structure function $S_2(\vec{k})$, which is related to the radial distribution function $g_2(\vec{r})$ by[19,20]

$$S_2(\vec{k})-1=\rho\int d^3r\,e^{i\vec{k}\cdot\vec{r}}[g_2(\vec{r})-1]\ , \tag{4.1}$$

where ρ is the number density of the liquid-helium system. After an inverse Fourier transform, we obtain

$$g_2(\vec{r})=1+\frac{1}{\rho}\int\frac{d^3k}{(2\pi)^3}e^{-i\vec{k}\cdot\vec{r}}[S_2(\vec{k})-1]\ . \tag{4.2}$$

The form of $g_2(\vec{r})$ is rather well known and we show in Fig. 1 such a plot, where the radial distance is treated as a scalar, normalized by the unit $\sigma=2.556\times10^{-10}$ m, which is the radial distance at which the Lennard-Jones potential is zero. As $g_2(r)$ is to be related to the pair correlation function $u_2(r)$ while $u_2(r)$ and $v_2(r)$ are already approximately related, the $g_2(r)-r$ graph is considered to be the experimental data.

We shall use curve-fitting techniques to find a representative expression for $g_2(r)$. We first carry out a Laplace transform L on $g_2(G=Lg_2)$ and express G as a series of resonance terms. Then we take an inverse transform of G, arriving at

$$g_t\left[\frac{r+r_0}{\sigma}\right]=l\left[\frac{r}{\sigma}\right]+\alpha\left[\alpha_{12}+\frac{r}{\sigma}\right]^{-7}\exp\left\{-\alpha_{11}\left[\left[\alpha_{12}+\frac{r}{\sigma}\right]^{-12}-\left[\alpha_{12}+\frac{r}{\sigma}\right]\right]\right\}, \tag{4.3}$$

where

$$l(r)=1+\alpha-\alpha_0e^{-\alpha_1r}-[\alpha_2\sin(\alpha_3r)+\alpha_4\cos(\alpha_3r)]\times e^{-\alpha_5r}+\alpha_6re^{-\alpha_7r}+\alpha_8r^2e^{-\alpha_9r} \tag{4.4}$$

and the coefficients $\alpha,\alpha_0,\alpha_1,\ldots$ are given by set B of Table I as an example. As $g_t=0$ for $r<r_0$, in order to fit the experimental curve, the variable of g_t is $(r+r_0)/\sigma$ where σ is the normalization constant.

We would remark that the BDJ type of trial wave function for a many-boson system including only pair correlation is expressed as

$$\Phi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)=\prod_{i<j}^{N}\exp[\tfrac{1}{2}u(r_{ij})]$$
$$=\exp\left[\tfrac{1}{2}\sum_{i<j}u(r_{ij})\right]\ . \tag{4.5}$$

This form of the interacting wave function is shown to be true for a many-boson system if only pair correlation is considered.[2] In view of the fact that the radial distribution function is defined[19] as

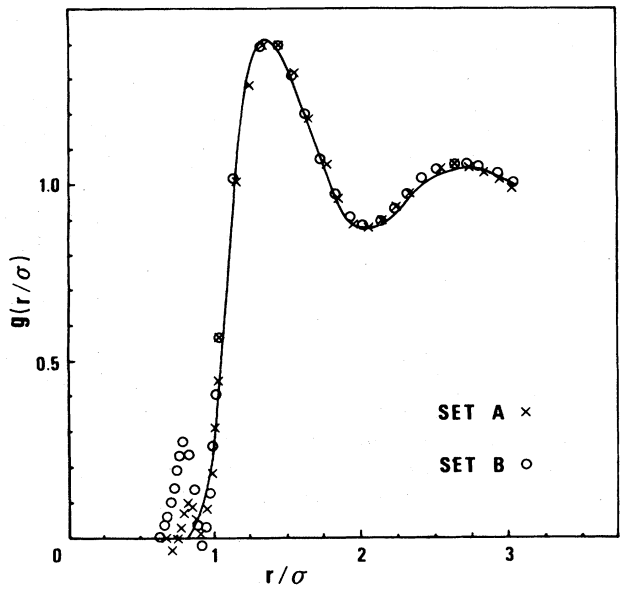

FIG. 1. Variation of the radial distribution function $g_2(r/\sigma)$ as a function of r/σ. The solid line indicates the neutron scattering experimental result of Henshaw (Ref. 12). We fit this curve by the stated curve-fitting techniques and two sets of coefficients from Table I: set A, $\times$; set B, $\circ$.

TABLE I. Parameters for fitting the radial distribution function.

Parameters	Set A	Set B
α	$1.720\,45\times10^{-38}$	$2.646\,84\times10^{-38}$
α_0	0.35	0.35
α_1	5.443 31	8.855 729
α_2	0.87	0.66
α_3	288	279
α_4	0.65	0.65
α_5	1.4636	1.3395
α_6	0.425	0.425
α_7	4.00	3.75
α_8	4.5	4.5
α_9	4.8	4.5
α_{10}	−0.26	−0.40
α_{11}	4.0	4.0
α_{12}	0.759 63	0.759 63
r_0/σ	0.6625	0.6425
Δ/σ	0.097 13	0.117 13

$$g_2(r_{12}=|\vec{r}_1-\vec{r}_2|) = \frac{N!}{(N-2)!\rho^2}\frac{\int d\vec{r}_3\cdots d\vec{r}_N\,|\Phi(\vec{r}_1,\ldots,\vec{r}_N)|^2}{\langle\Phi|\Phi\rangle}, \tag{4.6a}$$

it is easy to see from (4.5) and (4.6a) that we can write $g_2(r_{12})$ as

$$g_t(r_{12}/\sigma)=e^{u_2(r_{12}/\sigma)}f(r_{12}/\sigma), \tag{4.6b}$$

where $f(r_{12}/\sigma)$ is an algebraic function. In our analysis we have used $g_t(r/\sigma)$ to represent $g_2(r/\sigma)$. Clearly, to the order of approximation used in the curve-fitting process, inspection of (4.3) and (4.6a) gives

$$u_2(r/\sigma)=-\alpha_{11}\left[\frac{1}{\left[\frac{r+\Delta}{\sigma}\right]^{12}}-\frac{1}{\left[\frac{r+\Delta}{\sigma}\right]^{6}}\right], \tag{4.7}$$

$$\alpha_{11}=4.0$$

$$f(r/\sigma)=\Theta((r-r_0)/\sigma)g_0\left[\frac{r-r_0}{\sigma}\right] \tag{4.8}$$

in which

$$g_0(r/\sigma)=\left\{l(r/\sigma)+\alpha\left[\alpha_{12}+\frac{r}{\sigma}\right]^{-7}\exp\left\{-\alpha_{11}\left[\left[\alpha_{12}+\frac{r}{\sigma}\right]^{-12}-\left[\alpha_{12}+\frac{r}{\sigma}\right]\right]\right\}\right\}$$
$$\times\exp\left[\alpha_{11}\left[\frac{1}{\left[\alpha_{12}+\frac{r}{\sigma}\right]^{12}}-\frac{1}{\left[\alpha_{12}+\frac{r}{\sigma}\right]^{6}}\right]\right] \tag{4.9}$$

and the parameter Δ is given by

$$\Delta/\sigma=\alpha_{12}-r_0/\sigma, \tag{4.10}$$

while Θ is a step function, defined by

$$\Theta((r-r_0)/\sigma)=\begin{cases}1 & \text{for } r>r_0\\ 0 & \text{for } r\le r_0\end{cases} \tag{4.11}$$

in order to take care of the fact that the radial distribution function deduced experimentally starts from $r/\sigma=r_0/\sigma$ (Fig. 2). Thus once we find a set of parameters α, $\alpha_0,\alpha_1,\ldots$ (like set B in Table I) for a good fitting of $g_2(r/\sigma)$, we arrive at an explicit expression u_2 as a function of r, given by (4.7). In Fig. 2 we also plot the function $f(r/\sigma)$ versus r/σ.

V. SWITCHING PROCESS AND THE TWO-PARTICLE POTENTIAL FUNCTION

We now need to specify the integral

$$I=\int_{-\xi}^{0}S_w(t)dt \tag{5.1}$$

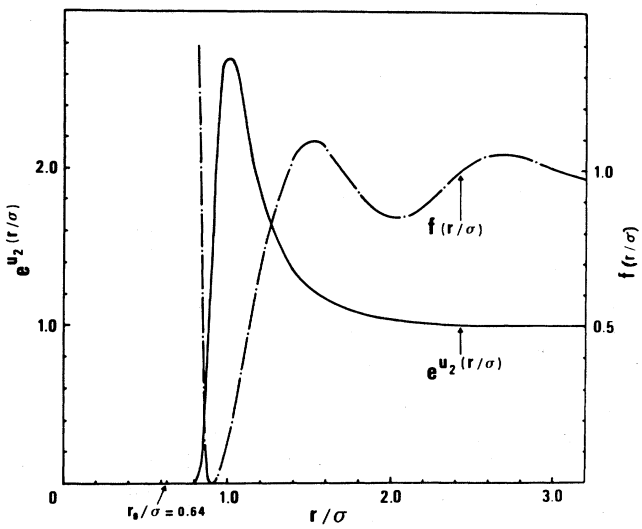

FIG. 2. Features of the functions $\exp[u_2(r/\sigma)]$ and $f(r/\sigma)$. u_2 is given by (4.7). Note that $\exp u_2 = 0$ when $r = r_0$. In fact $\exp u_2$ is very close to zero for $r_0 < r < 0.785$.

in Eq. (3.26) before we can deduce our potential v_2 as a final goal of this investigation.

In analyzing relation (3.26) we notice that the imaginary number i appears. If we express $u_2(r_{ij})$ as the sum of the real and imaginary parts, then the real part vanishes and the imaginary part

$$u_I(r_{ij}) = -\frac{1}{\hbar}\left[\int_{-\xi}^{0} S_w(t)dt\right] v_2(r_{ij};0) \ .$$

In other words, $u_I(r_{ij})$ must be equal to the $u_2(r_{ij})$ given in the Eq. (4.6b). Therefore $u_2(r_{ij})$ and $v_2(r_{ij};0)$ differ generally by a negative sign, apart from a certain shift in scale, which we know is due to the contribution of the switching integral (5.1)

$$u_2(r_{ij}) = -\frac{1}{\hbar}\left[\int_{-\xi}^{0} S_w(t)dt\right] v_2(r_{ij}) \ , \tag{5.2}$$

where the zero in $v_2(r_{ij};0)$ has been omitted for simplicity.

For numerical evaluation, we propose a model for the switching function $S_w(t)$. In the spirit of the new U-matrix theory, the switching function introduces the interaction Hamiltonian in a certain time interval (which could be zero, if the switching process is sudden). Suppose we express $S_w(t)$ as a "gradual model" first, and let other physical conditions decide the more specific nature of the switching process. More precisely, we propose to write $S_w(t)$ as

$$S_w(t) = \exp\left[-\gamma\left[\frac{b}{b+t} - 1\right]\right] , \tag{5.3}$$

where $(-b)$ refers to the time when the interaction Hamiltonian starts to be introduced and γ is a parameter specifying the gradual degree of switching to be determined later. In Fig. 3 we show that variation of $S_w(t)$ as a function of normalized time t/b, for γ is either large or small, the switching process becomes more "sudden."

Based on (5.3), (5.1) has the explicit form

$$I(b,\xi,\gamma) = b - (b-\xi)\exp\left[-\gamma\left[\frac{\xi}{b-\xi}\right]\right] + b\gamma e^{\gamma}\left\{\ln\left[\frac{b-\xi}{b}\right] + \sum_{n=1}^{\infty}\frac{1}{n!n}(-\gamma)^n + \left[-\left[\frac{b}{b-\xi}\right]^n\right]\right\} . \tag{5.4}$$

In view of (4.7) we plot $u_2(r)$ as function of r (Fig. 4) in units of the parameter σ, which represents the value of r at which the Lennard-Jones potential is just zero, so that the dotted line crosses the r axis at the value 1σ. Now, we need to consider some subtle physical ideas before we can calculate I. First, we note that the potential function $v_2 = -(\hbar/I)u_2$. The correlation function is dimensionless, while the integral I has the dimension of time. For convenience in discussion, we normalize the integral I by the SI (Systéme Internationale) value of $\hbar$, but in seconds; namely, we set $I = 1.0546 \times 10^{-34}$ s so that $v_2 = -u_2$. Using such a value of I, we plot in Fig. 4 the potential function v_2 versus r (in units of σ). We would emphasize that whatever value of I we come to later, it only affects the scale of v_2, but does not affect the points where v_2 is minimum or when v_2 is zero. In our deduced potential function, the minimum of v_2, or its depth, is specified by $r/\sigma = 1.005$, corresponding to OP in Fig. 5. For $v_2 = 0$, $r/\sigma = d_{hc}/\sigma = 1 - \Delta/\sigma = 0.883$ [see Eq. (4.7) and Table I for value of Δ]. We have used the subscript hc to indicate that d_{hc} can be taken to represent the hard-core diameter. The absolute value of the hard-core radius deduced here is $r_{hc} = 1.1282$ Å.

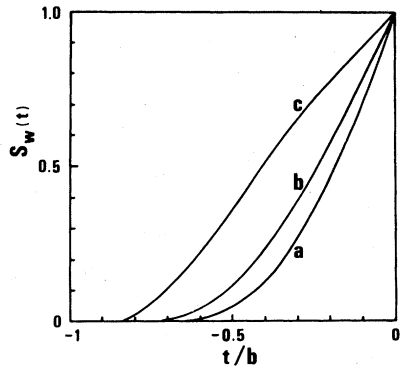

FIG. 3. The variation of the switching function $S_w(t)$ as a function of normalized time t/b, for (a) $\gamma = 3.0$, (b) $\gamma = 2.164$, and (c) $\gamma = 1.0$.

Now consider a helium atom at O as shown in Fig. 5. When another helium atom is in the vicinity of the potential of the first atom it experiences a force. We assume that the interaction among two atoms can be described by phonon interaction between the centers of the atoms. In other words, we take the view that if a phonon travels with the speed v_g in the liquid-helium system, the time taken for an atom to receive a "complete message" of interaction is given by $t = R/v_g$, where R is the center-to-center distance.

For convenience of quantitative analysis we transform the time parameter b [in Eq. (5.3)] according to

$$\beta = b \Big/ \left[\frac{\sigma}{v_g} \right] \tag{5.5}$$

and the characteristic time scale ξ in (5.4) according to

$$\zeta = \xi \Big/ \left[\frac{\sigma}{v_g} \right] \tag{5.6}$$

so that

$$I = \int_{-\xi}^{0} S_w(t)dt = \alpha(\beta,\zeta,\gamma)\frac{\sigma}{v_g} , \tag{5.7}$$

where β, ζ, and γ are all dimensionless parameters, and

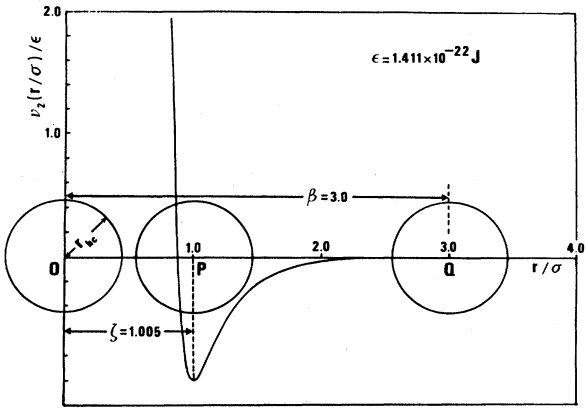

FIG. 5. Schematic representation of the interaction between two helium atoms, in which the two-particle potential function v_2 has been normalized, i.e., $v_2 = -u_2$, where v_2 is expressed in units of J.

$$\alpha(\beta,\zeta,\gamma) = \beta - (\beta-\zeta)\exp\left[-\gamma\left[\frac{\zeta}{\beta-\zeta}\right]\right] + \gamma\beta e^{\gamma}\left\{\ln\left[\frac{\beta-\zeta}{\beta}\right] + \sum_{n=1}^{\infty}\frac{1}{n!n}(-\gamma)^n\left[1-\left[\frac{\beta}{\beta-\zeta}\right]^n\right]\right\} . \tag{5.8}$$

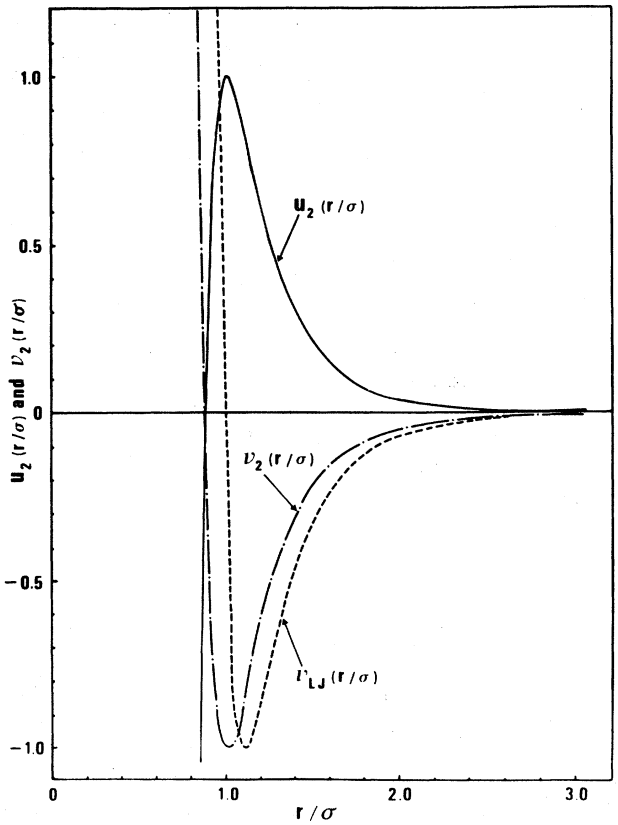

FIG. 4. Variation of the pair correlation function $u_2(r/\sigma)$ —— and the normalized two-particle potential $v_2(r/\sigma)$ —·—·— with normalized radial distance r/σ. Here $\sigma = 2.556\times10^{-10}$ m. u_2 is given by Eq. (4.7) and $v_2 = -u_2(\hbar/I) = -u_2$, where the integral I is taken to be 1.0546×10^{-34} s. For comparison, the normalized Lennard-Jones potential v_{LJ}/ϵ is also plotted — — — with $\epsilon = 1.411\times10^{-22}$ J.

Thus $\alpha(\sigma/v_g)$ represents the time taken by a phonon to travel a distance $\alpha\sigma$. In Fig. 5, when $\beta=3$, we assume that the "test atom" at Q begins to "feel" the interaction due to the atom at the origin.[21] As the potential is attractive until $v_2=0$, the test atom approaches towards 0. When the center of the test atom is at d_{hc}/σ, the "hard cores" of the two atoms touch. Then the second atom will be pushed back due to the repulsive force. The second atom will oscillate in the potential well and eventually arrives at an equilibrium position, where the center coincides with the point P. In describing phonon interaction, we do not assume, of course, that the phonon "passes through" the helium atom to its center, but we take the physical picture that it takes time for an atom to absorb a phonon and vibrates as it does so, and a rough estimation of the center-to-center interaction time is given by

$$\xi = \frac{OP}{v_g} = 1.005\frac{\sigma}{v_g} . \tag{5.9}$$

To have an idea of how the function $\alpha(\beta,\zeta,\gamma)$ in (5.7) behaves with respect to the dimensionless parameter β, we plot the α-β graph for three values of $\gamma = 1.0$, 1.868 and 3.0 in Fig. 6(a) using our potential $v_2 = -(\hbar/I)u_2$. For comparison we also plot the α-β graph Fig. 6(b) using the Lennard-Jones potential. Note that when the potential model changes, the value of ξ changes accordingly. Using our potential, $\xi = 1.005(\sigma/v_g)$, while using the Lennard-Jones potential, $\xi = 1.1225(\sigma/v_g)$.

Suppose before interaction, the system has energy E_0. According to the uncertainty principle in quantum mechanics, if we take the measurement of energy of a quantum system in a time interval $\Delta t = \alpha(\sigma/v_g)$ [see (5.7)], then the uncertainty in the measurement of energy of the final state (namely, the state including interaction) of the system would be $\Delta E \approx E_0 + \epsilon - E_0 = \epsilon$, where ϵ represents the depth of the potential well. While we need

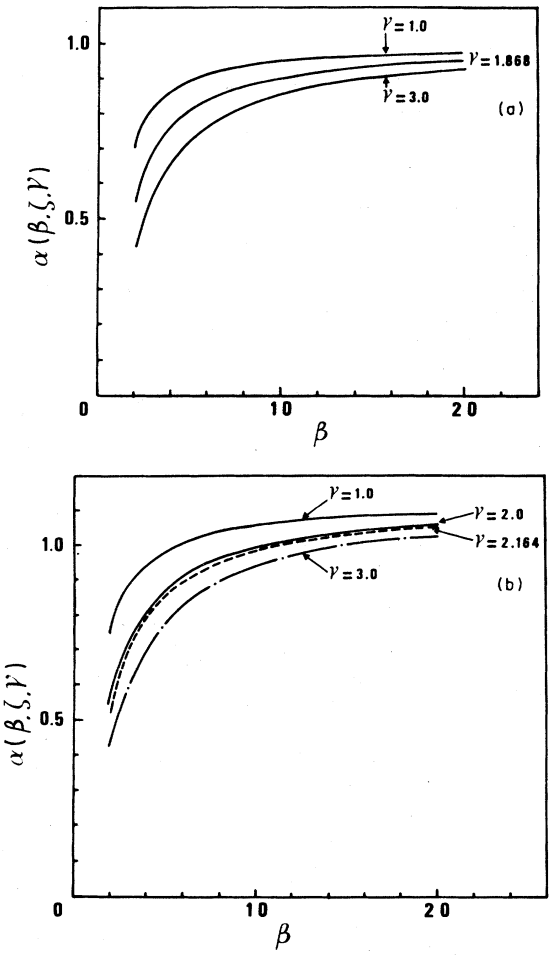

FIG. 6. (a) A plot of $\alpha(\beta,\xi,\gamma)$ vs β for our deduced two-particle potential function and some different values of the parameter γ as indicated. (b) A plot of $\alpha(\beta,\xi,\gamma)$ vs β for the Lennard-Jones potential function and some different values of the parameter γ.

the value of the switching integral I to find the depth of our potential well, we, however, need the value of ϵ to evaluate I. For the purpose of estimation, ϵ is taken tentatively to be that of the Lennard-Jones potential. The "deduced" depth can then be compared to the *ad hoc* estimated depth afterwards. Thus we take[20,22]

$$\Delta E \approx \epsilon = 1.411 \times 10^{-22}\ \text{J}\ ,$$

$$v_g = 237\ \text{m s}^{-1}\ .$$

By the uncertainty principle,

$$\Delta E\, \Delta t \geq \hbar$$

or

$$\epsilon\alpha \frac{\sigma}{v_g} \geq \hbar\ . \tag{5.10}$$

Taking the lower bound, we get

$$\alpha = 0.6930\ . \tag{5.11}$$

So far we have taking γ as a parameter. Since we have already estimated α above, we can plot a graph of α versus γ in Fig. 7(a) for our potential. From Figs. 7(a) and 7(b), we estimate that the value of γ for our potential is 1.868 and that for the Lennard-Jones potential it is 2.164, respectively.

Finally, in view of relation (4.7) and (5.2), the deduced potential is given by

$$v_2(r/\sigma) = -\frac{\hbar}{\alpha(\sigma/v_g)} u_2(r/\sigma)$$

$$= 4.0 \times \epsilon \left[\left[\frac{r+\Delta}{\sigma} \right]^{12} - \left[\frac{r+\Delta}{\sigma} \right]^{-6} \right]\ . \tag{5.12}$$

A comparison of our deduced potential to the Lennard-Jones potential is given in Fig. 4. It is interesting to note that these two potential functions have similar forms, and they differ only in the small-r range. The normalized depth of our "deduced" potential is also the same as that of the Lennard-Jones potential. There are two more interesting features: our potential is softer and it does *not* diverge at $r=0$. The last feature enables us to carry out Fourier transformation on v_2 (and also u_2), and such a

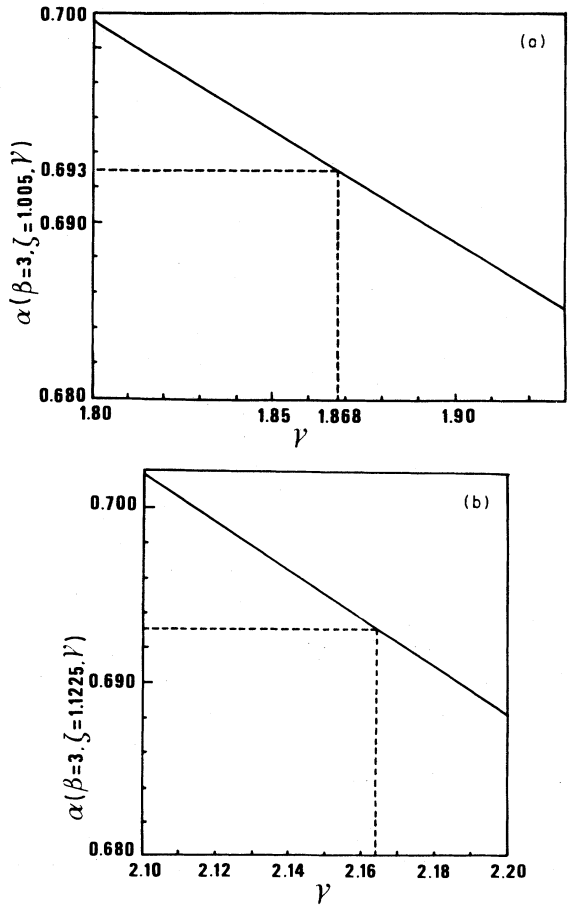

FIG. 7. (a) The variation of $\alpha(\beta=3,\xi,\gamma)$ vs γ for our deduced two-particle potential function. From this figure we obtain $\gamma=1.868$, which corresponds to $\alpha=0.6930$. (b) The variation of $\alpha(\beta=3,\xi,\gamma)$ vs γ for the Lennard-Jones potential function. From this figure $\alpha=0.6930$ corresponds to $\gamma=2.164$.

procedure is important in analyzing a dense helium system.

VI. CONCLUSION

In this investigation we have applied the U-matrix theory to a many-boson system, and established the correspondency between the correlation functions and the interaction potential functions. We would like to remark on the following main features of our study.

(1) We consider that in a neutral dense system like a liquid-helium system, the characteristics of the potential around each particle determine what a physical state the many-body system would correlate and settle in after a transient period of interaction. Based on this basic concept, the interaction wave function of a many-body system resulting from our new U-matrix theory is identified as the same wave function, including effects of correlations in the Wong-Fung many-body theory. Consequently, we have found that the pair correlation operator $\hat{Q}_2$ and pair correlation function $u_2(r_{ij})$ are simply related to the two-particle interaction potential operator $\hat{v}_2(t)$ and two-particle potential function $v_2(r_{ij};t)$, respectively, by

$$\begin{aligned}\hat{Q}_2 &= -\frac{i}{\hbar}\hat{g}_2(0,-b) \\ &= -\frac{i}{\hbar}\int_{-b}^{0} S_w(t)\left[\hat{v}_2(t)+\sum_{r=1}^{\infty}\frac{(it/\hbar)^r}{r!}\hat{\Gamma}_r(2,t)\right]dt \\ &= -\frac{i}{\hbar}\left[\int_{-\xi}^{0} S_w(t)dt\right]\hat{v}_2(0)\end{aligned}$$

and

$$u_2(r_{ij}) = -\frac{1}{\hbar}\left[\int_{-\xi}^{0} S_w(t)dt\right]v_2(r_{ij}) ,$$

where $(-b)$ specifies the "starting time" of the interaction and ξ is a characteristic time parameter for the two-particle interaction potential.

(2) Based on experimental data on the liquid-structure function $S(k)$ and an inverse Fourier transform of $S(k)$, one can obtain the experimental two-particle radial distribution function $g_2(r)$. In order to facilitate a more thorough investigation, we have used curve-fitting techniques to deduce a mathematical expression [namely, $g_t(r)$] to represent $g_2(r)$. According to the definition of $g_2(r)$ given in (4.6a), and the form of the Wong-Fung wave function including only pair correlation (to this order, this is identical to the BDJ trial wave function) given in (4.5), we know that $g_2(r)$ can be written in the form

$$g_2(r/\sigma) = e^{u_2(r/\sigma)} f(r/\sigma) .$$

Comparing $g_t(r/\sigma)$ with $g_2(r/\sigma)$, we deduce that the pair correlation function has the form

$$u_2(r/\sigma) = -\alpha_{11}\left[\left(\frac{r+\Delta}{\sigma}\right)^{-12} - \left(\frac{r+\Delta}{\sigma}\right)^{-6}\right] ,$$

where

$$\alpha_{11} = 4.0 .$$

Here we would note two significant aspects of this u_2.

(i) Our deduced pair correlation function gives the same asymptotic approach as that of the pair correlation function model previously used[23–27] for $r\to\infty$. However, for $r\to 0$, our pair correlation function tends to a very large negative value, but still finite, whereas the previous models tend to infinity. This last property of our pair correlation function makes it Fourier transformable.

(ii) The form of our deduced pair correlation function is rather similar to that used in Refs. 26 and 27, but reverse in sign.

(3) We have proposed a model for the switching process, described by

$$S_w(t) = \exp\left[-\gamma\left[\frac{b}{b+t}-1\right]\right] ,$$

where γ is a parameter specifying the gradual degree of switching on the interaction Hamiltonian, and $(-b)$ refers to the time when the interaction starts to be introduced. The effective integral of the switching function $S_w(t)$, i.e.,

$$\begin{aligned}I &= \int_{-\xi}^{0} S_w(t)dt \\ &= \int_{-\xi}^{0}\exp\left[-\gamma\left[\frac{b}{b+t}-1\right]\right]dt\end{aligned}$$

serves as a bridge between the interaction-potential function and the correlation function. We assume, as an estimate that the test particle begins to be influenced by the source particle when the center-to-center distance is 3σ, implying that we have to take $\beta=3.0$ in (5.5). Consequently, the parameter b in the switching integral is $b=\beta\sigma/v_g$.

The distance between the origin and the point corresponding to the minimum of the potential is $\zeta=OP/\sigma=1.005$ (Fig. 6). Taking the uncertainty in energy measurement to be equal to ϵ, the depth of the LJ potential as an estimate, we have determined the function $\alpha(\beta=3,\zeta=1.005,\gamma)$ in (5.10) which is 0.693. Then we have found out that for $\alpha=0.693$, $\gamma=1.868$. We have thus specified all the parameters in the switching process. We would emphasize that if we only know the value of integral I, we can determine the depth of the potential. Therefore we can use our deduced pair correlation function to find the two-particle interaction potential, which has been shown to be similar in form to that of the Lennard-Jones potential, has the same depth ϵ.

It is interesting to remark, however, that the hard-core diameter according to the deduced potential is $d_{hc}=2r_{hc}=0.8836=2.257$ Å, slightly smaller than that obtained from the Lennard-Jones potential, which is equal to $d_{hc}(\mathrm{LJ})=1\sigma=2.556$ Å.

(4) It appears that the U-matrix theory works in a many-boson system as well. Previously, different models for the pair correlation function and the potential func-

tion have to be used separately in order to calculate the relevant physical quantities. It seems that correlation functions and the potential functions were treated as if ar ing from different physical sources in the past. The application of U-matrix theory reported here appears to indicate that we have opened the door for the study of potential function around a particle much more directly.

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