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Maximum-overlap Jastrow wave function for liquid ^{4}He

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The maximum-overlap Jastrow wave function is computed for real liquid ^{4}He and for a model Bose fluid interacting with a realistic pair potential, the so-called HFDHE2 one. We propose a method for obtaining information on the interparticle interaction starting from the radial distribution function $g(r)$ and maximum-overlap Jastrow wave function. The method is tested by use of the results for the Lennard-Jones and HFDHE2 systems.

I. INTRODUCTION

The variational method based on minimization of the expectation value of the Hamiltonian is a standard approach to the study of dense quantum fluids such as the helium liquids. Complementary to this, another variational principle has been recently applied to quantum fluids,[1,2] one based on the maximization of the overlap integral $\langle \psi_{\mathrm{mod}} \mid \psi_0 \rangle$ between the exact ground state ψ_0 and a model wave function ψ_{mod}. The extremum condition leads to a certain equality between correlation functions, the simplest of which is the radial distribution function (RDF) $g(r)$ of the system and of the model.

Use of a second variational principle is justified by two main reasons. First, a variational wave function is interesting not only for the computation of the quantity on which the variational principle is based, the energy, for instance, but as the starting point for computation of other observables of the system, such as the momentum distribution or the correlation functions. Comparison of such quantities derived from different variational principles gives an indication of how good the family of trial wave functions used is. Second, the variational principle based on $\langle \psi_{\mathrm{mod}} \mid \psi_0 \rangle$ requires, in a certain approximation, only knowledge of the true $g(r)$ of the fluid and this can be obtained from the experimentally known structure factor $S(q)$. No assumption is needed for the form of the Hamiltonian of the system. This opens the possibility that from the maximum-overlap computation we can obtain information on the interatomic interaction.

In this paper we study the case of Bose fluids, for which it is known[3] that a Jastrow function

$$\psi_J(\{\mathbf{r}_i\} \mid u) = \prod_{i<j} e^{-u(r_{ij})/2} \tag{1}$$

represents a rather good approximation of the ground state when the Jastrow pseudopotential $u(r)$ has been suitably chosen. We compute the maximum-overlap Jastrow pseudopotential $\bar{u}(r)$ for liquid Helium starting from both the experimental $S(q)$ and from the $g(r)$ obtained from exact simulations[4,5] of a Bose fluid interacting with a realistic pair potential, the so-called HFDHE2.[6]

It is clear that the Jastrow pseudopotential mirrors, in a certain way, the interatomic potential. In the ideal gas $u(r)=1$ and deviations from unity are caused by the interaction. In a dense fluid, as in liquid helium, many particle effects are important and it is known that certain features, such as the long-range tail of $u(r)$, are specifically related to collective effects. On the other hand, energy-variational computations[7,8] give good evidence that the short-range structure of $u(r)$ is dominated by two-body effects through the interatomic interaction. Suppose we have two quantum fluids, A and B, which have a slightly different interaction. Since the collective effects should be very similar in the two systems when the density is the same, we can expect that the difference $u_A - u_B$ between the two Jastrow pseudopotentials reflects essentially the difference $v_A - v_B$ between the two interatomic potentials. The observation is not very useful if u_A and u_B are derived from an energy computation, since this requires already the knowledge of the potentials. The situation is different if u_A and u_B are obtained from a maximum-overlap computation which requires as input only the radial distribution functions g_A and g_B. Then, if for the A system we know *both* v_A and g_A but for the B system only g_B, there is the possibility of obtaining information on $v_B - v_A$ from $u_B - u_A$. In this paper we test this idea using two maximum-overlap pseudopotentials; the first is the one we obtain here for the model Bose fluid interacting with the accurate HFDHE2 pair potential for ^{4}He and the second is the $u(r)$ already computed[2] for a Lennard-Jonnes (LJ) Bose fluid.

The contents of the paper are the following. In Sec. II we discuss our method for obtaining the maximum-overlap pseudopotential starting from a given RDF $g(r)$. In Secs. III and IV we present the results for a Bose fluid interacting with the HFDHE2 potential and for liquid ^{4}He, respectively. In Sec. V we investigate to what extent the difference between the pseudopotentials for the HFDHE2 and Lennard-Jones potentials reflects the difference of the relative pair interactions. Our conclusions are contained in Sec. VI.

II. MAXIMUM-OVERLAP JASTROW PSEUDOPOTENTIAL

It was shown by one of us[1] that the normalized Jastrow function $\psi_J(\{r_i\} \mid u)$ which has the maximum overlap with the exact ground state ψ_0 of a Bose fluid is obtained from that pseudopotential, which we call $\bar{u}(r)$, for which

$$g_0(r)=g_{\mathrm{mxd}}(r \mid \bar{u}) \ . \tag{2}$$

$g_0(r)$ is the RDF corresponding to the probability distribution ψ_0^2, and $g_{\mathrm{mxd}}(r \mid \bar{u})$ is the RDF corresponding to the suitably normalized product $\psi_0\psi_J(\bar{u})$. It has been verified empirically[3] on the basis of Green-function Monte Carlo (GFMC) computations that a Jastrow function is closed enough to ψ_0 that the difference ψ_0-ψ_J can be treated as a perturbation to linear order. In this case[3]

$$g_0(r)=2g_{\mathrm{mxd}}(r \mid u)-g_J(r \mid u) \ . \tag{3}$$

$g_J(r)$ is the RDF corresponding to $\psi_J^2(u)$. Use of this relation in (2) gives the approximate maximum-overlap condition

$$g_0(r)=g_J(r \mid \bar{u}) \ , \tag{4}$$

i.e., $\bar{u}(r)$ is such that it leads to a RDF which coincides with the exact one. Formally, this is equivalent to the solution of the so-called inverse problem for *classical* fluids, i.e., the determination of the pair interaction which reproduces a given RDF. This equivalence simply follows from the identity of $\psi_J^2(\{r_i\} \mid u)$, with the probability distribution in configuration space of classical particles at temperature T interacting with a pair potential $v^*(r)=k_B T u(r)$, where T is an arbitrary temperature.

In paper I (Ref. 2) we solved the functional equation (4) with an iterative predictor-corrector method. For the predictor[1] we used either the random-phase approximation (RPA) or the modified hypernetted-chain (MHNC) equation. The RPA states that, given a pseudopotential $u^{(0)}$,

$$\delta c(r) \equiv c_J(r \mid u^{(0)}+\delta u)-c_J(r \mid u^{(0)})=-\delta u(r) \ , \tag{5}$$

where $c_J(r \mid u^{(0)})$ is the Ornstein-Zernike (OZ) direct correlation function corresponding to $g_J(r \mid u^{(0)})$, and $\delta u(r)$ is an arbitrary (small) variation of the pseudopotential. Use of (5) with $\delta u=\bar{u}-u^{(0)}$ with the OZ relation

$$g(r)-1=c(r)+\rho\int d^3r' c(r')[g(\mid \mathbf{r}-\mathbf{r}' \mid)-1] \ ,$$

and use of (4) leads to the RPA result

$$\bar{u}_{\mathrm{RPA}}(r)=u^{(0)}(r) + \frac{1}{\rho(2\pi)^3}\int d^3k\, e^{i\mathbf{k}\cdot\mathbf{r}}[S_J^{-1}(k \mid u^{(0)})-S_0^{-1}(k)] \ . \tag{6}$$

$S(k)$ is the structure factor

$$S(k)=1+\rho\int d^3r\, e^{i\mathbf{k}\cdot\mathbf{r}}[g(r)-1] \tag{7}$$

corresponding to any chosen $g(r)$. The RPA, in general, is a reasonable but not very accurate approximation, so that (6) is not taken as the final prediction of u. Instead, (6), which now we call $\bar{u}^{(1)}$, is used only as a first estimate of $\bar{u}$. With this pseudopotential $\bar{u}^{(1)}$, we compute the "exact" RDF with a Monte Carlo simulation. Then (5) can be used again, with $\bar{u}^{(1)}$ replacing $u^{(0)}$, and the scheme can be repeated, giving

$$\bar{u}^{(i)}(r)=\bar{u}^{(i-1)}(r)+\delta_{\mathrm{RPA}}^{(i)}(r) \ , \tag{8}$$

where

$$\delta_{\mathrm{RPA}}^{(i)}(r)=\frac{1}{\rho(2\pi)^3} \times \int d^3k\, e^{i\mathbf{k}\cdot\mathbf{r}}[S_J^{-1}(k \mid \bar{u}^{(i-1)})-S_0^{-1}(k)] \ . \tag{9}$$

The MHNC equation (Ref. 9) states that the so-called bridge function $E(r \mid u)$ remains unchanged for small variations of $u(r)$ and this leads to

$$\bar{u}^{(i)}(r)=\bar{u}^{(i-1)}(r)+\delta_{\mathrm{MHNC}}^{(i)}(r) \ , \tag{10}$$

$$\delta_{\mathrm{MHNC}}^{(i)}(r)=\delta_{\mathrm{RPA}}^{(i)}+\ln[g_J(r \mid k^{(i-1)})/g_0(r)] +g_J(r \mid u^{(i-1)})-g_0(r) \ , \tag{11}$$

where $\delta_{\mathrm{RPA}}^{(i)}$ is the same functional form as in (9).

A typical computation proceed as follows. As starting $u^{(0)}$ we take a pseudopotential obtained from some previous variational computation of the energy for a pair interaction similar to that of the system under examination. We have verified[10] that the choice of $u^{(0)}$ is not crucial. Then a number of iterations are performed, first computing the correction to the previous pseudopotential, either by (11) or by (9), and second, running a MC simulation with the new pseudopotential. The cycle is repeated until the differences

$$\Delta_i g = \mid g_J(r \mid \bar{u}^{(i)})-g_0(r) \mid$$

and

$$\Delta_i S = \mid S_J(k \mid u^{(i)})- -S_0(k) \mid$$

are below a set of standard errors; for instance, the statistical error associated with the MC simulation. In order to obtain good accuracy in $\bar{u}$, it is important to control the deviations both in r and k space since this allows one to discriminate between small systematic deviations in r space and those of random nature. Of the two predictors, the MHNC one is known to be very accurate at short distances in the region of the core. On the other hand, the MHNC predictor is more affected by any noise contained in g_0 or g_J due to the presence of the logarithmic term in (11). The RPA predictor is less affected by the noise, but it is accurate only for the slowly varying components of the pseudopotential. In order to optimize the result, we usually start with some cycles with the MHNC predictor until the short-range part of $g_0(r)$ is well reproduced, and then we switch to the RPA predictor to obtain full convergence. Since the successive $u^{(i)}$ have a tendency to oscillate around the solution, in the later cycles we add only $\frac{1}{2}\delta_{\mathrm{RPA}}$ or $\frac{1}{2}\delta_{\mathrm{MHNC}}$ to the previous pseudopotential. Both

δ_{RPA} and δ_{MHNC} require knowledge of $g_J(r)$ and $S_J(k)$. With simulation, $g_J(r)$ is obtained only up to a maximum distance $L/2$, where L is the side of the simulation cube, so that $S_J(k)$ cannot be obtained directly by a Fourier transform of this $g_J(r)$, but the RDF must be extended to larger distances in order to avoid truncation errors. It is not known how to do this exactly and various approximations have been proposed. We have used a method[4] found satisfactory with GFMC computations: The RDF is fitted in the tail region $r \lesssim L/2$ with the function $\mathrm{Re}[Ar^{-1}\exp(zr)]$ with respect to the complex numbers A and z, and the resulting function is used to represent the RDF for $r > L/2$. This method of extension introduces a certain error in the deduced pseudopotential, but this error can be minimized if the same method of extension is used for both g_J and g_0.

III. MAXIMUM-OVERLAP PSEUDOPOTENTIAL FOR THE HFDHE2 FLUID

The maximum-overlap pseudopotential for the LJ fluid at liquid-helium density has already been computed in paper I. Here we compute $u(r)$ for Bose particles interacting with a potential which is more realistic for ^{4}He, the HFDHE2 (Ref. 6) potential (see Fig. 1). Results of a GFMC computation are available for this potential,[4] as well as a computation of the properties at finite temperature based on a path-integral method.[5] Both computations are supposedly exact.

We have started our computation with $g_0(r)$ from the GFMC computation. Unfortunately, this $g_0(r)$ is rather irregular, with fluctuations from one point to the next on the grid in r space which are much larger than the results of the similar GFMC computation[11] for the LJ potential. We have tried to perform some smoothing of $g_0(r)$, but the large amount of noise did not allow the determination of a reasonably stable result with respect to the parameters of the smoothing function. The RDF of the path-integral method is more regular and we have used the $g_0(r)$ computed at the lowest temperature, $T = 1.176$ K, as the "exact" RDF of the ground state. This temperature is small enough that essentially no rotons are excited. Due to the small size of the system used in the path-integral computation (64 particles), also long-wavelength phonons cannot be present, so that this finite-temperature RDF should represent a very good approximation of the ground state.

In our MC simulation we have used the same number of particles and both $g_0(r)$ and $g_J(r\,|\,u^{(i)})$ have been extended at $r > L/2$ with the same algorithm. In order to achieve good precision, we have performed very long MC runs of 15 000 moves per particle at each iteration.

The trend of the computation turns out to be very similar to that of the LJ fluid. After three iterations the basic structure of $g_0(r)$ and $S_0(r)$ is well reproduced and after another five iterations one gets convergence to the level of the MC noise: The deviation $g_i(r)$ is less than 0.5% when $g_0 > 0.2$ and less than 4% in the inner-core region. The deviations $\Delta S_i(k)$ are less than 1%, with an average value of 0.3%. The pseudopotential at convergence is shown in Fig. 2, together with that of the LJ fluid. The shape is rather similar, a sharp rise at short distances followed by a structure in the intermediate range 4–7 Å. The local maximum at 5.3 Å is very close to the position of the minimum of $g(r)$ and this structure is slightly more pronounced than in the case of the LJ potential. In particular, the minimum at ~7 Å is more pronounced for the HFDHE2 potential, but this distance is close to $L/2$, so that this result might be affected by the extension of the RDF.

It is interesting to compare $\bar{u}$ with the pseudopotential obtained from an energy computation. The best Jastrow pseudopotential obtained from the Lagrange-Euler equa-

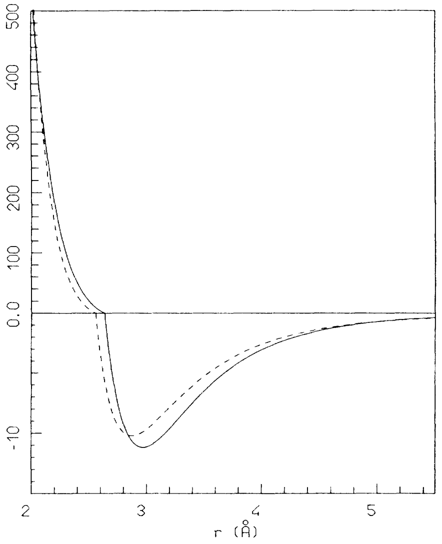

FIG. 1. HFDHE2 pair potential (solid line) and the LJ one (dashed line). Notice the change of scale.

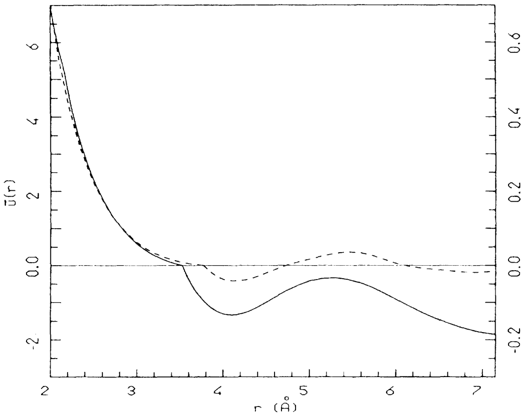

FIG. 2. Maximum-overlap Jastrow pseudopotential for the HFDHE2 potential (solid line) and for LJ (dashed line) at the equilibrium density of ^{4}He. Left-hand scale is up to the first zero of $u(r)$ and the right-hand scale is beyond.

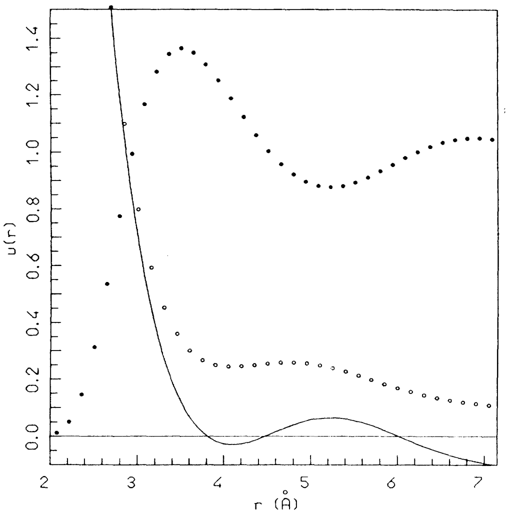

FIG. 3. Maximum-overlap pseudopotential (solid line) and optimum pseudopotential from energy computation (Ref. 12) (open dots). Solid dots represent $g_0(r)$ (Ref. 5).

tion in the HNC approximation[12] is shown in Fig. 3. This result is for an infinite system and it has built in the long-range r^{-2} tail[13] due to the zero-point motion of long-wavelength phonons. This contribution is absent in $g_0(r)$ as well as in our computation due to the finite size of the system. We have estimated $\bar{u}$ for an infinite system by adding to the computed maximum-overlap pseudopotential the missing phonon contribution evaluated by

$$\delta_{\rm ph}(r)=\rho^{-1}(2\pi)^{-1}\int d^3k\, e^{i\mathbf{k}\cdot\mathbf{r}}[\tilde{S}_0^{-1}(k)-S_0^{-1}(k)]\ , \qquad (12)$$

where $\tilde{S}_0(k)=\hbar k/2mc$, c being the sound velocity, for $k<k_c$, and $\tilde{S}_0(k)=S_0(k)$ for $k>k_c$. k_c is the crossing point between $S_0(k)$ and the Feynman form $\hbar k/2mc$ appropriate for small k. At short distances, $\bar{u}(r)$ is rather similar to the energy variational pseudopotential, and both have the same basic structure at intermediate distance. This structure, however, is much more pronounced in $\bar{u}(r)$, where a well-defined maximum and minimum appear. This is similar to what was found[2] for the LJ fluid.

IV. MAXIMUM-OVERLAP PSEUDOPOTENTIAL FOR REAL LIQUID ^{4}He

In this computation we have used, as input, the measured $S(k)$ by neutron scattering[14] at the equilibrium density and at the lowest temperature, $T=1$ K. As already discussed in the preceding section, this temperature is low enough that $S(k)$ should essentially coincide with the ground state $S_0(k)$, apart from the very-small-k region. In this first computation of an exploratory nature, we wanted to use the same number of particles (64) as in the previous computations for model systems. For this reason we cannot use directly the measured $S(k)$, but rather we must subtract the contribution coming from long-range correlations. These are estimated as follows: We start from the RDF, which has been already computed[14] from the measured $S(k)$; $g(r)$ is truncated at the distance $r=L/2=7.15$ Å corresponding to our simulation cube. This truncated $g(r)$ is extended at $r>L/2$ with the algorithm discussed in Sec. II. A Fourier transformation of this extended $g(r)$ gives a structure factor which we take as $S_0(k)$. As expected, this $S_0(k)$ differs significantly at small k; for instance, $S_0(0)=0.07$ in place of $S(0)=\rho k_B T K_T=0.04$ (K_T is the isothermal compressibility), but at larger k the difference between $S_0(k)$ and the measured one becomes small. For instance, it is 1% at the main maximum of $S(k)$.

As our starting pseudopotential we have used u computed for the HFDHE2 potential. After five iterations a reasonable convergence was reached [average deviation of 2% in $g(r)$ and $S(k)$], and in view of the uncertainty in $S_0(k)$ we have not pushed the computation further. The resulting pseudopotential, shown in Fig. 4, is rather close to that of the HFDHE2 potential and this is not surprising in view of the good agreement[4] found between the RDF computed with the HFDHE2 potential and the experimental RDF. At short distances $u(r)$ follows the trend of the maximum-overlap pseudopotentials of the LJ and HFDHE2 fluids, but $u(r)$ is rather irregular at shorter distances, where $g_0(r)\lesssim 0.2$. Presumably, this reflects the uncertainty in the deduction of the radial distribution function at short distances starting from a structure factor which is known only over a finite range of wave vectors (0.8–6.7 Å^{-1} in the present case).

V. INVERSE PROBLEM IN BOSE QUANTUM FLUIDS

The short-range behavior of the Jastrow pseudopotential reflects close encounters of pairs of particles. If the interference effect due to the presence of a third particle very close by can be neglected (at typical liquid-helium density, the probability of such three-body collisions is very small), then the Jastrow factor $\exp[-u(r)/2]$ is expected[7,8] to be close to the solution of the two-body Schrödinger equation at some characteristic energy. It is

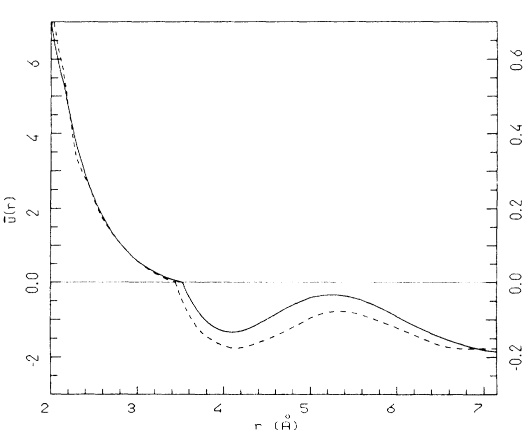

FIG. 4. Same as in Fig. 2. For the HFDHF2 potential (solid line) and for real ^{4}He (dashed line).

not obvious *a priori* how far in the distance r between the pair of particles this similitude will hold, but energy-variational computations have shown[8] that this similitude extends over a significant range of distances, i.e., up to a distance of order of the position of the first peak of the RDF. The effect of the presence of the other particles is taken into account by introducing a boundary condition $\exp[-u(d)/2]=1$ at a characteristic healing length d. On the other hand, the optimal Jastrow pseudopotentials coming from energy or from maximum-overlap computations show a structure at intermediate distances which is not present in the solution of the two-body Schrödinger equation. The position of this structure depends on density and it roughly scales like $\rho^{-1/3}$, so that it must be a collective effect.[15,2] At larger distances the pseudopotential goes over smoothly to the r^{-2} tail, again a collective effect.[13]

Before we can try to extract information on the pair interaction from the maximum-overlap pseudopotential, we must separate—in $u(r)$—the collective contribution from the two-body one. We are not able to do this, in general, because we do not yet have a theory of the intermediate-range structure of $u(r)$. However, we can do this approximately if we know the pseudopotential of a system with a pair interaction close to that of the system under examination. Let us call $v_A(r)$ and $v_B(r)$ the two pair interactions and $\bar{u}_A(r)$ and $\bar{u}_B(r)$ the corresponding maximum-overlap pseudopotentials. Let us split the $\bar{u}$ into a pair term $W(r)$ and a collective contribution $Z(r)$:

$$\bar{u}_A(r)=W_A(r)+Z_A(r), \quad \bar{u}_B(r)=W_B(r)+Z_B(r) \ . \tag{13}$$

The pair Jastrow factors

$$l_\alpha(r)=\exp[-W_\alpha(r)/2], \quad \alpha=A,B \tag{14}$$

are assumed to be a solution of the two-body Schrödinger equation[8]

$$\left[-\frac{\hbar^2}{m}\frac{\partial^2}{\partial r^2}+v_\alpha(r)\right]l_\alpha(r)=0, \quad \alpha=A,B \tag{15}$$

with the boundary condition $l_\alpha(d)=1$, $l'_\alpha(d)=0$ at a suitable healing length d. The collective effects enter $\bar{u}$ in two places, directly in the $Z(r)$ term and indirectly in $W(r)$ via the healing length. If the two pair potentials v_A and v_B are similar and the density is the same, we can assume that to a first approximation the collective effects in the two systems are the same, so that

$$Z_A(r)=Z_B(r), \quad d_A=d_B \ . \tag{16}$$

Taking the difference of Eq. (15) for A and B, expressing l_α in terms of W_α, and using (13) and (16), we can obtain $v_B(r)$ in the form

$$v_B(r)=v_A(r)+H_{AB}(r)+K_{AB}(r) \ , \tag{17}$$

$$H_{AB}(r)=\frac{\hbar^2}{m}\left[\tfrac{1}{2}\bar{u}''_A+\tfrac{1}{4}(\bar{u}'_A)^2+\frac{1}{r}\bar{u}'_A -\tfrac{1}{2}\bar{u}''_B+\tfrac{1}{4}(\bar{u}'_B)^2+\frac{1}{r}\bar{u}'_B-\tfrac{1}{2}\bar{u}'_A\bar{u}'_B\right] , \tag{18}$$

$$K_{AB}(r)=\frac{\hbar^2}{2m}(\bar{u}'_A-\bar{u}'_B)W'_A(r) \ , \tag{19}$$

where $u'=du(r)/dr$ and $u''=d^2u(r)/dr^2$.

Suppose that we know, for the system A, both the pair interaction $v_A(r)$ and the RDF $g_0^A(r)$, from which we can obtain $\bar{u}_A(r)$. For the system B, we know only $g_0^{(B)}(r)$ and the relative $\bar{u}_B(r)$. Then, Eq. (17) gives us the unknown pair interaction $v_B(r)$. There is one problem in using (17): The term H_{AB} can be computed from $\bar{u}_A$ and $\bar{u}_B$ alone, but the term K_{AB} also requires knowledge of the pair contribution $W'_A(r)$, which is only a part of $\bar{u}_A$. Explicit calculation shows that the K_{AB} term is much smaller than H_{AB}, so that it makes essentially no difference if K_{AB} is approximately by

$$K_{AB}(r)=\hbar^2/2m(\bar{u}'_A-\bar{u}'_B)\bar{u}'_A(r) \ . \tag{20}$$

Equation (17) for $v_B(r)$ relies on two approximations, namely that the collective terms for the two systems are the same and that the pair term $W(r)$ is a solution of Eq. (15). In order to test if these approximations are acceptable, we have used the computed maximum-overlap pseudopotentials for the LJ and HFDHE2 systems. As reference system A, we use the LJ fluid and we compare v_B-v_A as given by (17) with the known difference between the two potentials. As shown in Fig. 5, $H_{AB}(r)+K_{AB}(r)$ is very noisy, but the basic trend of

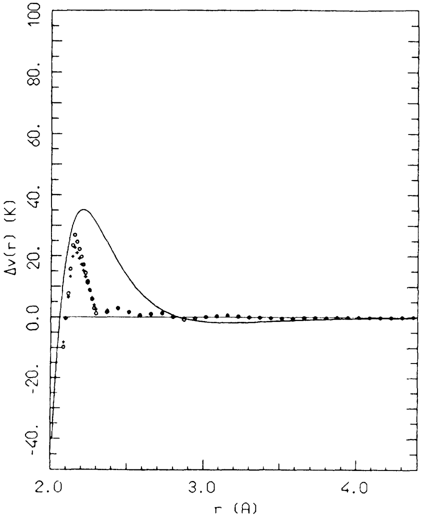

FIG. 5. Difference between the HFDHE2 and LJ potentials (solid line) and the quantity $H(r)+K(r)$ as given in Eqs. (18) and (19) computed with the maximum-overlap pseudopotentials for the two systems. ○ and + are the results of the last two iterations of the computation of $u(r)$.

$v_B - v_A$ is reproduced. The level of the noise, however, does not allow one to give a definite answer on the level of accuracy of (17).

This noise has two sources which are of comparable importance. On one hand, some noise is introduced in our computation of $\bar{u}$ by the simulation stage of the iterative method. The deviations between $H_{AB}+K_{AB}$ computed at two successive iterations of $\bar{u}$ [the MHNC predictor (11) was used] give an idea of this effect. The differential operations performed on $\bar{u}$ required to build $H_{AB}+K_{AB}$ amplify enormously any noise, and this is particularly significant at short distances, where $g(r) \lesssim 0.1$. Either longer simulations in computing g_J are required or a method of solving the functional equation (4) which does not use simulation is. Notice that in computing $H_{AB}+K_{AB}$ we have used the $\bar{u}_A$ and $\bar{u}_B$ as given by the predictors (9) and (10), and no smoothing has been applied to $\bar{u}$ or g_J.

A second source of error is due to the RDF g_0 used as input. These come from computations of the quantum problem which are exact but statistical in nature. Therefore, g_0 is affected by some noise. In paper I we applied a five-point spline smoothing to the function $g_0(r)\exp[u(r)]$, where $u(r)$ is the McMillan pseudopotential.[16] The weights attributed to the different points change smoothly from 1% for $r > \sigma = 2.556$ Å to 10% for $r < \sigma$. The precise value used for the smoothing parameters has a small but significant effect on the smoothed $g_0(r)$ and this leads to a variation in the resulting $H_{AB}+K_{AB}$ which is of the order of the oscillations present in the result given in Fig. 5. We suspect that the origin of the short-wavelength oscillations present in $H_{AB}+K_{AR}$ are due to the smoothing procedure. Clearly, this problem will be avoided when we will have available results of exact simulations of quantum systems with a lower level of noise.

VI. DISCUSSION

We have computed the maximum-overlap Jastrow pseudopotential $\bar{u}$ for the HFDHE2 fluid and real liquid ^{4}He at the equilibrium density. The two pseudopotentials turn out to be rather similar and there is a small but significant deviation from the pseudopotential of the LJ fluid.

We have explored the possibility of deducing the difference between the pair interactions of two slightly different systems from the difference between the relative maximum-overlap pseudopotentials. The LJ fluid is used as reference and we have tried to deduce the HFDHE2 potential starting from the exact RDF of this system. The algorithm is based on the assumption that the pseudopotential contains a part of collective origin which is weakly dependent on the detailed shape of the pair interaction, and that the remaining part of two-body origin is solution of a Schrödinger-like equation. The extracted potential has the basic feature of the correct one, but the level of noise is too large to reach a quantitative conclusion. In order to decrease the amount of noise, we need a better way of solving the functional equation (4) for $\bar{u}$, so that the result is less affected by the statistical noise of simulation and that the exact simulations of the quantum fluid increase the accuracy of their RDF. It is also important to perform computations on systems larger than the present ones is order to minimize the effect of the extension of the RDF.

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