

## Momentum distribution of liquid helium

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We have obtained the one-body density matrix and the momentum distribution  $n(p)$  of liquid  ${}^4\text{He}$  at  $T=0$  K from diffusion Monte Carlo (DMC) simulations, using trial functions optimized via the Euler Monte Carlo (EMC) method. We find a condensate fraction smaller than in previous calculations. Though we do not explicitly include long-range correlations in our calculations, we obtain a momentum distribution at long wavelength which is compatible with the presence of long-range correlations in the exact wave function. We have also studied  ${}^3\text{He}$ , using fixed-node DMC, with nodes and trial functions provided by the EMC. In particular, we analyze the momentum distribution  $n(p)$  with respect to the discontinuity  $Z$  as well as the singular behavior at the Fermi surface. We also show that an approximate factorization of the one-body density matrix  $\rho(r) \approx \rho_0(r)\rho_B(r)$  holds, with  $\rho_0(r)$  and  $\rho_B(r)$ , respectively, the density matrix of the ideal Fermi gas and the density matrix of a Bose  ${}^3\text{He}$ . [S0163-1829(97)05901-8]

### I. INTRODUCTION

The momentum distribution  $n(p) = \langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle$  is a fundamental quantity for the study of both the static and the dynamical properties of quantum liquids, as it gives direct information about the high-momentum components of the ground-state wave function.<sup>1</sup> Experimentally, access to  $n(p)$  is provided by deep inelastic neutron scattering at a large momentum transfer  $\hbar Q$ . The extraction of  $n(p)$  from the measured scattered intensity, however, is affected by the limitations imposed by the experimental resolution and the final-state interactions. Thus the most accurate information on the momentum distribution of  ${}^4\text{He}$  available to date is likely to be the one obtained through accurate, microscopic calculations, such as those presented in this study.

At  $T=0^\circ$  K the momentum distribution  $n(p)$  of an ideal Bose gas is given by a delta function  $\delta(\mathbf{p})$ , corresponding to all particles being in the condensate. Conversely, the condensate fraction of  ${}^4\text{He}$  at the equilibrium density is less than 10%, implying that the effects of the strongly repulsive core of the interatomic interaction is nonperturbative. Similarly for  ${}^3\text{He}$  the discontinuity of  $n(p)$  at the Fermi momentum  $\hbar p_F$ , which gives the strength of the quasiparticle pole, is  $\sim 0.2$  at equilibrium instead of 1, as in the ideal Fermi gas. In fact, it has been always difficult to carry out *ab initio* calculations of the momentum distribution for these systems within the field-theoretical approach.<sup>2</sup>

Modern, realistic, quantitative calculations only started with the development of variational Monte Carlo (VMC) methods<sup>3</sup> and the hypernetted-chain (HNC, FHNC) equations<sup>4,5</sup> for Jastrow models of both Bose and Fermi liquids. FHNC and HNC equations for the momentum distribu-

tion have been numerically solved in variational calculations of nuclear matter,<sup>6</sup> liquid  ${}^4\text{He}$ ,<sup>7,1</sup> and liquid  ${}^3\text{He}$ ,<sup>8-10</sup> for which triplet and backflow correlations were also taken into account. To improve upon the above variational estimates of  $n(p)$ , nonconventional perturbative techniques, based on correlated basis functions<sup>11</sup> (CBF's), have been developed, and applied to liquid  ${}^4\text{He}$  (Ref. 7) and nuclear matter.<sup>6,1</sup>

HNC and FHNC theories have the merit to allow for fine details of interparticle correlations, such as long-range behavior, spin dependence, and anisotropies in inhomogeneous systems. However, not all cluster diagrams resulting from the theory and involved in the HNC formalism, can be summed in closed form, and in FHNC formulation the procedure to estimate the elementary diagrams with exchange bonds is not completely under control. Therefore, approximations like scaling,<sup>12</sup> interpolation,<sup>8</sup> or truncated summations<sup>13-15</sup> must be invoked, and, in liquid-helium calculations, these result in a non-negligible loss of accuracy with respect to a fully variational treatment.<sup>16,17</sup>

The momentum distribution of liquid  ${}^4\text{He}$  and  ${}^3\text{He}$  has also been calculated, at zero temperature, by using the Green-function Monte Carlo (GFMC) method.<sup>18,1</sup> At finite temperature, calculations have been performed for  ${}^4\text{He}$  by the path integral Monte Carlo (PIMC) method,<sup>19,1</sup> and, more recently, by the VMC method with trial functions of the Shadow type.<sup>20</sup> The available theoretical estimates of the momentum distribution of liquid  ${}^4\text{He}$  provided by variational and GFMC methods are in reasonably good agreement among themselves, except for low momenta and for the condensate fraction. For liquid  ${}^3\text{He}$  the situation is less satisfactory.

The GFMC and the diffusion Monte Carlo (DMC)

methods,<sup>21,22,17</sup> afford to date the most precise tools to perform ground-state calculations for many-particle systems. For bosons they provide energy estimates that are virtually exact, within statistical accuracy. In fact the same is true for the averages of ( $R$ ) diagonal operators [not the case for  $n(p)$ ], for which algorithms exist, like the so-called forward walking method,<sup>23,24</sup> which yield *pure* estimates. On the other hand, the estimates of observables that do not commute with the Hamiltonian are usually obtained from *mixed* averages—through an extrapolation procedure whose accuracy depends on the quality of the trial function  $\Psi$  used for the importance sampling.<sup>3</sup> The extrapolation introduces a bias in the estimates which is second order in the difference between  $\Psi$  and the ground-state wave function  $\Phi_0$ . For fermions there is an additional source of error related to the existence of the so-called *sign problem*. To date, to obtain a numerically stable algorithm it is customary to approximate the unknown nodes of the sought ground state  $\Phi_0$  with those of the trial function  $\Psi$  [the *fixed-node* approximation<sup>22</sup>]. This imposes a bias on any average, which for nondiagonal observables cumulates with the one arising from the extrapolation procedure. Therefore, to minimize systematic errors, especially in the evaluation of properties such as the momentum distribution, it is necessary to achieve maximum accuracy in the optimization of the trial function.

Recently, an optimization procedure based on Monte Carlo calculations and denoted as the Euler Monte Carlo (EMC) method has been proposed.<sup>25,17</sup> This EMC method has been successfully applied to both liquid  $^4\text{He}$  and  $^3\text{He}$ .<sup>16,17</sup> The EMC wave functions have pair and triplet correlations fully optimized, and provide the lowest available energy upper bounds. Moreover, their use in DMC calculations<sup>21,22,17</sup> has led to results of unprecedented accuracy for the energy, pair function, and static structure function.

In this paper we present results for the one-body density matrix  $\rho(r)$  and the momentum distribution  $n(p)$  of liquid  $^4\text{He}$  and  $^3\text{He}$ , at various densities, obtained with DMC calculations based on EMC wave functions. The plan of the paper is as follows. In Sec. II we summarize the computational details involved in the calculation of  $n(p)$ . We then present the results for liquid  $^4\text{H}$  in Sec. III, and those for liquid  $^3\text{He}$  in Sec. IV. We finally offer a summary and conclusions in Sec. V.

## II. COMPUTATIONAL DETAILS

In DMC simulations<sup>21,22</sup> the ground-state wave function  $\Phi_0$  is sampled through a random walk in configuration space, guided by a trial function  $\Psi$ . In practice one samples the mixed probability  $f = \Phi_0\Psi$ . We chose  $\Psi = SF$  for  $^4\text{He}$  and  $\Psi = D_\uparrow D_\downarrow F$  for  $^3\text{He}$ , with the *correlation* part  $F$  symmetric in the particle coordinates,  $S$  a symmetrized product of one-particle orbitals, and  $D_\uparrow$  and  $D_\downarrow$  Slater determinants of one-particle orbitals for particles of up- and down-spin. In the homogeneous liquid  $S = \text{const}$ , and  $D_\sigma$  is built from plane waves (PW's), or from plane waves with short- (SBF) or long- (LBF) ranged backflow corrections. As a full account has already been given elsewhere<sup>16,17</sup> of both the EMC method, which we employ to construct and optimize the trial wave function  $\Psi$ , and of the use of EMC wave functions in

DMC simulations, here we shall restrict to essential details.

All calculations (variational and diffusion) presented in this paper, unless explicitly noted, have been performed using EMC wave functions with fully optimized pair and triplet pseudopotentials<sup>17</sup> (OJOT), and modeling helium with the HFDHE2 pair potential of Aziz *et al.*<sup>26</sup> A cubic simulation box and periodic boundary conditions were used. For  $^3\text{He}$ , backflow correlations have been included,<sup>17</sup> in the usual way,<sup>27–29</sup> by replacing the plane waves  $\exp(i\mathbf{k}_i \cdot \mathbf{r}_j)$  in the Slater determinants with  $\exp(i\mathbf{k}_i \cdot \mathbf{x}_j)$ , where  $\mathbf{x}_j = \mathbf{r}_j + \sum_{k \neq j} \eta(r_{jk})(\mathbf{r}_j - \mathbf{r}_k)$ . The function  $\eta(r)$  is taken either short ranged,<sup>27</sup>

$$\eta_S(r) = \lambda_B \exp(-(r - r_B)^2 / \omega_B^2) ((2r - L)/L)^3, \quad (1)$$

or long ranged<sup>30</sup>

$$\eta_L(r) = \lambda_B \exp(-(r - r_B)^2 / \omega_B^2) + \lambda'_B / r^3, \quad (2)$$

where  $\lambda_B$ ,  $r_B$ ,  $\omega_B$ , and  $\lambda'_B$  are variational parameters. The long-ranged backflow function is smoothly cut off at the boundary of the simulation box of size  $L$  by replacing the expression given in Eq. (2) with  $\eta'_L(r) = \eta_L(r) + \eta_L(L - r) - 2\eta_L(L/2)$ . In practice, we first simultaneously optimize the pair and triplet pseudopotentials with the backflow parameters as specified in Refs. 27 and 30, and then we optimize  $\eta(r)$  at fixed pseudopotentials.

The  $^3\text{He}$  results presented below were obtained with short-ranged backflow, unless otherwise specified. Also, DMC simulations were performed within the fixed-node approximation, whereby the nodes of the ground state  $\Phi_0$  are assumed to coincide with those of the EMC trial function.

In a uniform liquid in a state described by the wave function  $\Psi$ , the one-body density matrix can be defined as

$$\rho(r) = \frac{V \int d\mathbf{r}_2 \dots d\mathbf{r}_N \Psi^*(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)}{\int d\mathbf{r}_1 \dots d\mathbf{r}_N |\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)|^2}, \quad (3)$$

so that, having imposed periodic boundary conditions to the  $N$  particles in the volume  $V$ ,

$$\rho(0) = 1, \quad (4)$$

and the independence from  $\mathbf{r}_1$  follows from translational invariance. For fermions, the integration over the variable  $\mathbf{r}_i$  is understood also to imply the a over spin projection. If we denote with  $R$  and  $R'$ , respectively the configurations  $(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$  and  $(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)$ , and we exploit the translational invariance, we can rewrite Eq. (3) as

$$\rho(r) = \frac{\int dR \Psi^*(R) \Psi(R')}{\int dR |\Psi(R)|^2} = \int dR P(R) \frac{\Psi(R')}{\Psi(R)}, \quad (5)$$

with

$$P(R) = \frac{|\Psi(R)|^2}{\int dR |\Psi(R)|^2}, \quad (6)$$

the probability induced by the wave function  $\Psi$ . Using Eq. (5), the variational density matrix (i.e., the one defined in

term of the trial wave function  $\Psi$ ) may be conveniently calculated by the Monte Carlo method as

$$\rho_{\text{VMC}}(r) \approx \frac{1}{N} \sum_{i=1}^N \frac{\Psi(R'_i)}{\Psi(R_i)}, \quad (7)$$

with the configurations  $R_i$  drawn from the probability  $P(R)$ . The DMC-extrapolated estimate  $\rho(r)$  is given by

$$\rho(r) = 2\rho_{\text{mix}}(r) - \rho_{\text{VMC}}(r), \quad (8)$$

where the mixed estimate  $\rho_{\text{mix}}(r)$  is calculated from an expression identical with that of Eq. (7), with the configurations  $R_i$  drawn, however, from the mixed probability  $P_{\text{mix}}(R) = f(R)/\int dR f(R)$  and  $f(R) = \Phi_0(R)\Psi(R)$ . In practice, the auxiliary configurations  $R'$  appearing in Eq. (7) are generated from a given  $R$  by moving a particle either of fixed increments along a random direction (FM) or to points randomly distributed in the simulation box (RM). It turns out that the two methods give more accurate results at small and at large  $r$ , respectively.

The momentum distribution is defined as  $n(p) = \langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \rangle$ , where an average on spin projections is also implied for unpolarized  $^3\text{He}$ . It is simply related to the one-body density matrix by a Fourier transform

$$n(p) = \frac{\rho}{\nu} \int d\mathbf{r} e^{i\mathbf{p}\cdot\mathbf{r}} \rho(r) = \frac{\rho}{\nu} \left( n_0 \delta(\mathbf{p}) + \int d\mathbf{r} e^{i\mathbf{p}\cdot\mathbf{r}} (\rho(r) - n_0) \right), \quad (9)$$

where  $\rho = N/V$  is the density of the system,  $\nu$  is the degeneracy factor, which is 1 for  $^4\text{He}$  and the fully polarized  $^3\text{He}$ , and 2 for normal  $^3\text{He}$ ; and  $n_0$  is the large- $r$  limit of the density matrix,  $n_0 = \rho(\infty)$ . In fact,  $\rho(r)$  vanishes for large values of  $r$  in  $^3\text{He}$ , whereas for  $^4\text{He}$  it saturates to  $n_0 \neq 0$ , due to the macroscopic occupation of the state with zero momentum.  $n_0$  is the condensate fraction, i.e., the fraction of  $^4\text{He}$  atoms occupying the state with  $p=0$ .

Evidently, the normalization of the density matrix given in Eq. (4) implies, for the momentum distribution, the normalization sum rule

$$\frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{p} n(p) = \rho(0) = 1. \quad (10)$$

The momentum distribution has been calculated in two different manners. Having sampled the density matrix as function of  $r$ , one can just take its Fourier transform according to Eq. (9). Alternatively, restricting to the RM method, one can also directly accumulate

$$n(\mathbf{p}) = \frac{\rho}{\nu} \frac{1}{N} \sum_{i=1}^N \frac{e^{i\mathbf{p}\cdot\mathbf{r}} \Psi(R'_i)}{\Psi(R_i)}. \quad (11)$$

At first sight it seems that the  $\mathbf{r}$  integration is missing in Eq. (11) above. However, a little reflection shows that accumulating the estimator of Eq. (11) correctly implements the integration (average) over  $\mathbf{r}$ , which appears in definition (9) of the momentum distribution, since  $\mathbf{r}$  is chosen at random for each configuration  $R_i$ , with a uniform distribution in the

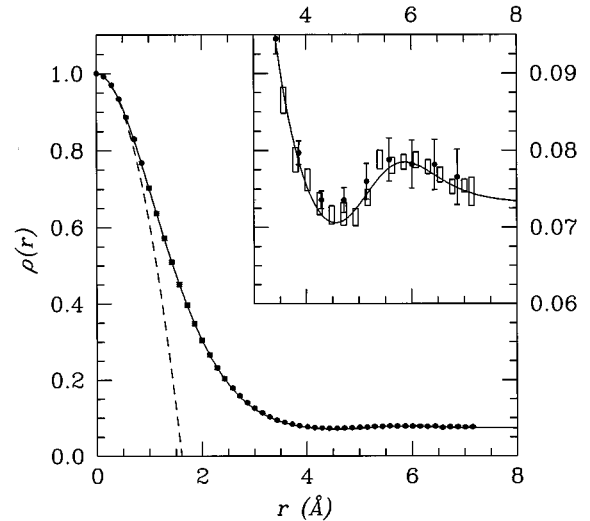


FIG. 1. One-body-density matrix of  $^4\text{He}$  at the equilibrium density  $\rho(\text{\AA}^{-3})=0.02186$ . The full curve is the fit of Eq. (14) to our DMC results (extrapolated estimates), with the dashed curve showing the parabola  $1 - (MT/3\hbar^2)r^2$ , which satisfies the kinetic-energy sum rule. The solid circles and rectangles respectively give our DMC results obtained with the FM and RM methods. A comparison of the estimates yielded by the two methods in the tail region is given in the inset.

simulation box. This second calculation of  $n(\mathbf{p})$  is implemented for  $\mathbf{p}$ 's that are reciprocal-lattice vectors of the simulation cell. Equation (11) is employed to accumulate variational and mixed estimators, from which the extrapolated estimator is then obtained, as explained above. From Eqs. (3) it follows that the kinetic energy per particle  $T$  can be related to the curvature of the density matrix at the origin, according to

$$T = - \left[ \frac{\hbar^2}{2M} \nabla^2 \rho(r) \right]_{r=0}, \quad (12)$$

which also implies the kinetic-energy sum rule [see Eq. (9)]

$$T = \frac{\hbar^2}{2M} \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{p} p^2 n(p). \quad (13)$$

### III. LIQUID $^4\text{He}$

We have carried out DMC calculations of the one-body density matrix and of the momentum distribution of  $^4\text{He}$  at four densities, using EMC trial functions and 64 atoms in the simulation box. Selected runs with up to 232 particles have been performed to check for finite-size effects. In Fig. 1 we show our results for the one-body density matrix  $\rho(r)$  at the equilibrium density. The kinetic-energy sum rule (13) is manifestly satisfied, and the saturation to a finite  $n_0$  at large  $r$  is evident, in spite of the fact that with 64 particles only distances up to about 7  $\text{\AA}$  are accessible. In the inset we also give a comparison between estimates obtained with the FM and RM methods. The greater accuracy of the latter method at large distances is apparent. In Fig. 2 we report, also at the equilibrium density, extrapolated estimates of the momentum distribution  $n(p)$ , obtained using Eq. (11). Due to the finite

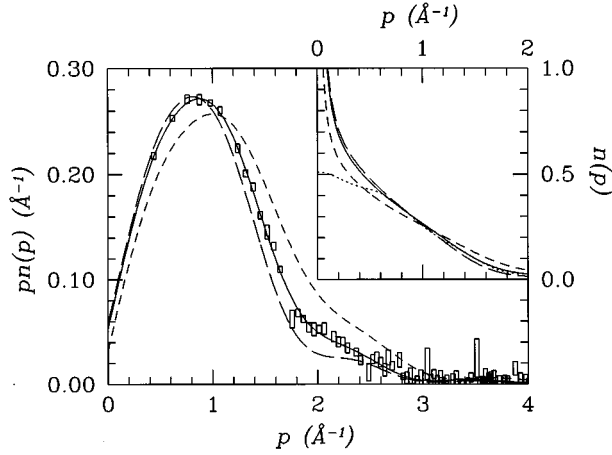


FIG. 2. Momentum distribution of  ${}^4\text{He}$  at  $T=0^\circ\text{K}$ . Long dashes, full curve, and short dashes are fits to the DMC results at  $\rho(\text{\AA}^{-3})=0.019\,64$ ,  $0.021\,86$ , and  $0.026\,22$ , whereas the rectangles give the DMC extrapolated estimates at the equilibrium density  $\rho(\text{\AA}^{-3})=0.021\,86$ . The inset shows the long-wavelength behavior of  $n(p)$ , with the dotted curve reporting the results of the GFMC method (Ref. 18).

size of the system only wave vectors larger than  $\sim 0.4\text{\AA}^{-1}$  are accessible. We note that a shoulder is discernible in  $pn(p)$  at  $p \geq 2\text{\AA}^{-1}$ .

In order to extract the condensate fraction  $n_0$  from our DMC results, as well as to facilitate applications, we have fitted our DMC-extrapolated estimates of the density matrix and momentum distribution, obtained with the RM method, to the following analytic formula:

$$n(p) = (2\pi)^3 \rho \delta(\mathbf{p}) n_0 + \left[ n_0 \frac{p_1}{p} + n_1 \cos^2\left(\frac{p}{p_2}\right) \right] e^{-(p/p_3)^\alpha} + n_2 e^{-(p-p_4)^2/p_5^2}. \quad (14)$$

The first two terms in Eq. (14) account for the existence of the condensate, while the third suitably models the shoulder in  $pn(p)$ . The fourth and last term accounts for the gross main structure of the momentum distribution.

We have simultaneously fitted  $n(p)$  and  $\rho(r)$ , which must be obtained numerically by Fourier transforming the function of Eq. (14), imposing as well the normalization condition (10) and the kinetic energy sum rule (13). Moreover, we set  $p_1 = Mc/2\hbar$  to satisfy the long-wavelength behavior

$$\lim_{p \rightarrow 0} pn(p) = \frac{n_0 Mc}{2\hbar}, \quad (15)$$

induced by long-range correlations, as first discussed by Gavoret and Nozieres.<sup>31</sup> Above  $M$  is the mass of the  ${}^4\text{He}$  atom and  $c$  the sound velocity, which we estimate from the DMC (Ref. 17) equation of state (EOS). Thus we fit at each density six independent parameters to more than 100 MC points, obtaining a reduced  $\chi^2$  between 0.98 and 1.20. The resulting fit parameters are recorded in Table I.

In principle one could also take  $c$  as unknown, and obtain an independent estimate of the sound velocity. We have tried this alternative, at the equilibrium density, obtaining an esti-

TABLE I. Parameters of the fit (14) to the DMC momentum distribution and density matrix of  ${}^4\text{He}$  at  $T=0^\circ\text{K}$ , at various densities.  $\rho$  is in  $\text{\AA}^{-3}$  and  $p_1$ - $p_5$  are in  $\text{\AA}^{-1}$ .

$\rho$	0.019 64	0.021 86	0.024 01	0.026 22
$n_0$	0.111 63	0.071 673	0.046 227	0.027 079
$\alpha$	1.6941	1.7634	2.2342	1.9976
$n_1$	0.055 274	0.038 282	0.019 157	0.021 497
$n_2$	0.402 85	0.398 93	0.366 95	0.384 83
$p_1$	0.499 57	0.733 94	0.959 34	1.1964
$p_2$	0.389 71	0.385 25	0.404 35	0.405 88
$p_3$	1.4900	1.6744	2.2153	2.1832
$p_4$	0.297 13	0.205 38	0.284 94	0.062 765
$p_5$	0.851 28	1.0016	1.0132	1.2549

mate of  $c$  which is about 10% lower than experimental and DMC-EOS estimates, and has, however, a very large uncertainty ( $\sim 50\%$ ), reflecting the absence of DMC points for  $p \leq 0.4\text{\AA}^{-1}$ , where the singular term in  $n(p)$  is important. We may conclude that our data are compatible with the presence of singular term in  $n(p)$ ,<sup>31</sup> in spite of the lack of long-range terms in the pseudopotentials that we used.<sup>17</sup> In Fig. 3 we show the density matrix at the four densities that we studied, as given by the fit of Eq. (14) with the parameters of Table I.

The DMC momentum distribution and density matrix are compared with the fit of Eq. (14) in Figs. 1, 2, and 4, at the equilibrium density. The fit appears to be very good. A similar conclusion holds at the other densities that we studied.

The condensate fraction  $n_0$  is mostly constrained by the large- $r$  behavior of  $\rho(r)$ , which results in a term proportional to  $\delta(\mathbf{p})$  in the momentum distribution. As we already mentioned, the singular behavior of  $n(p)$  at small  $p$ , implied by Eq. (15), is much less effective in determining  $n_0$ , because of the absence of DMC estimates for  $p \leq 0.4\text{\AA}^{-1}$ . From the

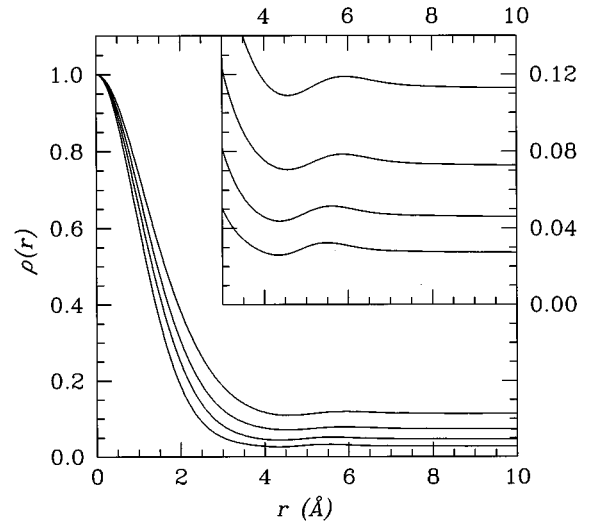


FIG. 3. One-body-density matrix  $\rho(r)$  of  ${}^4\text{He}$ . The curves from the topmost to the lowest, give the analytical fit of Eq. (14) to our DMC results (extrapolated estimates), respectively at  $\rho(\text{\AA}^{-3})=0.019\,64$ ,  $0.021\,86$ ,  $0.024\,01$ , and  $0.026\,22$ . The inset shows  $\rho(r)$  in the tail region.

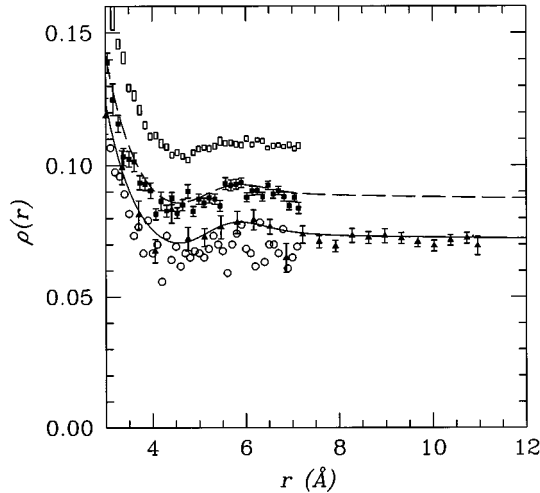


FIG. 4. Dependence on the quality of the wave function and on the method (VMC vs DMC) of the one-body-density matrix of  ${}^4\text{He}$ , at the equilibrium density  $\rho(\text{\AA}^{-3})=0.02186$ . The full curve is the fit to our DMC results (extrapolated estimates) for 64 particles, using our best trial function (OJOT), while the dashed curve gives the fit to the VMC results obtained with this trial function. Empty rectangles and solid squares, respectively, give VMC and DMC results obtained from a simple OJ trial function, which embodies only pair pseudopotentials. Finally, the triangles are the DMC results obtained using the OJOT trial function and 232 particles, and the circles report the finding of PIMC at  $T=1.18^\circ\text{K}$  (Ref. 19).

inset of Fig. 1 one might conclude that the range  $r \leq 7 \text{\AA}$ , accessible with 64 atoms is not large enough to unambiguously assess the value of  $n_0$ . However, simulations with 232 atoms yield, in the extra range  $7 \text{\AA} \leq r \leq 11$ , DMC estimates that are in perfect agreement with the fit to the 64 particles results, as is clear from Fig. 4. We also illustrate in this figure the dependence of the large- $r$  limit of the density matrix, i.e.,  $n_0$ , on the quality of the wave function. In particular it is apparent that improving the MC description, either changing from VMC to DMC methods, for a given trial function, or changing to a better trial function in the DMC method, results in a decrease of  $n_0$  in the case considered.

In Fig. 5 and Table II we compare our predictions for  $n_0$  with those from other theoretical treatments, as well as with experimental results at low temperature. Consistently with the observation made above, our use of very accurate trial functions<sup>17</sup> yields DMC predictions for the condensate fraction which are lower than previously obtained by GFMC (Ref. 18) and HNC (Ref. 7) methods. On the theoretical side the only prediction that agrees with our own, though it has a much larger statistical error, is the PIMC one at  $T=1.18^\circ\text{K}$ .<sup>19</sup> We should remind the reader that in fact PIMC method has no trial function bias. We find instead a sizable discrepancy from the experimental estimates of Snow, Wang, and Sokol,<sup>32</sup> who determined  $n_0$  by fitting a model  $n(p)$  to the measured Compton profile  $J(Y)$ —a procedure, however, which appears to be model dependent. Different choices for  $n(p)$  produce equivalently good fits of  $J(Y)$ ,<sup>33</sup> though embodying very different condensate fractions, all the way from  $n_0=0$  to  $n_0=10\%$ . In fact, our DMC momentum distribu-

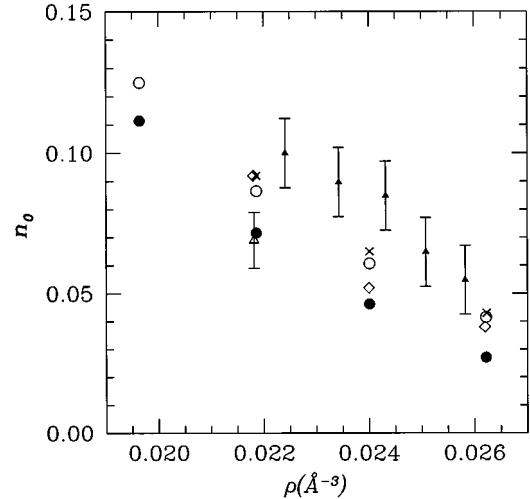


FIG. 5. Condensate fraction of liquid  ${}^4\text{He}$ , as a function of the density. DMC (solid circles); EMC (open circles); GFMC (Ref. 18) (diamonds); HNC (Ref. 7) (crosses); experimental estimates at  $T=0.75^\circ\text{K}$  (Ref. 32) (solid triangles); PIMC at  $T=1.18^\circ\text{K}$  (Ref. 19) (empty triangle).

tion yields prediction for the Compton profile which agrees well with the experiments, as we show below.

The inelastic neutron-scattering cross section at high momentum transfer  $\hbar Q$  can be approximated by its impulse approximation (IA) expression, which is proportional to the Compton profile<sup>33</sup>

$$J(Y) = \frac{1}{4\pi^2\rho} \int_{|Y|}^{\infty} dp \, pn(p). \quad (16)$$

The scattering in the IA does not depend on the energy  $\omega$  and the momentum transfer  $\hbar Q$  separately, but only through the scaling variable  $Y$ , given by

$$Y = (M/\hbar Q)(\omega - \omega_r), \quad (17)$$

where  $\omega_r = \hbar^2 Q^2/2M$  is the recoil energy of the scattering atom. The dynamical response function  $S(Q, \omega)$ , in the IA, is given by  $J(Y)$  times the factor  $M/(\hbar Q)$ . Final-state effects (FSE's) of the medium on the scattered atom as well as experimental resolution (ER), broaden the Compton profile, particularly its  $\delta$  peak at  $p=0$ , which is due to the Bose condensation. In Fig. 6 Compton profiles, calculated with our DMC momentum distributions, are compared with observed scattering data<sup>34</sup> at  $T=0.35^\circ\text{K}$ , converted to  $J(Y)$ . Once ER and FSE are taken into account,<sup>34</sup> good agreement with the experiment is obtained.

TABLE II. Condensate fraction  $n_0$  in  ${}^4\text{He}$ . DMC, GFMC (Ref. 18), and HNC (Ref. 7) predictions are at  $T=0$ . The PIMC (Ref. 19) result is at  $T=1.18^\circ\text{K}$ , and the density is in  $\text{\AA}^{-3}$ . The figure in parentheses is the uncertainty on the last figure, whenever available.

$\rho$	0.019 64	0.021 86	0.024 01	0.026 22
DMC	0.112(1)	0.0717(5)	0.0462(6)	0.02.71(6)
PIMC		0.069(10)		
GFMC		0.092(1)	0.052(1)	0.037(2)
HNC		0.092	0.065	0.043

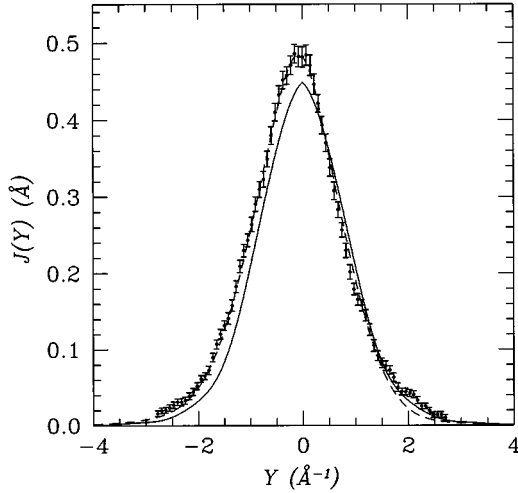


FIG. 6. Compton profile  $J(Y)$  of  ${}^4\text{He}$  at the equilibrium density  $\rho(\text{\AA}^{-3})=0.02186$  compared with experimental (solid circles) data at  $Q=23\text{\AA}^{-1}$  and  $T=0.35^\circ\text{K}$  (Ref. 34). The dashed (solid) curve is obtained from our fit to the DMC  $n(p)$  allowing (not allowing) for both the experimental broadening and the final state interactions of Ref. 34. In calculating the dashed curve, a shift of  $-0.1\text{\AA}$  in  $Y$  has been also used as in Ref. 34.

#### IV. LIQUID ${}^3\text{He}$

For normal  ${}^3\text{He}$ , DMC simulations using EMC trial functions with backflow and the fixed-node approximation have been performed at five densities, with 54 atoms in the simulation box. We investigated the dependence of the momentum distribution on the size of the system and on the range of the backflow, respectively, with runs for 114 atoms and with runs using trial functions embodying long-range backflow.

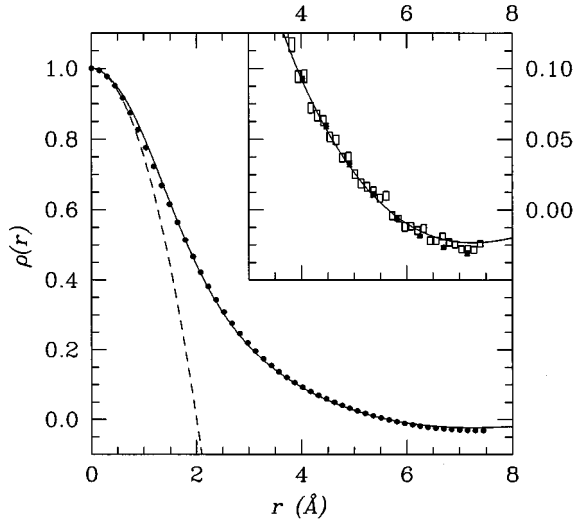


FIG. 7. One-body-density matrix of  ${}^3\text{He}$  at the equilibrium density  $\rho(\text{\AA}^{-3})=0.01635$ . The full curve is the fit of Eq. (19) to our DMC results (extrapolated estimates), with the dashed curve showing the parabola  $1 - (MT/3\hbar^2)r^2$ , which satisfies the kinetic-energy sum rule. The solid circles and rectangles, respectively, give our DMC results obtained with the FM and RM methods. A comparison of the estimates yielded by the two methods in the tail region is given in the inset.

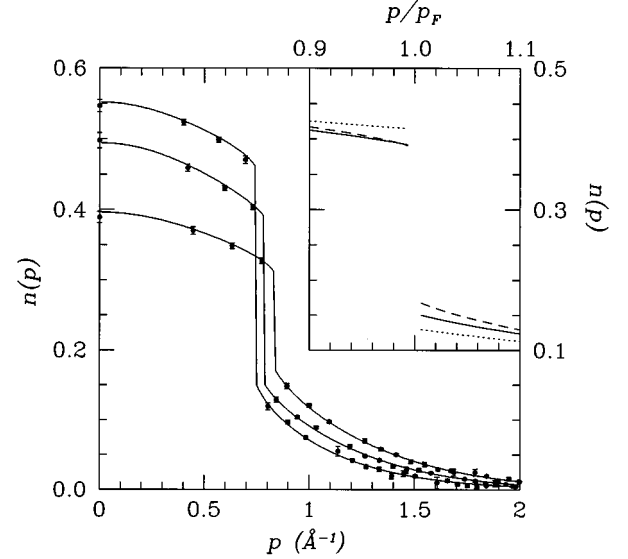


FIG. 8. Momentum distribution of  ${}^3\text{He}$  at  $T=0^\circ\text{K}$  and  $\rho(\text{\AA}^{-3})=0.01413, 0.01635,$  and  $0.01946$ : dots are DMC (fixed-node) extrapolated estimates; full curves are fits to the DMC results. Larger densities correspond to lower curves at  $p=0$ . The inset shows the behavior around the Fermi momentum at the equilibrium density  $\rho(\text{\AA}^{-3})=0.01635\text{\AA}^{-3}$ , using PW ( $\cdots$ ), SBF ( $\text{---}$ ), and LBF ( $\text{- - -}$ ) trial functions.

In Fig. 7 we give our DMC estimates for the density matrix at the equilibrium density. It is clear that the kinetic-energy sum rule (13) is satisfied. The size of the system allows for a determination of  $\rho(r)$  through its first zero and up to the first minimum. A comparison between results obtained with FM and RM methods is also given in the inset. The smaller error on the FM results, compared with that on the RM estimates, is due to the much longer runs used to accumulate the FM  $\rho(r)$  in this case.

In Fig. 8 we report, at three different densities, the momentum distribution  $n(p)$  obtained using Eq. (11). Clearly, the discontinuity  $Z$  at the Fermi wave vector  $p_F$  is substantially reduced, with respect to its value  $Z=1$  in the noninteracting system, and moreover it systematically shrinks, as the system becomes denser and the effects of the interaction become more important.  $Z$  is also slightly reduced when the nodes of the trial function are improved from PW to SRB and then to LBF. Size effects on the momentum distribution appear to be negligible, as it is clear from the comparison between variational results for 54 and 114 particles given in Fig. 9, at the equilibrium density.

In a normal Fermi liquid such as  ${}^3\text{He}$  the momentum distribution, in addition to the discontinuity, has infinite slopes<sup>35,36</sup> at  $p_F$ . To leading order in  $p-p_F$ ,

$$n(p \rightarrow p_F^\pm) \approx n(p_F^\pm) + A \frac{p-p_F}{p_F} \ln \left| \frac{p-p_F}{p_F} \right|, \quad (18)$$

with the coefficient  $A$  related to imaginary part of the self-energy  $\Sigma(\mathbf{p}, E)$ .

To extract  $Z$  from the calculated momentum distribution and to check that our results are consistent with the presence of the singular term of Eq. (18), we fitted our data for  $\rho(r)$  and  $n(p)$  to the real-space form

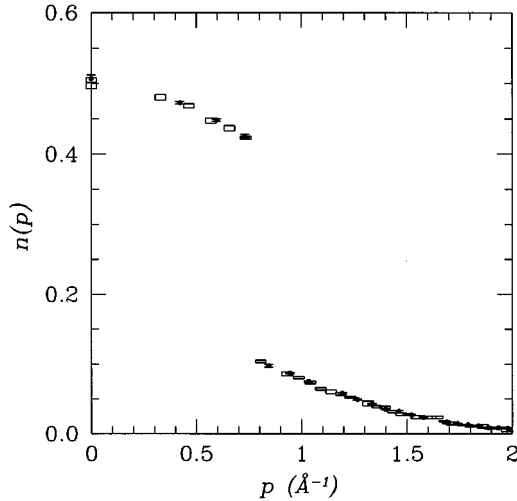


FIG. 9. Momentum distribution of  ${}^3\text{He}$  at equilibrium density  $\rho(\text{\AA}^{-3})=0.016\,35$  with the VMC method, using OJ trial functions, with 54 (solid circles) and 114 (rectangles) particles.

$$\rho(r) = Z\rho_0(x) + a_1 \frac{\rho_0(x)}{x} + a_2 \frac{x\rho_0(x) - \sin(x)}{x^3} - a_1 \frac{e^{-b_1x}}{x} + (a_3 + a_4x + a_5x^2 + a_6x^3)e^{-b_2x}, \quad (19)$$

with  $x = p_F r$ , and

$$\rho_0(r) = \frac{3}{x^3}(\sin x - x \cos x), \quad (20)$$

the density matrix of the ideal Fermi gas. The first two terms in Eq. (19) account, respectively, for the discontinuity and the infinite slope of  $n(p)$  at  $p_F$ . The third term allows for finite discontinuities in the first and second derivatives of  $n(p)$  at  $p_F$ . Finally, the fourth term is needed to eliminate the divergence that the term  $\rho_0(x)/x$  produces at the origin. We impose the normalization condition (10) and the kinetic-energy sum rule (13), as well as the vanishing of the first and third derivatives of  $\rho(r)$  at  $r=0$ . Thus we fit at each density five independent parameters to more than 100 MC points, with a reduced  $\chi^2$  between 0.87 and 1.15. The resulting fit parameters are recorded in Table III.

TABLE III. Parameters of the fit (19) to the fixed-node DMC momentum distribution and density matrix of  ${}^3\text{He}$  at  $T=0^\circ\text{K}$ , at various densities.  $\rho$  is in  $\text{\AA}^{-3}$ .

$\rho$	0.011 98	0.014 13	0.016 35	0.017 97	0.019 46
$Z$	0.459 77	0.305 98	0.236 16	0.143 28	0.135 66
$a_1$	0.142 48	0.286 12	0.193 76	0.416 99	0.246 13
$a_2$	-0.119 73	-0.219 12	-0.123 81	-0.281 25	-0.239 82
$a_3$	-0.732 00	-0.807 32	-0.643 05	-2.1780	-0.962 72
$a_4$	3.2095	1.9033	3.2723	4.1029	3.9981
$a_5$	-1.5905	0.648 01	-0.098 765	-2.4600	-0.647 25
$a_6$	7.6229	1.5582	4.6639	6.8026	6.2113
$b_1$	9.0415	5.3494	7.3460	7.3676	7.5530
$b_2$	3.5907	2.7487	3.0716	3.3316	3.1652

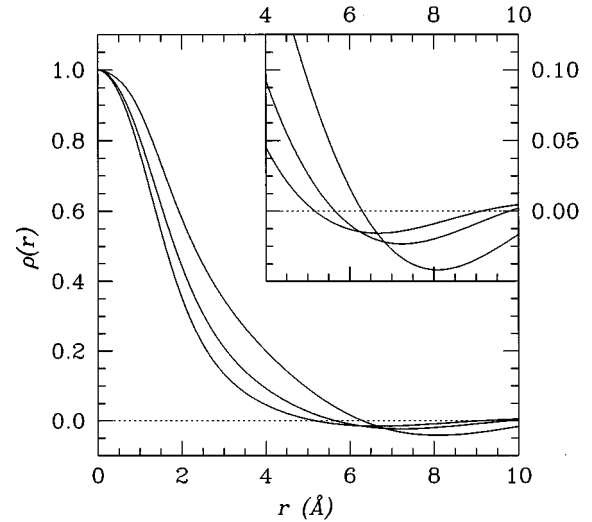


FIG. 10. One-body density matrices  $\rho$  of  ${}^3\text{He}$ . The curves, from the least to the most steep, give the analytical fit of Eq. (19) to our fixed-node DMC results (extrapolated estimates), respectively at  $\rho(\text{\AA}^{-3})=0.011\,98$ ,  $0.016\,35$ , and  $0.019\,46$ . The inset shows  $\rho(r)$  in the tail region.

We compare fit and DMC estimates for  $\rho(r)$  and for  $n(p)$ , respectively, in Figs. 7 and 8. Evidently, Eq. (19) is fully consistent with our DMC results. In Fig. 10 we show the one-body density matrix at three of the densities that we studied, as given by the fit of Eq. (19). As for the noninteracting case,  $\rho(r)$  becomes steeper with increasing density, and its first zero moves toward the origin.

A comparison of our results for the momentum distribution of  ${}^3\text{He}$  with those from some other calculations is given in Fig. 11 and Table IV. HNC results<sup>10</sup> are in close agreement with our variational  $n(p)$ , for  $p \geq p_F$  as well as with the estimate of  $Z$ , while small differences are present at small momenta, which are, however, of little relevance in the density of states  $\propto n(p)p^2$ . The evident discrepancies between

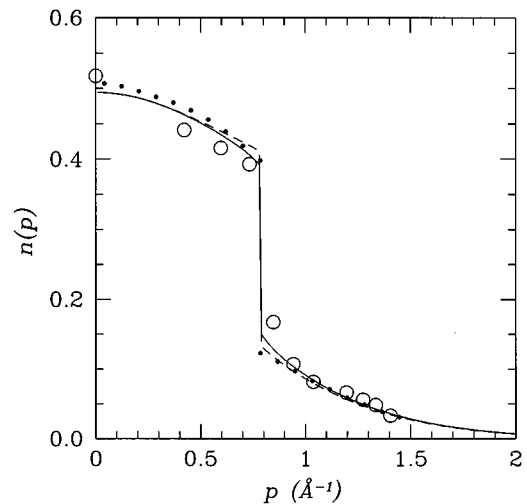


FIG. 11. Momentum distribution of  ${}^3\text{He}$  at equilibrium density  $\rho(\text{\AA}^{-3})=0.016\,35$ : comparison of the present DMC (—) and VMC (- -) fits with the predictions of GFMC (Ref. 18) (circles) and HNC (Ref. 10) (solid circles).

TABLE IV. Discontinuity of the momentum distribution at  $p_F$ ,  $Z$ , as function of the density, from various calculations. SBF and LBF denote the DMC estimates, obtained using the fit of Eq. (19), and results for EMC wave functions with short- and long-range backflow, respectively. VMC gives the variational estimate for the SBF wave function.

$\rho$	0.011 98	0.014 13	0.016 35	0.017 97	0.019 46
HNC <sup>a</sup>		0.348	0.275	0.244	0.221
VMC			0.272(2)		
GFMC <sup>b</sup>			$\leq 0.2$		
SBF	0.46(2)	0.31(2)	0.24(1)	0.14(1)	0.14(1)
LBF			0.21(2)		

<sup>a</sup>Reference 10.

<sup>b</sup>Reference 18.

our results and those of the GFMC method<sup>37</sup> around the Fermi surface are probably due to the poorer trial function used in the GFMC method,<sup>37</sup> as well as to statistical errors.

As we already mentioned, the functional form of Eq. (19) implies for  $n(p)$  a singular term at  $p_F$  of the form Eq. (18), with  $A = a_1/\pi$ . For instance, at the equilibrium density  $\rho(\text{\AA}^{-3}) = 0.016\,35$ , we find  $A = 0.06(2)$ , being, however, unable at present to assess the size dependence of such estimate. An independent estimate of  $A$  is given by a perturbation calculation<sup>36</sup> for a dilute, hard-sphere, Fermi gas. To order  $(p_F R)^2$ ,

$$A_0 = 2 \frac{\nu - 1}{\pi^2} (p_F R)^2, \quad (21)$$

with  $R$  the radius of the Fermi particle. Evidently  ${}^3\text{He}$  at equilibrium is not at all dilute. Nevertheless, taking  $R = \sigma/2 \approx 1.3 \text{\AA}$ , one obtains  $A_0 \approx 0.20$ , which is of the same order of magnitude as our DMC estimate. In CBF theory one obtains,<sup>6</sup> instead,

$$A_{\text{CBF}} = \frac{2W_0}{\pi} p_F \frac{de^v(p_F)}{dp}, \quad (22)$$

where  $e^v(p)$  is the variational energy and  $W_0$  is an inverse energy parameter characterizing the imaginary part  $W(p, E)$  of the self-energy  $\Sigma(p, E)$ , close to the Fermi energy,

$$W(p, E) \approx W_0(E - e_F)^2, \quad E \rightarrow e_F. \quad (23)$$

If one takes  $W_0 \approx 2.5^\circ \text{K}^{-1}$  and  $de^v(p_F)/dp = \hbar^2 p_F / M_v$ ,  $M_v/M = 0.76$  from earlier work<sup>38</sup> where a model form of  $W(p, E)$  was fitted to the measured specific heat in  ${}^3\text{He}$ ,  $A_{\text{CBF}} \approx 21$  is obtained, which is two orders of magnitude larger than both the DMC and the perturbative estimate.

The effective mass  $M^*$  is related to the dispersion at  $p_F$  of the quasiparticle energy<sup>2</sup>

$$e(p) = \frac{\hbar^2 p^2}{2M} + \text{Re}\Sigma(p, e(p)), \quad (24)$$

according to  $\hbar^2 p_F / M^* = de(p_F)/dp$ . Thus<sup>39,6,10</sup>  $M^*/M = M_E M_K$ , with the  $K$  mass

$$M_K^{-1} = 1 + \frac{M}{\hbar^2 p_F} \frac{\partial}{\partial p} \text{Re}\Sigma(p, E)|_{E=e_F, p=p_F}, \quad (25)$$

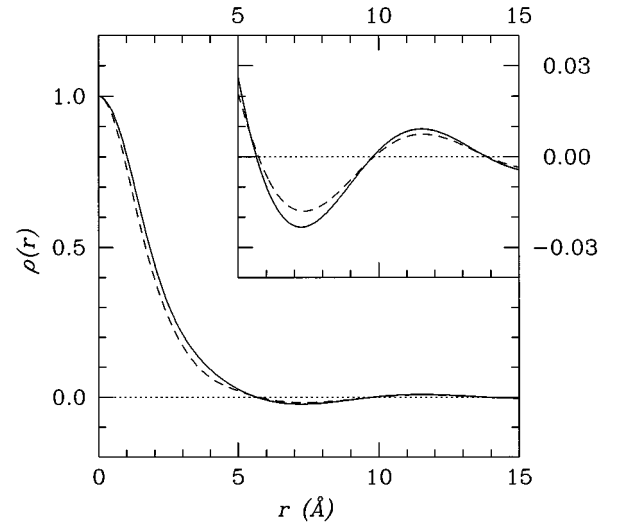


FIG. 12. The one-body density matrix  $\rho(r)$  of  ${}^3\text{He}$  at  $T=0^\circ \text{K}$  and  $\rho_e = 0.016\,35 \text{\AA}^{-3}$  (full curve). The dashed curve gives the product  $\rho_0(r)\rho_B(r)$ , with  $\rho_0(r)$  and  $\rho_B(r)$ , respectively, the density matrix for the ideal (uncorrelated) Fermi gas and the density matrix of a Bose  ${}^3\text{He}$ . The inset shows  $\rho(r)$  in the tail region.

and the  $E$  mass

$$M_E = 1 - \frac{\partial}{\partial E} \text{Re}\Sigma(\mathbf{p}, E)|_{E=e_F, p=p_F} = Z^{-1}. \quad (26)$$

Thus, the  $E$  mass is nothing but  $Z^{-1}$ , i.e., the strength of the quasi-particle pole at  $p_F$ .<sup>40,41</sup> However, we lack an estimate of the  $K$  mass to predict  $M^*$ . Hence we are planning to perform variational and transient estimate calculations of  $M^*$ , along the lines of an equivalent calculation for the two-dimensional electron gas.<sup>42,43</sup>

At the Fermi wave vector  $p_F$ , the momentum distribution  $n(p)$  has a discontinuity and, according to perturbation theory and to CBF's, at least the additional singular behavior of Eq. (18). It is known<sup>44</sup> that singularities dominate the large distance behavior of the Fourier transform of a generalized function, such as  $n(p)$ . This implies in particular that as  $r \rightarrow \infty$   $\rho(r) \approx Z\rho_0(r)$ , to leading order. On the other hand, using the parameters given in Table III, one can show that the first zero of the DMC density matrix at the equilibrium density (see also Fig. 7) is at  $p_F r = 5.62$ , which is not very different from  $p_F r = 5.72$ —the location of the first zero of  $\rho_0(r)$ . We therefore consider the approximate decoupling

$$\rho(r) = \rho_0(r)\rho_B(r), \quad (27)$$

where the function  $\rho_B(r)$  must satisfy  $\rho_B(0) = 1$ ,  $\lim_{r \rightarrow \infty} \rho_B(r) = Z$ , and we further choose it to be non-negative everywhere. It is tempting to take  $\rho_B(r)$  as the density matrix of a suitable Bose system, with a condensate fraction  $Z$ .

We have thus simulated a system of  ${}^3\text{He}$  with Bose statistics, at the equilibrium density of real  ${}^3\text{He}$ . We find a condensate fraction of 0.208(5), which within error bars agrees with our best estimate of  $Z = 0.21(2)$ . In Fig. 12 we compare our fit to the density matrix of  ${}^3\text{He}$  with the prediction of the approximate formula (27), using for  $\rho_B(r)$  the fit to the simulated density matrix of a Bose  ${}^3\text{He}$ . It is apparent



that the decoupling of Eq. (27) approximately holds. In fact Eq. (27) overestimates the kinetic energy by 14%, while underestimating the envelope of the tail of  $\rho(r)$  by about a 20%. Thus statistics and correlations in  ${}^3\text{He}$  decouple, within a reasonable accuracy, into those of an ideal (uncorrelated) Fermi gas and a Bose  ${}^3\text{He}$ , as far as  $\rho(r)$  is concerned.

## V. CONCLUSIONS

In this paper we have presented DMC calculations of the one-body density matrix and of the momentum distribution of liquid  ${}^4\text{He}$  and liquid  ${}^3\text{He}$  based on accurate trial wave functions with fully optimized pair and triplet pseudopotentials. For  ${}^3\text{He}$  the fermion sign problem has been avoided, by resorting to the fixed-node approximation. In particular, we used backflow nodes, which are more accurate than the simpler plane-wave nodes. We recorded our data in a form suitable for future use, in terms of analytical fits.

Our prediction for the condensate fraction of  ${}^4\text{He}$  is lower than in previous microscopic calculations, and we argued that these seem to be consistently related to the improved description of  ${}^4\text{He}$  afforded by the calculations presented here. We also found that our results are statistically consistent with the presence of a singular term in  $n(p)$ , as predicted earlier by Gavoret and Nozieres, in spite of the absence of explicit long-range correlations in our trial functions.

The discontinuity  $Z$  of  $n(p)$  at  $p_F$  in  ${}^3\text{He}$  is also predicted from our calculations to be sensibly lower than in previous variational calculation, and in substantial agreement with GFMC estimates. We have investigated the presence in the

$n(p)$  of logarithmic singularities, as predicted by approximate treatments. We find that our results are compatible with the presence of such terms. However, the strength of such a term agrees in order of magnitude with perturbation theory, whereas a CBF treatment with empirical parameters for the imaginary part of the optical potential implies a strength which differs from our prediction by two orders of magnitude.

We have also demonstrated that an approximate decoupling  $\rho(r) \approx \rho_0(r)\rho_B(r)$  holds, with  $\rho_0(r)$  and  $\rho_B(r)$ , respectively, the density matrix for the ideal Fermi gas and the density matrix of a Bose  ${}^3\text{He}$ . Thus statistics and correlation effects seem to decouple in  ${}^3\text{He}$ , as far as the density matrix is concerned. The Bose  ${}^3\text{He}$  has in fact a condensate fraction which agrees within error bars with the discontinuity  $Z$  found in the Fermi  ${}^3\text{He}$ .

We believe that the estimates given in this paper provide the most accurate information available to date for this kind on He. This is of particular importance for the condensate fraction in  ${}^4\text{He}$ , as its extraction from deep inelastic neutron scattering seems still not feasible. Using our accurate EMC trial functions, we also studied partially polarized  ${}^3\text{He}$ . We shall report on this study elsewhere.<sup>45</sup>

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