Final-State Effects on the Deep-Inelastic Response of Liquid ^{4}He

C. Carraro and S. E. Koonin
W. K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California 91125
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We calculate the deep-inelastic response of liquid ^{4}He. Using a universality hypothesis for the bridge function, we obtain a new, highly consistent ground-state Jastrow wave function with condensate fraction $n_0 \simeq 0.081$. The dynamics of final-state interactions is accounted for by a Monte Carlo sampling of the scattering wave function of the recoiling He atom. The results, in excellent agreement with recent neutron-scattering measurements, indicate that the response has a more complicated dependence on the structure of the ground state than is assumed by all previous theories.

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Deep-inelastic neutron scattering (DINS) from liquid ^{4}He (LHe) at very high momentum transfer offers the possibility of measuring the single-particle momentum distribution $n(k)$, and thus the Bose-Einstein condensate fraction n_0.[1] However, the naively expected signature of the condensate, a δ-function peak in the scaled structure factor $F \equiv (q/M)S(\mathbf{q},\omega)$ at energy transfer $\omega = q^2/2M$, is not seen in experiments performed at momentum transfers q as high as 23 Å^{-1}. This is because of finite experimental resolution and because of final-state interactions (FSI), i.e., strong scattering of the recoiling He atom in the liquid, resulting in the broadening of the free-particle recoil spectrum. Hence, comparison of experiment to theory requires the calculation not only of static properties, such as $n(k)$, but also of the dynamics that determine the FSI. Whereas the former can be essentially computed exactly [e.g., through Green's function[2] or path-integral Monte Carlo[3] (PIMC) methods], the latter have so far eluded all attempts of (stochastically) exact evaluation, except for the case of few-body systems.[4]

In this Letter, we report a calculation of the dynamic structure factor of LHe (at $T=0$ and saturated vapor pressure) in the high-momentum-transfer limit. An essential ingredient, and the starting point of our calculation, is a good ground-state wave function. We take the Jastrow form, $\psi = \prod_{i \neq j} f(r_{ij})$, which suitably describes the strong correlations between particles while offering great computational advantages. The pair-correlation function, which is known experimentally, is related to f by

$$g(r) = f^2(r)\exp[-g(r)+1+c(r)+B(r)],$$

where the direct correlation function c is obtained from g through the Ornstein-Zernicke equation, and B is an infinite set of elementary diagrams, termed the "bridge function." A common assumption (the hypernetted-chain approximation) is to take B to be at most the sum of a handful of diagrams, and to choose f to minimize the variational ground-state energy. This is known to describe rather poorly the structure of systems with strong short-range repulsion.[5] A better assumption, based on the short-range character of B, is the universality hypothesis of Rosenfeld and Ashcroft,[6] who showed that, with great accuracy, the bridge function, suitably scaled, is independent of the details of the short-range potential. Thus, B for LHe can be taken to be that of a hard-sphere gas at packing fraction 0.2.[6] Given this B, we can extract f from the experimental g. The latter is obtained as the Fourier transform of the static structure factor $S(k)$, measured by neutron scattering[7] ($0.8 \leq k \leq 10.8$ Å^{-1}), x-ray scattering[8] ($0.13 \leq k \leq 1.12$ Å^{-1}), and extrapolated linearly for $k \to 0$ to give the proper phonon spectrum. Consistency checks can assess the quality of our wave function. The pair-correlation function calculated by MC sampling of $|\psi|^2$ shows very good agreement with the input experimental g (Fig. 1). The total energy per particle is $E/N = -6.4$ K (close to the experimental value of -7.2 K).

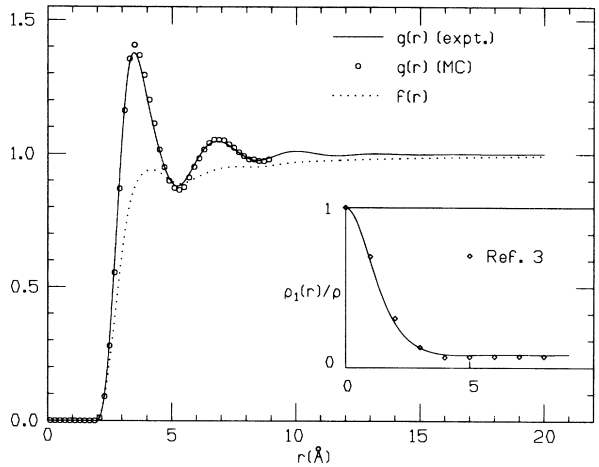

FIG. 1. Pair-correlation function for ^{4}He. The solid line is the experimental result at 1 K. The circles are the ground-state calculation, assuming a Jastrow wave function and the universal bridge function (the Jastrow factor is the dotted line). Inset: The calculated one-body off-diagonal density matrix (the diamonds are the PIMC results at $T = 1.18$ K).

Success in the computation of the dynamical effects hinges on the essentially one-dimensional character of the problem. Although our expressions can be given a firm theoretical foundation,[9] they can be derived intuitively as follows. In the impulse approximation (IA) (i.e., in the limit of scattering-free recoil), one finds

$$\frac{q}{M}S_{\mathrm{IA}}(\mathbf{q},\omega)\equiv F_{\mathrm{IA}}(Y)=\frac{1}{2\pi\rho}\int_{-\infty}^{+\infty}ds\,\rho_1(s\hat{\mathbf{z}})e^{isY}, \qquad (1)$$

where $\rho_1(\mathbf{r})$ is the one-body density matrix, related to $n(\mathbf{k})$ by Fourier transformation, ρ is the number density, $\hat{\mathbf{z}}\equiv\mathbf{q}/q$ is the direction of recoil, and $Y=M\omega/q-q/2$ is the component of the momentum of the He atom along $\hat{\mathbf{q}}$ before it is struck by the neutron. Thus, in the IA, DINS simply measures the longitudinal one-body momentum distribution of the ground state.

If we now allow for interactions during the recoil, it is easy to show that the only relevant scattering events at high q are those in which the recoiling atom strikes a background atom. We therefore need the propagator for a single atom moving in the instantaneous potential generated by the static background. At high momentum transfers, we express this propagator through the scattering wave functions of the recoiling particle,[9] obtaining a q-dependent scaled response (hereafter, we assume ψ to have unit norm, and set $\hbar=1$)

$$F(q,Y)=\int_{-\infty}^{+\infty}\frac{ds}{2\pi}e^{isY}\int d^3r_1\cdots d^3r_N\,\psi(\mathbf{r}_1+s\hat{\mathbf{z}},\ldots,\mathbf{r}_N)\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\frac{\phi_q(z_1+s)}{\phi_q(z_1)}\exp\left[-is\left[q-\frac{MV(z_1+s)}{q}\right]\right], \qquad (2)$$

where ϕ_q is the 1D outgoing scattering state of the recoiling particle in the potential

$$V(z)=\sum_{j=2}^{N}V_{1j}[x_{j1}^2+y_{j1}^2+(z_j-z)^2]^{1/2}$$

due to all other particles along the straight line of recoil. This state satisfies

$$\left[\frac{d^2}{dz^2}+q^2-2MV(z)\right]\phi_q(z)=0, \qquad (3)$$

which is reminiscent of the eikonal scattering equation (to which it reduces with further approximations). Traditionally, the effects of FSI are described by a "broadening" function $R(q,Y)$ defined as

$$F(q,Y)=\int_{-\infty}^{+\infty}dY'F_{\mathrm{IA}}(Y')R(q,Y-Y'). \qquad (4)$$

It is most useful to visualize the scattering process in real space, where the MC calculation is done. Thus we Fourier transform (1) to get

$$\hat{F}_{\mathrm{IA}}(s)=\rho_1(s\hat{\mathbf{z}})=\int d^3r_1\cdots d^3r_N\,\psi(\mathbf{r}_1+s\hat{\mathbf{z}},\mathbf{r}_2,\ldots,\mathbf{r}_N)\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N). \qquad (5)$$

Here s represents the recoil distance of the struck particle, and $\hat{F}_{\mathrm{IA}}(s)$ is the overlap of the ground-state wave function with itself, after displacing an atom by a distance s. The presence of the condensate is signaled by a nonzero limit of this overlap as $s\rightarrow\infty$: $\lim_{s\rightarrow\infty}\hat{F}(s)=n_0$. Similarly, from (2) we find

$$\hat{F}(q,s)=\int d^3r_1\cdots d^3r_N\,\psi(\mathbf{r}_1+s\hat{\mathbf{z}},\ldots,\mathbf{r}_N)\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\frac{\phi_q(z_1+s)}{\phi_q(z_1)}\exp\left[-is\left[q-\frac{MV(z_1+s)}{q}\right]\right]. \qquad (6)$$

Thus $\hat{F}(q,s)$ probes not only the overlap of two ground-state configurations, but also the extent to which the recoiling He atom scatters while it moves from the initial to the final position. Weak scattering will slightly dephase the initial and final states, giving $\hat{F}$ an imaginary part. Strong scattering will deflect an atom away from the straight-line recoil, effectively resulting in absorption (i.e., in a decrease in the real part of $\hat{F}$ with respect to $\hat{F}_{\mathrm{IA}}$). Both effects are governed by the presence of the surrounding medium and by its structure, as is evident from Eqs. (2) and (3). The interplay between ground-state structure and FSI, whose importance has been previously pointed out by Silver,[10] can be properly accounted for only by a fully consistent treatment of Eqs. (3) and (6).

We readily cast Eq. (6) in a form suitable for MC evaluation. We simulate a cubic box ($L=18.05$ Å, $N=128$) with periodic boundary conditions. Ground-state configurations can be generated according to $|\psi|^2$ with the Metropolis algorithm. Once this is done, atom i is displaced in the z direction by a distance $s_{\max}=L/2$, and Eq. (3) is integrated backwards, from $z_i+s_{\max}$ to z_i, imposing outgoing boundary conditions at $z_i+s_{\max}$.[11] We use the Aziz pair potential.[12]

Figure 2 shows the results of calculations of $\hat{F}$ for

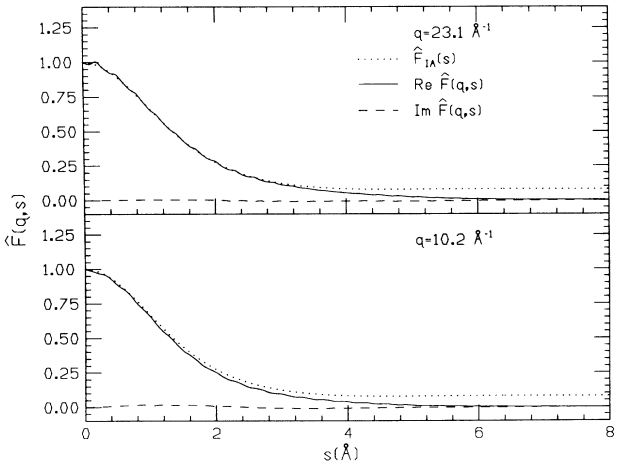

FIG. 2. Y Fourier transform of the structure factor at $q=23.1$ and 10.2 Å^{-1}. The IA coincides with $\rho_1(s)/\rho$ (Fig. 1, inset).

$q=10.2$ and 23.1 Å^{-1}, together with the IA, Eq. (5).[13] Note that a signature of long-range order is completely absent in the dynamic response [$\lim_{s\to\infty}\hat{F}(s)=0$]. Comparison to experiment is possible after convolving the calculated response with the measured instrumental resolution,[14] $R_q^{\rm expt}(Y)$. This is essential at the higher values of q, where $R_q^{\rm expt}(Y)$ is rather broad. For lower q's, FSI account for essentially all the broadening of the condensate peak; therefore, a theory of FSI is most stringently tested in this regime. The predicted response is shown in Fig. 3, together with the experimental data.[15] In each case, we show for comparison the results obtained with the IA [broadened by $R_q^{\rm expt}(Y)$] without FSI.

Multiple-scattering (MS) series have been derived for the FSI, and finite-order truncations thereof have been compared to the DINS data.[16] In these theories the $\delta(Y)$ condensate peak is ultimately broadened only by the instrumental resolution. Our calculations, which contain all orders of a MS expansion, show that this is incorrect, and that the peak is broadened by FSI even in the case of infinite instrumental resolution (Fig. 2), preventing the straightforward extraction of n_0 from experiment.

In Fig. 4, we present calculations of the FSI broadening $R(q,Y)$ for various q. Note that $R(q,Y)$ becomes sharper as q increases from 10 to 23 Å^{-1}. In contrast, hard-core perturbation theory[10] (HCPT) shows very little change in $R(q,Y)$ as a function of q, therefore predicting that $F(q,Y)$ is too large and narrow at the lowest q's.[14] This is perhaps not surprising, because HCPT appears to be valid only in the $q\to\infty$ limit for strictly hard-core interactions, whereas Eqs. (2) and (3) are exact through $O(1/q)$ for arbitrary potentials.

The most significant feature of the present work is that the full many-body density matrix is retained.[17] All previous theories of FSI involve a reduction to the two-body density matrix ρ_2, which is usually in turn approximated through ρ_1 and $g(r)$.[18] This approximation allows $R(q,Y)$ to be expressed solely in terms of $g(r)$, which is known experimentally, and thus, in principle, one can extract the momentum distribution from Eq. (4). Unfortunately, our calculations show that the FSI have a more complicated dependence on the structure of the initial state than is naively accounted for by the radial pair correlation $g(r)$, at least at the smaller momentum transfers where the experimental resolution is sharpest. High-resolution measurements at larger q are needed if one is to attempt an extraction of n_0 uniquely from experimental input. At present, the condensate fraction remains a theoretical input to calculations that are compared to the data *a posteriori*.

In summary, we have carried out the first consistent calculations of deep-inelastic neutron scattering from liquid ^{4}He and have shown that both the q and the Y

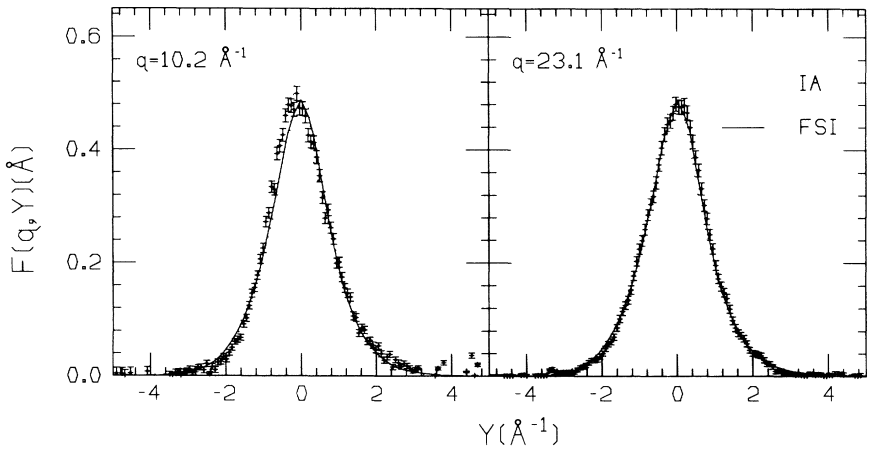

FIG. 3. The deep-inelastic response at $q=23.1$ and 10.2 Å^{-1} (data points at $T=0.75$ K from Ref. 15). Both our ground-state calculations (solid line) and the impulse approximation (dotted line) have been broadened by the measured instrumental resolution $R_q^{\rm expt}(Y)$ (note that the latter is much sharper at the lower q, as shown by the IA).

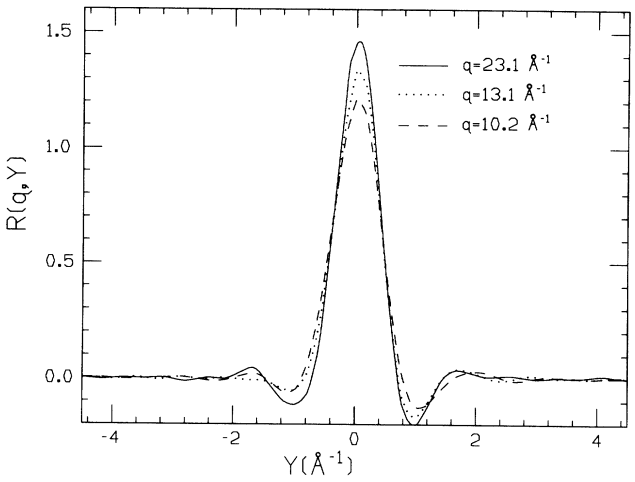

FIG. 4. Calculated FSI broadening function.

dependence of the data are very well reproduced by a (modified) eikonal description of the final-state interactions and by a ground-state wave function with condensate fraction $n_0 \simeq 0.081$.

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[17]Our Jastrow pair wave function omits triplet correlations, which are known to be essential to the quantitative variational determination of the ground-state energy. This should not be a serious problem in DINS calculations, which are far more dependent on the ground-state structure than on the energy. The former is described very well by our wave function. Triplet correlations might significantly influence the condensate fraction. Further investigations should focus on this possibility and on whether it is the cause of the small discrepancy between experiment and calculations that remains visible in Fig. 3.

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