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Antisymmetric part of the dynamic structure function of liquid ^{4}He

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At large momentum transfers it is convenient to express the dynamic structure function $S(k,\omega)$ as the sum of a symmetric part about $\omega=k^2$ and an antisymmetric part. The latter is zero in the impulse approximation, and its leading contribution is given by $S_A(y)/(2k)^2$, where $y=(\omega-k^2)/2k$ is the usual scaling variable. We calculate the integrals of $S_A(y)$, weighted with y, y^3, and y^5 in liquid ^{4}He using sum rules as suggested by Sears. Polynomial expansions are used to construct models of $S_A(y)$ which appear to be in qualitative agreement with the observed antisymmetric part at large values of k.

Deep inelastic neutron scattering experiments[1-7] measure the dynamic response function $S(k,\omega)$ at large values of k and ω. If the impulse approximation[8] (IA) becomes valid at large k and ω, then these data can be directly used to extract the momentum distribution $n(p)$ of atoms in the target. However, it is well known[9-16] that, in many systems like helium liquids, corrections to the IA must be taken into account in order to extract the $n(p)$ from the available data. Many theorists[10,17,18] have predicted that in helium liquids these corrections would persist over the entire range of momentum transfers of practical interest, and thus, have generated a significant interest in their calculation.

It is convenient to introduce the scaling variable[19] y:

$$\omega\equiv k^2+2ky\ , \tag{1}$$

in units $\hbar^2/2m=1$, or equivalently $A^{-2}=6.06$ K in liquid ^{4}He, and following Sears,[9,10] obtain the expression

$$2kS(k,\omega)=S_{\mathrm{IA}}(y)+\frac{1}{2k}S_A(y)+\Delta_S(k,y)+\Delta_A(k,y)\ , \tag{2}$$

where

$$S_{\mathrm{IA}}(y)=\frac{1}{4\pi^2\rho}\int_{|y|}^{\infty}pdp\,n(p)\ , \tag{3}$$

is symmetric in y, ρ is density of atoms, $S_A(y)/2k$ gives the leading antisymmetric part,

$$S_A(y)=-S_A(-y)\ , \tag{4}$$

and $\Delta_S(k,y)$ and $\Delta_A(k,y)$ give corrections to the leading symmetric and antisymmetric parts. When the interparticle interactions are well behaved these corrections are of order k^{-2}; their asymptotic behavior, when the interaction contains a strong repulsive core, is being studied by many authors.[14-18]

The $S_A(y)$ is particularly important in nuclear physics,[20] where only the response at negative values of y, measured by scattering of high-energy electrons, can be used to study the $n(p)$ of nucleons in a nucleus. In helium liquids the antisymmetric part of the correction can be eliminated by symmetrizing the data. Nevertheless it is, at least for well-behaved interactions, the leading k^{-1} correction to IA, and thus, must be included in any realistic treatment of the corrections to the IA.

It is well known[21] that the ω^n weighted integrals of $S(k,\omega)$, the so-called sum rules, can be calculated from the ground-state wave function,

$$\int_0^\infty S(k,\omega)\omega^n d\omega=\frac{1}{N}\langle 0|\rho_k[H,\ldots,[H,\rho_k^{+}],\ldots]|0\rangle\ , \tag{5}$$

where N is the total number of atoms,

$$\rho_k=\sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}\ , \tag{6}$$

and there are n commutators on the right-hand side. The sums $\bar{S}_n(k)$, for odd values of n,

$$\begin{aligned}\bar{S}_n(k)&\equiv\frac{1}{(2k)^n}\int_0^\infty S(k,\omega)(\omega-k^2)^n d\omega\\&=\frac{1}{2k}\int_{-k/2}^{\infty}S_A(y)y^n dy+\int_{-k/2}^{\infty}\Delta_A(k,y)y^n dy\ ,\end{aligned} \tag{7}$$

can also be calculated from the Eq. (5), and they give direct information about $S_A(y)$. We obtain

$$\bar{S}_n(k)=\frac{1}{2k}(-1)^{(n+1)/2}\sum_{m=1}^{n-1}(n-m)\begin{pmatrix}n\\m-1\end{pmatrix}\sum_{j(\neq i)}\langle 0|[\partial_{z,i}^{n-m}v(r_{ij})]\partial_{z,i}^{m-1}|0\rangle+O(k^{-2})\ . \tag{8}$$

The terms of order k^{-2} (and higher) contain two (or more) interactions v; they give the contribution of $\Delta_A(k,y)$ to $\bar{S}_n(k)$, and are not studied in the present paper.

If we define quantities s_n to be the odd moments of $S_A(y)$,

$$s_n\equiv\int_{-k/2}^{\infty}S_A(y)y^n dy\ , \tag{9}$$

we find

$$s_1 = 0\,, \tag{10}$$

$$s_3 = \tfrac{1}{2} \sum_{j(\neq i)} \langle 0 | [\partial^2_{z,i} v(r_{ij})] | 0 \rangle\,, \tag{11}$$

$$s_5 = \sum_{j(\neq i)} \{ \langle 0 | [\partial^4_{z,i} v(r_{ij})] | 0 \rangle - 5 \langle 0 | [\partial^2_{z,i} v(r_{ij})] \partial^2_{z,i} | 0 \rangle \}\,. \tag{12}$$

The s_3 depends only upon the pair distribution function $g(r)$:

$$s_3 = \frac{1}{2} \frac{4\pi\rho}{3} \int_0^\infty \left[v''(r) + \frac{2v'(r)}{r} \right] g(r) r^2 dr\,, \tag{13}$$

and it has been calculated with realistic potentials and the exact $g(r)$ obtained with the Green's function Monte Carlo (GFMC) method.[22,23]

The s_5, and higher sum rules, involve gradients of the ground-state wave function, and thus cannot be obtained from distribution functions alone. In the present work we estimate s_5 with the simplest Jastrow approximation,

$$\Psi_0 = \prod_{i<j} f_2(r_{ij})\,, \tag{14}$$

for the ground-state wave function of liquid ^{4}He. It is convenient to define

$$s_5 = A - 5B\,; \tag{15}$$

$$A = \frac{4\pi\rho}{5} \int_0^\infty \left[v''''(r) + \frac{4v'''(r)}{r} \right] g(r) r^2 dr\,, \tag{16}$$

can be calculated easily from the GFMC $g(r)$. The term B, with the Jastrow approximation, is given by

$$B = B_1 + B_2 + B_3\,, \tag{17}$$

$$B_1 = \rho \int d^3r\, g(r) [\partial^2_z v(r)] \frac{\partial^2_z f_2(r)}{f_2(r)}\,, \tag{18}$$

$$B_2 = \rho^2 \int d^3r_{ij} d^3r_{ik}\, g_3(\mathbf{r}_{ij},\mathbf{r}_{ik}) [\partial^2_{z,i} v(r_{ij})] \left[\frac{\partial^2_{z,i} f_2(r_{ik})}{f_2(r_{ik})} + 2 \frac{\partial_{z,i} f_2(r_{ij})}{f_2(r_{ij})} \frac{\partial_{z,i} f_2(r_{ik})}{f_2(r_{ik})} \right], \tag{19}$$

$$B_3 = \rho^3 \int d^3r_{ij} d^3r_{ik} d^3r_{il}\, g_4(\mathbf{r}_{ij},\mathbf{r}_{ik},\mathbf{r}_{kl}) [(\partial^2_{z,i} v(r_{ij})] \frac{\partial_{z,i} f_2(r_{ik})}{f_2(r_{ik})} \frac{\partial_{z,i} f_2(r_{il})}{f_2(r_{il})}\,. \tag{20}$$

It is easy to calculate B_1 exactly, and the superposition approximation

$$g_3(\mathbf{r}_{ij},\mathbf{r}_{ik}) \approx g(r_{ij}) g(r_{ik}) g(r_{jk})\,, \tag{21}$$

$$g_4(\mathbf{r}_{ij},\mathbf{r}_{ik},\mathbf{r}_{kl}) \approx g(r_{ij}) g(r_{ik}) g(r_{il}) g(r_{jk}) g(r_{jl}) g(r_{kl})\,, \tag{22}$$

is used for the three- and four-body distribution functions in B_2 and B_3. The calculation of B_3 is further approximated by expanding g_4 in powers of short-ranged functions $h_{ij} = g(r_{ij}) - 1$:

$$g_4(\mathbf{r}_{ij},\mathbf{r}_{ik},\mathbf{r}_{kl}) \approx g(r_{ij}) g(r_{ik}) g(r_{il}) (1 + h_{jk} + h_{jl} + h_{kl} + h_{jk}h_{jl} + h_{jk}h_{kl} + h_{jl}h_{kl} + h_{jk}h_{jl}h_{kl})\,. \tag{23}$$

The three terms 1, h_{jk}, and h_{jl} give zero contribution; the h_{kl} term gives the largest contribution ($\sim -8A^{-6}$), the terms quadratic in h give contributions of order $2.5\,A^{-6}$ each, and the contribution of the $h_{jk}h_{jl}h_{kl}$ term, expected to be $\sim -1A^{-6}$, is neglected.

The calculated values are given in Table I for the Aziz[24] and Lennard-Jones (LJ) models of the interatomic potential. The appropriate GFMC $g(r)$ of the Courant group[22,23] are used. The McMillan $f_2(r)$,

$$f_2(r) = \exp[-\tfrac{1}{2}(b/r)]^5\,, \tag{24}$$

$$b = 1.17\sigma = 2.99A\,, \tag{25}$$

is used for calculations with the LJ potential, and an optimized $f_2(r)$ obtained by the paired phonon analysis[25] is used with the Aziz potential.

The calculation of s_5 can be significantly improved by considering ground-state wave functions with pair and triplet correlations,[26] and by using exact many-body distribution functions via a Monte Carlo integration of the expectation values. The triplet correlations influence the pair distribution functions and the binding energy by $\sim 10\%$, and assuming that they have a similar effect on s_5, we can expect the present results to change by $\sim 10\%$.

The values of s_3 and s_5 can be used to test calculations of $S_A(y)$. They can also be used to construct crude models of $S_A(y)$ as follows. Let $S_A(y)$ be given by

$$S_A(y) = \sum_{\text{odd}\,n} b_n \mathcal{P}_n(y) S_{\text{IA}}(y)\,, \tag{26}$$

TABLE I. The s_3 and s_5 in liquid ^{4}He.

Term	Aziz	LJ
s_3	$12.4A^{-4}$	$10.1A^{-4}$
s_5	$198A^{-6}$	$133A^{-6}$
A	$462A^{-6}$	$498A^{-6}$
B	$53A^{-6}$	$73A^{-6}$
B_1	$111A^{-6}$	$126A^{-6}$
B_2	$-57A^{-6}$	$-52A^{-6}$
B_3	$-1A^{-6}$	$-1A^{-6}$

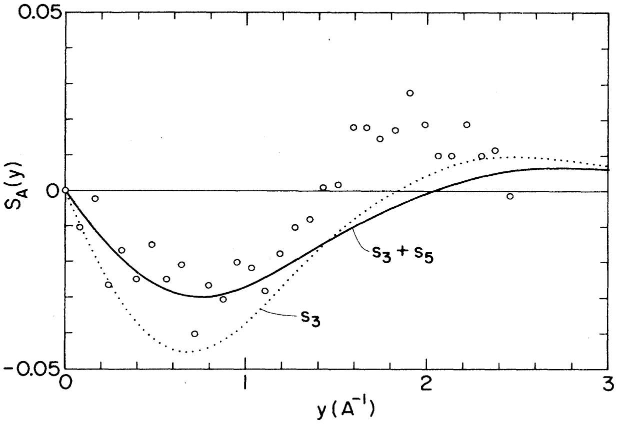

FIG. 1. The two approximations to $S_A(y)$ calculated with the Aziz potential compared with the antisymmetric part of $S(k,\omega)/(2k)^2$ measured at $k=10A^{-1}$ from Ref. 1.

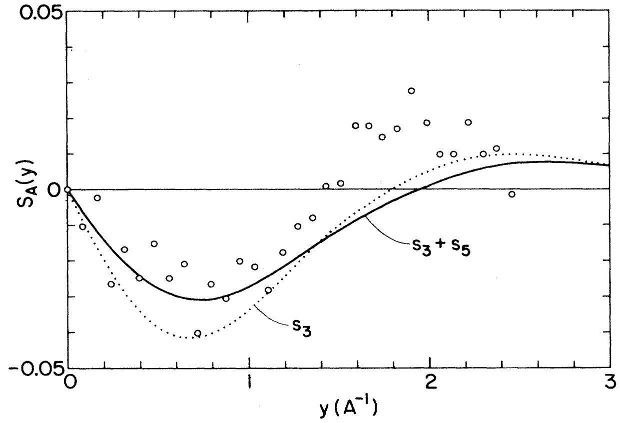

FIG. 2. The same as in Fig. 1, calculated with the LJ potential.

where P_n are polynomials:

$$\mathcal{P}_n(y)=\sum_{\text{odd}\,m<n}\xi_{n,m}y^m\,, \tag{27}$$

$$\langle\mathcal{P}_m|\mathcal{P}_n\rangle\equiv\int_{-\infty}^{+\infty}\mathcal{P}_m(y)\mathcal{P}_n(y)S_{\mathrm{IA}}(y)dy=\delta_{m,n}\,, \tag{28}$$

so that

$$b_n=\sum_{\text{odd}\,m<n}\xi_{n,m}s_m\,. \tag{29}$$

We have obtained two approximations to $S_A(y)$. In the first $b_{n>3}=0$ and $b_1(=0)$ and b_3 are determined from s_1 and s_3, and in the second $b_{n>5}=0$ and $b_{n<5}$ are determined from $s_{n\leq 5}$. The variational[27] $n(p)$, which has recently been shown to fit experimental data,[7] is used to generate the weight function $S_{\mathrm{IA}}(y)$. With the Aziz potential we obtain $b_3=4.42$ and $b_{n\neq 3}=0$ in the first approximation, and $b_3=4.42$, $b_5=1.83$, and $b_{n\neq 3,5}=0$ in the second. The two approximations are compared with the antisymmetric part of measured[1] $S(k,\omega)$ at $k=10A^{-1}$, divided by $(2k)^2$ in Figs. 1 and 2. While the second approximation (solid line) is clearly better than the first one, it does not completely fit the data; the position of the zero of $S_A(y)$, in particular, is shifted from the experimental value.

There is a large class of systems (hydrogen atom, for example) such that $S(k,\omega)$ has divergent ω^n weighted moments for big enough n. On the other hand, in systems with LJ-like interactions, these moments exist to all orders due to e^{-c/r^5} behavior of the many-body distribution functions at small interatomic distances r. Usefulness of these moments in reconstruction of $S(k,\omega)$ via some sort of orthogonal polynomial expansion has recently been questioned.[16]

However, the results of the present calculations suggest that just the lowest few terms of these expansions provide a qualitative description of the $S_A(y)$. A few more values of s_n for $n=7, 9, \ldots$ may be needed to obtain a quantitative description of the $S_A(y)$. Unfortunately, it appears that calculations of $s_{n>3}$ are not trivial. For example, there is a large cancellation between the leading two-body integrals A and B_1 that contribute to s_5. A wrong negative value of s_5 is obtained if only the two-body integrals are retained and B_2 and B_3 are neglected. These cancellations appear to persist for higher s_n.

Comparison of the present results with experimental data suggests that at $k=10A^{-1}$, the $S_A(y)/(2k)^2$ gives a large part of the total antisymmetric part of $S(k,\omega)$. Thus, at $k>10A^{-1}$ it may be possible to treat $\Delta_A(k,y)$ as a correction. In principle the s_n are sensitive to the interatomic potentials; however, comparison of values obtained with the Aziz and LJ potentials indicates that the s_3 and s_5 need to be determined with errors smaller than 10% to study models of interatomic potentials.

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