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## THEORETICAL LIQUID STRUCTURE FUNCTION FOR LIQUID $He^4$ AT $T=0$†

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The Bijl-Feynman dispersion relation

$$\mathcal{E}(K)=\hbar^2K^2/2mS(K) \tag{1}$$

expresses the energy of an elementary excitation in a condensed boson system at $T=0$ in terms of the liquid structure function $S(K)$. For small values of $K$ the excitations are phonons governed by the linear relation $\mathcal{E}(K)=\hbar KC$ (in which $C$ is the velocity of first sound). Consequently, in the phonon region,

$$S(K)=\hbar K/2mC. \tag{2}$$

Equation (2) determines the slope of the liquid structure function at the origin.

The experimentally measured $S(K)$ for liquid $He^4$ (experimental values extend down to $K=0.8$ Å$^{-1}$) may be extrapolated to the origin by a fairly smooth curve. However, the slope at the origin determined in this manner does not agree with Eq. (2). This apparent discrepancy was noticed sometime ago by Jackson[1] and independently by Miller, Pines, and Noziéres.[2] The latter authors developed the consequences of the apparent discrepancy and pointed out that the experimental evidence is consistent with the occurrence of a shoulder on the $S(K)$ curve in the neighborhood of $K=0.6$ Å$^{-1}$ and indeed strongly supports the existence of such a shoulder.

The purpose of this Letter is to report a theoretical calculation of $S(K)$ which exhibits the shoulder at the predicted position. I start from an assumed Lennard-Jones 6-12 type potential for the interaction between two helium atoms and attempt to determine the best possible Jastrow-type trial function to describe the ground state. The actual calculations begin with an assumed form $g(r,\alpha)$, for the radial distribution function. The free parameters $\alpha$ generate a family of possible radial distribution functions. For given $\alpha$, the expectation value of the kinetic energy is computed by an iteration-variation algorithm based on finding the maximum value of the Wu-Feenberg functional $J$.[3] The expectation value of the potential energy is given immediately in terms of $g(r,\alpha)$. Thus the expectation value of the Hamiltonian $H$ is found as a function of $\alpha$. The minimum value of this function in the $\alpha$ space then selects out a best radial distribution function from the $g(r,\alpha)$ family of functions. These results will be reported in greater detail at the conclusion of calculations now in progress.

The liquid structure function is computed from the relation

$$S(K,\alpha)=1+\rho\int e^{i\vec{K}\cdot\vec{r}}[g(r,\alpha)-1]d\vec{r}$$
$$=1+\frac{4\pi\rho}{K}\int_0^\infty r\sin Kr[g(r,\alpha)-1]dr. \tag{3}$$

Several families of trial functions, $g(r,\alpha)$, have been studied. The functions $S(K)$ generated by the more successful of these all exhibit the shoulder mentioned earlier. The common features of the trial functions which put a shoulder on the $S(K)$ curve in the predicted neighborhood are (1) the range over which $g(r)$ is effectively zero, (2) the rising slope of $g(r)$, and (3) the mag-

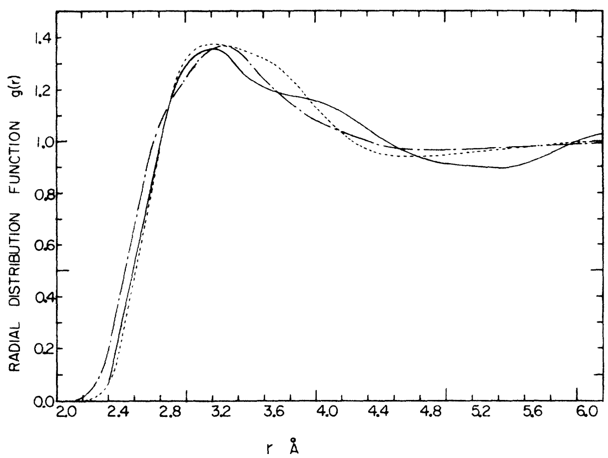


FIG. 1. Radial distribution function $g(r)$; solid line: experimental data of Goldstein and Reekie as normalized by Wu; dashed line: form *B* in text; dash-dot line: form *A* in text.

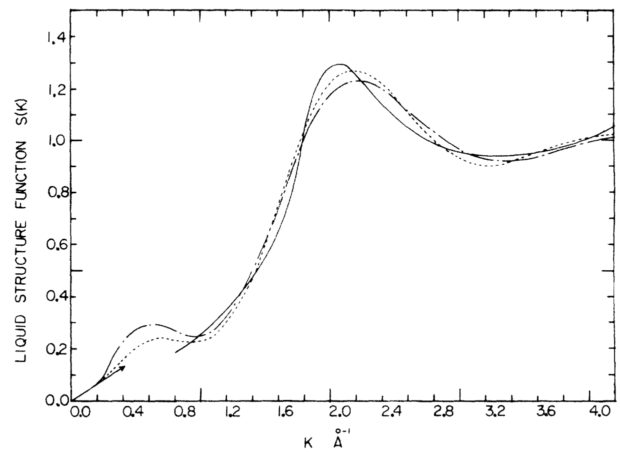


FIG. 2. Liquid structure function $S(K)$; solid line: experimental data of Goldstein and Reekie as normalized by Wu; dashed line: calculated from form *B* of $g(r)$; dash-dot line: calculated from form *A* of $g(r)$; arrow: small-$K$ behavior of $S(K)$ given by Eq. (2).

nitude and width of the nearest neighbor peak. These also are the features in which the trial functions resemble closely the experimentally determined $g(r)$ [as the Fourier transform of the observed $S(K)$]. Two of the functions used are shown in Fig. 1 along with the experimental curve of Goldstein and Reekie[4] as normalized by Wu.[3]

The theoretical forms are written

$$g(r)=g_0(r)+\delta_1(r), \tag{4}$$

subject to the normalization conditions

$$\rho\int[g_0(r)-1]d\vec{r}=-1,$$
$$\int\delta g_1(r)d\vec{r}=0. \tag{5}$$

Form A is

$$g_0(r)=(C+1)\exp\left[-\left(\frac{d}{r}\right)^{10}\right] -c\exp\left[-(1+z)\left(\frac{d}{r}\right)^{10}\right],$$

$$\delta g_1(r)=A\left\{\left(\frac{d}{r}\right)^{16}\exp\left[-(1+y)\left(\frac{d}{r}\right)^{10}\right] -B\left(\frac{d}{r}\right)^{8}\exp\left[-(1+q)\left(\frac{d}{r}\right)^{10}\right]\right\}, \tag{6}$$

with $d=2.6$ Å, $z=4$, $A=70$, $y=20$, $q=350$ giving the lowest energy found so far. The parameters $C$ and $B$ are determined by the normalization conditions of Eq. (5). Form *B* is

$$g_0(r)=\exp\left[-\left(\frac{d}{r}\right)^{6}\right]\left[1+a\left(\frac{d}{r}\right)^{6}+b\left(\frac{d}{r}\right)^{12}\right],$$

$$\delta g_1(r)=A\exp\left[-(1+z)\left(\frac{d}{r}\right)^{6}\right] \times\left(\frac{d}{r}\right)^{6}\left[1-B\left(\frac{d}{r}\right)^{6}+C\left(\frac{d}{r}\right)^{12}\right], \tag{7}$$

with $d=3.34$ Å, $a=0.8$, $A=0.2$, $B=100$, $z=6$. As before, the remaining parameters $b$ and $C$ are fixed by the normalization conditions.

The liquid structure functions resulting from Eqs. (6) and (7) are shown in Fig. 2 along with the Goldstein and Reekie curve as normalized by Wu.[3] Since the asymptotic behavior of the trial functions is essentially arbitrary, the computed $S(K)$ are not expected to have the correct slope at the origin. For this reason the functions $S(K)$ are computed only down to $K=0.2$ Å$^{-1}$ and continued to the origin by the smooth interpolation.

These results should help to direct attention to the difficult experimental problem of measuring $S(K)$ down to $K=0.4$ Å$^{-1}$ at $T\leq 1$°K.

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