Scaling and final-state interactions in deep-inelastic neutron scattering

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The momentum distributions of atoms in condensed matter can be determined by neutron inelastic scattering experiments if the momentum transfer $\hbar q$ is large enough for the scattering to be described by the impulse approximation. This is strictly true only in the limit $q \to \infty$ and, in practice, the experimentally determined momentum distributions are distorted by final-state interactions by an amount that is typically 2% to 8%. In this paper we develop a self-consistent method for correcting for the effect of these final-state-interaction effects. We also discuss the Bjorken-scaling and y-scaling properties of the thermal-neutron scattering cross section and demonstrate, in particular, the usefulness of y scaling as an experimental test for the presence of residual final-state interactions.

I. INTRODUCTION

In the last few years there has been a growing interest in the experimental determination of atomic momentum distributions in condensed matter by means of neutron inelastic scattering experiments at large momentum transfer, $\hbar q$. These deep-inelastic neutron scattering experiments, which have been mostly confined to the range $5 \lesssim q \lesssim 20$ Å^{-1}, have yielded momentum distributions for liquid[1–5] and solid[6] helium and liquid neon.[7] The most notable achievement of this work has been the determination[3–5] of the condensate fraction of superfluid helium from the observed temperature variation of the momentum distributions. This work is certain to increase in the future as high-resolution neutron inelastic scattering measurements become possible at even larger values of q using the high epithermal neutron fluxes available from spallation sources. For example, Brugger *et al.*[8] have recently measured the inelastic scattering in liquid helium at $q = 83$ Å^{-1} with an energy resolution of a few percent. They have also determined the momentum distributions for hydrogen in various chemical environments and for pyrolytic graphite.

The experimental determination of atomic momentum distributions by deep-inelastic neutron scattering is based on the impulse approximation.[9] This approximation is asymptotically exact[10,11] as $q \to \infty$, but for the finite values of q at which the experiments are performed the scattered neutron distributions are distorted by interatomic interference and final-state-interaction effects that limit the accuracy with which the momentum distributions can be determined. The interatomic interference effects have an oscillatory dependence on q and, hence, can be largely eliminated[3] by averaging the data over a suitable range of q values. The final-state-interaction effects are[10,11] of order q^{-1}. However, if the scattered neutron distributions are symmetrized about the recoil energy, the q^{-1} terms all cancel,[2] and one is left with residual final-state-interaction effects that are of order q^{-2}. The main purpose of the present paper is the development of a self-consistent method of correcting for these residual q^{-2} effects.

The use of deep-inelastic scattering for the experimental determination of momentum distributions is, of course, not limited to thermal-neutron scattering. The Compton scattering of x rays,[12–23] γ rays,[24,25] and electrons[26,27] has long been used for the determination of electron momentum distributions in atoms, molecules, and crystals. For example, it was Compton scattering that provided the first experimental verification[12] of the Fermi-Dirac distribution for the conduction electrons in metals. The momentum distributions of nucleons in nuclei have similarly been determined by inelastic scattering experiments with high-energy protons[28–31] and electrons,[32–35] and the momentum distribution of quarks in nucleons has been studied by the deep-inelastic scattering of electrons,[36–38] muons,[39–41] and neutrinos.[42] In fact, deep-inelastic lepton-nucleon scattering provides the most direct proof for the actual existence of quarks.[43]

In all the above applications of deep-inelastic scattering the general expressions for the scattering cross section have a similar basic structure, so that the method developed in this paper for correcting for final-state interactions in the context of thermal-neutron scattering may also be applicable elsewhere. Conversely, some of the results obtained in these other fields are applicable to the analysis of thermal-neutron scattering data. A case in point is the scaling of the deep-inelastic scattering cross section (e.g., Bjorken scaling[44,45] and y scaling[46]), which we shall discuss later in this paper.

II. DEEP-INELASTIC NEUTRON SCATTERING

We begin with a brief review of the theory of deep-inelastic neutron scattering in the impulse approximation.

A. Dynamic structure factor

The double differential cross section for the scattering of a neutron by a system of N identical atoms is given by[47]

$$\frac{d^2\sigma}{d\Omega' d\epsilon'} = Nb^2(k'/k)S(q,\omega) , \tag{2.1}$$

where b is the bound scattering length per atom and $S(q,\omega)$ is the dynamic structure factor in which $\vec{q}$ and ω

are the momentum and energy, in units of $\hbar$, that are transferred from the neutron to the system in the collision,

$$\vec{q}=\vec{k}-\vec{k}' ,$$
$$\omega=\epsilon-\epsilon' . \tag{2.2}$$

Here $\vec{k}$ and $\vec{k}'$ are the incident neutron and scattered neutron wave vectors, and $\hbar\epsilon=(\hbar k)^2/2m_n$ is the incident neutron energy in which m_n denotes the neutron mass.

The dynamic structure factor is given by

$$S(q,\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-i\omega t)F(q,t)dt , \tag{2.3}$$

where

$$F(q,t)=\frac{1}{N}\sum_{i,j=1}^{N}\langle\exp[-i\vec{q}\cdot\vec{r}_i(0)]\exp[i\vec{q}\cdot\vec{r}_j(t)]\rangle . \tag{2.4}$$

Here $\vec{r}_j(t)$ denotes the position operator for the jth atom in the Heisenberg picture and the brackets $\langle\cdots\rangle$ denote a thermodynamic average.

B. Incoherent approximation

In deep-inelastic scattering $q\gg 2\pi/d$, where d is the nearest-neighbor distance. As a result, the $i\neq j$ terms in (2.4) can be neglected and

$$F(q,t)=\langle\exp[-i\vec{q}\cdot\vec{r}(0)]\exp[i\vec{q}\cdot\vec{r}(t)]\rangle , \tag{2.5}$$

where $\vec{r}(t)$ denotes the position of one particular atom which we can call the scattering atom.

Equation (2.5) is referred to as the incoherent approximation, since one neglects interatomic interference effects and regards each atom as scattering independently of the others. Note, however, that although $F(q,t)$ depends only on the position of the scattering atom, the remaining $N-1$ atoms are not merely spectators in the collision since, as a result of interatomic forces, these other atoms will influence the time variation of $\vec{r}(t)$ and, hence, of $F(q,t)$.

C. Impulse approximation

For a classical system (2.5) can be expressed as

$$F(q,t)=\langle\exp[i\vec{q}\cdot\{\vec{r}(t)-\vec{r}(0)\}]\rangle$$
$$=\left\langle\exp\left[i\vec{q}\cdot\int_0^t\vec{v}(t')dt'\right]\right\rangle , \tag{2.6}$$

where $\vec{v}=d\vec{r}/dt$ is the velocity of the scattering atom. This equation is not valid quantum mechanically since $\vec{r}(0)$ and $\vec{r}(t)$ then no longer commute. Nevertheless, if the interatomic forces are velocity independent, $F(q,t)$ can be expressed[10] in the closely related form

$$F(q,t)=\exp(i\omega_r t)\left\langle\mathcal{T}\exp\left[i\vec{q}\cdot\int_0^t\vec{v}(t')dt'\right]\right\rangle , \tag{2.7}$$

where $\mathcal{T}$ is a time-ordering operator and $\hbar\omega_r=(\hbar q)^2/2m$ is the recoil energy, m being the mass of an atom.

In the limit $q\to\infty$ the right-hand side of (2.7) is appreciably different from 0 only if $t\to 0$, in which case $\vec{v}(t')$ can be replaced by $\vec{v}(0)=\vec{v}$. Thus, as $q\to\infty$,

$$F(q,t)\to\langle\exp[i(\omega_r+\vec{q}\cdot\vec{v})t]\rangle\equiv F_\infty(q,t) , \tag{2.8}$$

and

$$S(q,\omega)\to\langle\delta(\omega-\omega_r-\vec{q}\cdot\vec{v})\rangle\equiv S_\infty(q,\omega) . \tag{2.9}$$

One can easily verify that the delta function in Eq. (2.9) expresses conservation of energy and momentum in the collision of a neutron with an atom having initial velocity $\vec{v}$.

For a finite value of q the approximation

$$S(q,\omega)\simeq S_\infty(q,\omega) \tag{2.10}$$

is called the impulse approximation[9] and is based on the assumption that the scattering atom recoils as if it were free. It is important to note that in the impulse approximation interatomic forces are neglected only in the final state, but not in the initial state, since the thermodynamic average in (2.9) refers to the interacting system and not to an ideal gas.

D. Final-state interactions

We present a brief heuristic discussion of final-state interactions. A more rigorous treatment will be given later in Sec. IV. Let us first introduce a quantity τ such that

$$qv_0\tau=1 , \tag{2.11}$$

where v_0 is the rms velocity of an atom. According to (2.7) we can then interpret τ as the time of interaction of the neutron with the system. If F_0 denotes the rms force that the atoms exert on the scattering atom, then the latter will receive an impulse of the order of $F_0\tau$ during the time of interaction. For the impulse approximation to be valid we therefore require that

$$F_0\tau\ll mv_0 \tag{2.12}$$

TABLE I. Values of quantities for some representative liquids. The values are obtained from data given in Refs. 7, 10, and 48–50.

	m (g/mol)	T (K)	K_0/k_B (K)	p_0 (Å^{-1})	F_0 (pN)	F_0/K_0 (Å^{-1})	q_s (Å^{-1})	q_a (Å^{-1})
^{4}He	4.0026	1	14.0	1.52	8.9	4.6	0.82	1.53
Ne	20.183	27	48.2	6.33	55	8.3	1.47	1.18
Ar	39.948	85	128	14.5	118	6.7	1.18	0.33
Rb	85.47	473	710	50.0	237	2.4	0.43	0.013

and, hence, that

$$q \gg F_0/mv_0^2 = F_0/2K_0 , \tag{2.13}$$

where $K_0 = mv_0^2/2$ is the average kinetic energy per atom. Values of F_0/K_0 for some representative liquids are listed in Table I.

III. SCALING

A. y scaling

Equation (2.9) can be expressed equivalently as

$$S_\infty(q,\omega) = \int \delta[\omega - \omega_r - (\hbar/m)\vec{q}\cdot\vec{p}]n(\vec{p})d\vec{p} , \tag{3.1}$$

where $\hbar\vec{p} = m\vec{v}$ is the momentum of the scattering atom and $n(\vec{p})$ is the momentum distribution function which is defined such that $n(\vec{p})d\vec{p}$ is the fraction of atoms in the initial state with momenta in $d\vec{p}$ so that

$$\int n(\vec{p})d\vec{p} = 1 . \tag{3.2}$$

Taking the z axis to be the direction of $\vec{q}$, we then get

$$S_\infty(q,\omega) = (m/\hbar q)\int \delta(y - p_z)n(\vec{p})d\vec{p} , \tag{3.3}$$

where

$$y = (m/\hbar q)(\omega - \omega_r) = m\omega/\hbar q - q/2 . \tag{3.4}$$

Hence

$$S_\infty(q,\omega) = (m/\hbar q)J(y) , \tag{3.5}$$

where $J(y)$ is the longitudinal momentum distribution function,

$$J(p_z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} n(p_x,p_y,p_z)dp_x\,dp_y . \tag{3.6}$$

For an isotropic system such as a gas or liquid, in which $n(\vec{p})$ depends only on the magnitude of $\vec{p}$, it is easily shown that

$$J(y) = 2\pi\int_{|y|}^{\infty} n(\vec{p})p\,dp \tag{3.7}$$

and hence that

$$n(\vec{y}) = -(2\pi y)^{-1}dJ(y)/dy . \tag{3.8}$$

In the case of x-ray scattering, where $n(\vec{p})$ is the momentum distribution function for the electrons, the quantity $J(y)$ is the Compton profile.[23] The expression (3.8) for the momentum distribution in terms of the derivative of the Compton profile is originally due to DuMond.[12]

It follows from (2.9) that

$$\lim_{q\to\infty}[qS(q,\omega)] = (m/\hbar)J(y) . \tag{3.9}$$

More precisely, (3.9) involves the simultaneous limit $q\to\infty$ and $\omega\to\infty$ such that y remains constant. In this limit $qS(q,\omega)$ depends only on the scaling variable y and not on q and ω separately. This asymptotic property of the dynamic structure factor, which was first emphasized by West[46] in the context of electron scattering, is now usually referred to as y scaling.

This y-scaling property provides great flexibility in the experimental determination of atomic momentum distribution functions in condensed matter by means of neutron inelastic scattering measurements at large q. For example, for a constant-q scan, in which $S(q,\omega)$ is measured as a function of ω for a fixed value of q,[2–4,7]

$$yn(\vec{y}) = \lim_{q\to\infty}\left[-\frac{1}{2\pi}\left[\frac{\hbar q}{m}\right]^2\frac{\partial}{\partial\omega}S(q,\omega)\right] . \tag{3.10}$$

Alternatively, for a constant-ω scan, in which $S(q,\omega)$ is measured as a function of q for a fixed value of ω,

$$yn(\vec{y}) = \lim_{\omega\to\infty}\left[\frac{\hbar}{\pi m}\left[\frac{\omega_r}{\omega_r+\omega}\right]\frac{\partial}{\partial q}qS(q,\omega)\right] . \tag{3.11}$$

The momentum distribution can also be obtained from time-of-flight experiments[1,5,6] in which $S(q,\omega)$ is measured as a function of the scattered neutron wavelength $\lambda' = 2\pi/k'$ for fixed values of the incident neutron wavelength λ and the angle of scattering ϕ so that q and ω both vary over the scan.

Finally, we point out that for an isotropic system the momentum distribution function also determines the distribution of kinetic energy, $K = (\hbar p)^2/2m$. Thus if $n(K)dK$ is the fraction of atoms in dK, so that

$$\int_0^\infty n(K)dK = 1 , \tag{3.12}$$

then

$$n(K)dK = n(\vec{p})4\pi p^2\,dp , \tag{3.13}$$

and

$$n(K) = (4\pi m/\hbar^2)pn(\vec{p}) . \tag{3.14}$$

Hence, it follows from (3.10) that

$$n(K) = \lim_{q\to\infty}\left[-\left[\frac{4\omega_r}{\hbar}\right]\frac{\partial}{\partial\omega}S(q,\omega)\right] , \tag{3.15}$$

where

$$K = (\hbar/4\omega_r)(\omega - \omega_r)^2 . \tag{3.16}$$

B. Bjorken scaling

It follows from (3.1) that

$$S_\infty(q,\omega) = \frac{1}{|\omega|}\int \delta(1 - x(1 + 2p_z/q))n(\vec{p})d\vec{p} , \tag{3.17}$$

where

$$x = \omega_r/\omega = \hbar q^2/2m\omega . \tag{3.18}$$

Hence

$$\lim_{q\to\infty}[\omega S_\infty(q,\omega)] = \delta(1-x) , \tag{3.19}$$

and so

$$\lim_{q\to\infty}[\omega S(q,\omega)] = \delta(1-x) . \tag{3.20}$$

More precisely, (3.20) involves the simultaneous limit $q\to\infty$ and $\omega\to\infty$ such that x remains constant. In this limit $\omega S(q,\omega)$ depends only on the scaling variable x and

not on q and ω separately. This asymptotic property of the dynamic structure factor is the nonrelativistic analog of Bjorken scaling[44,45] which was originally introduced in the context of deep-inelastic lepton-nucleon scattering.

The x- and y-scaling properties differ not only in the nature of the limits involved but also in the fact that $S_\infty(q,\omega)$ has the y-scaling property for all q while it has the x-scaling property only in the limit $q\to\infty$. In other words, y scaling is a property of the impulse approximation itself, while x scaling, or Bjorken scaling, is merely an asymptotic property of the impulse approximation.

Bjorken scaling simply means that as $q\to\infty$,

$$S(q,\omega)\to\delta(\omega-\omega_r)\ . \tag{3.21}$$

Physically, this means that for sufficiently large momentum transfer, the scattering atom is effectively at rest in the initial state, and $S(q,\omega)$ then describes the free recoil of this atom. In deep-inelastic lepton-nucleon scattering[36–43] the observation of Bjorken scaling is regarded as direct experimental evidence for the existence of quarks. By the same token the observation of Bjorken scaling in thermal-neutron scattering by condensed matter can be regarded as direct experimental evidence for the existence of atoms. However, since the existence of atoms is no longer a controversial question, Bjorken scaling is not of such fundamental interest here.

If $n(\vec{p})$ and, hence, $J(y)$ and $S_\infty(q,\omega)$ are Gaussian functions, as they are classically or in a harmonic crystal, then $S_\infty(q,\omega)$ has a full width at half maximum given by

$$\Delta\omega=\left[\frac{8\ln 2}{3}\right]^{1/2}\left[\frac{\hbar p_0}{m}\right]q\ , \tag{3.22}$$

where $\hbar p_0$ is the rms momentum,

$$p_0^2=\int p^2 n(\vec{p})d\vec{p}\ . \tag{3.23}$$

Hence, the relative width of the peak is

$$\frac{\Delta\omega}{\omega_r}=\left[\frac{32\ln 2}{3}\right]^{1/2}\frac{p_0}{q}\ . \tag{3.24}$$

The condition for Bjorken scaling is that $\Delta\omega\ll\omega_r$ and, hence, that $q\gg 2.72p_0$. On the other hand, the condition for y scaling is, as we have argued earlier in Sec. II D, that $q\gg F_0/2K_0$.

Table I lists the values of p_0 for some representative liquids. In liquid ^{4}He, for example, $p_0=1.52$ Å^{-1} and, in the experiments of Ref. 8, $q=83$ Å^{-1} so that $\Delta\omega/\omega_r=5\%$, which is roughly the same as the instrumental width in these experiments. Thus from a practical point of view one might say that the Bjorken scaling limit has been reached in these experiments.

To obtain the energy resolution necessary to obtain accurate momentum distributions from deep-inelastic neutron scattering experiments it is at present usually necessary to use smaller values of q than above, typically 5–20 Å^{-1}, and in this case one must allow for the effect of final-state interactions which is the subject of the next section.

IV. FINAL-STATE INTERACTIONS

The dynamic structure factors $S(q,\omega)$ obtained from neutron inelastic scattering measurements in the range $5\lesssim q\lesssim 20$ Å^{-1} for liquid[1–5,51–57] and solid[6,58] helium, liquid neon,[59] and liquid rubidium[60] are qualitatively consistent with the impulse approximation to the extent that they give $S(q,\omega)$ distributions that are approximately symmetrical about ω_r and that have full widths at half maximum which increase more or less linearly with increasing q.

Nevertheless, significant discrepancies exist, particularly at the smaller values of q. For example, the measured $S(q,\omega)$ distributions exhibit small but definite asymmetry such that the high-energy wings are enhanced and the low-energy wings are depressed. Also, positions of the peaks lie somewhat below ω_r and the widths are slightly less than one would expect on the basis of the impulse approximation. These distortions can be attributed to the effects of final-state interactions which are neglected in the impulse approximation and which will be discussed in the following sections.

The peak positions and widths are also observed to have a slight oscillatory dependence on q. This can be attributed to interatomic interference effects which are neglected in the incoherent approximation and which we shall continue to ignore in what follows.

A. General expression for $S(q,\omega)$

We begin by defining a quantity $\tilde{R}(q,t)$ such that

$$F(q,t)=\tilde{R}(q,t)F_\infty(q,t)\ . \tag{4.1}$$

Then

$$S(q,\omega)=\int_{-\infty}^{\infty}R(q,\omega')S_\infty(q,\omega-\omega')d\omega'\ , \tag{4.2}$$

where

$$R(q,\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-i\omega t)\tilde{R}(q,t)dt\ . \tag{4.3}$$

It then follows from (2.8) that

$$\lim_{q\to\infty}\tilde{R}(q,t)=1\ , \tag{4.4}$$

and, hence, that

$$\lim_{q\to\infty}R(q,\omega)=\delta(\omega)\ . \tag{4.5}$$

For a finite value of q the function $R(q,\omega)$ has a finite width and characterizes the distortion of $S(q,\omega)$ due to final-state interactions.

In previous works, a number of authors[2,61–63] have described final-state interactions in terms of an expression of the form (4.2) with explicit models for $R(q,\omega)$. We shall adopt a different approach which begins with the observation that since $R(q,\omega)$ is approximately equal to a delta function at large q, we expect that a convergent expansion will be obtained by expanding $S_\infty(q,\omega-\omega')$ in a Taylor series in powers of ω'. Hence, (4.2) becomes

$$S(q,\omega)=\sum_{n=0}^{\infty}\frac{(-)^n}{n!}R_n(q)\frac{\partial^n}{\partial\omega^n}S_\infty(q,\omega)\ , \tag{4.6}$$

where

$$R_n(q)=\int_{-\infty}^{\infty}\omega^n R(q,\omega)d\omega\ . \tag{4.7}$$

It then follows from (3.5) that

$$S(q,\omega)=(m/\hbar q)\sum_{n=0}^{\infty}(-)^n A_n(q)d^nJ(y)/dy^n\ , \tag{4.8}$$

where

$$A_n(q)=\frac{1}{n!}(m/\hbar q)^n R_n(q)\ . \tag{4.9}$$

Equation (4.8) provides a formally exact expression for the dynamic structure factor in terms of the longitudinal momentum distribution function $J(y)$ and the coefficients $A_n(q)$ which we now proceed to calculate.

B. Sum rules

It follows from (4.2), with the help of the binomial theorem

$$(a+b)^n=\sum_{m=0}^{n}\begin{bmatrix}n\\m\end{bmatrix}a^{n-m}b^m\ , \tag{4.10}$$

that

$$S_n(q)=\sum_{m=0}^{n}\begin{bmatrix}n\\m\end{bmatrix}R_{n-m}(q)S_{\infty,m}(q)\ , \tag{4.11}$$

where $S_n(q)$ is the nth central moment of $S(q,\omega)$,

$$S_n(q)=\int_{-\infty}^{\infty}(\omega-\omega_r)^n S(q,\omega)d\omega\ , \tag{4.12}$$

and $S_{\infty,m}(q)$ is the corresponding mth central moment of $S_\infty(q,\omega)$.

The moments of $S(q,\omega)$ have been calculated in Refs. 64–66 for $n=0$ to 4 and in Ref. 10 for $n=5$ and 6. It is found that $S_n(q)$ is a polynomial in q^2,

$$\begin{aligned}
&S_0(q)=1\ ,\\
&S_1(q)=0\ ,\\
&S_2(q)=a_{22}q^2\ ,\\
&S_3(q)=a_{32}q^2\ ,\\
&S_4(q)=a_{42}q^2+a_{44}q^4\ ,\\
&S_5(q)=a_{52}q^2+a_{54}q^4\ ,\\
&S_6(q)=a_{62}q^2+a_{64}q^4+a_{66}q^6\ .
\end{aligned} \tag{4.13}$$

In general,

$$a_{nn}=\langle v_z^n\rangle\ , \tag{4.14}$$

where the z axis is again taken to be the direction of $\vec{q}$. For an isotropic system,[64,65]

$$\begin{aligned}
&a_{32}=\hbar\langle\Delta V\rangle/6m^2\ ,\\
&a_{42}=\langle\vec{F}^2\rangle/3m^2\ ,
\end{aligned} \tag{4.15}$$

and expressions for the remaining coefficients can be found in Ref. 10. Here Δ denotes the Laplacian with respect to the position of the scattering atom, V is the total potential energy of the system, and $\vec{F}=-\vec{\nabla}V$ is the interatomic force on the scattering atom.

The moments of $S_\infty(q,\omega)$ follow immediately from (2.9) and we see that

$$S_{\infty,n}(q)=a_{nn}q^n\ , \tag{4.16}$$

where a_{nn} is again given by (4.14) and vanishes when n is odd. Hence it follows from (4.11) that

$$\begin{aligned}
&R_0(q)=1\ ,\\
&R_1(q)=0\ ,\\
&R_2(q)=0\ ,\\
&R_3(q)=a_{32}q^2\ ,\\
&R_4(q)=a_{42}q^2\\
&R_5(q)=a_{52}q^2+(a_{54}-10a_{32}a_{22})q^4\ ,\\
&R_6(q)=a_{62}q^2+(a_{64}-15a_{42}a_{22})q^4\ .
\end{aligned} \tag{4.17}$$

The fact that $R_0(q)$ and $R_4(q)$ are both positive while $R_2(q)$ equals zero implies that $R(q,\omega)$ cannot be a positive function, such as a Gaussian or a Lorentzian, but must have an oscillatory tail. The existence of such a tail has also been found in some model calculations[63] of $R(q,\omega)$.

Finally, it follows from (4.9) that

$$A_n(q)=\begin{cases}1\ , & n=0\\ 0\ , & n=1,2\\ O(q^{-1})\ , & n=3,5\ldots\\ O(q^{-2})\ , & n=4,6,\ldots\end{cases}\ . \tag{4.18}$$

In particular,

$$\begin{aligned}
&A_3(q)=m\langle\Delta V\rangle/36\hbar^2 q\ ,\\
&A_4(q)=m^2\langle\vec{F}^2\rangle/72\hbar^4q^2\ .
\end{aligned} \tag{4.19}$$

Hence, (4.8) becomes

$$S(q,\omega)=\frac{m}{\hbar q}\left[1+\sum_{n=3}^{\infty}(-)^n A_n(q)\frac{d^n}{dy^n}\right]J(y)\ , \tag{4.20}$$

in which the first term gives the impulse approximation (3.5) and the remaining terms are the corrections for final-state interactions.

It must be emphasized that (4.20) is merely a formal expansion and that there are, in fact, situations in which it will fail. One such situation is the case of superfluid ^{4}He which we discuss later in Sec. IV E. Another is the case of a hard-sphere fluid for which $S(q,\omega)$ has long high-energy wings that cause[48] $S_n(q)$, and hence $A_n(q)$, to diverge when $n\geq 3$. The hard-sphere fluid has also been studied recently by Weinstein and Negele,[11] who showed on the basis of time-ordered perturbation theory that although $qS(q,\omega)$ is a function only of y in the limit $q\to\infty$, this function is no longer $J(y)$.

C. Symmetrization

We begin by decomposing (4.20) into two parts,

$$S(q,\omega)=S_s(q,\omega)+S_a(q,\omega) , \tag{4.21}$$

where

$$S_s(q,\omega)=\frac{m}{\hbar q}\left[1+\sum_{n=2}^{\infty}A_{2n}(q)\frac{d^{2n}}{dy^{2n}}\right]J(y) ,$$
$$S_a(q,\omega)=\frac{m}{\hbar q}\left[-\sum_{n=1}^{\infty}A_{2n+1}(q)\frac{d^{2n+1}}{dy^{2n+1}}\right]J(y) . \tag{4.22}$$

It then follows from (4.18) that

$$qS_s(q,\omega)=(m/\hbar)J(y)+O(q^{-2}) ,$$
$$qS_a(q,\omega)=O(q^{-1}) . \tag{4.23}$$

Since $J(y)$ is an even function of y for an isotropic system it is evident that $S_s(q,\omega)$ is an even function of $\omega-\omega_r$ (symmetric) and $S_a(q,\omega)$ is an odd function of $\omega-\omega_r$ (antisymmetric). Thus

$$S_s(q,\omega)=\tfrac{1}{2}[S(q,\omega)+S(q,2\omega_r-\omega)] ,$$
$$S_a(q,\omega)=\tfrac{1}{2}[S(q,\omega)-S(q,2\omega_r-\omega)] . \tag{4.24}$$

Such a decomposition of $S(q,\omega)$ into symmetric and antisymmetric parts has previously been made[2] on the basis of a Gram-Charlier expansion,[10,48,49] which likewise shows that the final-state interaction effects are of order q^{-1} in $qS_a(q,\omega)$ and of order q^{-2} in $qS_s(q,\omega)$.

The relations (4.24) can be used to decompose measured $S(q,\omega)$ distributions into symmetric and antisymmetric parts. Examples of such decompositions can be found in Ref. 2 for liquid helium and in Ref. 7 for liquid neon. Momentum distributions for liquid helium[2-5] and liquid neon[7] have been obtained from the measured $S_s(q,\omega)$ distributions by neglecting the q^{-2} correction for final-state interactions. A test of the validity of this procedure is, according to (4.23), whether $qS_s(q,\omega)$ depends only on y for the range of q values employed. This is demonstrated for the case of liquid neon in Fig. 1 which shows $qS_s(q,\omega)$ as a function of y for the eleven values of q in the range 5.0—10.0 Å^{-1} that were used in the analysis in Ref. 7. It is seen that in first approximation $qS_s(q,\omega)$ is indeed a universal function of y. The discrepancies that occur are due not only to effects of final-state interactions but also to interatomic interference effects and counting statistics.

A quantitative measure of the magnitude of the final-state interactions is provided by the quantities

$$\eta_s=A_4(q)/y_0^4 ,$$
$$\eta_a=A_3(q)/y_0^3 , \tag{4.25}$$

in which y_0 denotes the rms value of y,

$$y_0^2=\int_{-\infty}^{\infty}y^2J(y)dy . \tag{4.26}$$

Here η_s is a measure of the relative distortion of $S_s(q,\omega)$ due to final-state interactions, and η_a indicates the magnitude of $S_a(q,\omega)$ relative to $S_\infty(q,\omega)$. Since $y_0^2=p_0^2/3$, it follows from (4.19) that

$$\eta_s=(q_s/q)^2 ,$$
$$\eta_a=q_a/q , \tag{4.27}$$

where

$$q_s=F_0/(4\sqrt{2}K_0) ,$$
$$q_a=\langle\Delta V\rangle/(8\sqrt{3}K_0p_0) . \tag{4.28}$$

Here $F_0^2=\langle\vec{F}^2\rangle$ is the mean-square force on the scattering atom and $K_0=(\hbar p_0)^2/2m$ is the average kinetic energy. A necessary condition for final-state interactions to be negligible is that $q\gg q_s$, which agrees with the heuristic result (2.13).

The relation

$$F_0^2=\tfrac{2}{3}K_0\langle\Delta V\rangle \tag{4.29}$$

is rigorously true for a classical system,[67] for which $K_0=\frac{3}{2}k_BT$, and also for a simple harmonic oscillator.[10] We regard it as a useful approximation quite generally, in which case

$$q_a=2\sqrt{3}q_s^2/p_0 . \tag{4.30}$$

The values of q_s and q_a are listed in Table I for some representative liquids. The momentum distributions for

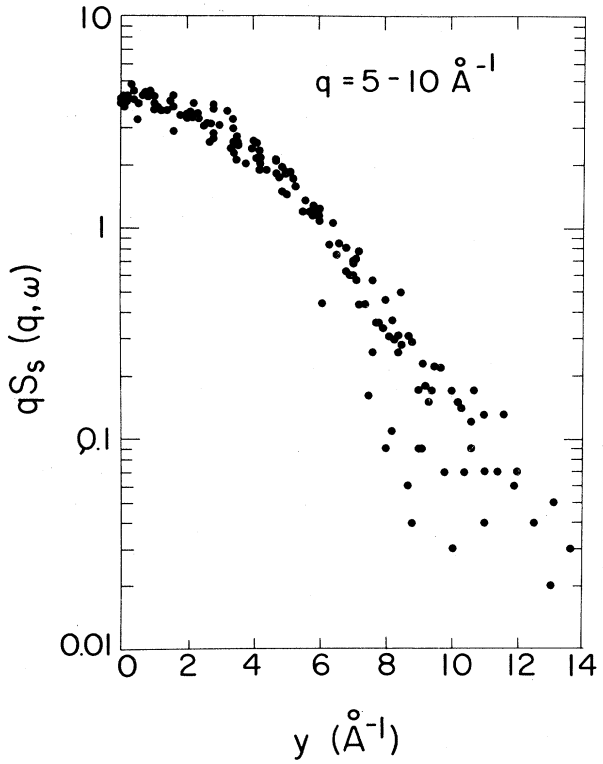

FIG. 1. y scaling in liquid neon. $qS_s(q,\omega)$ is shown in arbitrary units as a function of $y=(m/\hbar q)(\omega-\omega_r)$ for liquid neon at $T=26.9$ K for the eleven values of q in the range 5.0—10.0 Å^{-1}, which were used in the determination of the momentum distribution in Ref. 7. The data are from Ref. 59.

liquid helium, which were obtained in Refs. 4 and 5, were based on data for which $5.0 \leq q \leq 7.0$ Å^{-1} so that η_s varies from 1.4% to 2.7%. For the corresponding work on liquid neon,[7] $5.0 \leq q \leq 10.0$ Å^{-1} and η_s varies from 2.2% to 8.6%.

D. Self-consistent correction procedure

Keeping only the leading correction terms in (4.22) we get

$$S_s(q,\omega)=\frac{m}{\hbar q}\left[1+A_4(q)\frac{d^4}{dy^4}\right]J(y)\ ,$$

$$S_a(q,\omega)=\frac{m}{\hbar q}\left[-A_3(q)\frac{d^3}{dy^3}\right]J(y)\ , \tag{4.31}$$

so that

$$J(y)=\frac{\hbar q}{m}\left[S_s(q,\omega)+\alpha\frac{\partial}{\partial\omega}S_a(q,\omega)\right]\ , \tag{4.32}$$

in which

$$\alpha=\left[\frac{\hbar q}{m}\right]\frac{A_4(q)}{A_3(q)}=\frac{\langle\vec{F}^2\rangle}{2\hbar\langle\Delta V\rangle}\ , \tag{4.33}$$

and is independent of q. Hence, it follows from (3.8) that

$$yn(\vec{y})=-\frac{1}{2\pi}\left[\frac{\hbar q}{m}\right]^2\left[\frac{\partial}{\partial\omega}S_s(q,\omega)+\alpha\frac{\partial^2}{\partial\omega^2}S_a(q,\omega)\right]\ . \tag{4.34}$$

In (4.32) and (4.34) the information about the final-state interactions that is contained in $S_a(q,\omega)$ is used to correct for the final-state interaction effects in $S_s(q,\omega)$.

To the extent that (4.29) is valid, we get

$$\alpha=\frac{K_0}{3\hbar}=\frac{\hbar}{6m}\int p^2 n(\vec{p})d\vec{p}\ . \tag{4.35}$$

Thus (4.34) and (4.35) provide a self-consistent pair of equations for the determination of the momentum distribution from the measured dynamic structure factor. If the approximation (4.29) is not valid, the value of α can be estimated from the criterion that the right-hand sides of (4.32) and (4.34) should depend only on y.

E. Superfluid helium

For superfluid ^{4}He it has been established theoretically[68–72] that as $p\to 0$,

$$n(\vec{p})=n_0\left[\delta(\vec{p})+\frac{a}{p^2}+\frac{b}{p}+\cdots\right]\ , \tag{4.36}$$

where n_0 is the condensate fraction and

$$a=mk_BT/8\pi^3\hbar^2\rho n_s\ ,$$
$$b=mc/16\pi^3\hbar\rho\ , \tag{4.37}$$

in which ρ is the number density, n_s the superfluid fraction, and the c the velocity of sound. Hence, it follows from (3.7) that as $y\to 0$,

$$J(y)=n_0[\delta(y)-2\pi(a\ln|y|+b|y|+\cdots)]\ , \tag{4.38}$$

and from (3.5) that as $\omega\to\omega_r$,

$$S_\infty(q,\omega)=n_0\left[\delta(\omega-\omega_r)-\frac{\pi m}{\hbar}\left[\frac{2a}{q}\ln\left|\frac{m}{\hbar q}(\omega-\omega_r)\right|+b|\omega/\omega_r-1|+\cdots\right]\right]\ . \tag{4.39}$$

In the theory of final-state interactions developed in Sec. IV A it was tacitly assumed that $S_\infty(q,\omega)$ is analytic for all ω. Since (4.39) is, however, singular at $\omega=\omega_r$, the expansion (4.6) will not be valid in the neighborhood of this singularity. Thus, for example, one would not expect (4.34) to yield a momentum distribution with a well-resolved condensate peak if this peak were not present in $S_s(q,\omega)$.

Substituting (4.39) into (4.2), we see that in general

$$S(q,\omega)=n_0R(q,\omega-\omega_r)+S'(q,\omega)\ , \tag{4.40}$$

in which the first term is the condensate peak and the second term the contribution from the uncondensed atoms. Hohenberg and Platzman have assumed[9] that the broadening of the condensate peak is a simple lifetime effect in which case the full width at half maximum of $R(q,\omega)$ will be given by

$$\Delta\omega=\frac{1}{\tau(q)}=\rho(\hbar q/m)\sigma(q)\ , \tag{4.41}$$

where $\tau(q)$ is the mean time between collisions for the recoiling ^{4}He atom and $\sigma(q)$ is the collision cross section. This estimate is consistent[4] with the observed temperature variation of $S(q,\omega)$ for liquid ^{4}He. On the other hand, if the broadening of the condensate peak were a simple lifetime effect one would expect $R(q,\omega)$ to have a Lorentzian shape which, as noted earlier, would violate the sum rules (4.17). Thus the effect of final-state interactions on the condensate peak in $S(q,\omega)$ is still an open question, and the use of (4.41) to estimate[2,9] how large q must be in order to resolve this peak experimentally must be treated with caution.

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