Quantum effects in deep inelastic neutron scattering

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In the impulse approximation (IA), which is used to interpret deep inelastic neutron scattering measurements, the predicted scattering is identical to that which would be obtained from a gas of noninteracting atoms, with the momentum distribution of atoms in the target system. The validity of the IA rest on the approximation that the struck particle recoils freely after the collision with the neutron. Departures from the IA are usually attributed to final-state effects (FSE), which are caused by the breakdown of this approximation. A second implicit assumption of the IA, which has received little attention in the literature, is that the atoms in the target system have a distribution of energies in the initial state, i.e., before the collision. This is not true in a quantum system at zero temperature, where, although there is a distribution of atomic momenta, the initial state has a unique energy. It is shown that "initial-state effects" (ISE), which are caused by the breakdown of the latter assumption at low temperatures, largely account for observed asymmetries and peak shifts from the IA prediction for $S(\mathbf{q},\omega)$. It is shown that if FSE's are negligible, ISE's are negligible when $q \gg p_i$, where q is the momentum transfer and p_i is the root-mean-square atomic momentum. Finally, it is shown that FSE's are negligible when $q \gg p_i$, in systems other than quantum fluids and that, since in this regime ISE's are also negligible, the IA is reached for such systems when $q \gg p_i$.

I. INTRODUCTION

The technique of deep inelastic neutron scattering (DINS) was first proposed by Hohenberg and Platzmann[1] over 20 years ago, as a method of directly observing the Bose condensate in superfluid ^{4}He. They suggested that at sufficiently high momentum transfers, the impulse approximation (IA) can be used to interpret neutron scattering data. In the IA, the scattering cross section is simply related to the single-particle momentum distribution of atomic nuclei in the target system, and DINS provides a unique probe of the atomic momentum distribution function. A considerable number of DINS experiments on ^{4}He have been performed,[2–9] but the analysis of data is complicated by the presence of departures from the IA. There is an extensive theoretical literature on this question,[10–22], but no consensus of opinion on a number of fundamental points.

It has recently also become more important to determine the validity of the IA for neutron scattering from other condensed matter systems, due to the development of spallation neutron sources. DINS requires the use of relatively high-energy neutrons (>1 eV). Spallation sources[23] have much more intensity at these energies than reactor sources and should facilitate more precise measurements of atomic momentum distribution functions, with much improved resolution and counting statistics. Thus measurements on samples containing light atoms other than ^{4}He will become more attractive. The advantages of spallation neutron sources in DINS have already been demonstrated in definitive measurements on ^{4}He, performed at the Intense Pulse Neutron Source (IPNS) at Argonne National Laboratory,[9] and in measurements on other systems at the National Laboratory for High Energy Physics (KEK) (Refs. 24 and 25) source in Japan. The advent of more intense sources such as Isis at Rutherford Appleton Laboratory, United Kingdom and Los Alamos Neutron Scattering Center (LANSCE) at Los Alamos National Laboratory, should bring further increases in both attainable momentum transfers and the sensitivity of measurements. DINS measurements at the present time have similar count rates and resolutions to those made 20 years ago in Compton scattering,[26] a technique which is closely related to DINS (DINS is sometimes referred to as "neutron Compton scattering"). The sensitivity of Compton scattering measurements improved rapidly following the early work, and the technique has subsequently developed into a fruitful branch of research. DINS measurements can be expected to show similar rapid improvements.

In this paper a new approach to determining the form and magnitude of departures from the IA, which was suggested by the work of Gunn, Andreani, and Mayers,[27] is developed. Most theoretical treatments of the IA are formulated in terms of the behavior of the single-particle correlation function $I(\mathbf{q},t)$ at short times t. In this paper a formulation is given in terms of $\mathbf{r}$, the position coordinate of the struck particle. This is in many ways a more natural approach for a determination of momentum distributions, since $\mathbf{r}$ rather than t is the conjugate variable to $\mathbf{p}$. The validity of the approach for scattering from a many-body system relies essentially on the incoherent approximation, which ensures that $S(\mathbf{q},\omega)$ is independent of the coordinates of other particles (see the Appendix). Indeed it is implicit, in the assumption that DINS measures the momentum distribution of a single particle, that this is so. The formal simplicity of the treatment, which contrasts with rather complex many-body treatments, allows for the clear physical interpretation of a number of

features that have been observed in experimental data and numerical calculations.

Perhaps the main advantage of the approach is that two essentially different approximations inherent in the IA can be separated and their individual effects examined. In the IA it is assumed both that the struck particle recoils freely in the final state and that the initial state of the scattering system can, in a sense, be described as a collection of free particles. The scattering cross section is identical to that which would be obtained for a fictitious gas of noninteracting particles, with a momentum distribution identical to that of the atoms in the target system. The "initial state" is the state of the target system before the scattering event, and the "final state" that after. "State" is synonymous with "condition" in this paper, although often a single quantum state is referred to. Precisely which meaning is taken should be evident from the context.

Departures from the IA caused by interactions of the struck atom in the final state are generally referred to as "final-state effects" (FSE's). Correspondingly, in this paper departures from behavior of the scatterer as a collection of free atoms in the initial state are referred to as "initial-state effects" (ISE's). It is shown that significant departures from the IA occur at low temperatures because of ISE's. The physical origin of these departures is the quantum nature of the initial state. Calculations on exactly soluble models and comparison with experimental data shows that ISE's largely account for observed inaccuracies in the IA prediction.

In Sec. II an introduction to the IA is given, and the main physical approximations inherent therein are examined. In Sec. III ISE's are treated by representing the atom as a free particle in the final state, but using the exact form of the initial state and comparing the resultant scattering cross section with that calculated in the IA. The treatment is illustrated in Sec. IV by a calculation on an exactly soluble model system. In Sec. V the main conclusions and implications for measurements are discussed. Throughout the paper the calculation of $S(\mathbf{q},\omega)$ is treated as a single-particle problem. The justification of this approach in a many-particle system is given in the Appendix.

II. THE IMPULSE APPROXIMATION

A. Introduction to impulse approximation

In a classical system, the IA is valid when the condition

$$q \gg F_i \Delta t \tag{2.1}$$

is satisfied. q is the momentum transfer, Δt is the approximate time interval during which the interaction between the incident and struck particles is significant, and F_i is the force exerted on the struck particle by other particles in the scattering system. When (2.1) is satisfied, the cross section for scattering from a single particle is proportional to

$$S(\mathbf{q},\omega)=\int n(\mathbf{p})\delta(\omega-(\mathbf{p}+\mathbf{q})^2/2M+p^2/2M)d\mathbf{p}\ , \tag{2.2}$$

where $n(\mathbf{p})$ is the probability that the target particle has momentum $\mathbf{p}$, ω is the energy transferred to the particle, and M is the mass of the particle. The cross section is identical to that obtained in scattering from a gas of free particles with momentum distribution $n(\mathbf{p})$. The physical rationale behind the IA is that F_i can be neglected during the collision. Thus, the potential energy of the struck particle is also neglected in the δ function, which expresses energy conservation, and the particles appear as free during the collision process. It should be stressed that the effects of the interaction between the target particle and its environment are still significant, as together with the temperature they determine the momentum distribution $n(\mathbf{p})$. Conversely a measurement of $n(p)$ provides information on interatomic interactions.

In neutron scattering in the IA, the scattering is also determined by the expression (2.2). In this case $S(\mathbf{q},\omega)$ is the incoherent neutron scattering function, and the partial differential cross section is[28]

$$\frac{d^2\sigma}{d\Omega\, dE_1}=(k_1/k_0)|b|^2S(\mathbf{q},\omega)\ , \tag{2.3}$$

where k_1 and k_0 are the wave numbers of the scattered and incident neutrons, E_1 is the energy of the scattered neutron, and b is the scattering length.

The preceding argument given for the validity of the IA is difficult to apply to neutron scattering. For example the definition of the "interaction time" Δt is unclear. Mott and Massey[29] define the interaction time as

$$\Delta t=\Delta r/v\ , \tag{2.4}$$

where v is the velocity of the incident particle, and Δr is the range of the force between the incident and target particles. Although this criterion gives reasonable results for collisions between atoms, it fails for neutron scattering because of the short range of the interaction between the neutron and the target nucleus. There is also a problem of principle in that the argument implies that the incident neutron can be described by a wave packet, and suggests that the validity of the IA is linked to the wavelength spread of the incident beam. No such dependence occurs in theoretical derivations of the neutron cross section, which assume that the incident neutron can be represented as a plane wave.

It is shown in Sec. III that a better criterion for the validity of the IA in neutron scattering is (with $\hbar=1$)

$$q \gg p_i\ , \tag{2.5}$$

where p_i is the root-mean-square atomic momentum. Dimensional arguments can be used to obtain order of magnitude estimates, in terms of p_i and M, for other quantities characterizing the atomic motion, e.g., (1) length, $r_i \simeq 1/p_i$ (in a solid this is approximately the rms displacement of the atom from its mean position), (2) the mean kinetic energy, $\kappa_i=p_i^2/2M$, which is approximately (in a harmonic system exactly) equal to the mean potential energy, and (3) the mean force on the atom $F_i \simeq \kappa_i/r_i$.

Within the accuracy of these estimates (2.5) agrees with criteria obtained by other authors, who have used a

variety of treatments. For example Reiter and Silver[19] give

$$q \gg (F_i M/\Delta p)^{1/2} , \tag{2.6}$$

where Δp is the width of the atomic momentum distribution. Equating Δp and p_i gives (2.5). Similarly conditions given by Sears[17]

$$q \gg F_i/2\kappa_i , \tag{2.7}$$

and Platzmann and Tsoar[30]

$$q \gg (2ME_B)^{1/2} , \tag{2.8}$$

where $E_B \simeq E_i$ is the binding energy, reduce to (2.5).

We note that although these criteria depend only upon the magnitude of q and the equilibrium properties of the initial state, it is generally assumed that they indicate when FSE's are small. It is shown in Sec. III that (2.5) is applicable only at low temperatures and in fact indicates when ISE's are small. FSE's were discussed in the original paper of Hohenberg and Platzmann,[1] who argued that the observed momentum distribution in ^{4}He would be broadened due to the finite lifetime of the final state, introduced by collisions of the recoiling atom with other atoms. This finite lifetime makes any measurement of the energy transfer, and hence the momentum transfer, uncertain. Their argument gives a broadening of the observed momentum distribution by $\Delta p_c \simeq 1/r_c$, where r_c is the mean distance between collisions. In this case the magnitude of the broadening does indeed depend upon the final rather than initial state as $r_c \simeq 1/(\rho_0 \sigma)$, where ρ_0 is the number of atoms per unit volume and σ is the atom-atom collision cross section. The cross section σ is a function of the relative velocities of the colliding atoms that has only a weak dependence on the initial state at high q.

Final-state broadening of the observed momentum distribution (or to be more precise the Compton profile) is one manifestation of FSE's. The other is the introduction of distortions into the measured $n(\mathbf{p})$. Roughly speaking, the physical origin of the former is the confinement of the struck atom in the final state by the "cage" of neighboring atoms, while that of the latter is departures from free atom behavior in the interior of the cage. These departures are caused by the longer-range component of the interatomic potential, which introduces a nonuniform potential within the cage. The combination of these two processes introduces an asymmetric "resolution function," which is independent of any instrumental resolution but is determined by $\mathbf{q}$ and ω, and the properties of the target system. It will be shown that the asymmetries introduced by the latter process become small at high q. In Sec. V a brief argument is given that shows that final-state broadening is small at high q in systems other than quantum fluids. A more detailed discussion of final-state broadening is planned for a subsequent paper.

B. Formulation of the impulse approximation in neutron scattering

The standard expression for $S(\mathbf{q},\omega)$ for neutron scattering from a system of identical atoms in the Born approximation is[28]

$$S(\mathbf{q},\omega) = (1/N) \sum_i g_i \sum_f \left| \sum_n \langle i | \exp(-i\mathbf{q}\cdot\mathbf{r}_n) | f \rangle \right|^2 \times \delta(\omega + E_i - E_f) , \tag{2.9}$$

where $|i\rangle$ and $|f\rangle$ are the initial and final quantum states, E_i and E_f are the corresponding energies, $\mathbf{r}_n$ is the position coordinate of atom n, and N is the number of atoms. g_i is the Boltzmann factor for occupation of quantum state $|i\rangle$, and $\sum_i$, which denotes a sum over initial states, performs a thermal average. It is assumed in the IA that the scattering is incoherent so that terms containing products of the form

$$\exp(i\mathbf{q}\cdot\mathbf{r}_j)\exp(-i\mathbf{q}\cdot\mathbf{r}_k)$$

with $k \neq j$ give negligible contribution. Then each atom gives an identical contribution to $S(\mathbf{q},\omega)$ and

$$S(\mathbf{q},\omega) = \sum_i g_i \sum_f |\langle i | \exp(-i\mathbf{q}\cdot\mathbf{r}) | f \rangle|^2 \delta(\omega + E_i - E_f) . \tag{2.10}$$

Following the standard treatments[28] $S(\mathbf{q},\omega)$ can be written as

$$S(\mathbf{q},\omega) = 1/(2\pi) \int I(\mathbf{q},t) \exp(-i\omega t) dt , \tag{2.11}$$

where

$$I(\mathbf{q},t) = \langle \exp[-i\mathbf{q}\cdot\hat{\mathbf{r}}(0)] \exp[i\mathbf{q}\cdot\hat{\mathbf{r}}(t)] \rangle . \tag{2.12}$$

$\hat{\mathbf{r}}(t)$ is the Heisenberg operator for the position of the nucleus at time t, and $\langle\ \rangle$ denotes a thermal average over possible initial states of the scattering system. The IA consists of approximating $\hat{\mathbf{r}}(t)$ by

$$\hat{\mathbf{r}}(t) = \hat{\mathbf{r}}(0) + (t/M)\hat{\mathbf{p}} , \tag{2.13}$$

where $\hat{\mathbf{p}}$ is the momentum operator conjugate to $\hat{\mathbf{r}}$. With the approximation (2.13), it is straightforward[28] to show that $S(\mathbf{q},\omega)$ reduces to the expression given in (2.2). As in the classical case, for a gas of free particles (2.13), and consequently (2.2), are exact. This equation will also be accurate if $I(\mathbf{q},t)$ is small unless t is small, since the right-hand side (RHS) of (2.13) consists of the two highest-order terms in a Taylor expansion of $\hat{\mathbf{r}}(t)$ in t. Equation (2.13) has no explicit behavior on the potential energy of interaction, and clearly describes the motion of a free particle with momentum $\mathbf{p}$.

Equation (2.2) can also be derived in a more elementary fashion by directly treating the scattering system as a collection of free particles. For scattering from a single particle in a given quantum state $|i\rangle$, (2.9) gives

$$S(\mathbf{q},\omega) = \sum_f \left| \int \psi_i^*(\mathbf{r}) \exp(-i\mathbf{q}\cdot\mathbf{r}) \psi_f(\mathbf{r}) d\mathbf{r} \right|^2 \times \delta(\omega + E_i - E_f) , \tag{2.14}$$

where ψ_i and ψ_f are the initial and final state wave functions of the particle. For a free particle, with momentum $\mathbf{p}$ and normalized in a box of volume V,

$$\psi_i(\mathbf{r}) = V^{-1/2} \exp(i\mathbf{p}\cdot\mathbf{r}) \tag{2.15}$$

and $E_i = p^2/2M$. Similarly the final state is described by a plane wave with wave vector $\mathbf{k}_f$ and energy $E_f = k_f^2/2M$. The integral in (2.14) is then zero unless $\mathbf{k}_f = \mathbf{p}+\mathbf{q}$, and unity otherwise. Thus

$$S(\mathbf{q},\omega) = \delta(\omega - (\mathbf{p}+\mathbf{q})^2/2M + p^2/2M) \ . \tag{2.16}$$

The extension to (2.2) is obvious.

C. Assumptions of the impulse approximation

The main physical assumptions that are used to derive the IA are as follows.

(1) The scattering is incoherent, i.e., the scattering is insensitive to the effects of correlations between atomic positions (except insofar as these influence the momentum distribution).

(2) The final-state wave function of the particle can be treated as a plane wave, with wave number k_f and energy $k_f^2/2M$.

(3) The initial state of the scattering system is treated as a collection of free particles with momentum distribution $n(\mathbf{p})$.

Assumption (1) is valid for scattering from a hypothetical perfect rigid crystal when[28]

$$q \gg 1/a \ , \tag{2.17}$$

where a is the nearest-neighbor interatomic separation. In this case Bragg peaks become closely spaced and merge into an incoherent background. As previously mentioned, for other approximations in the IA to be valid $q \gg p_i$ must be satisfied, and, since in most systems at low temperatures $p_i \gg 1/a$, (2.17) should be well satisfied in the impulse regime. It is assumed throughout this paper, as in previously published work, that the incoherent approximation is satisfied in any DINS measurement.

It is implicit in the formulation of assumption (2) that the notion of a single-particle wave function for the struck particle in the final state has meaning in a many-particle system. This seems plausible, since, at energy transfers much greater than those of typical collective modes within the scattering system, one would expect excitations to have a single-particle nature. Even if this is allowed, then it may still appear that assumption (2) is never valid in a real system, since the final-state wave function will be confined to a region of space of the order of atomic dimensions by collisions with other atoms. However, from the form of (2.14),[27] it is clear that all that is necessary for an accurate calculation of $S(\mathbf{q},\omega)$ is that $\psi_f(\mathbf{r})$ is plane wave like over the region of space, where $\psi_i(\mathbf{r})$ has significant amplitude. When $\omega \gg V_i$, deviations from plane-wave behavior in this region should be small, and since $S(\mathbf{q},\omega)$ is insensitive to departures from free particle behavior of ψ_f, which occur outside this region, assumption (2) is again plausible.

Assumption (3) will be valid at high temperatures, where the effects of interatomic interactions are less important and the behavior of the scattering system approaches that of a gas of free atoms. However this region is correspondingly of less experimental interest, since $S(\mathbf{q},\omega)$ is insensitive to the interatomic interactions that are the object of investigation. At low temperatures assumption (3) is more questionable. It is shown in Sec. III that at high q the IA is reached in the absence of FSE's, and that therefore ISE's are negligible under these conditions, but that at lower q assumption (3) can be a serious source of error at low temperature, even when FSE's are negligible.

III. INITIAL-STATE EFFECTS

A. The plane-wave impulse approximation

From (2.10) the neutron scattering function for scattering from a single particle at zero temperature is

$$S(\mathbf{q},\omega) = \sum_f \left| \int \psi_i^*(\mathbf{r}) \exp(-i\mathbf{q}\cdot\mathbf{r}) \psi_f(\mathbf{r}) d\mathbf{r} \right|^2 \times \delta(\omega - E_f + E_i) \ . \tag{3.1}$$

From assumption (2),

$$\psi_f(\mathbf{r}) = \exp(i\mathbf{k}_f\cdot\mathbf{r}) \tag{3.2}$$

and

$$E_f = k_f^2/2M \ . \tag{3.3}$$

Normalization constants are neglected throughout, as they are not relevant to the discussion. The magnitude of $S(\mathbf{q},\omega)$ can always be derived from the condition $\int S(\mathbf{q},\omega)d\omega = 1$, which is rigorously true in the incoherent approximation.[31] Substituting (3.2) and (3.3) in (3.1) gives

$$S(\mathbf{q},\omega) = \sum_f |\bar{\psi}_i(\mathbf{k}_f - \mathbf{q})|^2 \delta(\omega + E_i - k_f^2/2M) \tag{3.4}$$

$$= \sum_f n(\mathbf{k}_f - \mathbf{q}) \delta(\omega + E_i - k_f^2/2M) \ . \tag{3.5}$$

$\bar{\psi}_i$ is the Fourier transform of ψ_i, and $n(\mathbf{p}) = |\bar{\psi}_i(\mathbf{p})|^2$ is the momentum probability distribution of an atom in state i. Converting the sum over final states to an integral over $\mathbf{k}_f$, and remembering that when the final state is a plane wave the density of points in $\mathbf{k}_f$ space is independent of $\mathbf{k}_f$, we obtain

$$S(\mathbf{q},\omega) = \int n(\mathbf{k}_f - \mathbf{q}) \delta(\omega + E_i - k_f^2/2M) d\mathbf{k}_f \ . \tag{3.6}$$

Making the substitution $\mathbf{p} = \mathbf{k}_f - \mathbf{q}$ gives

$$S(\mathbf{q},\omega) = \int n(\mathbf{p}) \delta(\omega[(\mathbf{p}+\mathbf{q})^2/2M + E_i]) d\mathbf{p} \ . \tag{3.7}$$

The difference between (3.7), which has been derived by explicitly neglecting FSE's, and (2.2) is entirely caused by ISE's. In the derivation of (2.2), it is assumed that the momentum and energy of the struck atom are related via $E_i = p^2/2M$, so that a distribution of momenta implies a distribution of initial-state energies. The presence of E_i rather than $p^2/2M$ in the δ function of (3.7) is due to the quantum nature of the initial state. As zero temperature the system is quantum dominated and there is a precise ground-state energy, but a distribution of momentum values. Following the terminology of quasielastic electron-nucleon scattering, where similar arguments

have been used,[32–34] we henceforward refer to (3.7) and its variations discussed later as the plane-wave impulse approximation (PWIA).

In the work of Gunn, Andreani, and Mayers,[27] a WKB approach was used to investigate departures from plane-wave behavior in the final state. The necessary condition of validity for the description of $\psi_f(r)$ in the WKB approximation is[35]

$$|1/(k_f^2)(dk_f/dx)|^2 \ll 1 \ . \tag{3.8}$$

In this case a description of the form (3.2) is permissible, with

$$k_f(x)=\{2M[\omega+E_i-V(x)]\}^{1/2} \ . \tag{3.9}$$

As mentioned previously, it is only necessary for (3.2) and (3.3) to be a good approximation in the region of space where $\psi_i(r)$ has significant amplitude (i.e., $r \simeq r_i$) for a good approximation to $S(q,\omega)$ to be obtained. At large energy transfers (3.9) clearly satisfies (3.8), in this region.

A simple approximation to (3.9) is

$$k_f=[2M(\omega+E_i-V_f)]^{1/2} \ , \tag{3.10}$$

where the x dependence of k_f is neglected and V_F is a constant parameter that represents some average of $V(x)$ over the trajectory of the particle in the final state. In this case E_i in (3.7) is replaced by α where

$$\alpha=E_i-V_f \ . \tag{3.11}$$

If it is assumed that V_f is equal to V_i, the mean potential energy in the initial state, then $\alpha=\kappa_i$, where κ_i is the mean kinetic energy of a particle in the initial state and

$$S(\mathbf{q},\omega)=\int n(\mathbf{p})\delta(\omega(\mathbf{p}+\mathbf{q})^2/2M+\kappa_i)d\mathbf{p} \ . \tag{3.12}$$

This equation was first given, without derivation, by Stringari.[36] He justified the choice of κ_i in the δ function by the observation that this gave the correct first moment of $S(q,\omega)$. It is rigorously true that[31]

$$\int \omega S(q,\omega)d\omega=q^2/2M=\omega_R \ , \tag{3.13}$$

where this equation defines the "recoil energy," ω_R. However, the second moment of $S(q,\omega)$ must also satisfy the "ω^2 sum rule," which is satisfied in the incoherent approximation,[31]

$$\int \omega^2 S(q,\omega)d\omega=\tfrac{4}{3}\omega_R\kappa_i+\omega_R^2 \ , \tag{3.14}$$

and (3.12) overestimates the second moment by

$$\int n(p)(p^2/2M-\kappa_i)^2dp \ .$$

The choice $\alpha<\kappa_i$, which is equivalent to $V_f>V_i$, must be made to satisfy (3.14). It is physically more reasonable that $V_f>V_i$, since the struck particle will tend to move away from a potential minimum, to regions of higher potential energy than those occupied in the initial state. In the intermediate q range, where approximations that are only expected to be valid at high q are used, it is not surprising that the form of $S(q,\omega)$ derived in (3.7) cannot simultaneously satisfy both sum rules. Despite this, one would still expect that (3.7) should be a better approximation than the IA, since only FSE's are neglected in the derivation of the former, whereas both FSE's and ISE's are neglected in that of the latter. It is also worth noting that, as will be shown, at high q (3.12) reduces to the IA, which does satisfy both sum rules.

B. High q behavior

It can be seen from (2.2) that in the IA the δ function in $S(q,\omega)$ is only nonzero for points $\mathbf{p}$ in atomic momentum space which satisfy

$$\mathbf{p}\cdot\hat{\mathbf{q}}=(M/q)(\omega-q^2/2M) \ , \tag{3.15}$$

where $\hat{\mathbf{q}}$ is the unit vector along q, whereas from (3.12) only points

$$\mathbf{p}\cdot\hat{\mathbf{q}}=(M/q)(\omega-q^2/2M)+(M/q)(\kappa_i-p^2/2M) \tag{3.16}$$

contribute to $S(\mathbf{q},\omega)$. Assuming that $n(p)$ is small when $p \gg p_i$, only points for $p \simeq p_i$ need be considered. In this case, when $q \gg p_i$, the second term on the RHS of (3.16) can be neglected, and $p^2/2M$ and κ_i in the δ functions of (2.2) and (3.12) can be interchanged with negligible error. The insensitivity of $S(\mathbf{q},\omega)$ to an interchange of $p^2/2M$, κ_i, or α in the δ function at high q is used at a number of points in this paper. The essential argument is that the δ function determines which points in atomic momentum space contribute to $S(\mathbf{q},\omega)$. At high q the change in the position of these points and in the corresponding value of $n(\mathbf{p})$ introduced by the interchange can be neglected. The PWIA thus reduces to the IA when $q \gg p_i$. This is the justification for the criterion (2.5).

C. Scaling

In an isotropic system (3.12) reduces to[36]

$$S(q,\omega)=(M/q)\int_{|p_-|}^{|p_+|} pn(p)dp \ , \tag{3.17}$$

where

$$p\pm=q\pm[2M(\omega+\kappa_i)]^{1/2} \ . \tag{3.18}$$

When $q \gg p_i$, $p_+ \simeq 2q$, so $n(p_+)\simeq 0$ and p_+ can be taken as infinite. Then

$$S(q,\omega)=(M/q)J(y_1) \ , \tag{3.19}$$

where

$$y_1=p_-=q-[2M(\omega+\kappa_i)]^{1/2} \tag{3.20}$$

and

$$J(y_1)=\int_{|y_1|}^{\infty} pn(p)dp \ . \tag{3.21}$$

The dependence of $qS(q,\omega)$ on the single variable y_1, rather than q and ω separately, is known as "y_1 scaling."[36]

In the IA it can similarly be shown from (2.2) (Refs. 17 and 37) that in an isotropic system $S(q,\omega)$ obeys y scaling

$$S(q,\omega)=(M/q)J(y) \ , \tag{3.22}$$

where

$$y=(M/q)(\omega-q^2/2M)\ . \tag{3.23}$$

The function $J(y)$ is analagous to the Compton profile in Compton scattering. It can be interpreteted physically as the probability that an atom has the momentum component y along the direction of $\mathbf{q}$. The dependence of J on the variable y_1 rather than y has two important consequences. (i) $J(y)$ and $J(y_1)$ are peaked at y or $y_1=0$, i.e., at constant q the position of the peak in $S(q,\omega)$ is at the "recoil energy" $\omega_R=q^2/2M$ in the IA, and $\omega=q^2/2M-\kappa_i$ in the PWIA. (ii) Since $J(y)=J(-y)$, $S(q,\omega)$ at constant $\mathbf{q}$ in the IA is symmetric in ω about its peak. The PWIA is not symmetric about its peak. $S(q,\omega)$ rises sharply at $\omega<\omega_R$, and falls off more slowly at $\omega>\omega_R$. (see Figs. 2 and 3).

. As expected from the discussion following (3.16), for $q\gg p_i$, y_1 and y become identical since,

$$y_1=(2m/p_+)(q^2/2M-\omega-\kappa_i)\ . \tag{3.24}$$

When $q\gg p_i$, $p_+\simeq 2q$, and $\kappa_i/p_+\simeq 0$, so that $y_1\simeq y$.

D. The validity of the PWIA

Comparison with experimental data and calculations on exactly soluble models shows that $S(q,\omega)$ scales with y_1 rather than y at low temperatures. For example Stringari[36] showed that (3.12) gave remarkably good agreement with the ^{4}He data of Martel *et al.*[3] The results given in Sec. V for a particle confined in a box with rigid walls and previously published calculations on a Debye solid,[38,39] show that the PWIA is a much better approximation at low temperatures than the IA in these model systems. The assymetry in graphite data[40] is also well described by a harmonic Debye model, and hence this system must also give better agreement with the PWIA. That the PWIA gives much better agreement than the IA, with data and calculations on systems with such different potentials, together with the demonstration above that, the PWIA relies on a less restrictive set of approximations, provides strong evidence that the PWIA is a better approximation than the IA.

E. Final-state effects

Equation (3.7) predicts that ISE's cause the peak of $S(q,\omega)$ to move to ω_R-E_i, compared with ω_R in the IA. Shifts in the recoil peak to lower energies are usually attributed to FSE's. In fact it appears from the treatment above that interactions in the final state move the peak to higher energies. The potential energy in the final state was treated by replacing E_i with $\alpha=E_i-V_f$. α decreases in magnitude as the final-state interaction potential V_f increases and this causes the peak (at $\omega_R-\alpha$) to move to higher ω values. The tendency for FSE's to move the peak to higher ω can also be seen in a very direct manner from the form of (3.1). The dominant effect of the interatomic potential will be to slow the recoiling atom as it approaches other atoms. This will introduce longer wavelength Fourier components into $\psi_f(\mathbf{r})$, and hence lower q components into $S(\mathbf{q},\omega)$. Thus, at a given energy transfer $S(q,\omega)$ will shift to lower values of q, while conversely at fixed q, $S(q,\omega)$ will move to higher values of ω. A peak shift to higher ω has been predicted in previous calculations of FSE's,[11,22] which have taken account of the energy of interaction between particles. In contrast the calculation of Silver and Reiter[19] on FSE's in a system of quasiclassical hard spheres, where there is no interaction energy, predicts no shift of the peak to larger values of ω, in agreement with the aformentioned interpretation.

F. High-temperature behavior

At high temperatures one expects the ISE's should be small, since interactions between particles become less significant, and the initial state approximates more closely to a gas of free particles. Proof of this can be seen from the following argument. At finite temperatures the momentum distribution in an isotropic system is

$$n(p)=\sum_i g_i n_i(p)\ , \tag{3.25}$$

where $n_i(p)$ is the momentum distribution of an atom in the state i, and g_i is the Boltzmann factor as before. If $n(p)$ is approximated by

$$n(p)=\sum_i g_i \delta(p-2M\kappa_i)^{1/2})\ , \tag{3.26}$$

then Eqs. (2.2) and (3.12) give identical results, i.e., the PWIA is identical to the IA. Equation (3.26) will be a good approximation at high temperatures, where it is equivalent to replacing the exact, continuous $n(p)$, by a series of closely spaced discrete values. The fact that peak shifts and asymmetries in $S(q,\omega)$ become small at high temperature does not appear to be widely known, possibly due to the generally held assumption that these features are caused by FSE's, which depend only weakly on temperature.

It is clear from the preceding argument that (3.12) is valid only at low temperatures. The use of (3.12) at high temperatures replaces a thermal distribution of possible energies by a single averaged value, and is a poor approximation. Calculations on a Debye solid[38] show that the temperature at which the IA starts to give a better description than the PWIA approximately corresponds to the energy of zero-point motion. Rinat[41] has also shown that (3.12) gives poor agreement with liquid neon data at temperatures close to the classical limit.

IV. PARTICLE IN A BOX AT ZERO TEMPERATURE

The calculation of $S(\mathbf{q},\omega)$ for neutron scattering from a single particle confined in a cubic box with rigid walls, provides clear illustrations of the formalism and conclusions of Sec. III. Taking the x,y, and z axes perpendicular to the cube faces, the scattering cross section at zero temperature, from a particle in a cubic box of side $2a$, is given by Eq. (3.1) with

$$\psi_i(\mathbf{r})=\psi_1(x)\psi_1(y)\psi_1(z) \tag{4.1}$$

and

$$\psi_f(\mathbf{r})=\psi_n(x)\psi_m(y)\psi_j(z)\ , \tag{4.2}$$

where

$$\psi_n(x)=(1/a^{1/2})\Pi_a(x)\cos(k_n x) \quad n \text{ odd} ,$$
$$=(1/a^{1/2})\Pi_a(x)\sin(k_n x) \quad n \text{ even} , \tag{4.3}$$

$\Pi_a(x)$ is defined as

$$\Pi_a(x)=1 \quad |x|<a ,$$
$$=0 \quad |x|>a . \tag{4.4}$$

The energies of the initial and final states are, respectively,

$$E_i=3k_1^2/2M \tag{4.5}$$

and

$$E_f=(k_n^2+k_m^2+k_j^2)/2M , \tag{4.6}$$

where

$$k_n=n\pi/(2a), \quad n=1,2,3,\ldots . \tag{4.7}$$

When x is taken parallel to q the integration over y and z yields the product $\delta_{j1}\delta_{m1}$ and we obtain

$$S(q,\omega)=\sum_n \left| \int \psi_1^*(x)\exp(iqx)\psi_n(x)dx \right|^2 \delta(\omega+E_1-E_n) , \tag{4.8}$$

i.e., the problem reduces to one dimension and is identical to that of scattering from a particle in an infinite square-well potential.

From (4.3) the Fourier transform of the function $\psi_n(x)$ is

$$\bar{\psi}_n(p)=a^{1/2}\{ \operatorname{sinc}[(p+k_n)a]$$
$$+(-1)^{n+1}\operatorname{sinc}[(p-k_n)a]\} , \tag{4.9}$$

where $\operatorname{sinc}(p)=\sin(p)/p$. $|\bar{\psi}_1(p)|^2$, which is the probability that an atom in the state ψ_1 will be found to have momentum p along **q** (i.e., the Compton profile) is shown in Fig. 1.

In the PWIA and the IA, the distribution of final states is assumed to be continuous, whereas the allowed levels in a square-well potential are discrete. The density of states in a square well is

$$\rho_d(k_f)=\sum_n \delta(k_f-k_n) , \tag{4.10}$$

where k_n is defined in (4.7). The assumed continuous density of states is given by a similar expression,

$$\rho_c(k_f)=\sum_m \delta(k_f-k_m) , \tag{4.11}$$

where $k_m=n\pi/2b$. In the limit $b\to\infty$ this approaches a continuous function.

We now calculate expressions for $S(q,\omega)$ in the IA and the PWIA, and compare these expressions with those obtained by exact calculation.

A. Exact calculation

From (4.3) and (4.8)

$$S(q,\omega)=1/(a)\sum_n [\bar{\psi}_1(q-k_n)+(-1)^{n+1}\bar{\psi}_1(q+kn)]^2$$
$$\times\delta(\omega+E_1-E_n) . \tag{4.12}$$

Since k_n is positive by definition, the δ function can be expressed as follows:

$$\delta(\omega+E_1-E_n)=\delta(\omega+E_1-k_n^2/2M)=(M/\beta)\delta(k_n-\beta) , \tag{4.13}$$

where

$$\beta=[2M(E_1+\omega)]^{1/2} . \tag{4.14}$$

Thus

$$S(q,\omega)=M/(a\beta)\sum_n [\bar{\psi}_1(q-\beta)+(-1)^{n+1}\bar{\psi}_1(q+\beta)]^2$$
$$\times\delta(k_n-\beta) . \tag{4.15}$$

From (4.10) this reduces to

$$S(q,\omega)=[\rho_d(\beta)/a]\{(M/\beta)[\bar{\psi}_1(q-\beta)$$
$$+(-1)^{n+1}\bar{\psi}_1(q+\beta)]^2\} . \tag{4.16}$$

B. Impulse approximation

Assuming that the initial state can be represented as a gas of free particles with momentum distribution $|\psi_1(p)|^2$,

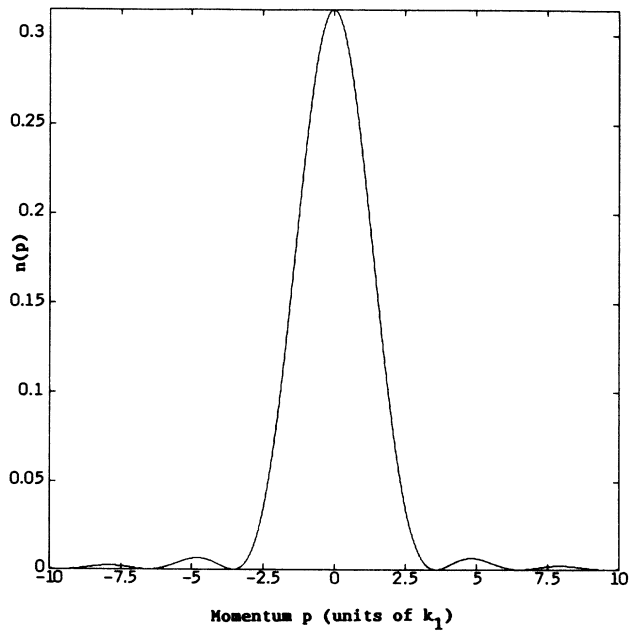

FIG. 1. Compton profile of an atom in the ground state of an infinite square-well potential. $J(p)=|\bar{\psi}_1(p)^2$, where $\bar{\psi}_1(p)$ is given by Eq. (4.9).

that the final states are also plane waves,

$$\psi_f(x)=(1/b^{1/2})\exp(ik_f x)$$

and using (4.11) gives,

$$S(q,\omega)=[\rho_c(y)/b]\{(M/q)|\psi_1(y)|^2\}\ , \tag{4.17}$$

where y is defined by (3.23). The expression within braces { } in (4.17) can also be derived very easily from the one-dimensional analogue of (2.2)

C. Plane-wave impulse approximation

Assuming that the final state is a plane wave as in Sec. III A, then from (4.8),

$$S(q,\omega)=[\rho_c(\beta)/b]\{(M/\beta)[|\bar{\psi}_1(q+\beta)|^2 + |\bar{\psi}_1(q-\beta)|^2]\}\ , \tag{4.18}$$

where β is defined by (4.14). The expression within braces { } can also be directly calculated from the one-dimensional form of (3.12) (note that in this model $E_i=\kappa_i$).

D. Comparison of IA and PWIA with exact calculation

The results (4.17) and (4.18) differ from (4.16) in that they contain a factor ρ_c/b rather than ρ_d/a. These factors describe the occupation of states in k_f space, when the allowed final states have continuous and discrete distributions, respectively. The weight of the contribution to $S(q,\omega)$, per unit volume of k_f space, is the same in the two cases, because of the presence of the factors $1/a$ and $1/b$, but in the continuous case this weighting is uniformly distributed over k_f space, whereas when the levels are discrete it is concentrated at the values $k_f=k_n$. For a comparison of the different results we omit ρ_f. A similar approach was taken by Rieter and Silver[19] in their discussion of a harmonic oscillator. The functions plotted are the envelopes that determine the relative magnitudes of the contributions to $S(q,\omega)$ made at allowed energy transfers.

The error introduced by treating the initial state as a collection of free particles appears particularly clearly in this model. In Figs. 2 and 3 the functions within braces { } in the different formulations, normalized so that $\int S(q,\omega)=1$, are shown for $q=4k_1$ and $q=11k_1$ as a function of ω. It can be seen that the PWIA is a much more accurate approximation than the IA at $q=4k_1$. At $q=11k_1$, the PWIA is almost identical to the exact result, while the IA still gives significant error. The asymmetry and the peak shift to lower values of ω are well reproduce by the PWIA.

The exact expression (4.16) for $S(q,\omega)$ consists of two identical contributions of width $\simeq 2k_1$, centered at $q\pm\beta$. These contributions correspond to the two Fourier components of the final-state wave function ψ_n, given by (4.3). At high ω, β is large, and the overlap between these two contributions is correspondingly small. Thus only one of these contributions is significant for the calculation of $S(q,\omega)$ at positive q. It is therefore a good approximation to neglect one of the Fourier components of $\psi_i(x)$ so that

$$\psi_n(x)\simeq(1/a^{1/2})\Pi_a(x)\exp(ik_n x)\ . \tag{4.19}$$

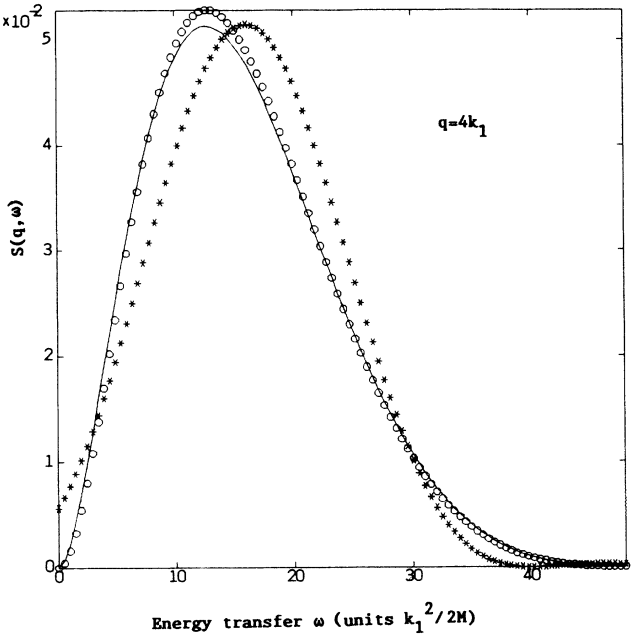

FIG. 2. Comparison of exact solution for a particle in an infinite square-well potential, at a momentum transfer $q=4k_1$, with the various approximations discussed in the text: Solid line: exact solution (4.16); ***: impulse approximation (4.17); ○○○: plane-wave impulse approximation (4.18).

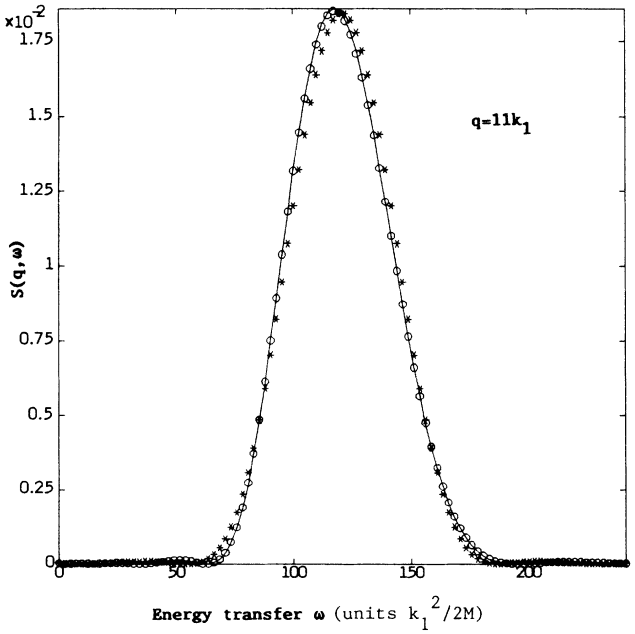

FIG. 3. As Fig. 2 but for $q=11k_1$.

Substituting (4.19) in (4.8) and using $\Pi_a(x)=[\Pi_a(x)]^2$ gives exactly the same envelope function as the PWIA. This explains why the PWIA gives such accurate agreement with the exact calculation in Fig. 3. The differences between the PWIA and the exact calculation in Fig. 2 are entirely caused by the overlap of the two contributions to $S(q,\omega)$ at lower q, which are the only consequence of FSE's in this model.

The model illustrates very clearly that the importance of FSE's is determined by the probability that an atom in the initial state occupies regions of space where significant departures from plane-wave behavior occur. At high q, where (4.19) is a good approximation, departures from plane-wave behavior occur only for $|x|>a$, where $\psi_i(x)=0$ and thus FSE's are negligible.

V. SUMMARY AND IMPLICATIONS FOR REAL SYSTEMS

It has been shown that when final-state effects (FSE's) are neglected, significant departures from the impulse approximation occur at low temperatures because of the quantum nature of the initial state of the target system. These "initial-state effects" (ISE's) cause the peak of $S(\mathbf{q},\omega)$ to move to lower values of ω compared with the impulse approximation (IA) prediction and introduce asymmetries into $S(\mathbf{q},\omega)$. Such features are observed in experimental data and numerical calculations but have generally been attributed to FSE's. In contrast it has been shown that FSE's in fact move the peak to higher values of ω.

The PWIA, in which FSE's are neglected, has been used to derive an expression for $S(\mathbf{q},\omega)$, which was first given by Stringari.[36] This expression predicts that $S(\mathbf{q},\omega)$ scales with y_1, compared with the y scaling predicted by the IA. It has been shown that at either high q or high temperature, the PWIA and the IA are identical, and that therefore y scaling is obeyed in these regimes when FSE's are absent. Thus, if experimental data y scales, this can be taken as evidence that ISE's are negligible.

The discussion of Sec. IV D illustrates that FSE's are significant only when departures of the final-state wave function from plane-wave behavior occur in the region of space which has significant probability of occupation by a particle in the initial state. Typical interatomic potentials consist of a relatively weak long-range interaction combined with a short-range repulsive interaction, e.g., the Lennard-Jones potential. At high momentum transfers q, any departures from plane-wave behavior will be small, except in regions of space where the hard-core component of the potential is dominant.

The model of Sec. IV crudely describes the high q regime, where an individual atom is confined within a box, the volume of which is defined by the hard-core component of the interatomic potential. Within the box the longer-range component of the potential can be neglected, and one expects that the final-state wave function at high q is given approximately by the form (4.19), with a the interatomic separation. The region of space with significant probability of occupation in the initial state is $r\simeq 1/p_i$, where p_i is the mean atomic momentum. In for example a Debye solid at zero temperature,[40] the mean square atomic displacement is $\langle r^2\rangle \simeq 108(M\Theta_D)$, where Θ_D is the Debye temperature in K, and M is the atomic mass in amu. Even for a light element such as Li, the probability that an atom will occupy regions of space with $r>a$ is $\simeq\exp(-100)$. Thus FSE's should be small at high q and low temperatures. This conclusion is not limited to solids, since on the time scale of DINS measurements ($\simeq 1/\omega$), atoms in a liquid are effectively static. Reiter and Silver[19] have arrived at a similar conclusion using a very different argument. Although in anharmonic systems such as solid He $a\simeq 1/p_i$, the model of Sec. IV, which is an extreme case of an anharmonic potential [$V(x)=\lim_{n\to\infty}|x/a|^n$], suggests that in anharmonic systems FSE's are also small. We note that this argument cannot be applied to ^{4}He in the presence of a Bose condensate since, as shown in the Appendix, off-diagonal long-range order implies that the initial-state wave function has significant amplitude at $r\gg a$. However, DINS should be a reliable method of determining momentum distributions in systems other than quantum fluids. Such systems are likely to become the object of more intensive experimental investigation with the development of spallation neutron sources and improved instrumentation.

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APPENDIX: VALIDITY OF SINGLE-PARTICLE TREATMENT IN A MANY-BODY SYSTEM

It is shown that if the scattering is incoherent and the struck particle does not interact with other particles in the final state, [assumptions (1) and (2) of Sec. II C], then $S(\mathbf{q},\omega)$ can be calculated as if the scattering system were composed of a single particle. A "wave function" and a corresponding energy can be defined, which when substituted in the full many-body expression for $S(\mathbf{q},\omega)$ give an apparently single-particle problem.

The exact expression for the incoherent $S(\mathbf{q},\omega)$ in an N particle system at zero temperature is,

$$S(\mathbf{q},\omega)=\sum_f \left|\int \Psi_i^*(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\exp(-i\mathbf{q}\cdot\mathbf{r}_1)\Psi_f(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)d\mathbf{r}_1,d\mathbf{r}_2,\ldots,d\mathbf{r}_N\right|^2\delta(\omega+E_i-E_f)\,, \tag{A1}$$

where $\mathbf{r}_1,\mathbf{r}_2$, etc., denote particle positions and Ψ is the many-particle wave function. If there are no interactions between the struck particle and other particles in the final state, the final-state wave function can be written as the product of a plane wave with the $N-1$ particle wave function Θ describing the other particles.

$$\Psi_f(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\exp(i\mathbf{k}_f\cdot\mathbf{r}_1)\Theta(\mathbf{r}_2,\ldots,\mathbf{r}_N)\,. \tag{A2}$$

Correspondingly, the final-state energy is a sum,

$$E_f = k_f^2/2M + E \ , \tag{A3}$$

where $k_f^2/2M$ is the energy of the recoiling particle, and E the energy of all other particles. The initial-state "wave function" is formally defined as

$$\psi_i(\mathbf{r}_1) = \int \Psi_i(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)\Theta(\mathbf{r}_2, \ldots, \mathbf{r}_N) d\mathbf{r}_2, \ldots, d\mathbf{r}_N \ . \tag{A4}$$

From Eqs. (A1) to (A4),

$$S(\mathbf{q},\omega) = \sum_f \left| \int \psi_i^*(\mathbf{r}_1) \exp[i(\mathbf{q}+\mathbf{k}_f)\cdot\mathbf{r}_1] d\mathbf{r}_1 \right|^2 \times \delta(\omega - k_f^2/2M + \alpha) \ , \tag{A5}$$

where $\alpha = E_i - E$.

Assuming that the parameter α is a constant as in Sec. III, is equivalent to the assumption that all the energy transfer is to the struck particle, i.e., that

$$k_f^2/2M - \omega = \text{const} \ . \tag{A6}$$

This is clearly implied by the assumption that the struck particle does not interact with other particles in the final state. Alternatively this can be regarded as an additional approximation that has a similar accuracy to the replacement of (3.9) by (3.10).

It can be shown [cf. (3.4) and (3.7)] that (A5) reduces to

$$S(\mathbf{q},\omega) = \int |\bar{\psi}_i(\mathbf{p})|^2 \delta(\omega - (\mathbf{p}+\mathbf{q})^2/2M + \alpha) d\mathbf{p} \ , \tag{A7}$$

and furthermore it is shown in Sec. III that when q is sufficiently large, compared with the width of $\bar{\psi}_i(\mathbf{p})$, α can be relaced by $p^2/2M$ with negligible error. Thus at high q (A7) reduces to a form identical to the IA except that $n(p)$ is replaced by $|\bar{\psi}_i(\mathbf{p})|^2$. The evidence for assuming that $n(p)$ is identical to $|\bar{\psi}_i(\mathbf{p})|^2$ at high q in any system seems overwhelming. It is true by definition, in a quantum system composed of a single particle in a potential. It is also true in a many-body system, providing that in the absence of FSE's, the IA is reached at sufficiently large q.

The further interpretation of $\psi_i(\mathbf{r})$ is of some physical interest, although unnecessary for the validity of the discussion in the text. The single-particle momentum distribution is

$$n(\mathbf{p}) = \int \rho(\mathbf{r}_a, \mathbf{r}_b) \exp[i\mathbf{p}\cdot(\mathbf{r}_a - \mathbf{r}_b)] d(\mathbf{r}_a - \mathbf{r}_b) \ , \tag{A8}$$

where the single-particle density matrix is defined by,

$$\rho(\mathbf{r}_a, \mathbf{r}_b) = \int \Psi_i^*(\mathbf{r}_a, \mathbf{r}_2, \ldots, \mathbf{r}_N) \times \Psi_i(\mathbf{r}_b, \mathbf{r}_2, \ldots, \mathbf{r}_N) d\mathbf{r}_2, \ldots, d\mathbf{r}_n \ . \tag{A9}$$

In a system with translational invariance $\rho(\mathbf{r}_a - \mathbf{r}_b) = \rho(\mathbf{r})$, with $\mathbf{r} = \mathbf{r}_a - \mathbf{r}_b$ and

$$n(\mathbf{p}) = \int \rho(\mathbf{r}) \exp(i\mathbf{p}\cdot\mathbf{r}) d\mathbf{r} \ . \tag{A10}$$

However, the function $\psi_i(\mathbf{r})$ satisfies,

$$n(\mathbf{p}) = \left| \int \psi_i(\mathbf{r}) \exp(i\mathbf{p}\cdot\mathbf{r}) d\mathbf{r} \right|^2 \ . \tag{A11}$$

From Eqs. (A10) and (A11) it follows that

$$\rho(\mathbf{r}) = \psi_i^*(\mathbf{r}) * \psi_i(\mathbf{r}) \ , \tag{A12}$$

where $*$ denotes convolution, thus the presence of off-diagonal long-range order in the single-particle density matrix is associated with $\psi_i(\mathbf{r})$ having significant amplitude for a large range of $\mathbf{r}$.

The physics suggests that the function $\Theta(\mathbf{r}_2, \ldots, \mathbf{r}_N)$ in (A2) is the ground-state wave function of the $N-1$ particle system, composed of the original system in the absence of the struck particle. In the absence of final-state interactions no energy is transferred to other particles, and if the N particle system is in its ground state, then the $N-1$ particle system must also be in its ground state. ($\psi_i(\mathbf{r})$ defined in this way has similarities to the ground-state average of the field creation operator.[43]) However, I know of rigorous proof that $\rho(\mathbf{r})$ is obtained from (A2) and (A12), if this interpretation is assumed.

$\psi_i(\mathbf{r})$ and $\psi_f(\mathbf{r})$ can be physically interpreted as follows. At the high-energy transfers required for the IA to be valid, the static approximation of neutron scattering can be used, since the time scale of atomic motions is short compared to $1/\omega$. One imagines that with other particles instantaneously fixed at the positions $\mathbf{r}_2, \ldots, \mathbf{r}_N$, single-particle initial- and final-state wave functions for the struck particle exist, which are solutions to the Schrödinger equation in the potential of these fixed atoms. These wave functions will tend to be localized at the position of the struck atom, which sits in the potential minimum created by the "cage" of surrounding atoms. $\psi_i(\mathbf{r})$ and $\psi_f(\mathbf{r})$ are then averages over all possible configurations of the other atoms. The probability of these configurations is determined by correlations between particles in the initial state, i.e., by the pair correlation function $g(\mathbf{r})$. Of course this picture cannot explain the extension in space of $\psi_i(\mathbf{r})$ when a Bose condensate is present.

[1] P. C. Hohenberg and P. M. Platzmann, Phys. Rev. **152**, 198 (1966).

[2] H. A. Mook, Phys. Rev. Lett. **32**, 1167 (1974).

[3] P. Martel, E. C. Svensson, A. D. B. Woods, V. F. Sears, and R. A. Cowley, J. Low Temp. Phys. **23**, 285 (1976).

[4] A. D. B. Woods and V. F. Sears, Phys. Rev. Lett. **39**, 415 (1977).

[5] V. F. Sears, E. C. Svensson, P. Martel, and A. D. B. Woods, Phys. Rev. Lett. **49**, 279 (1982).

[6] H. A. Mook, Phys. Rev. Lett. **51**, 1454 (1983).

[7] R. O. Hilleke, P. Chaddah, R. O. Simmons, D. L. Proce, and S. K. Sinha, Phys. Rev. Lett. **52**, 847 (1984).

[8] W. G. Stirling, E. F. Talbot, B. Tanatar, and H. R. Glyde, J. Low Temp. Phys. (to be published); J. Low Temp. Phys. **73**, 33 (1988).

[9] T. Sosnick, W. M. Snow, and P. E. Sokol, Proceedings of the Workshop on Momentum Distributions, Argonne National Laboratory, 1988, edited by R. N. Silver and P. E. Sokol (Ple-

num, New York, in press).
[10]H. A. Gersch and L. J. Rodriguez, Phys. Rev. A **8**, 905 (1973).
[11]L. J. Rodriguez, H. A. Gersch, and H. A. Mook, Phys. Rev. A **9**, 2085 (1974).
[12]J. J. Weinstein and J. W. Negle, Phys. Rev. Lett. **49**, 1016 (1982).
[13]P. M. Platzmann and N. Tsoar, Phys. Rev. B **30**, 6397 (1984).
[14]T. R. Kirkpatrick, Phys. Rev. B **30**, 1266 (1984).
[15]G. Reiter and T. Becher, Phys. Rev. B **32**, 4492 (1985).
[16]B. Tanatar, E. F. Talbot, and H. R. Glyde, Phys. Rev. B **36**, 2425 (1987).
[17]V. F. Sears, Phys. Rev. B **30**, 44 (1984).
[18]H. R. Glyde, J. Low Temp. Phys. **59**, 561 (1985).
[19]G. Reiter and R. N. Silver, Phys. Rev. Lett. **54**, 1047 (1985).
[20]R. N. Silver and G. Reiter, Phys. Rev. B **35**, 3647 (1987).
[21]R. N. Silver, Phys. Rev. B **38**, 2283 (1988).
[22]R. N. Silver, Phys. Rev. B **39**, 4022 (1989).
[23]W. G. Williams and S. W. Lovesey, Contemp. Phys. **30**, 35 (1989).
[24]S. Ikeda and N. Watanabe, Phys. Lett. A **121**, 34 (1987).
[25]S. Ikeda, M. Misawa, S. Tomiyoshi, and T. Suzuki, Phys. Lett. A **134**, 191 (1988).
[26]*Compton Scattering,* edited by B. Willams (McGraw-Hill, New York, 1977).
[27]J. M. F. Gunn, C. Andreani, and J. Mayers, J. Phys. C **19**, 1835 (1986).
[28]S. W. Lovesey, *Theory of Neutron Scattering from Condensed Matter* (Oxford University Press, London, 1987), Vol. 1.
[29]N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, London 1949).
[30]P. Platzmann and N. Tsoar, in *Compton Scattering,* Ref. 26, Sec. 2.4.
[31]G. L. Squires, *Introduction to the Theory of Thermal Neutron Scattering* (Cambridge University Press, London 1978), Chap. 4.
[32]I. Sick, D. Day, and I. S. McCarthy, Phys. Rev. Lett. **45**, 871 (1980).
[33]I. Sick, Commun. Part. Nucl. Phys. **18**, 109 (1989).
[34]C. Ciofi degli Atti, E. Pace, and G. Salme, Phys. Rev. C **36**, 1208 (1987).
[35]R. H. Dicke and J. P. Wittke, *Introduction to Quantum Mechanics* (Addison-Wesley, New York, 1960), Chap. 14.
[36]S. Stringari, Phys. Rev. B **35**, 2038 (1987).
[37]G. B. West, Phys. Rep. **18**, 263 (1975).
[38]J. Mayers, C. Andreani, and G. Baciocco, Phys. Rev. B **39**, 2022 (1989).
[39]J. M. F. Gunn and M. Warner, Z. Phys. B **56**, 13 (1984).
[40]M. P. Paoli and R. S. Holt, J. Phys. C **21**, 3633 (1989).
[41]A. S. Rinat, Phys. Rev. B **36**, 5171 (1987).
[42]A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, *Theory of Lattice Dynamics in the Harmonic Approximation* (Academic, New York, 1971).
[43]P. W. Anderson, *Basic Notions of Condensed Matter Physics* (Benjamin-Cummings, Menlow Park, 1984), p. 233.