Initial state effects in deep inelastic neutron scattering

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We demonstrate that a modified form of the impulse approximation (IA), proposed by Stringari, follows in a natural way from the analysis of Gunn, Andreani, and Mayers. An exact calculation of $S(q,\omega)$, for a harmonic system with a Debye density of states, is compared with the prediction of the IA and the Stringari form (SIA). The SIA gives a better description for temperatures less than $0.3\Theta_D$, where Θ_D is the Debye temperature. We derive a simple quantitative criterion for the validity of the IA in terms of the ratio of the atomic kinetic energy and the recoil energy. We argue that the deviations from the IA at low temperatures are primarily due to the quantum nature of the initial state, rather than final-state effects.

I. INTRODUCTION

There has been a considerable recent revival of interest in the determination of momentum distribution of atoms by neutron scattering at high momentum transfers.[1–5] Initial interest in condensed-matter research was aroused by Hohenberg and Platzman,[6] who considered the condensate in ^{4}He. The technique is known as neutron scattering in the impulse approximation (IA) or often as deep inelastic neutron scattering. The recent interest has been stimulated by measurements performed at Intense Pulsed Neutron Source, Argonne National Laboratory and by the advent of more intense spallation neutron sources such as ISIS at the Rutherford Appleton Laboratory (UK) and LANSCE at Los Alamos. Such sources have a much higher intensity at the neutron energies required for deep inelastic neutron scattering (>1 eV), than reactor sources.[7] It is likely that the technique will provide valuable information for the determination of atomic motions.

There is still controversy in the literature over the criteria which must be satisfied for the impulse approximation to be valid. In particular, deviations from the IA, which are usually attributed to final-state effects (i.e., deviations from free-atom recoil) introduce uncertainties in measured momentum distributions. In the standard derivations of the IA two assumptions are made. The first is that the momentum transfer is sufficiently large, that there are no interference effects between different atoms, i.e., the scattering is incoherent. This should be valid when $q \gg 1/a$, where a is the mean spacing between nearest-neighbor atoms and $\hbar q$ is the momentum transfer. The second is that the struck atom gains sufficient energy from the neutron that its recoil appears to be that of a free atom.

Stringari[8] has observed that the standard form of the IA does not correctly treat the bound nature of the initial state. By initial state we mean the state of the target system before the collision with the neutron. We show in Sec. II that a modified form of the IA, derived heuristically by Stringari, follows in a natural way from the approach of Gunn *et al.*[9]

In Secs. III and IV we present a comparison of $S(q,\omega)$, calculated exactly within the harmonic approximation, with the standard IA and the modified Stringari form. We use the modified Stringari form of the IA to derive a simple quantitative criterion for the validity of the IA. We then argue that many of the deviations from the impulse approximation, which have previously been attributed to final-state effects, are in fact due to an inadequate treatment of the quantum nature of the initial state.

II. THEORY

We first present a brief review of relevant theory. The double differential cross section for scattering at zero temperature from a single particle is[9,10]

$$\frac{d^2\sigma}{d\Omega\, dE} = |b|^2(k'/k) \times \sum_n \left| \int \psi_n(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) \psi_0(\mathbf{r}) d\mathbf{r} \right|^2 \times \delta(\hbar\omega + E_0 - E_n) = |b|^2(k'/k) S(\mathbf{q},\omega) , \tag{2.1}$$

where $\psi_0(\mathbf{r})$ is the ground-state wave function of the particle, $\psi_n(\mathbf{r})$ is that for the nth state, E_0 and E_n are their respective energies, $\hbar\omega$ is the energy transfer, $\hbar q$ the momentum transfer, and b the scattering length of the

particle. The second equality in (2.1) defines the neutron scattering function $S(q,\omega)$.

We consider scattering into a final state n and assume that the form of the final wave function approximates to a plane wave of wave vector $\mathbf{k}_f$, then

$$S(\mathbf{q},\omega)\sim \left|\int \psi_0(\mathbf{r})\exp[i(\mathbf{q}-\mathbf{k}_f)\cdot\mathbf{r}]d\mathbf{r}\right|^2 \times\delta(\hbar\omega+E_0-E_n) =|\tilde{\psi}_0(\mathbf{q}-\mathbf{k}_f)|^2\delta(\hbar\omega+E_0-E_n)\ , \tag{2.2}$$

where $\tilde{\psi}_0$ is the Fourier transform of ψ_0. Thus $S(\mathbf{q},\omega)$ in this approximation samples the momentum distribution of the initial atomic state at momentum $\hbar(\mathbf{q}-\mathbf{k}_f)$. The value of $\mathbf{k}_f$ is determined by ω and the condition for conservation of energy expressed in the δ function of Eq. (2.2).

An alternative derivation of $S(\mathbf{q},\omega)$ in the impulse approximation starts with an expression for $S(\mathbf{q},\omega)$ expressed in terms of the single-particle correlation function $I(\mathbf{q},t)$:[10]

$$S(q,\omega)=[1/(2\pi\hbar)]\int dt\ \exp(-i\omega t)I(\mathbf{q},t)\ , \tag{2.3}$$

where

$$I(\mathbf{q},t)=\langle\exp[-i\mathbf{q}\cdot\hat{\mathbf{r}}(0)]\exp[i\mathbf{q}\cdot\hat{\mathbf{r}}(t)]\rangle\ , \tag{2.4}$$

$\hat{\mathbf{r}}(t)$ is the Heisenberg operator for the particle at time t, and $\langle\ \rangle$ denotes thermal averaging over the target state. It is then assumed that the impulse approximation is valid for short times, i.e., in (2.4) we can make the replacement

$$\hat{\mathbf{r}}(t)=\hat{\mathbf{r}}(0)+(t/M)\hat{\mathbf{p}}\ , \tag{2.5}$$

where M is the mass of the particle and $\hat{\mathbf{p}}$ the momentum operator conjugate to $\hat{\mathbf{r}}$. The form of the operator $\hat{\mathbf{r}}(t)$ is then identical to that for a free particle. Approximation (2.5) treats the particle as free both before and after the collision with the neutron, but the initial momentum distribution of the atoms is modified from its free-gas form by the interactions between the atoms.[11] With the approximation (2.5) it is straightforward to obtain the standard impulse approximation to $S(q,\omega)$, namely,

$$S_I(\mathbf{q},\omega)=\int n(\mathbf{p})\delta(\hbar\omega-(\hbar^2/2M)(\mathbf{p}+\mathbf{q})^2 +(\hbar^2/2M)p^2)d\mathbf{p}\ , \tag{2.6}$$

where $n(\mathbf{p})$ is the atomic momentum distribution. The two formulations of the IA, Eqs. (2.2) and (2.6), are very different in form. However they reduce to the same expression at sufficiently high momentum transfers.[9]

It can be seen from Eq. (2.6) that a particular point in $\mathbf{q},\omega$ space samples the atomic momentum distribution of an isotropic system at the momentum

$$y_0=(M/\hbar q)(\omega-\hbar q^2/2M)\ . \tag{2.7}$$

Conversely, $S_I(\mathbf{q},\omega)$ scales with y_0.[12] This behavior is well known in Compton scattering and high-energy physics (see Ref. 11 and Sears[12] for further details).

Stringari[8] has suggested that an expression of the form

$$S_s(q,\omega)=\int n(\mathbf{p})\delta(\hbar\omega-(\hbar^2/2M)(p+q)^2+\langle K_i\rangle)d\mathbf{p} \tag{2.8}$$

is an improvement to the IA (2.6). Here $\langle K_i\rangle$ is the average kinetic energy per atom and the subscript i refers to properties of the target before it is struck by the neutron, i.e., the initial state. In this case the point (q,ω) corresponds to

$$\hbar p\pm=[2M(\hbar\omega+\langle K_i\rangle]^{1/2}\pm\hbar q\ . \tag{2.9}$$

The $p+$ term makes a negligible contribution to $S_s(q,\omega)$ at high-q values and so $S_s(q,\omega)$ samples the atomic momentum space at

$$y_1=[2M(\hbar\omega+\langle K_i\rangle)]^{1/2}-q\ . \tag{2.10}$$

In this approximation, y_1 is the scaling variable, rather than y_0. Stringari showed that Eq. (2.8) gave a good description of the ^{4}He data presented by Martel *et al.*[13] In their data analysis, Martel *et al.* divided $S(q,\omega)$ into symmetric and antisymmetric parts with respect to the recoil energy. The antisymmetric part of $S(q,\omega)$ is due entirely to deviations from the IA, so that the symmetric part alone approaches the impulse approximation more closely than the sum of the two parts.[12] They derived $n(p)$ using the symmetric part alone in Eq. (2.6). Stringari obtained a good description of the antisymmetric part using their derived $n(p)$ and Eq. (2.8).

The form $S_s(\mathbf{q},\omega)$ given by Stringari follows in a natural way from Eq. (2.2). If the energy transfer is sufficiently large, [see Eq. (5.4)] the final-state wave function will indeed be plane-wave-like, as assumed in (2.2), with a wave number which varies weakly with $\mathbf{r}$.

In one dimension,

$$k_f(x)=(2M/\hbar^2)^{1/2}[E_i+\hbar\omega-V(x)]^{1/2}\ , \tag{2.11}$$

where E_i is the energy of the initial state and $V(x)$ is the potential in which the particle sits. To derive Eq. (2.8), we assume that the effect of the potential is to shift the final wave number to that of an average over the probability density of the initial atomic state,

$$\langle k_f\rangle=\int k_f(x)|\psi_0(x)|^2dx\ . \tag{2.12}$$

A tentative physical interpretation of this is that $|\psi_0(x)|^2$ determines the probability of a collision occurring at x. The time of interaction between the neutron and the nucleus is sufficiently short that the nucleus moves only a short distance during the interaction. Thus the neutron will only be sensitive to values of $\mathbf{k}_f$ near the collision point.[11] However, the concept of interaction time is difficult to justify in any formal sense, and this semiclassical picture must be treated with caution.

For large $\hbar\omega$, from (2.11),

$$k_f(x)\sim(2M\omega/\hbar)^{1/2}\{1+[E_i-V(x)]/2\hbar\omega\}\ , \tag{2.13}$$

and we obtain

$$\langle k_f\rangle\sim(2M/\hbar^2)^{1/2}(\hbar\omega+\langle K_i\rangle)^{1/2}\ , \tag{2.14}$$

where

$$\langle K_i \rangle = E_i - \langle V_i \rangle \tag{2.15}$$

and

$$\langle V_i \rangle = \int V(x)|\psi_0(x)|^2 dx \tag{2.16}$$

are, respectively, the kinetic energy and the potential energy of the initial state. From Eqs. (2.2) and (2.14), $S(q,\omega)$ samples the atomic momentum space at y_1 in agreement with Eq. (2.10).

III. HARMONIC SOLID

The harmonic approximation gives a good description of many systems at low temperature. It also has the distinct advantage that the single particle $S(q,\omega)$ and $n(p)$ can be calculated exactly from the density of states. It might be objected that a particle in a harmonic potential can never be free, as the potential is unbounded. However Gunn *et al.*[9] have argued, from the form of Eq. (2.1), that the recoiling atom need only display free-particle behavior in the region of space where the initial-state wave function has significant amplitude. The numerical results presented here and previously[14] show that a harmonic solid does approach the impulse approximation at large-q values.

For an isotropic system, the incoherent scattering function in the harmonic approximation is given by[10,15]

$$S_H(q,\omega) = [1/(2\pi\hbar)] \int_{-\infty}^{+\infty} dt \exp(-i\omega t) \times \exp\{(\hbar q^2/2M) \times [\gamma(t) - \gamma(0)]\} , \tag{3.1}$$

where

$$\gamma(t) = \int_{-\infty}^{+\infty} d\omega [Z(\omega)/\omega] n(\omega) \exp(-i\omega t) . \tag{3.2}$$

$Z(\omega)$ is the normalized phonon density of states and $n(\omega)$ is the Bose-Einstein occupation factor

$$n(\omega) = [\exp(\hbar\omega/k_B T) - 1]^{-1} \tag{3.3}$$

in which k_B is Boltzmann's constant.

The method used by Maradudin *et al.*[16] to calculate the distribution in space of an atom in a harmonic solid can easily be adapted to give the momentum distribution. The momentum distribution of an individual atom is

$$n(\mathbf{p}) = \langle \delta(\hat{\mathbf{p}}' - \mathbf{p}) \rangle , \tag{3.4}$$

where $\langle\ \rangle$ denotes a thermal average of the operator $\delta(\hat{p}' - p)$ over all phonon occupations, as in (2.4).

Writing the δ function as a Fourier integral,

$$\delta(\hat{\mathbf{p}}' - \mathbf{p}) = [1/(2\pi)^3] \int \exp[i\mathbf{r}\cdot(\hat{\mathbf{p}}' - \mathbf{p})] d\mathbf{r} \tag{3.5}$$

and using the identity for a harmonic system[10]

$$\langle \exp(i\hat{\mathbf{p}}'\cdot\mathbf{r}) \rangle = \exp[-\tfrac{1}{2}\langle(\hat{\mathbf{p}}' - \mathbf{r})^2\rangle] \tag{3.6}$$

we obtain for an isotropic system

$$n(p) = [1/(2\pi M k_B T^*)^{3/2}] \exp[-p^2/(2M k_B T^*)] , \tag{3.7}$$

where

$$k_B T^* = \tfrac{2}{3}[\langle p^2 \rangle / 2M] . \tag{3.8}$$

This is identical to the expression for a free gas of Boltzmann particles, except that the temperature is replaced by an effective temperature T^* which is $\frac{2}{3}$ of the average kinetic energy per particle. In terms of the density of states,

$$T^* = (\hbar/k_B) \int_0^{\infty} \omega Z(\omega) \coth(\hbar\omega/k_B T) d\omega . \tag{3.9}$$

From Eqs. (2.6) and (3.7) we obtain the IA for $S(q,\omega)$:

$$S_I(q,\omega) = 1/(4\pi E_R k_B T^*)^{1/2} \times \exp[-(\hbar\omega - E_R)^2/(4E_R k_B T^*)] , \tag{3.10}$$

where

$$E_R = \hbar^2 q^2/2M \tag{3.11}$$

is the recoil energy of the particle. From Eqs. (2.8), (2.10), and (3.7) and neglecting the contribution from p_+ we obtain

$$S_s(q,\omega) = [1/(4\pi E_R k_B T^*)^{1/2} \times \exp[-y_1^2/(2M k_B T^*)] \tag{3.12}$$

as the Stringari formulation of the IA, hereafter referred to as SIA.

IV. NUMERICAL SIMULATIONS

A FORTRAN program has been written to calculate the harmonic scattering function $S_H(q,\omega)$ exactly from the density of states. A fast Fourier transform routine has been used to evaluate the Fourier transforms in Eqs. (3.1) and (3.2). We chose to use a Debye density of states

$$Z(\omega) = \begin{cases} 3\omega^2/\omega_D^3, & \omega < \omega_D , \\ 0, & \omega > \omega_D . \end{cases}$$

At the large-q values needed to approach the IA, where $S(q,\omega)$ is dominated by multiphonon processes, the exact form of $Z(\omega)$ should have no significant effect. This conclusion is supported by simulations on vanadium using the measured vanadium density of states. The program correctly reproduces the one phonon $S(q,\omega)$ at low-q values. We have also compared its predictions with the formalism of Nelkin and Parks.[17] Although this approximation does not reproduce the sharp features in $S(q,\omega)$ shown in Fig. 1, at higher-q values it gives very good agreement. As a final check, we calculated neutron differential cross sections $d\sigma/d\Omega$ as a function of incident neutron energy and scattering angle. A comparison with the predictions of the Placzek expansion[18] gave good agreement for neutron energies $\gtrsim \hbar\omega_D$.

Some results of the program are shown as solid lines in Figs. 1 and 2. We have used reduced units, i.e., temperature is given in units of Debye temperature (Θ_D) and energy in units of Debye energy. The dashed lines show the

predictions of the IA [Eq. (3.10)] and the dotted-dashed lines those of the SIA [Eq. (3.12)]. Note that, as can be seen directly from Eq. (3.10), the conventional IA is symmetric about a maximum at $\hbar\omega = E_R$. The SIA has its maximum at $\hbar\omega = E_R - \langle K_i \rangle$ and is not symmetric.

Figure 1(a) shows a comparison at $T=0$ for a recoil energy of $E_R = 1$. The presence of two, three, and four phonon peaks is clearly visible in the exact $S_H(q,\omega)$. The influence of the discontinuity in the Debye density of states at $\hbar\omega = 1$ is seen in $S_H(q,\omega)$ at $\hbar\omega = 1,2,3$. At higher values of $\hbar\omega$, the presence of multiphonon effects blurs the discontinuities, which eventually become unobservable. It can be seen that even at a value of E_R as low as 1, where the IA is not expected to be valid, the SIA gives on the average a better description of $S_H(q,\omega)$ particularly at larger values of $\hbar\omega$. At a recoil energy of 3 [Fig. 1(b)] the SIA is clearly better than the IA over the entire ω range. At a recoil energy of 5 [Fig. 1(c)] although there are still significant deviations from the conventional IA, the SIA gives a good description of $S_H(q,\omega)$ over most of the energy range. There is still some slight evidence of the discontinuity in the density of states at $\hbar\omega = 1$ and 2, but at higher values of ω, where the response is dominated by multiphonon processes,

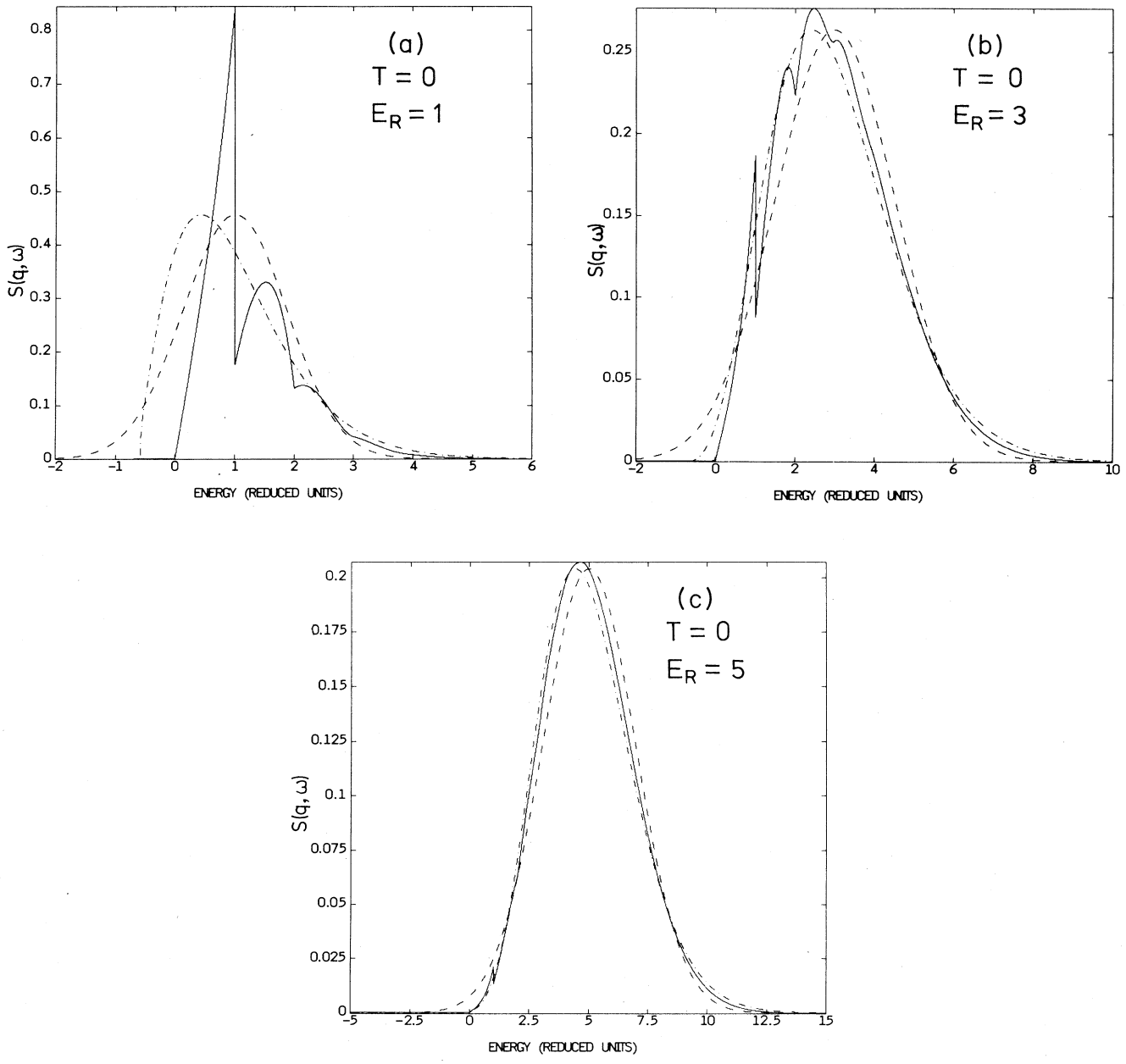

FIG. 1. $S(q,\omega)$ calculated exactly within the harmonic approximation (solid line) is compared with the IA (dashed line) and with the SIA (dashed-dotted line) at $T=0$. T is in units of Debye temperature, recoil energy E_R in units of Debye energy.

$S_H(q,\omega)$ is smooth and well approximated by Eq. (3.12).

In Fig. 2 we show the results of simulations at $T=1$. In contrast to the zero-temperature case, the IA clearly gives a better description of $S_H(q,\omega)$ than the SIA, at all values of recoil energy. The IA works well even at $E_R=1$. We interpret this as a manifestation of increasingly free-particle-like behavior, as the temperature is raised (at the Debye temperature T^* and T differ by less than 6%). At high temperatures there is a thermal distribution of $\langle K_i \rangle$ values. The Stringari approximation is equivalent to replacing this distribution by a single, thermally averaged K_i. It appears that assuming a free-particle initial momentum distribution is a better approximation when $T=\Theta_D$. The cross-over temperature, at which the IA starts to give a better description than the SIA, occurs at $\sim 0.3\Theta_D$. This is close to $3\Theta_D/8$, the temperature at which the thermal energy is equal to the kinetic energy of zero point motion, in a Debye solid.

V. VALIDITY OF THE IMPULSE APPROXIMATION

There is still controversy in the literature as to which conditions must be satisfied for the IA to be valid. For example, Sears[12] derives an interaction time $\tau=1/qv_0$,

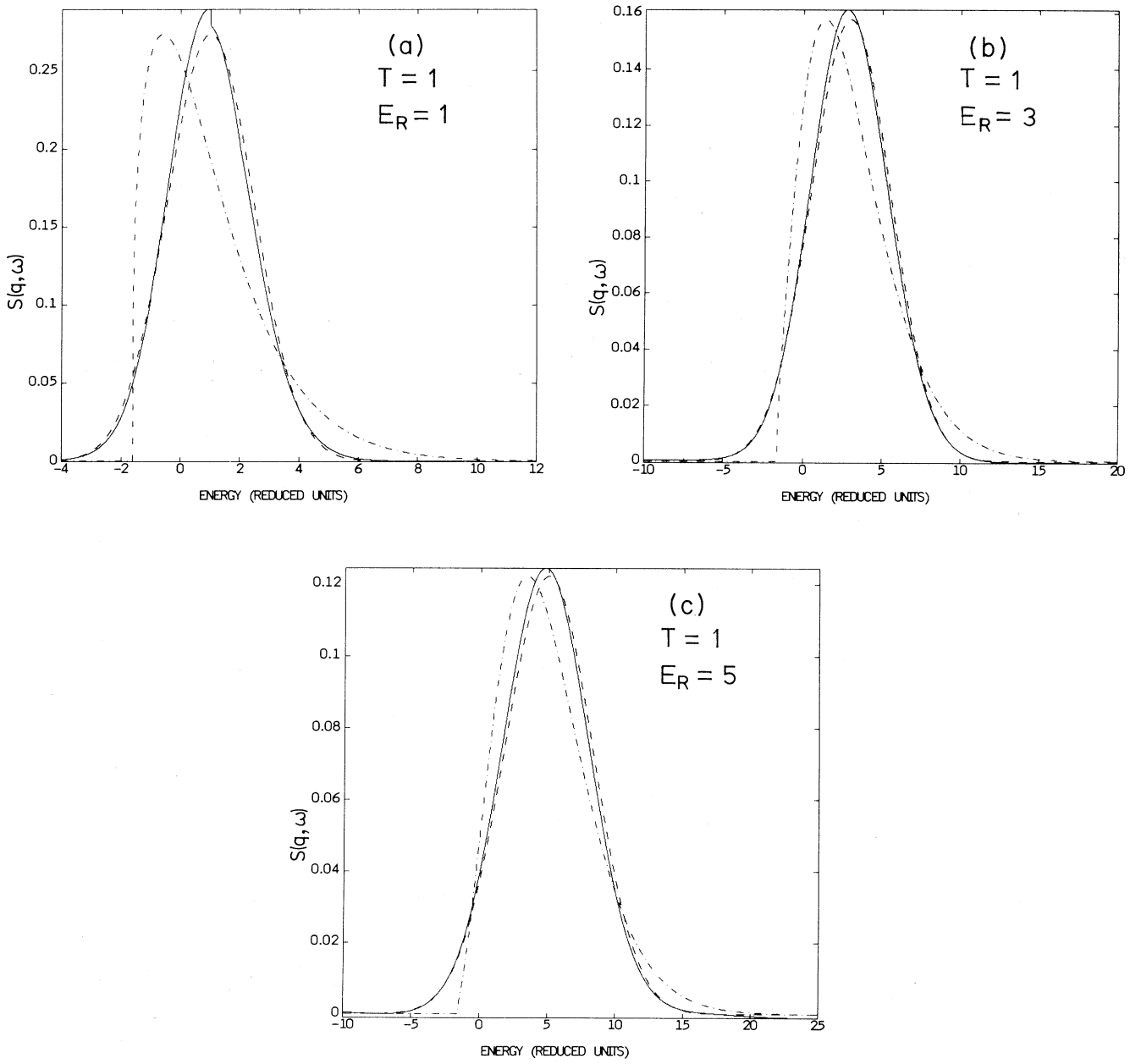

FIG. 2. As in Fig. 1 but at temperature $T=\Theta_D$.

where v_0 is the mean velocity of the atom in the initial state. The IA is then said to be valid if

$$F_0\tau \ll Mv_0 \ , \tag{5.1}$$

where F_0 is the mean force exerted on the atom by surrounding atoms. This leads to the condition

$$q \gg F_0/2\langle K_i\rangle \ . \tag{5.2}$$

Reiter and Silver[3] also derive a condition for validity of the IA using an interaction time. For the approach of Eq. (2.2) to be valid, the condition

$$|(1/k_f^2)(dk_f/dx)| \ll 1 \tag{5.3}$$

must be satisfied. This condition is well known from the WKB approximation.[19] If it is not satisfied, the final-state wave function will not approximate to a plane wave. When applied to Eq. (2.13) and with $\hbar\omega \sim \hbar^2q^2/2M$, this gives

$$q \gg [(M/\hbar^2)dV/dx]^{1/3} \tag{5.4}$$

as a necessary condition for the final state to be approximately plane-wave-like.

Platzman and Tzoar[11] present an expansion of $S(q,\omega)$ in terms of E_B/E_R, where E_B is the binding energy. Their conclusion is that the IA is valid to an accuracy of $(E_B/E_R)^2$. As a final example, the expansion of Nelkin and Parks[17] predicts that the ratio $\langle K_i\rangle/E_R$ determines the validity of the IA. The latter criterion is easiest to apply to experimental data. E_R is known, and $\langle K_i\rangle$ can be approximately determined from the width of the measured $S(q,\omega)$, or the exact sum rule

$$\langle K_i\rangle = \lim_{q\to\infty}(3\hbar/4E_R) \times \int_{-\infty}^{+\infty}[\omega-(E_R/\hbar)]^2 S(q,\omega)d\omega \ . \tag{5.5}$$

In the exact expansion for $S(q,\omega)$ in the harmonic approximation [Eq. (3.1)], q appears only in the recoil energy E_R. Thus for a harmonic solid it is rigorously true that E_R determines when the IA is reached, rather than q. It is worth pointing out that Debye temperatures do not have a strong systematic variation with atomic mass. For example, calcium and platinum, both fcc structures, have identical Debye temperatures, but masses which differ by a factor of 5. One would therefore expect that the q value required to reach the IA is roughly proportional to $M^{1/2}$. We now present a simple quantitative criterion for the validity of the IA in terms of the ratio $\langle K_i\rangle/E_R$.

It appears both from the analysis of experimental ^{4}He data by Stringari and the harmonic calculations presented in the last section, that the SIA accounts for most of the observed asymmetry in $S(q,\omega)$. Stringari showed that by expanding the scaling variable y_1 to first order in $1/q$, $S_s(q,\omega)$ could be divided into symmetric and antisymmetric parts. The symmetric part is identical to the IA

$$S_s^{(s)}(q,\omega) = S_I(q,\omega) \ . \tag{5.6}$$

The antisymmetric part is

$$S_s^{(a)}(q,\omega) = [2\pi M y_0 n(y_0)/\hbar^4q^2] \times (M\langle K_i\rangle - \tfrac{1}{2}\hbar^2y_0^2) \ . \tag{5.7}$$

For a Gaussian momentum distribution such as Eq. (3.7) and noting that $\langle K_i\rangle = (3/2)k_BT^*$, we obtain

$$S_s^{(s)}(q,\omega) = [4\pi\langle K_i\rangle M^2/3\hbar^2q^2]n(y_0) \ . \tag{5.8}$$

The ratio of the antisymmetric and symmetric parts is

$$S_s^{(a)}/S_s^{(s)} = (3y_0/2q\langle K_i\rangle M)[M\langle K_i\rangle - (\tfrac{1}{2})\hbar^2y_0^2] \ . \tag{5.9}$$

For a given value of q, this ratio has extrema at

$$\hbar\omega_\pm = E_R \pm (2\hbar^2q^2\langle K_i\rangle/3M)^{1/2} \ , \tag{5.10}$$

where, as before, E_R is the recoil energy $\hbar^2q^2/2M$.

From Eqs. (2.7), (5.8), and (5.10) the ratio of $S_s^{(s)}(q,\omega)$ at the extrema to that at the recoil frequency ω_R is

$$S_s^{(s)}(q,\omega_\pm)/S_s^{(s)}(q,\omega_R) = e^{-1/2} \ , \tag{5.11}$$

i.e., the maximum asymmetry occurs close to the maximum of $S(q,\omega)$. At $\omega_\pm$, Eqs. (5.9) and (5.10) give

$$S_s^{(a)}(q,\omega_\pm)/S_s^{(s)}(q,\omega_\pm) = \pm(\langle K_i\rangle/3E_R)^{1/2} \ . \tag{5.12}$$

Equation (5.12) should provide a good estimate of the maximum degree of asymmetry which is to be expected as a result of deviations from the IA.

The momentum distributions of ^{4}He is not expected to be Gaussian in form, both from theoretical considerations and experimental evidence. However, given that the results of Stringari agree well with data on ^{4}He, it seems reasonable to expect that Eq. (5.11) should be a useful guide to the degree of asymmetry expected in ^{4}He data. Taking $\langle K_i\rangle = 1.8$ meV we obtain $S_S^{(a)}/S_S^{(s)} = \pm 0.11$ from Eq. (5.11) at a q of 10 Å^{-1}. This agrees well with the data of Martel *et al.*[13]

VI. CONCLUSIONS

We have shown that the modified form of the IA proposed by Stringari (SIA) follows in a natural way from the formulation of the IA given by Gunn *et al.* A comparison of the predictions of the IA and the SIA with an exact calculation of $S(q,\omega)$ for a harmonic solid shows that at low temperatures the SIA is a better approximation to $S(q,\omega)$ than the IA. The analysis of the data of Martel *et al.* by Stringari also gives a good description of ^{4}He data. The fact that the SIA works well for two systems with very different atomic interactions, together with the derivation presented in Sec. II, provides strong support for its validity.

The aim of neutron scattering in the impulse approximation is to provide information on interatomic interactions. The effect of these will be strongest at low temperatures, and the low-temperature regime is therefore of greatest experimental interest. Since the SIA appears to account for most of the asymmetry observed in the measured $S(q,\omega)$ for liquid ^{4}He and the calculated $S_H(q,\omega)$ for a harmonic solid, we feel justified in using it to derive a condition for the validity of the IA. We find that at low temperatures, the quantity $(\langle K_i\rangle/3E_R)^{1/2}$ gives a mea-

sure of the maximum degree of asymmetry in $S(q,\omega)$ due to deviations from the IA.

For temperatures greater than $0.3\Theta_D$ the IA gives a better description of a Debye solid than the SIA. The energy corresponding to this temperature is close to the kinetic energy due to zero-point motion. We interpret this as evidence of increasingly classical, free-particle-like behavior of the initial state as the temperature is raised. The IA [Eq. (2.6)] describes the scattering from a system of free particles, where momentum and energy are conserved. At zero temperature the atomic momentum distribution is nonzero due to quantum effects, and the IA gives a finite probability that the target system will lose energy. However in reality such energy-loss processes are forbidden as the target system is already in its ground state. We suggest that these properties of the initial state, rather than effects of interatomic interactions on the recoiling atom, are primarily responsible for deviations from the IA at low temperatures.

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