PHYSICAL REVIEW B VOLUME 40, NUMBER 10 1 OCTOBER 1989

Approach to the asymptotic limit in inclusive scattering of neutrons from quantum liquids

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(Received 28 June 1988; revised manuscript received 20 April 1989)

We study the approach to the asymptotic limit in inclusive scattering in case the interaction between the constituents possesses a hard core. An extensive discussion is given of leading contributions to the linear response and of their dependence on various input components. The theory is applied to liquid ^{4}He at $T=1.2°$ K, $q=10$ Å^{-1}.

I. INTRODUCTION

In both condensed-matter and nuclear physics, continuing efforts are aimed at the study of the linear response, which constitutes an important source of information on matter. The starting point is frequently the response under asymptotic conditions which, roughly speaking, coincide with large momentum and energy transfers q,ω. One is then, in general, permitted to use the impulse approximation (IA) and the response becomes a simple expression in terms of $n(p)$, the single-particle momentum distribution. The extraction of the latter is frequently considered to be the primary goal of these studies.

In spite of the fact that conditions in some experiments are seemingly close to the asymptotic ones, data are not always in satisfactory agreement with IA predictions. Conversely, if from measurements of the response for large q one wishes to extract rare, large p components of $n(p)$, one needs a refined theory which permits a reliable isolation of the pure IA contribution in data.

One of the reasons for the mentioned disagreements is the apparently insufficient modeling of the approach to the asymptotic regime as described by the simplest of all final-state interactions (FSI's). The latter is caused by collisions of a high momentum knocked-on constituent with a partner in the medium. References 1–4 contain some descriptions of FSI's in liquid ^{4}He close to $T=0$ K as well as lists of references.

In the process many authors have apparently overlooked, or did not sufficiently emphasize, formally exact expressions for the response expanded in a series of inverse powers of q. These were published 15 years ago by Gersch and his co-workers[5,6] who, at the time, lacked sufficiently accurate input for realistic applications. In this context it is of interest to mention a recent semiclassical treatment of the response by Rosenfelder, whose FSI contribution coincides with the same in Gersch *et al.*[5] to lowest order in q^{-1}. His application to inclusive electron scattering on ^{12}C is to our knowledge the only one to date.[7]

A possible second cause for the mentioned disagreements may have its root in the presence of a short-range repulsion in the elementary interaction: the asymptotic expansion of the response of Gersch *et al.* and of Rosenfelder only holds for regular interactions. Weinstein and Negele then demonstrated numerically that the IA is not the correct asymptotic limit when interactions contain a hard core.[8] Reference 9 contains explicit expressions for these corrections.

Without the habitual emphasis on scaling, the following note focuses on FSI contributions to the response if the elementary interaction is strong, possesses a hard core, or both. Within a nonrelativistic Hamiltonian framework we shall use a multiple-scattering approach and first rederive in Sec. II for regular interactions the leading order correction to the IA and discuss some sum rules. Next we reformulate in Sec. III the theory for interactions with a strong repulsive component at short distances. Approximate expressions are given which permit applications in practice. Among others, these affect the intervening nondiagonal, two-particle density matrix, and we suggest (and later apply) quality tests for some approximations (Sec. IV). In Sec. V we discuss modifications of the theory in the presence of a superfluid component in ^{4}He. The theory is then applied to data for liquid ^{4}He for $q=10$ Å^{-1} at $T=1.2$ K (Sec. VI).

II. ASYMPTOTIC SERIES FOR THE LINEAR RESPONSE

We shall derive in this section some known formal results pertinent to the linear, longitudinal response of a many-body system at $T=0$ K close to the asymptotic region. We shall employ standard multiple-scattering techniques, which are suited for a generalization of the known results in case the elementary interaction possesses a hard core.

Consider a nonrelativistic system, which is described by a Hamiltonian H_A. Ground-state wave function and energy are denoted by Φ_A^0 and ε_A^0. The definition of the response in terms of a momentum and frequency parameter q,ω then reads ($\hbar=c=1$)

$$AS(q\omega)=(2\pi)^{-1}\int\int\int d\mathbf{r}\,d\mathbf{r}'\,dt\,e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\times e^{i\omega t}\langle\Phi_A^0|\hat\rho(\mathbf{r}t)\hat\rho(\mathbf{r}'0)|\Phi_A^0\rangle$$
$$=-\pi^{-1}\mathrm{Im}\langle\Phi_A^0|\hat\rho_{\mathbf{q}}^{\dagger}G(\omega+\varepsilon_A^0+i\eta)\hat\rho_{\mathbf{q}}|\Phi_A^0\rangle\,, \quad (2.1)$$

where

$$\hat\rho(\mathbf{r}t)=\exp(iH_At)\hat\rho(\mathbf{r})\exp(-iH_At)\,.$$

S is usually measured in an inclusive scattering experiment $A(x,x')X$ induced by a projectile x and is then the ratio of inclusive and elementary cross sections

$$AS(q\omega)=\frac{k}{k'}\frac{d^2\sigma^{xA}}{dq\,d\omega}\Big/\frac{d\sigma^{xc}}{dq} ,$$

where $(\mathbf{q},\omega)$ are momentum and energy transferred to the target. A in (2.1) is the number of particles contained in a volume at equilibrium density

$$\rho\ (=\langle\hat{\rho}(\mathbf{r})\rangle)=\lim_{A,\Omega\to\infty}(A/\Omega) ,$$

and $\hat{\rho}_{\mathbf{q}}=\sum_{i=1}^{A}e^{i\mathbf{q}\cdot\mathbf{r}_i}$ is a longitudinal density fluctuation. Finally, $G(z)=(z-H_A)^{-1}$ is the Green's function of the system corresponding to the full Hamiltonian.

In the following we exclusively consider the dominant, incoherent part of S where [cf. Eq. (2.1)] the same particle acts in $\hat{\rho}_{\mathbf{q}}^{+}$ and in $\hat{\rho}_{\mathbf{q}}$. Thus $(S=S^{\text{incoh}})$

$$S(q\omega)=\langle\Phi_A^0|e^{-i\mathbf{q}\cdot\mathbf{r}_1}\delta(\omega+\varepsilon_A^0-H_A)e^{i\mathbf{q}\cdot\mathbf{r}_1}|\Phi_A^0\rangle . \quad (2.2)$$

It will be useful to write the Hamiltonian H_A as follows:

$$\begin{aligned}H_A&=H_0+V\\&=H_{A-1}+T_1+\sum_{j\geq 2}v_{1j} .\end{aligned} \quad (2.3)$$

In Eq. (2.3) one emphasizes the $A-1$ particle core (eigenstates and energies Φ_{A-1}^n and ϵ_{A-1}^n), an initially knocked-on particle ("1") and their interaction

$$V=\sum_{j\geq 2}v_j\ \left[=\sum_{j\geq 2}v_{1j}\right] .$$

A standard result gives S in the impulse approximation (IA) when V in (2.3) is neglected (m is the mass of a constituent),

$$\begin{aligned}(q/m)S^{\text{IA}}(q\omega)&=F_0\left[y_0^A\right]\\&=(2\pi)^{-2}\int_{|y_0^A|}^{\infty}n(p)p\,dp .\end{aligned} \quad (2.4)$$

For nonsingular interactions (2.4) can be shown to be the $q\to\infty$, fixed y limit of S which depends only on the single-particle momentum distribution $n(p)/(2\pi)^3$ and the corresponding IA scaling variable

$$y_0^A=-\frac{A-1}{A}q+\left[\frac{A-1}{A}\left[\xi_0^2-\frac{q^2}{A}\right]\right]^{1/2} . \quad (2.5)$$

In (2.5) $\xi_0^2=2m(\omega+\langle\Delta\rangle)$ and $\langle\Delta\rangle=\langle\varepsilon_A^0-\varepsilon_{A-1}^{(n)}\rangle$ some average separation energy. For later use we mention a frequently used, alternative variable $(\xi^2=2m\omega)$ (Ref. 10)

$$y_W=-(q/2)(1-\xi^2/q^2) . \quad (2.6)$$

Notice that

$$y_W-y_0^A=\frac{[A/(A-1)](y_0^A)^2+2m\langle\Delta\rangle}{2q}=O(q^{-1}) . \quad (2.7)$$

The division (2.3) of the Hamiltonian clearly entails the same for the response. Writing

$$G(z)=G_0(z)+G_0(z)T(z)G_0(z) \quad (2.8)$$

with $G_0(z)=(z-H_0)^{-1}$, one obtains

$$S=S^{\text{IA}}+\Delta S . \quad (2.9)$$

Evaluation of ΔS is possible when using expansions of the scattering operator T in (2.8), for instance in terms of the elementary pair interaction v or, alternatively, in terms of the corresponding scattering operator $t=v+vG_0t$,

$$T=\sum_{j\geq 2}v_j+\sum_{j\geq 2}v_jG_0\sum_{k\geq 2}v_k+\cdots \quad (2.10a)$$

$$=\sum_{j\geq 2}t_j+\sum_{j\geq 2}t_jG_0\sum_{j\neq k\geq 2}t_k+\cdots . \quad (2.10b)$$

Data on diverse systems frequently refer to kinematical (q,ω) or (q,y) regions which are thought to be close to the asymptotic regime. One is thus naturally interested in a series expansion of $S(qy)$ in inverse powers of q at some fixed $y_i=y_i(q,\omega)$. For the reduced response

$$\phi(qy_i)\equiv(q/m)S(qy_i)$$

one finds

$$\phi(qy_i)=F_0(y_i)+(m/q)F_1^{(i)}(y_i)+O(q^{-2}) . \quad (2.11)$$

The IA to ϕ clearly is F_0 in the variable y_0^A, (2.5). In order to see how the terms in (2.11) arise, it is useful to start with the lowest-order term in (2.10a), assuming of course that matrix elements of v exist. For its contribution to ΔS, Eq. (2.9), one finds

$$\begin{aligned}[\Delta S(q\omega)]^v&=-\pi^{-1}(A-1)\\&\times\text{Im}\sum_{n,n'}\int\int\frac{d\mathbf{p}_1}{(2\pi)^3}\frac{d\mathbf{p}_1'}{(2\pi)^3}\\&\times\frac{\langle\Phi_A^0|\Phi_{A-1}^n\mathbf{p}_1\rangle\langle\mathbf{p}_1+\mathbf{q},\Phi_{A-1}^n|v|\mathbf{p}_1'+\mathbf{q},\Phi_{A-1}^{n'}\rangle\langle\mathbf{p}_1',\Phi_{A-1}^{n'}|\Phi_A^0\rangle}{[\omega+\Delta_n-(\mathbf{p}_1+\mathbf{q})^2/2m-\mathbf{p}_1^2/2m(A-1)+i\eta][\omega+\Delta_{n'}-(\mathbf{p}_1'+\mathbf{q})^2/2m-\mathbf{p}_1'^2/2m(A-1)+i\eta]}\end{aligned} \quad (2.12)$$

Notice first that for each "free" propagator G_0 in (2.12)

$$G_0 \underset{\substack{q\to\infty \\ y_0^A \text{ fixed}}}{\longrightarrow} [(q/m)(y_0^A-\mathbf{p}_1\cdot\hat{\mathbf{q}}+i\eta)]^{-1} . \tag{2.13}$$

In this limit the dependence on the core energy disappears and one may perform the sums over n,n' in (2.12) leading to ($\hat{q}=\hat{1}_z$)

$$[\Delta S(qy)]^v=-\left[\frac{m}{q}\right]^2(\pi A)^{-1}\mathrm{Im}\int\frac{d\mathbf{p}_1}{(2\pi)^3}\cdots\int\frac{d\mathbf{p}_2'}{(2\pi)^3}\delta^3(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1'-\mathbf{p}_2')\rho_2(\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_1'\mathbf{p}_2')\langle\mathbf{p}_1+\mathbf{q},\mathbf{p}_2|v|\mathbf{p}_1'+\mathbf{q},\mathbf{p}_2'\rangle$$
$$\times(y_0^A-p_{1z}+i\eta)^{-1}(y_0^A-p_{1z}'+i\eta)^{-1} , \tag{2.14}$$

where $\rho_2(\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_1'\mathbf{p}_2')$ is the nondiagonal two-particle density matrix

$$\rho_2(\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_1'\mathbf{p}_2')=A(A-1)\left[\prod_{n\geq3}\int\frac{d\mathbf{p}_n}{(2\pi)^3}\right]\times[\Phi_A^{0*}(\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3\cdots\mathbf{p}_A)\times\Phi_A^0(\mathbf{p}_1'\mathbf{p}_2'\mathbf{p}_3\cdots\mathbf{p}_A)] . \tag{2.15}$$

Notice that matrix elements of v in (2.14) depend only on the momentum transferred in the scattering, i.e., $v(\mathbf{p}_1-\mathbf{p}_1')$, independent of q,y and consequently $(\Delta\phi)^v=(1/q)O(1)$. By the same token a second-order contribution of the type $G_0vG_0vG_0$ leads by means of (2.13) alone to a q^{-2} dependence of $\Delta\phi$, etc. One thus infers from Eqs. (2.11) and (2.14) that F_1 draws exclusively on the lowest-order term just discussed.

In order to enable a comparison with previous derivations, one first transforms the integrand in (2.14) to $\mathbf{r}$ space

$$AF_1(y_0^A)=\pi^{-1}\int_0^\infty\sin(y_0^As)ds\times\int\int\rho_2(\mathbf{r}_1-s\hat{\mathbf{q}},\mathbf{r}_2;\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1d\mathbf{r}_2\times\int_0^s v(\mathbf{r}_1-\mathbf{r}_2-\sigma\hat{\mathbf{q}})d\sigma . \tag{2.16}$$

Next one introduces the West variable y_W, (2.6). Substitution of y_W into (2.11) with $y_i=y_0^A$ produces an additional part $O(q^{-1})$ originating in F_0. Some algebra and use of translational invariance yields

$$F_1(y_W)=(\pi\rho)^{-1}\int_0^\infty ds\,\sin(y_Ws)\times\int\rho_2(\mathbf{r}-s\hat{\mathbf{q}},0;\mathbf{r},0)d\mathbf{r}\times\int_0^s[v(\mathbf{r}-\sigma\hat{\mathbf{q}})-v(\mathbf{r})]d\sigma . \tag{2.17}$$

Equation (2.17) is just the result of Gersch *et al.*[5] and is also implicit in Rosenfelder's semiclassical treatment of the response.[7] We emphasize that both derivations explicitly use the elementary interaction v as appearing in H_A and not effective ones like t.

We conclude this section with remarks on some sum rules which S, or alternatively selected F_n, have to satisfy[11]

$$\sigma_{00}=\int_{-\infty}^{\infty}F_0(y)dy=1 , \tag{2.18a}$$
$$\sigma_{02}=\int_{-\infty}^{\infty}F_0(y)y^2dy=\tfrac{4}{3}\langle p^2/2m\rangle , \tag{2.18b}$$
$$\sigma_{11}=\int_{-\infty}^{\infty}F_1(y)ydy=0 , \tag{2.19a}$$
$$\sigma_{13}=\int_{-\infty}^{\infty}F_1(y)y^3dy=\tfrac{1}{6}\langle\Delta V\rangle . \tag{2.19b}$$

One notices first from (2.4) that F_0, computed with an arbitrary, normalized momentum distribution will always satisfy (2.18a). The same is the case for the second moment of F_0: when the latter has the form (2.4), Eq. (2.18b) uses the definition of the average single-particle kinetic energy $\langle p^2/2m\rangle$ for the distribution $n(p)/(2\pi)^3$, as appearing in Eq. (2.4). The sum rules (2.18) are thus mere implementations of unitarity and have no predictive power. This is not the case with the third moment of F_1, which depends on the nondiagonal two-particle density matrix. For any approximation to the latter the sum rule (2.19b) provides a genuine restriction.

III. THE RESPONSE FOR INTERACTIONS WITH A SHORT-RANGE REPULSION

In Sec. II we assumed that matrix elements of v exist. Consider next a system interacting through forces with a short-range repulsion. A proper treatment will produce a two-particle density distribution or a pair-correlation function $g(r)$ with "holes" in the region $r<a$. As a consequence averages of singular operators like $\langle V\rangle$ or $\langle\Delta V\rangle$ which require gV and $g\Delta V$ at one and the same position, remain finite [cf. Eq. (2.19b)].

A glance at Eq. (2.17) shows the kind of problem a singular potential causes. There the arguments of v and ρ_2 do not coincide in general: the paths of particles during scattering may cross regions of strong repulsion which is reflected in diverging F_n, a fact of which Gersch and his co-workers were aware many years ago.[5,6]

Replacing the series (2.10a) by (2.10b) clearly remedies this deficiency and will produce a finite ΔS, Eq. (2.9), but the expansion (2.11) will not naturally emerge because the intervening t-matrix elements contain all powers of q^{-1}. We therefore suggest an algorithm with the purpose of isolating F_n in (2.11) even if v contains a hard core.

Assume the repulsive interaction to be so strong that it may be replaced by a hard core (hc) with some radius a_c. Writing

$$v=\begin{cases}v^{\mathrm{hc}}, & r\leq a_c\\ v^{\mathrm{reg}}, & r>a_c ,\end{cases} \tag{3.1}$$

one may use the series (2.10b) for T, regrouping terms in a self-explanatory form

$$T = T^{\rm hc} + T^{(1)} + T^{(2)} + \cdots ,$$
$$T^{\rm hc} = \sum_{j\geq 2} t_j^{\rm hc} + \sum_{j\geq 2} t_j^{\rm hc} G_0 \sum_{j\neq k\geq 2} t_k^{\rm hc} + \cdots , \tag{3.2}$$
$$T^{(1)} = \sum_{t\geq 2} t_j^{\rm reg} + \sum_{j\geq 2} t_j^{\rm reg} G_0 \sum_{j\neq k\geq 2} t_k^{\rm hc} + \sum_{j\geq 2} t_j^{\rm hc} G_0 \sum_{j\neq k\geq 2} t_k^{\rm reg} + \sum_{j\geq 2} t_j^{\rm reg} G_0 \sum_{j\neq k\geq 2} t_k^{\rm hc} G_0 \sum_{l\neq k\geq 2} t_l^{\rm hc} + \cdots .$$

$T^{\rm hc}$ contains all contributions generated by $t^{\rm hc}$ alone, $T^{(1)}$ those which are linear in $t^{\rm reg}$ but of arbitrary order in $t^{\rm hc}$, etc. As first emphasized in this context by Weinstein and Negele,[8] $t^{\rm hc} = bq + O(1)$, and using Eq. (2.13) one finds that $t^{\rm hc} G_0 = O(1)$. As a result all terms in (3.2) of the pure hard-core type are of order q and contribute $O(1)$ to $(q/m) G_0 T G_0$ as does F_0 itself. These corrections we call δF_0. In Ref. 9 we derived the following expressions for the first two terms due to all binary $1\to j$, and ternary hard-core collisions $1\to j,\ k\,(\boldsymbol{\xi}_1 = \boldsymbol{\beta}_1 \zeta_1 = \mathbf{r}_1 - \mathbf{r}_2;\ \boldsymbol{\xi}_2 = \boldsymbol{\beta}_2 \zeta_2 = \mathbf{r}_2 - \mathbf{r}_3)$:

$$\delta F_0^{1\to j} = -(\pi A)^{-1} \int d\xi_2 \int_0^a d^2\beta_1 \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_1' \cos[y(\zeta_1+\zeta_1')] \rho_2(\boldsymbol{\beta}_1\zeta_1, \boldsymbol{\xi}_2; \boldsymbol{\beta}_1 - \zeta_1', \boldsymbol{\xi}_2) ,$$
$$\delta F_0^{1\to j,k} = (\pi A)^{-1} \int_0^a d^2\beta_1 \int_{|\beta_1-\beta_2|<a} d^2\beta_2 \int_0^\infty d\zeta_2 \int_0^\infty d\zeta_1 \int_{-\infty}^\infty d\zeta_1' \cos[y(\zeta_1+\zeta_1')] \rho_2(\boldsymbol{\beta}_1\zeta_1, \boldsymbol{\xi}_2; \boldsymbol{\beta}_1 - \zeta_1', \boldsymbol{\xi}_2) . \tag{3.3}$$

Next we discuss all terms in (3.2) of first order in $t^{\rm reg}$ but of any order in $t^{\rm hc}$

$$T^{(1)} = (\Omega^{\rm hc})^\dagger \left[\sum_{j\geq 2} t_j^{\rm reg} \right] \Omega^{\rm hc} , \tag{3.4}$$

where we formally introduced the Møller hard-core wave operator $\Omega^{\rm hc}$

$$\Omega^{\rm hc} = 1 + \sum_{j\geq 2} G_0 t_j^{\rm hc} + \sum_{j\geq 2} G_0 t_j^{\rm hc} \sum_{j\neq k\geq 2} G_0 t_k^{\rm hc} + \cdots . \tag{3.5}$$

We now estimate the large-q behavior of $T^{(1)}$. We already know that replacing $t^{\rm reg} \to v^{\rm reg}$ in (3.2) will produce the dominant contribution of $t^{\rm reg}$ in the by now standard limit: the hard-core wave operator $\Omega^{\rm hc} = {\rm const} + O(q^{-1})$ will not change this asymptotic behavior. By means of Eq. (3.2), (3.5), and (2.17) the division (3.1) then leads to the isolation of the lowest terms in the series (2.11)

$$\phi(qy_w) \approx F_0(y_W) + \delta_{\rm hc} F_0(y_W) + (m/q)[F_1(y_W, v^{\rm reg})]^{\rm dist} + O(q^{-2}) \tag{3.6}$$

and constitutes the formal generalization of Gersch's result valid for singular potentials.

One easily shows from (3.3) and its generalizations that δF_0 is even in y: hc corrected terms F_n of even and odd order have the same y parity as for regular potentials. In addition, for a finite number of particles A there are $A-1$ terms contributing to $\delta F_0^{\rm hc}$ and $\Omega^{\rm hc}$. Consequently ϕ remains by construction an asymptotic series in powers of q^{-1}.

We now discuss the distorted F_1 contribution $[F_1^{\rm dist} = F_1(\Omega^{\rm hc\dagger} v^{\rm reg} \Omega^{\rm hc})]$. From its definition (3.1) $v^{\rm reg}$ vanishes for $r<a$, while $\Omega^{\rm hc}$ accounts for the full hc distortion. At first sight the action of the two seems to be the same; however, $\Omega^{\rm hc}$ prevents particles from traversing the singular region of v, and in addition effectively weakens $v^{\rm reg}$ outside $r=a$.

Since an accurate treatment of $\Omega^{\rm hc}$ is quite involved, a natural approximation is to neglect $\Omega^{\rm hc}-1$ and to add a further cut on $v^{\rm reg}$ for $r \leq a_c; a_c \geq a$ removing scatterings with unwanted impact parameters (cf. the Butler approximation in early nuclear reaction theory).

Finally we notice that since the IA approximation $F_0(y)$ for regular interactions satisfies (2.18a), one has by necessity

$$\int_{-\infty}^{\infty} \delta_{\rm hc} F_0(y)\, dy = 0 . \tag{3.7}$$

One checks from the y dependence of the parts in (3.3) and from the ζ, ζ' integration intervals there, that (3.7) indeed holds. The argument can easily be generalized for any part of δF_0.

IV. APPROXIMATIONS FOR ρ_2

Since corrections (3.3) to the IA are dominated by binary hard-core scatterings, a calculation of the latter as well as of F_1, Eq. (2.17), requires knowledge of the nondiagonal two-particle density matrix, $\rho_2(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2)$.[12] These elements are, in principle calculable in any approximate solution of the many-body problem.[13] Alternatively one may use a founded guess. We refer to Refs. 5 and 6 for the choice of Gersch *et al.* (hereafter referred to as G)

$$\rho_2(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2) = \rho \rho_1(0, \boldsymbol{\Delta}) g^{1/2}(r) g^{1/2}(\mathbf{r}+\boldsymbol{\Delta}) , \tag{4.1a}$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $\boldsymbol{\Delta} = \mathbf{r}_1' - \mathbf{r}_1$ and shall in addition investigate the approximation (hereafter denoted as R)

$$\rho_2(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2) = \rho \rho_1(0, \boldsymbol{\Delta}) g(\mathbf{r}+\boldsymbol{\Delta}/2) . \tag{4.1b}$$

Both have two features in common. (i) The nondiagonal single-particle distribution $\rho_1(0,\boldsymbol{\Delta})$ which is the properly normalized Fourier transform of the single-particle momentum distribution $n(p)$

$$\rho_1(0, \boldsymbol{\Delta}) = \rho \int \frac{d^3p}{(2\pi)^3} e^{i\boldsymbol{\Delta}\cdot\mathbf{p}} n(\mathbf{p}) . \tag{4.2}$$

(ii) The pair distribution function $g(r)$ defined by

$$\rho_2(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1\mathbf{r}_2)=\rho^2 g(r) ,$$
$$\rho\int d^3r[1-g(r)]=1 . \quad (4.3)$$

The approximations clearly have the correct limit for $|\Delta|\to 0$. Consider further the following relation out of a hierarchy linking ρ_n of consecutive order n

$$\rho_1(\mathbf{r}_1,\mathbf{r}_1')=(A-1)^{-1}\int\rho_2(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1'\mathbf{r}_2)d\mathbf{r}_2 . \quad (4.4)$$

Since the approximations (4.1) contain $\rho_1(\mathbf{r}_1,\mathbf{r}_1')$ as a factor, Eq. (4.4) becomes a consistency condition imposed on $g(r)$ which for (4.1a) and (4.1b) reads

$$\gamma_G(\Delta)\equiv\rho\int d\mathbf{r}[1-g^{1/2}(r)g^{1/2}(\mathbf{r}+\Delta)]=1 , \quad (4.4a)$$

$$\gamma_R(\Delta)\equiv\rho\int d\mathbf{r}[1-g(\mathbf{r}+\tfrac{1}{2}\Delta)]=1 . \quad (4.4b)$$

Equation (4.4a) cannot hold for all Δ, but (4.4b) does, as a change of the integration variable $\mathbf{r}\to\mathbf{r}+\frac{1}{2}\Delta$ shows.

Next we investigate the outcome of the nontrivial F_1 sum rules (2.19) when the approximations (4.1) are used as input for a calculation of F_1, Eq. (2.17). It is an advantage to follow a derivation which leads to Eq. (10) of Ref. 2. Using the same method, one shows that both Eqs. (2.19) are *exactly* satisfied for either approximation (4.1), with the numerical outcome of the third moment sum rule (2.19b) depending on the quality of the intervening pair distribution function of $g(r)$. This rather surprising result cannot hold for any conceivable or reasonable approximation (cf. the model discussed in Ref. 2) and provides some arguments in favor of the use of the ρ_2 approximations (4.1).

V. *T* DEPENDENCE

Many data on quantum liquids have been taken at low T, and their calculation requires in principle T-dependent input. The required information is occasionally available as is for instance the case for the pair distribution function,[14] but as a rule T dependence may be neglected. The outstanding exception is of course the momentum distribution for ^{4}He below the transition temperature $T_c=2.17$ K:

$$n(p,T)=[1-n_0(T)]n_n(p,T)+(2\pi)^3 n_0(T)\delta^3(\mathbf{p}) , \quad (5.1a)$$

$$n_0(T)=n_0(0)\left[1-\left[\frac{T}{T_c}\right]^{\alpha}\right] , \quad (5.1b)$$

with $n_0\approx 0.092$ and $\alpha\approx 3.6$. The distributions $n_0(T)$ and $n_n(p,T)$ are for given T the condensate fraction and the momentum distribution of the normal atoms and have been computed by Whitlock and Panoff for $T=0$ K (Ref. 15) and by Ceperley and Pollock for $4.0\gtrsim T(\mathrm{K})\gtrsim 1.18$.[16,17] (The calculated $n_n(p)$ around $T=1.2$ K for which an application is made below seems not to smoothly join the same for higher T and we therefore used the cited $T=0$ K distribution). We notice between parentheses that the momentum distribution of the normal atoms is surprisingly well represented by an old parametrization suggested by Woods and Sears:[18]

$$n_{\mathrm{WS}}(p)=\begin{cases} n_1(0)e^{-p/p_1} & p_1\geq p_c, \quad p_1=0.4\ \text{Å}^{-1} \\ & p_2=1.2\ \text{Å}^{-1} \\ n_2(0)e^{-(p/p_2)^2} & p_2\leq p_c, \quad p_c=1.5\ \text{Å}^{-1} . \end{cases} \quad (5.2)$$

All quantities in (3.6), depending either directly on $n(p)$ [like $F_0(y)$] or indirectly through an approximation for ρ_2 of the type, Eq. (4.1), will in principle reflect the peculiarities of the condensate as described by (5.1) for $T<T_c$. For instance, for an infinite system $F_0(y)$ will be singular as is $n(p)$. What ultimately renders that part finite is the instrumental resolution which is folded into the (reduced) response $S(\phi)$,

$$\phi^R(qy)=\int_{-\infty}^{\infty}\phi(qy')R(y-y')dy' . \quad (5.3)$$

$R(y)$ is frequently of Gaussian shape

$$R(y)=(\pi^{1/2}y_G)^{-1}\exp(-y/y_G)^2 \quad (5.4)$$

with a width y_G, dependent on the experimental setup, on T, etc.

Next one substitutes into Eq. (5.3) ϕ in the approximation (3.6) and separates the resulting ϕ^R into dominant parts odd and even in y (Ref. 19):

$$\phi^{e,R}(qy;T)=[1-n_0(T)][F_0^{n,R}(y;T)+\delta_{\mathrm{hc}}F_0^{n,R}(y;T)] + n_0(T)[R(y)+\delta_{\mathrm{hc}}F_0^{c,R}(y;T)]+O(q^{-2}) , \quad (5.5)$$

$$\phi^{o,R}(qy;T)=\frac{m}{q}\{[1-n_0(T)]F_1^{n,R}(y) + n_0(T)F_1^{c,R}(y;T)\}+O(q^{-3}) .$$

$\delta_{\mathrm{hc}}F_0^{n,R}$ and $\delta_{\mathrm{hc}}F_0^{c,R}$ are the resolution broadened contributions to F_0 due to pure hard-core collisions between an atom in, respectively, the normal and in the condensate fraction with a second atom. Substituting (4.1) into Eq. (3.3) and denoting by Γ the special choice of g in (4.1) one finds $[w=(a^2-b^2)^{1/2}]$

$$\delta_{\mathrm{hc}}F_0^{n,R}\approx -2\rho\int_a^b db\, b\int_w^{\infty}ds\int_w^{\infty}ds'\cos[y_W(s+s')]\rho_1(0,s+s')\exp\{-[(s+s')y_G/2]^2\}g(\{b^2+[(s-s')/2]\}^2)^{1/2} , \quad (5.6a)$$

$$\delta_{\mathrm{hc}}F_0^{c,R}\approx -2\rho\int_a^b db\, b\int_w^{\infty}ds\int_w^{\infty}ds'\cos[y_W(s+s')]\exp\{-[(s+s')y_G/2]^2\}g(\{b^2+[(s-s')/2]\}^2)^{1/2} . \quad (5.6b)$$

VI. NUMERICAL RESULTS

In the following we apply the theory developed here to a data set on liquid ^{4}He for $q=10$ Å^{-1} at $T=1.2$ K which spreads over $|y_W| \lesssim 2.4$ Å^{-1}.[20] These data are apparently precise enough to allow a separation of the reduced response into even and odd y parts.

We first see from Eq. (2.7) that over the relevant y range the relative difference between y_0^A and y_W is less than $\sim 15\%$. One thus concludes on kinematical grounds that one is presumably not far from the asymptotic regime where that difference tends to 0. At first sight one may fear that the presence of the strong short-range repulsion upsets this estimate. Yet, a dynamical measure, proposed by Sears[1] confirms this estimate, and we shall assume the following basic tenet: the experimentally separated parts of $S(qy)$ or $\phi(qy)$, even and odd in y, are given by their lowest-order contribution [cf. (5.5)].

The following information has been used in actual calculations: (a) the radial distribution function $g(r)$ as computed by Kalos *et al.*[21] for the Aziz potential[22] and which vanishes for $r<a=2.0$ Å; (b) the momentum distributions discussed in Sec. V; (c) regular parts of the Aziz[22] and Lennard-Jones[23] potentials cut off at $r=a_c$. [Regarding a_c a comment is in order. Since the attractive part $v^{\rm reg}$ acts beyond the hard-core radius a_c, $g(r)$ will "penetrate" to distances smaller than a_c and a is thus expected to be slightly in excess of a. The actual values to be used will be discussed]; and (d) nondiagonal single-particle density as the Fourier transform (4.2) of the chosen momentum distribution. In the following, we report the results.

A. The consistency test (4.4)

Figure 1 shows $\gamma_R(\Delta)-1$ [Eq. (4.4a) as a function of Δ. It is surprising to see (4.1a), when judged on the criterion (4.4), to be far worse an approximation than (4.1b). One would expect the converse since (4.1a) and not (4.1b) permits hard-core "holes" in the two relative coordinates present in the physical ρ_2.

B. Hard-core correction to the IA for the normal and condensed fractions of the ^{4}He fluid

Consider first the expressions (3.3) for the normal part of the fluid and which is common to all matter with a hard-core component in the interaction. Contrary to the general result of Ref. 8 (from which ^{4}He has explicitly been excluded) we obtain a nearly negligible correction. Insight can be obtained when ρ_1 is also represented by a Gaussian:

$$\rho_1(0,s)=\exp(-sp_0/2)^2 \; .$$

The latter strongly damps the integrand in the regions where it is largest, i.e., for $s,s'\approx a$.

$$\mathcal{R}_{\rm IA}^{n,R}(y)=\delta_{\rm hc}F_0^{n,R}(y)/F_0^{n,R}(y)$$

depends on all input elements and shows amplitude oscillations required by

$$\int_{-\infty}^{\infty}\delta_{\rm hc}F_0^{n,R}(y)dy=0 \; .$$

For $a_c=a$ the amplitudes are negligible, but these grow with a_c and may become 0.2–0.3 for large ya_c.

For y values available in the present $q=10$ Å^{-1} data ($y\le 2.4$ Å^{-1}), $\mathcal{R}_{\rm IA}^{n}$ reaches 6–7% only for $(a_c-a)/a \gtrsim 0.15$. Unless there are serious arguments in favor of a_c much in excess of a, $\delta_{\rm hc}F_0^{n,R}$ remains a nearly negligible correction.

The situation is different for the correction (5.6b) due to the condensate fraction where ρ_1 is replaced by one. The damping is now governed by the exponential coming from the resolution function R. However, since p_0 (≈ 1.3 Å^{-1}) is much larger than a typical resolution width y_G (≈ 0.4 Å^{-1}),

$$\delta_{\rm hc}F_0^{c,R}| >> |\delta_{\rm hc}F_0^{n,R}| \; .$$

In spite of the small weight n_0, there results for $y\approx 0$ a sizeable FSI due to pure hard-core interactions of atoms in the condensed fraction. Its actual value is unfortunately sensitive to the detailed functional forms of ρ_1 and the resolution function R.

C. The reduced response $\phi(qy)$

Figure 2 shows $\phi^o(qy)$, Eq. (2.11), computed for the range $2.1 \gtrsim a_c$ (Å) $\gtrsim 2.0$ using (i) the approximation (4.1b), (ii) the Aziz potential, and (iii) the Whitlock-Panoff distribution $n_{\rm WP}(p)$. Results for $n_{\rm WS}$, Eq. (5.2), and/or for the regular part of a Lennard-Jones potential are practically the same and are not separately shown. However, a major difference results when ϕ^o is computed with the Gersch *ansatz* (4.1a). For it, Fig. 2 shows a far smaller spread as function of a_c the results of which are only shown as a hatched area. The following observations can be made. For ϕ^o, (a) The positions of extrema in, and sign changes $y_{\rm sc}$ of ϕ^o are about the same for all R and G results. Stringari ascribed this for his model to the choice of a purely Gaussian $n(p)$ (Ref. 24) and the same is the case for the Sears series[1] used in Ref. 2. Figures 2 and 3 show that for a model, more precise than the one presently discussed, the position $y_{\rm sc}\neq 0$ where ϕ^o changes sign strongly depends on the approximation used for ρ_2: $y_{\rm sc}\gtrsim 1.6$ Å^{-1} for R and $\gtrsim 2.1$ Å^{-1} for G. (b) The same distinction between R and G holds for extrema of ϕ^o. (c) Once a realistic $g(r)$ is used, the precise form of the ele-

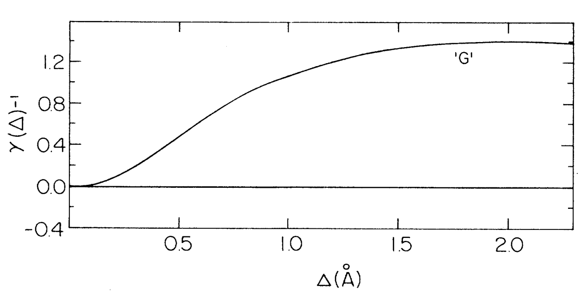

FIG. 1. Consistency defect $\gamma(\Delta)-1$, Eq. (4.4a), for approximation (4.1a) to ρ_2.

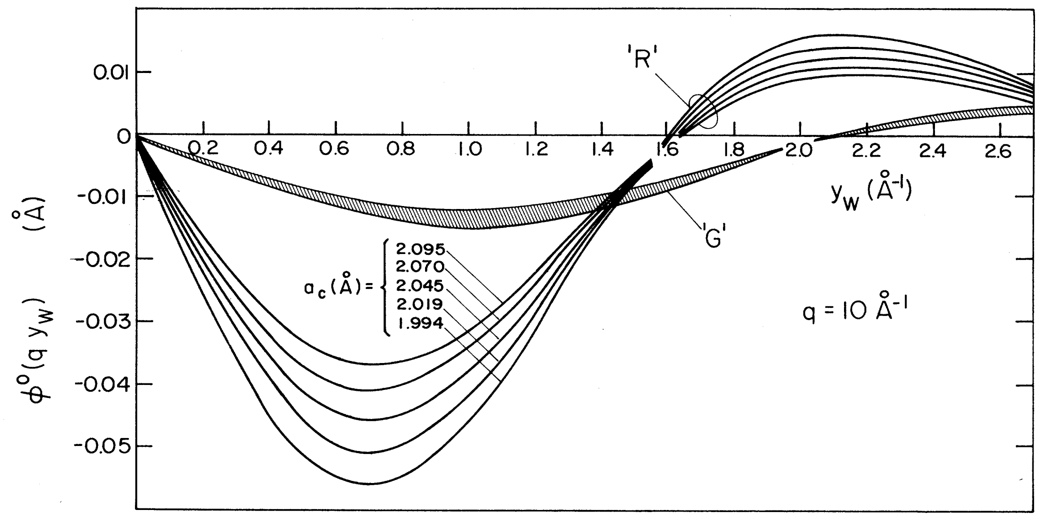

FIG. 2. $\phi^o(qy_w)$ using (4.1R) for $v_{\rm aziz}$, the distribution n_{WS}, Eq. (5.2), and a range of a_c values. The same for (4.1a) is given by a hatched band.

mentary interaction is only of secondary importance. (d) As expected, ϕ^o varies considerably with a_c. In the approximation (4.1b) a 6% change in a_c changes ϕ^o around the first extremum by $\approx 50\%$. The same for (4.1a) is appreciably smaller. It is clearly possible to fit ϕ^o for the $q=10$ Å^{-1} data[20] using the spread in results displayed in Figs. 2 and 3 with a_c, some 5% larger than $a=2.0$ Å. The same is the case for v_{LJ} and $a_c \sim 2.04$ Å. For, ϕ^e, inspection of Fig. 3 shows that theory reproduces ϕ^e very well except in the region of the quasielastic peak $y\approx 0$ where the influence of the condensate fraction is most marked. There $|\phi^o| \ll \phi^e$ is negligible and the same is the case for

$$|\delta_{\rm hc}F_0^{n,R}(0)| \ll F_0^{n,R} \; .$$

Thus with $\phi^R \approx \phi^{e,R}$ Eq. (5.5) becomes

$$\phi^R(q0;T) \approx [1-n_0(T)]F_0^{n,R}(0;T) + n_0(T)[R(0)+\delta_{\rm hc}F_0^{c,R}(0;T)] \; . \qquad (6.1)$$

Whether for $y\approx 0$ a condensate peak, broadened by instrumental resolution, will stand out against the normal quasielastic peak is apparently a matter of a few parameters. $F_0^{n,R}$ is maximally suppressed by $[1-n_0(0)]\approx 0.91$ and maximally enhanced by the condensate contribution

$$n_0(0)R(0) \approx 0.09 \approx (\pi^{1/2}y_G)^{-1}$$

[cf. (5.4)]. The latter in turn is reduced by the pure hard-core FSI part $\delta_{\rm hc}F_0^{c,R}$. As a result the net "peak," over and above the normal IA may amount to 10–15 % of the latter.

With little leeway to change the regular parts of $\phi^R(q,0,T)$, the only culprit for the disagreement between data and experiment around the quasielastic peak is likely to be the particular hard-core IA correction (5.6b) in (6.1), discussed in the preceding section. We have already noted the sensitivity of that correction (5.6b) to the damping influence of the resolution function replacing ρ_1 in (5.6a) by 1, and we are not overly worried by the discrepancy. Simultaneously one may have to discard the possibility of a *reliable* extraction of the condensate fraction $n_0(T)$ from a comparison of data and a theory around the quasielastic peak $y\approx 0$.

Comparison of Figs. 2 and 3 shows that the narrow spread in ϕ^o, when computed with the Gersch *ansatz* (4.16), does not permit a fit for any $a_c \gtrsim a$. One thus concludes that the ansatz (4.1a) is inferior on account of the outcome of the test (4.4) (cf. Fig. 1), as well as on the apparent impossibility to reproduce ϕ^o.

We conclude this section with a remark on the distribution of strength $y^3F_1(y)$ in the sum rule (2.19b). We

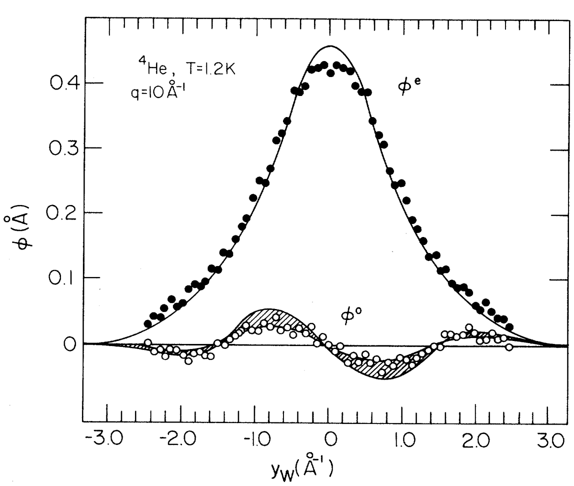

FIG. 3. Data for ϕ^e, ϕ^o.[20] The hatched area for $(\phi^o)_{\rm th}$ corresponds to $2.04 \lesssim a_c$(Å) $\lesssim 2.10$.

calculated the right-hand side to be

$$(\sigma_{13})_{\text{Aziz}}=0.257\times10^{-5}\ \text{Å}^{-3}\ ,$$
$$(\sigma_{13})_{LJ}=0.213\times10^{-5}\ \text{Å}^{-3}\ . \qquad (6.2)$$

For $a_c \lesssim a$, close to 95% of the strength is spread over the investigated range $y \leq 4$ Å^{-1}. Figures 2 and 3 show that for increasing a_c strength is shifted to larger y, as could indeed be checked numerically.

VII. CONCLUSIONS

In this paper we discussed a multiple-scattering theory for the linear, longitudinal response S in case the interaction between the constituents is strong or repulsive at short distances. For regular interactions v of relatively mild strength the reduced response $\phi(qy)$, Eq. (2.11), permits, for fixed y, an asymptotic expansion in q^{-1}, the coefficients of which depend on v and multiparticle density matrices.[5] In particular, a hard core upsets this neat and useful correspondence. For instance, in the presence of a strong, short-range repulsion, the impulse approximation F_0 acquires additive corrections $\delta_{\text{hc}}F_0$. In a similar fashion also all higher-order terms F_n, generated by the regular part of v, are modified by hard-core distorted wave corrections as multiplicative operands.

We have applied the theory to liquid ^{4}He at $T=1.2$ K, adopting the following corrections: (i) the dominant hc part of $\delta_{\text{hc}}F_0^n$, Eq. (3.3), due to binary hard-core collisions in the normal and condensed fraction and (ii) a model for hard-core distortions for the leading q^{-1} term with coefficient $F_1(y)$. For a collision between atoms in the normal fluid we found the first correction to be small for hard-core radii only slightly larger than $a=2.0$ Å, below which measurements[14] and theory[21] show the pair distribution function $g(r)$ to vanish. In view of the work by Weinstein and Negele[8] who obtained large hard-core corrections to the IA this seems to come as a surprise. However, the authors themselves warned that their results do not apply to parameters which govern liquid ^{4}He. The non-negligible hc correction to the IA comes from a unique source, namely, from hard-core collisions involving atoms in the condensed state.[25]

Without hc wave distortions, all F_n diverge. However, when as a model for hc wave distortions one retains v^{reg} only beyond a_c, all results will be finite. For ^{4}He at $q=10$ Å^{-1}, $(F_1)^{\text{dist}}$ alone produces for a narrow range around $a_c \sim 2.10$ Å satisfactory agreement for the odd y portion of the data. We further established the sensitivity of the numerical outcome to input elements like the single-particle momentum distribution function, the nondiagonal two-particle density matrix, and the choice for the regular part of v. Strongest affected by changes in input parameters are F_1, and in particular the hc correction $\delta_{\text{hc}}F_0^{c,R}$, Eq. (5.6b).

It is of further interest to confirm an earlier expectation. In Ref. 2 we attempted to approximate $F_1(y)$ using some terms in the so-called Sears series[1] and found rather poor agreement with the data. We suspected that this series converges slowly and recommended the use of an expression for the complete F_1 even when approximations would be needed for part of the input.

The reader will have noticed a deliberate deemphasis on the issue of y scaling with its immediate goal to extract from data single-particle momentum distributions. Here our primary goal has been the study of hard-core corrections $\delta_{\text{hc}}F_0$ and the dominant FSI contributions of order, $O(q^{-1})$. In the suggested approximations both require knowledge of the single-particle momentum distribution (or its Fourier transform $\rho_1(0,s)$ in a rather involved manner.

Yet, if the present model, or a suitable modification thereof, will describe future data over a wide q range, one might readdress the initial goal in a roundabout way. For instance, one first adopts an initial form for the $n(p)$ and computes with it $\delta_{\text{hc}}F_0$ and F_1. Those FSI terms may be subtracted from the data and the remainder, F_0, is then used to extract, a more accurate distribution. The procedure can be repeated till self-consistency has been reached.

A few words on some alternative descriptions of the response under similar kinematical conditions. First, for a regular interaction it is easy to show that through an expansion in powers of σ of the last integrand in Eq. (2.17) one generates the Sears series for F_1.[1] Parts calculated in Refs. 1 and 2 are thus contained in (2.17). We hope to return elsewhere to a comparison with the theory of Silver,[4] which appears to be of a different nature.

[1]V. F. Sears, Phys. Rev. B **30**, 44 (1984).

[2]A. S. Rinat, Phys. Rev. B **36**, 5171 (1987).

[3]B. Tanatar, E. F. Talbot, and H. R. Glyde, Phys. Rev. B **36**, 8376 (1987).

[4]R. N. Silver, Phys. Rev. B **37**, 3794 (1988); **38**, 2283 (1988); **35**, 3647 (1987).

[5]H. A. Gersch, L. J. Rodriguez, and R. N. Smith, Phys. Rev. A **5**, 1547 (1972).

[6]H. A. Gersch and L. J. Rodriguez, Phys. Rev. A **8**, 905 (1973); L. J. Rodriguez, H. A. Gersch, and H. A. Mook, *ibid.* **9**, 2085 (1974).

[7]R. Rosenfelder, Nucl. Phys. **A459**, 452 (1986).

[8]J. J. Weinstein and J. W. Negele, Phys. Rev. Lett. **49**, 1016 (1982).

[9]S. A. Gurvitz, A. S. Rinat, and R. Rosenfelder, Phys. Rev. C (to be published).

[10]G. B. West, Phys. Rep. **18C**, 263 (1975).

[11]See, e.g., R. Rosenfelder, Ann. Phys. (N.Y.) **128**, 188 (1980).

[12]We note that, while the exact response S [Eq. (2.1)] may be expressed in terms of diagonal elements of the dynamical two-particle density matrix, the lowest-order terms in terms of a $1/q$ expansion, F_1 (and δF_0), by themselves require nondiagonal elements of the static analogue.

[13]See, e.g., M. L. Ristig, Nucl. Phys. **A317**, 163 (1979).

[14]E. C. Svensson, V. F. Sears, A. D. B. Woods, and P. Martel, Phys. Rev. B **21**, 3638 (1980).

[15]P. Whitlock and R. Panoff, Can. J. Phys. **65**, 1409 (1987); and (private communication).

[16]D. M. Ceperly and E. L. Pollock, Can. J. Phys. **65**, 1416 (1987).
[17]An appreciably larger $n_0(0)$ is quoted by V. F. Sears, E. C. Svensson, P. Martel, and A. D. B. Woods, Phys. Rev. Lett. **49**, 279 (1982).
[18]A. D. B. Woods and V. F. Sears, Phys. Rev. Lett. **39**, 415 (1977).
[19]We recall that the terms retained in (5.5) are not the only ones of the indicated order [cf. Eq. (3.3)]. These dominate, though for not too dense systems.
[20]P. Martel, E. C. Svensson, A. D. B. Woods, V. F. Sears, and R. A. Cowley, J. Low Temp. Phys. **23**, 285 (1976).
[21]M. H. Kalos, M. A. Lee, P. A. Whitlock, and G. V. Chester, Phys. Res. **24**, 115 (1981).
[22]R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. **70**, 4430 (1969).
[23]G. K. Pollack, Rev. Mol. Phys. **36**, 748 (1964).
[24]S. Stringari, Phys. Rev. B **35**, 2038 (1987).
[25]Large corrections have been exactly evaluated for a model of a particle in a well (Ref. 9), which case cannot well be compared with an interacting many-particle system.