

Beyond the binary collision approximation for the large- q response of liquid ^4He

A. S. Rinat and M. F. Taragin

Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel

(Received 9 June 1998)

We discuss corrections to the linear response of a many-body system beyond the binary collision approximation. We first derive for smooth pair interactions an exact expression of the response $\propto 1/q^2$, considerably simplifying existing forms and present also the generalization for interactions with a strong, short-range repulsion. We then apply the latter to the case of liquid ^4He . We display the numerical influence of the $1/q^2$ correction around the quasielastic peak and in the low-intensity wings of the response, far from that peak. Finally we resolve an apparent contradiction in previous discussions around the fourth order cumulant expansion coefficient. Our results prove that the large- q response of liquid ^4He can be accurately understood on the basis of a dynamical theory. [S0163-1829(98)01346-0]

I. INTRODUCTION

High-energy pulsed neutrons from spallation sources have recently been used for the collection of good-quality cross sections data for the inclusive scattering of neutrons from liquid ^4He . Data are for temperatures below and above the transition temperature T_c .¹⁻³ The above cross sections are a direct measure of the dynamic response or structure function $S(q, \omega)$, where q, ω are the momentum and energy transferred to the system.

It appears convenient to consider the reduced response $\phi(q, y) = (q/M)S(q, \omega)$ instead of $S(q, \omega)$, where the energy loss parameter ω is replaced by an alternative kinematic variable y . The latter is a linear combination of (q, ω) . M is the mass of a constituent atom.

Virtually all dynamic calculations of the high- q response $S(q, \omega)$ (Refs. 4–11) have been based on the Gersch-Rodriguez-Smith (GRS) expansion of the reduced response in $1/q$ (Ref. 4) or modifications of it.^{5,6,8-10} The theory in principle employs only the elementary atom-atom interaction V and is otherwise free of parameters.

The dominant part of the large- q response is the asymptotic limit. It describes the response of a neutron striking an atom with given momentum. The absorption of the transferred momentum and energy-loss is not affected by other atoms in the medium. Final State Interactions (FSI) induced by V , produce corrections to the above limit which vanish for increasing q . The leading FSI $\propto 1/q$ is caused by binary collisions (BC) between a struck and an arbitrary second particle in the medium. For liquid ^4He , predictions for the reduced response $\phi(q, y)$ to order $1/q$ agree well with the data over a broad range around the central, quasielastic peak at $y=0$. In fact, the quality of the data hardly calls for refinements beyond the BC. The incentive to nevertheless consider the introduction of fine details is mainly of theoretical nature: A criterion for the expansion of a function of two variables $\phi(q, y)$ in $1/q$ must depend on y . In particular the large $|y|$ wings where the response is only a small fraction of the peak value, has been suspected before to be sensitive to details beyond the BC.

In this paper we treat $1/q^2$ corrections. Those are due to ternary collisions (TC) between a struck and two other par-

ticles. Their study is the major purpose of this paper.

A second topic to be discussed is related to the cumulant expansion of the response which has recently resulted in a successful, model-independent extraction of the single-atom momentum distribution in liquid ^4He .^{12-16,11} Our interest here is the resolution of an apparent discrepancy between the directly computed fourth cumulant coefficient and the value extracted in the BC approximation for a dynamically calculated response.¹¹

We start in Sec. II recalling some essentials of the GRS expansion for the reduced response, valid for smooth interparticle interaction⁴ and derive a formally simple representation of TC terms $\propto 1/q^2$. Next we mention modifications which are required if the pair-interaction has a strong, short-range repulsion. In Sec. III we present numerical values for TC contributions to the response of liquid ^4He and discuss its relative importance, in the peak region and the low-intensity wings. Section IV contains a brief discussion of the cumulant representation of the response which has recently been used to parametrize data for liquid ^4He . We report a complete calculation of the 4th order FSI cumulant coefficient, and thereby also resolve a previously existing discrepancy.

II. DOMINANT FSI PARTS IN THE RESPONSE FOR SMOOTH AND SINGULAR INTERACTIONS

Consider the response $S(q, \omega)$ per particle for an infinite system of point particles

$$S(q, \omega) = A^{-1} (2\pi)^{-1} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \Phi_0 | \rho_q^\dagger(t) \rho_q(0) | \Phi_0 \rangle. \quad (1)$$

$\rho_q(t)$ in Eq. (1) is the density operator, translated in time t by the Hamiltonian H

$$\rho_q(t) = e^{-iHt} \rho_q(0) e^{iHt},$$

$$\rho_q(0) = \sum_j e^{iq \cdot r_j(0)}. \quad (2)$$

Φ_0 is the ground state of the system with energy E_0 .

We shall work with the reduced response $\phi(q, y) = (q/M)S(q, \omega)$, where the energy loss ω is replaced by an alternative kinematic variable $y = y(q, \omega)$.^{4,17}

$$y = \frac{M}{q} \left(\omega - \frac{q^2}{2M} \right). \quad (3)$$

Substitution of Eq. (2) into Eq. (1) produces incoherent and coherent components. Considering high- q responses, it suffices to discuss the dominant incoherent part, where one tracks a single particle (for instance “1”) in its propagation through the medium.¹⁷

For the description of the large- q response we shall follow the formulation of Gersch, Rodriguez and Smith⁴ (GRS) and cite from there a few results. Details can be found in the bibliography.

It is convenient to introduce the Fourier transform (FT) of the reduced (incoherent) response

$$\tilde{\phi}(q, s) = \int_{-\infty}^{\infty} dy e^{-isy} \phi(q, y). \quad (4)$$

The variable $s = (q/M)t$ above is the distance traveled in the medium during a time t by a constituent, which moves with constant recoil velocity $v_q = q/M$: s is the length, canonically conjugate to the momentum y .

The density fluctuations ρ_q in Eq. (2) shift coordinates in the direction of \hat{q} , chosen to be the z direction. It leads to the following, standard expression, valid for local forces^{18,4} ($\mathbf{r} - \mathbf{s} = \mathbf{r} - s\hat{q}$)

$$\begin{aligned} \tilde{\phi}(q, s) &= (1/A) \langle \Phi_0(\mathbf{r}_1 - \mathbf{s}; \mathbf{r}_k) | T_\sigma \\ &\times \exp \left\{ (i/v_q) \int_0^s d\sigma [H(\mathbf{r}_1 - \boldsymbol{\sigma}; \mathbf{r}_k) - E_0] \right\} \\ &\times | \Phi_0(\mathbf{r}_1; \mathbf{r}_k) \rangle \\ &= \sum_n (1/v_q)^n \tilde{F}_n(s). \end{aligned} \quad (5)$$

The second line in Eq. (5) is the GRS series in $1/v_q$, which is generated by the expansion of the above, σ -ordered exponential. Here and in the following we shall denote by “ k ” all coordinates $\neq 1$, while “ l ” runs from 1 to A .

For local interactions, the Hamiltonian with shifted coordinate “1” can be written as

$$\begin{aligned} H(\mathbf{r}_1 - \boldsymbol{\sigma}; \mathbf{r}_k) &= \sum_l T_l + \sum_{\substack{l \neq 1 \\ k > l}} V(\mathbf{r}_l; \mathbf{r}_k) + \sum_{k > 1} V(\mathbf{r}_1 - \boldsymbol{\sigma}; \mathbf{r}_k) \\ &= \left[\sum_l T_l + \sum_{l, k > l} V(\mathbf{r}_l; \mathbf{r}_k) \right] \\ &+ \sum_{k > 1} [V(\mathbf{r}_1 - \boldsymbol{\sigma}; \mathbf{r}_k) - V(\mathbf{r}_1; \mathbf{r}_k)] \\ &= H(\mathbf{r}_1; \mathbf{r}_k) + U_1(\boldsymbol{\sigma}), \end{aligned} \quad (6)$$

with

$$\begin{aligned} U_1(\boldsymbol{\sigma}) [= U_1(\boldsymbol{\sigma}; \mathbf{r}_1, \mathbf{r}_k)] &= \sum_{k \neq 1} \delta_\sigma V(\mathbf{r}_1; \mathbf{r}_k), \\ \delta_\sigma V(\mathbf{r}_1; \mathbf{r}_k) &= [V(\mathbf{r}_1 - \boldsymbol{\sigma}; \mathbf{r}_k) - V(\mathbf{r}_1; \mathbf{r}_k)]. \end{aligned} \quad (7)$$

$\delta_\sigma V(\mathbf{r}_1; \mathbf{r}_k)$ is the difference between the interaction of a selected particle k and “1” with the latter, once at a shifted position $\mathbf{r}_1 - \boldsymbol{\sigma}$ and then at \mathbf{r}_1 ; $U_1(\boldsymbol{\sigma})$ is the same due to all particles $k \neq 1$. Using Eq. (6) one checks⁴

$$[H(\mathbf{r}_1 - \boldsymbol{\sigma}; \mathbf{r}_k) - E_0] \Phi_0(\mathbf{r}_1; \mathbf{r}_k) = U_1(\boldsymbol{\sigma}) \Phi_0(\mathbf{r}_1; \mathbf{r}_k). \quad (8)$$

It is convenient to introduce the FT of the GRS coefficient functions in Eq. (5). For example

$$\begin{aligned} \tilde{F}_0(s) &= \frac{1}{A} \int d\mathbf{r}_1 d\mathbf{r}_k \rho_A(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - \mathbf{s}, \mathbf{r}_k) = \frac{\rho_1(0; s)}{\rho} \\ &= \int \frac{d\mathbf{p}}{(2\pi)^3} e^{-i\mathbf{p} \cdot \mathbf{s}} n(\mathbf{p}). \end{aligned} \quad (9)$$

The dominant correction to the above asymptotic limit is ($\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$)

$$\begin{aligned} \frac{1}{v_q} \tilde{F}_1(s) &= \frac{i}{Av_q} \int d\mathbf{r}_1 d\mathbf{r}_k \rho_A(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - \mathbf{s}, \mathbf{r}_k) \\ &\times \int_0^s d\sigma [H(\mathbf{r}_1 - \boldsymbol{\sigma}) - E_0] \\ &= -\frac{i}{Av_q} \int d\mathbf{r}_1 d\mathbf{r}_k \rho_A(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - \mathbf{s}, \mathbf{r}_k) \\ &\times \int_0^s d\sigma U_1(\boldsymbol{\sigma}) \\ &= i \int d\mathbf{r} \frac{\rho_2(\mathbf{r}, \mathbf{r} - \mathbf{s}; 0)}{\rho} \tilde{\chi}_q(\mathbf{r}, s), \end{aligned} \quad (10)$$

where use has been made of Eq. (8). The function $\tilde{\chi}$ in Eq. (10)

$$\tilde{\chi}_q(\mathbf{r}, s) = -(1/v_q) \int_0^s d\sigma \delta_\sigma V(\mathbf{r}), \quad (11)$$

is the off-shell, eikonal phase in the coordinate representation, pertinent to the characteristic difference of interactions acting on “1” in Eq. (11). In order to obtain the appropriate on-shell phase one needs to replace the integration limits in Eq. (11) from $0, s$ to $-\infty, \infty$.

In all, $\tilde{F}_1(s)$ describes binary collisions (BC) of the struck particle “1” with any other particle in the medium. Its FT $F_1(y)$ is odd in y and for large q mainly shifts the position of the maximum of the even asymptotic $F_0(y)$ at $y = 0$.

The computation of the above quantities requires non-diagonal density matrices. We shall use a normalization, such that

$$\begin{aligned} \rho_n(1, \dots, n; 1', \dots, n') &= \frac{A!}{(A-n)!} \left(\prod_{j=n+1}^A \int d[j] \right) \\ &\times \Phi_0(1, \dots, n; n+1, \dots, n_A) \\ &\times \Phi_0(1', \dots, n'; n+1, \dots, n_A) \\ &= [(A-n-1)]^{-1} \int d[n+1] \rho_{n+1} \\ &\times (1, \dots, n, n+1; 1', \dots, n', n+1), \\ \rho_A(1, \dots, A; 1', \dots, A') &= A! \Phi_0^*(1, \dots, A) \Phi_0(1', \dots, A'), \end{aligned} \quad (12)$$

where we used a short-hand notation $1, n, 1' \dots$ for $\mathbf{r}_1, \mathbf{r}_n, \mathbf{r}_1', \dots$. The densities $\rho_n(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - \mathbf{s}, \mathbf{r}_k)$, required in

Eqs. (9), (10), are diagonal in all particles k , except in “1.” For example, $\rho_1(0;s) = \rho_1(\mathbf{r};\mathbf{r}-s)$ in Eq. (9) is the single-particle density matrix which has the single-particle momentum distribution $n(p)$ as its FT. Its diagonal part $\rho_1(0,0) = \rho$ is the number density.

The first two terms in the GRS series F_0, F_1 satisfactorily describe the data for the reduced response in a broad band around the quasi-elastic peak at $y=0$. Such a fit cannot be expected in the wings, where $F_1(y)$ occasionally reaches small negative values. In those wings $F_l(y)$, $l \geq 2$, competes for increasing $|y|$ with $F_0(y) + (1/v_q)F_1(y)$ of comparable size: ultimately $\phi(q,y) \geq 0$.

Partial expressions for the next-to-leading order terms $\tilde{F}_2(s), F_2(y)$ have been given before by Gersch *et al.*⁴ and by Besprosvany¹⁰ but those forms are not complete and are not always transparent. We shall derive below expressions for the exact \tilde{F}_2 , based on Eqs. (12), (15) in Ref. 4

$$\begin{aligned} \tilde{F}_2(s) &= \frac{i^2}{A!} \int d\mathbf{r}_1 d\mathbf{r}_k \rho_A(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - s, \mathbf{r}_k) \\ &\quad \times \int_0^s d\sigma [H(\mathbf{r}_1 - \boldsymbol{\sigma}, \mathbf{r}_k) - E_0] \int_0^{\sigma'} d\sigma' \\ &\quad \times [H(\mathbf{r}_1 - \boldsymbol{\sigma}', \mathbf{r}_k) - E_0]. \end{aligned} \quad (13)$$

Consider the operators in the brackets above, acting on the wave functions which compose ρ_A , Eq. (12), with shifted, respectively unshifted coordinate \mathbf{r}_1 . Their combined result is

$$\begin{aligned} \tilde{F}_2(s) &= \frac{i^2}{A!} \int d\mathbf{r}_1 d\mathbf{r}_k \rho_A(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - s, \mathbf{r}_k) \\ &\quad \times \int_0^s d\sigma [U_1(\boldsymbol{\sigma}) - U_1(s)] \int_0^{\sigma'} d\sigma' U_1(\boldsymbol{\sigma}') \\ &= \frac{i^2}{A!} \int d\mathbf{r}_1 d\mathbf{r}_k \rho_A(\mathbf{r}_1, \mathbf{r}_k; \mathbf{r}_1 - s, \mathbf{r}_k) \\ &\quad \times \left\{ \frac{1}{2} \left[\int_0^s d\sigma U_1(\boldsymbol{\sigma}) \right]^2 - U_1(s) \right. \\ &\quad \left. \times \int_0^s d\sigma \int_0^{\sigma'} d\sigma' U_1(\boldsymbol{\sigma}') \right\}. \end{aligned} \quad (14)$$

Since $\tilde{F}_2 \propto U^2$ and the latter $\propto V^2$ we dub \tilde{F}_2 the TC contribution to FSI.¹⁹

We start with the first term in the braces in Eq. (14). Using the definition in Eq. (7) one rewrites

$$\begin{aligned} \left[\int_0^s d\sigma U_1(\boldsymbol{\sigma}) \right]^2 &= \sum_{k \neq 1} \left[\int_0^s d\sigma \delta_\sigma V(\mathbf{r}_1 - \mathbf{r}_k) \right]^2 \\ &\quad + \sum_{1 \neq l \neq k \neq 1} \left[\int_0^s d\sigma \delta_\sigma V(\mathbf{r}_1 - \mathbf{r}_k) \right] \\ &\quad \times \left[\int_0^s d\sigma \delta_\sigma V(\mathbf{r}_1 - \mathbf{r}_l) \right]. \end{aligned} \quad (15)$$

The above components are distinct two- and three-particle operators and the same holds for the parallel decomposition

of the second term in the braces in Eq. (14). With $\bar{\mathbf{r}}_1 = \mathbf{r}_1 - \mathbf{r}_2$; $\bar{\mathbf{r}}_3 = \mathbf{r}_3 - \mathbf{r}_2$) one may reduce Eq. (14) to

$$\begin{aligned} \tilde{F}_2(s) &= \tilde{F}_2^{(2)}(s) + \tilde{F}_2^{(3)}(s), \\ \frac{1}{v_q^2} \tilde{F}_2^{(2)}(s) &= \int d\mathbf{r} \frac{\rho_2(\mathbf{r}-s, 0; \mathbf{r}, 0)}{\rho} \\ &\quad \times \left[\frac{1}{2} [i\tilde{\chi}_q(\mathbf{r}, s)]^2 + \frac{i}{v_q} \delta_s V(\mathbf{r}) \int_0^s d\sigma [i\tilde{\chi}_q(\mathbf{r}, \sigma)] \right], \end{aligned} \quad (16a)$$

$$\begin{aligned} \frac{1}{v_q^2} \tilde{F}_2^{(3)}(s) &= \int d\bar{\mathbf{r}}_1 d\bar{\mathbf{r}}_3 \frac{\rho_3(\bar{\mathbf{r}}_1 - s, 0; \bar{\mathbf{r}}_3; \bar{\mathbf{r}}_1, 0; \bar{\mathbf{r}}_3)}{\rho} \\ &\quad \times \left[\frac{1}{2} [i\tilde{\chi}_q(\bar{\mathbf{r}}_1, s)] [i\tilde{\chi}_q(\bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3, s)] \right. \\ &\quad \left. + \frac{i}{v_q} \delta_s V(\bar{\mathbf{r}}_1) \int_0^s d\sigma [i\tilde{\chi}_q(\bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3, \sigma)] \right], \end{aligned} \quad (16b)$$

with $\tilde{\chi}_q(\mathbf{r}, s)$ the off-shell phase as defined in Eq. (11). (Note that $\tilde{\chi} \propto 1/v_q$.)

For smooth, nonsingular local forces, the above completes the derivation of an exact expression for $\tilde{F}_2(s)$. However, if V possesses a strong, short-range repulsion, as is the case for atom-atom interactions, difficulties emerge. There are no problems if in integrands wave functions or density matrices and V have identical arguments, in which case large values of V are generally off-set by small values of ρ_n at common small \mathbf{r} . This is not the case in general. A prime example is Eq. (10) with \mathbf{r} -dependence through $V(\mathbf{r} - \boldsymbol{\sigma})$, $0 \leq |\boldsymbol{\sigma}| \leq s$, and $\mathbf{r} - \boldsymbol{\sigma}$ generally not coinciding with either $\mathbf{r} - s$ or \mathbf{r} in $\rho_2(\mathbf{r} - s, \mathbf{r}; 0)$: Large line integrals may result.

In the above case smooth expressions emerge again upon summation of a ladder of pair interactions $V(\mathbf{r})$, leading to V_{eff} which is the eikonal, off-shell t matrix.^{6,7,10} Effectively

$$i\tilde{\chi} \rightarrow \exp[i\tilde{\chi}] - 1 = i\tilde{\chi} + 1/2 [i\tilde{\chi}]^2 + \dots \quad (17)$$

Using Eqs. (10) and (17) we define

$$\tilde{G}_2(s, q[V]) \equiv \tilde{F}_2(s, V \rightarrow [t]) = \tilde{G}_2^{(2)}(s, q) + \tilde{G}_2^{(3)}(s, q), \quad (18)$$

with the following two- and three-particle components

$$\begin{aligned} \frac{1}{v_q^2} \tilde{G}_2^{(2)}(s, q) &= \int d\mathbf{r} \frac{\rho_2(\mathbf{r}-s, 0; \mathbf{r}, 0)}{\rho} \left[\frac{i}{v_q} \delta_s V(\mathbf{r}) \right. \\ &\quad \left. \times \int_0^s d\sigma (\exp[i\tilde{\chi}_q(\mathbf{r}, \sigma)] - 1) \right], \end{aligned} \quad (19a)$$

$$\begin{aligned} \frac{1}{v_q} \tilde{G}_2^{(3)}(s, q) &= \int d\bar{\mathbf{r}}_1 d\bar{\mathbf{r}}_3 \frac{\rho_3(\bar{\mathbf{r}}_1 - s, 0; \bar{\mathbf{r}}_3; \bar{\mathbf{r}}_1, 0, \bar{\mathbf{r}}_3)}{\rho} \\ &\times \left[\frac{1}{2} (\exp[i\tilde{\chi}_q(\bar{\mathbf{r}}_1, s)] - 1) \right. \\ &\times (\exp[i\tilde{\chi}_q(\bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3, s)] - 1) + \frac{i}{v_q} \delta_s V(\bar{\mathbf{r}}_1) \\ &\left. \times \int_0^s d\sigma (\exp[i\tilde{\chi}_q(\bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3, \sigma)] - 1) \right]. \quad (19b) \end{aligned}$$

Care should be exercised in the replacement $V \rightarrow V_{eff}$ for an ill-behaved V as we shall now illustrate by focusing on the first term in the brackets in Eq. (16a), $\frac{1}{2}[i\tilde{\chi}]^2$. It can be shown that *all* higher order terms $\tilde{F}_n(s, [V])$ contain a two-body component of the form

$$\frac{1}{v_q} \tilde{F}_n^{(1)}(s, [V]) = \int d\mathbf{r} \frac{\rho_2(\mathbf{r} - s, 0; \mathbf{r}, 0)}{\rho} [(i\tilde{\chi})^n / n!]. \quad (20)$$

Using Eq. (17) those may be summed up to

$$\sum_{n>1} \tilde{F}_n^{(1)}(s, [V]) = \tilde{F}_1(s, [t]). \quad (21)$$

If therefore $\tilde{F}_1(s, [V])$ has been regularized by $V \rightarrow V_{eff} = t$, the first part of $\tilde{F}_2^{(2)}(s)$ in Eq. (16a) is already contained in $\tilde{F}_1(s, [t])$ and in order to avoid double-counting it should be removed from $\tilde{G}_2(s, [V])$. We note that by construction, the remaining term in Eq. (19a) which emerges from TC is nevertheless of two-body character.

Equations (19a) and (19b) above are the exact TC contributions to the GRS series (5) for the reduced response. At this point we mention an alternative to the GRS series, namely the cumulant representation for the FT of the reduced response²⁰

$$\tilde{\phi}(q, s) = \tilde{F}_0(s) \tilde{R}(q, s) = \tilde{F}_0(s) \exp[\tilde{\Omega}(q, s)], \quad (22a)$$

$$\tilde{R}(q, s) = \sum_{n \geq 1} \left(\frac{1}{v_q} \right)^n \frac{\tilde{F}_n(s)}{\tilde{F}_0(s)}, \quad (22b)$$

$$\tilde{\Omega} = (\tilde{R} - 1) - (1/2)(\tilde{R} - 1)^2 + \dots, \quad (22c)$$

with all FSI effects contained in either \tilde{R} or $\tilde{\Omega}$

Below we report a calculation of TC contributions, using choices for the underlying densities.

III. TC CONTRIBUTIONS TO THE RESPONSE OF LIQUID ⁴He

Until now, dynamical calculations based on the GRS series were limited to FSI in the BC approximation, i.e.

$$\tilde{\Omega} \rightarrow \tilde{\Omega}^{BC} = \tilde{\Omega}_2 = \frac{\tilde{F}_1}{v_q \tilde{F}_0} - 1 \quad (23)$$

with the GRS series, cut at $n=2$, as in Ref. 11. We now report what apparently are the first results for the next-to-leading order TC corrections and which are contained in $\tilde{G}_2 = \tilde{G}_2^{(2)} + G_2^{(3)}$, Eqs. (18), (19).

We first recall the standard input described in Ref. 11. For the bare interaction we use the standard $V^{A_{ziz}}$, Ref. 21, and for the single-atom momentum distribution the results of Refs. 22,23. As regards semidiagonal two-particle density matrix $\rho_2(\mathbf{r} - s, 0; \mathbf{r}, 0)$, there exist results obtained with stochastic methods,^{24,9} but computationally it is unnecessarily time-consuming to evaluate those for each and every (\mathbf{r}, s) , as is required in calculations of the expressions (10) or (19a).

In the past relatively simple guesses have been made for ρ_2 . We shall use below the interpolation formula by GRS,^{4,6}

$$\begin{aligned} \rho_2(\mathbf{r} - s, 0; \mathbf{r}, 0) &= \rho \rho_1(0; s) \zeta_2(\mathbf{r} - s, \mathbf{r}), \\ \zeta_2(\mathbf{r} - s, \mathbf{r}) &\approx \sqrt{g(|\mathbf{r} - s|)g(r)} \end{aligned} \quad (24)$$

with $g(r)$ the pair-distribution function, chosen to be the one from Ref. 9.

A calculation of \tilde{G}_3 requires the 3-particle density matrix ρ_3 which, as before is nondiagonal in coordinate ‘‘1.’’ As an approximation we suggest

$$\begin{aligned} \rho_3(\bar{\mathbf{r}}_1 - s, 0, \bar{\mathbf{r}}_3; \bar{\mathbf{r}}_1, 0, \bar{\mathbf{r}}_3) &\approx \frac{(A-2)}{(A-1)} \frac{\rho_2(\bar{\mathbf{r}}_1 - s, 0; \bar{\mathbf{r}}_1, 0) \rho_2(\bar{\mathbf{r}}_3 - s, 0; \bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3, 0)}{\rho_1(0; s)} \\ &= \frac{(A-2)}{(A-1)} \rho^2 \rho_1(0; s) \zeta_2(\bar{\mathbf{r}}_1 - s, \bar{\mathbf{r}}_1) \zeta_2(\bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3 - s, \bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3), \end{aligned} \quad (25)$$

where use has been made of Eq. (24). The choice (25) has several advantages.

(i) With ‘‘1’’ paying a special role, it is symmetric in the other coordinates.

(ii) It exactly satisfies the ‘‘sum rule’’ (12).

(iii) It factorizes in parts dependent on $\bar{\mathbf{r}}_1, \bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_3$.

(iv) It causes ρ_3 to vanish for small values of the 4 coordinates which would otherwise produce large values for the factors in the operator in the brackets in Eq. (19b).

An immediate consequence of (iii) above is the reduction of the, effectively 5-dimensional integral in Eq. (19b) to the product of two, two-dimensional integrals

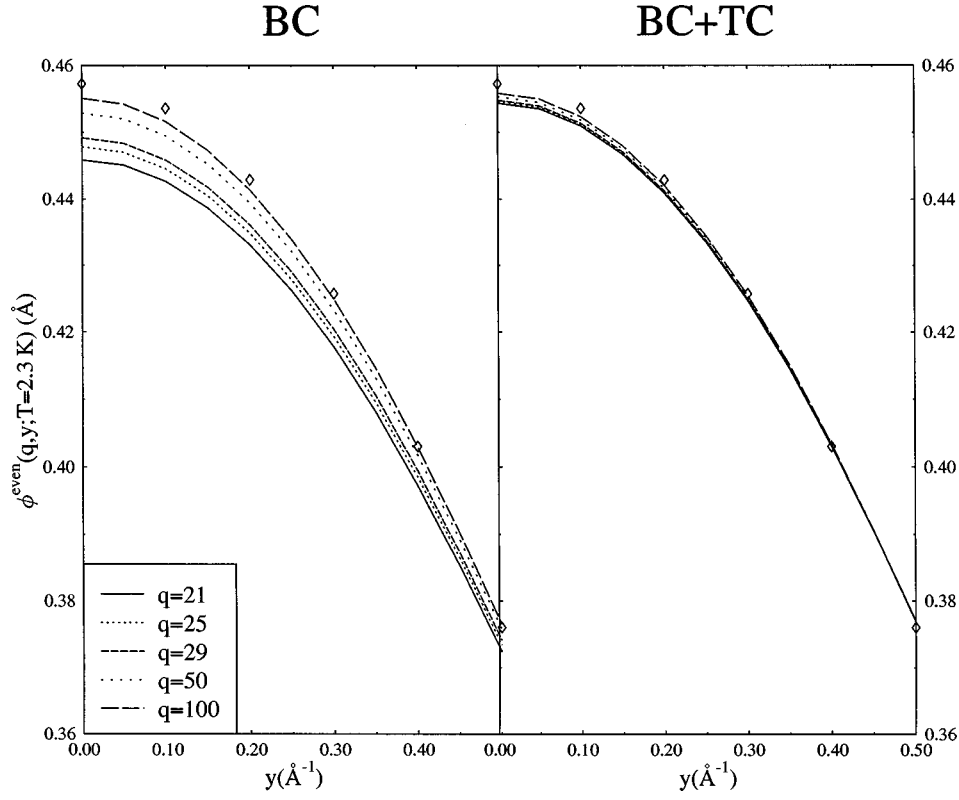


FIG. 1. (a),(b) The approach to the asymptotic limit $F_0(y)$ (diamonds) for small y of the calculated even part of the response without and with the (even) TC contributions.

$$\frac{1}{v_q^2} \frac{\tilde{G}_2^{(2)}(s, q)}{\tilde{F}_0(s)} = \rho \int d\mathbf{r} \zeta_2(\mathbf{r}-s, \mathbf{r}) \times \left[\frac{i}{v_q} \delta_s V(\mathbf{r}) \int_0^s d\sigma (\exp[i\tilde{\chi}_q(\mathbf{r}, \sigma)] - 1) \right], \quad (26a)$$

$$\frac{1}{v_q^2} \frac{\tilde{G}_2^{(3)}(s, q)}{\tilde{F}_0(s)} = \left[\frac{i}{v_q} \int d\bar{\mathbf{r}}_1 \zeta_2(\bar{\mathbf{r}}_1 - s, \bar{\mathbf{r}}_1) \delta_s V(\bar{\mathbf{r}}_1) \right] \times \left[\int d\bar{\mathbf{r}}_3 \zeta_2(\bar{\mathbf{r}}_3 - s, \bar{\mathbf{r}}_3) \right] \times \left[\int_0^s d\sigma (\exp[i\tilde{\chi}_q(\bar{\mathbf{r}}_3, \sigma)] - 1) \right]. \quad (26b)$$

Anticipating small TC corrections we approximate the cumulant representation (22)

$$\tilde{\Omega}^{TC} \approx \tilde{R}^{TC} - 1, \quad (27)$$

$$\tilde{R}^{TC} = \frac{\tilde{G}_2}{v_q^2 \tilde{F}_0}.$$

The thus defined TC contribution to the FSI phase has been added to the previously calculated BC part $\tilde{\Omega}^{BC}$, Eq. (23).

From Eq. (22a) and the inverse of Eq. (4), we compute the response for $T=2.3$ K to the corresponding order.

A first observation is the relative insignificance of 3-body TC contributions for the q -range investigated. A heuristic argument runs as follows: If the BC FSI contributions amounts to a fraction of the the dominant asymptotic limit, one estimates from the factorization (25) of the 3-body density matrix that TC FSI is approximately the square of that fraction of F_0 .

We now display some results for TC contributions. Figures 1(a) and 1(b) show for small y and $q = 21, 25, 29, 50, 100 \text{ \AA}^{-1}$ the even part of the calculated reduced response $\phi^{\text{even}}(q, y) = [\phi(q, y) + \phi(q, -y)]/2$ without, and including TC contributions (note that ϕ^{TC} is even). Even for $y=0$ there is an effect which for increasing $q \geq 21 \text{ \AA}^{-1}$ decreases from 2 to 0%.

Figures 2(a) and 2(b) show the fractional effect of TC contributions

$$\alpha(q, y) = 1 + \frac{\phi^{TC}(q, y)}{\phi^{BC}(q, y)} \quad (28)$$

calculated for $2.5 \leq |y|$ (in \AA^{-1}) ≤ 3.3 . The difference in sign of $\alpha - 1$ clearly shows the effect of the competition between the dominant even and odd parts in the wings of the response.

Finally, Figs. 3(a), 3(b), and 3(c) show for $q = 21, 25, 29 \text{ \AA}^{-1}$, $T=2.3$ K the effect of TC on the calculated response, including the unresolved effect of the instru-

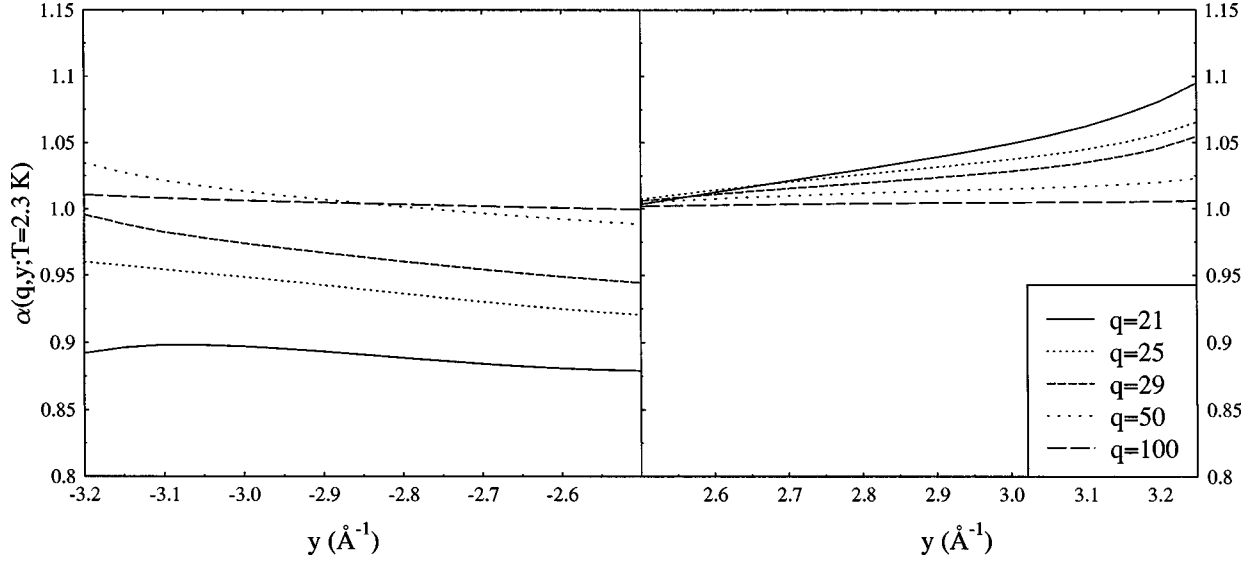


FIG. 2. (a),(b) The fractional effect $\alpha(q, y)$, Eq. (28) of TC contributions in the wings $2.5 \leq |y|$ (in \AA^{-1}) ≤ 3.3 .

mental resolution. The small TC contributions discernibly improve the agreement of predictions with data^{3,14,16} in the above y regions.

IV. ON THE FOURTH CENTRAL MOMENT OF THE RESPONSE

The preceding sections deal with the reduced response (22) up to, and including TC contributions and its, in principle exact, calculation. For the FT of those one needs $\tilde{F}_n(s), n \leq 2$ or [cf. Eq. (22)] $\tilde{\Omega}(q, s)$ to that order, both for all relevant s .

We now address a second topic which is related to the cumulant representations (22) and which is based on the small- s expansions

$$\tilde{F}_0(s) = \exp \left[\sum_{m \geq 2} \frac{(-is)^m}{m!} \bar{\alpha}_m \right], \quad (29a)$$

$$\tilde{\Omega}(q, s) = \sum_{m \geq 3} \frac{(-is)^m}{m!} \bar{\beta}_m(q). \quad (29b)$$

The above coefficients α_m are related to even moments of the momentum distribution $n(p)$, while the FSI coefficient functions $\bar{\beta}_m(q)$ in the expansion (29b) can be expressed in terms of central moments of the response (see for instance Ref. 25)

$$\begin{aligned} \mathcal{M}_n(q) &= \int d\omega (\omega - q^2/2M)^n S(q, \omega) \\ &= (v_q)^n \int dy y^n \phi(q, y) \equiv (v_q)^n \bar{\mathcal{M}}_n(q). \end{aligned} \quad (30)$$

For our purpose it suffices to give the following expressions for $n=3,4$ and valid for local interactions V^{26}

$$\bar{\beta}_3 = \bar{\mathcal{M}}_3 = \left(\frac{1}{6v_q} \right) \langle \nabla^2 V \rangle, \quad (31a)$$

$$\bar{\beta}_4 = \bar{\mathcal{M}}_4 - \bar{\alpha}_4 - 3\bar{\alpha}_2^2 = \left(\frac{1}{3v_q^2} \right) \langle \mathcal{F}_1 \cdot \mathcal{F}_1 \rangle. \quad (31b)$$

\mathcal{F}_1 above

$$\mathcal{F}_1 = \sum_{k \neq 1} \mathcal{F}_1(1, k) = -\nabla_1 \sum_{k > 1} V(\mathbf{r}_1 - \mathbf{r}_k), \quad (32)$$

distinct from $U_1(s)$, Eq. (7), is the true total force on a given particle ‘‘1.’’^{27,28} The expectation value in Eq. (31b) can thus be separated in two parts. The first contains the square of the force on ‘‘1’’ due to one particle and in the second part forces on ‘‘1’’ by two different particles

$$\begin{aligned} \langle \mathcal{F}_1 \cdots \mathcal{F}_1 \rangle &= \left\langle \sum_{j \neq 1} [\mathcal{F}_1(1, j)]^2 \right\rangle \\ &+ \left\langle \sum_{1 \neq j \neq k \neq 1} \mathcal{F}_1(1, j) \mathcal{F}_1(1, k) \right\rangle. \end{aligned} \quad (33)$$

The expansions (29) and (29b) provide a parametrization of the response, but the technique has been shown to have its problems.¹¹ One such problem is the convergence for growing s which is indispensable for the calculation of the inverse FT (4) from $\phi(q, y)$. Moreover, the cumulant expansion lacks a systematic ordering in powers of $1/q$ which is also remedied in GRS theory. Notwithstanding, there has recently been a renewed interest in the above small s -cumulant expansions as a vehicle to extract the single-atom momentum distribution $n(p)$ from response data for ⁴He and Ne.^{12–16,11} Around $\bar{\beta}_4$ an apparent contradiction arises, which we discuss below.

One may ‘‘invert’’ Eqs. (29) and (29b) in order to find alternative expressions for

$$\bar{\beta}_m(q) = m! i^m \lim_{s \rightarrow 0} [\tilde{\Omega}(q, s)/s^m].$$

In particular

$$\bar{\beta}_3(q) = 6 \lim_{s \rightarrow 0} [\text{Im} \tilde{\Omega}(q, s)/s^3], \quad (34a)$$

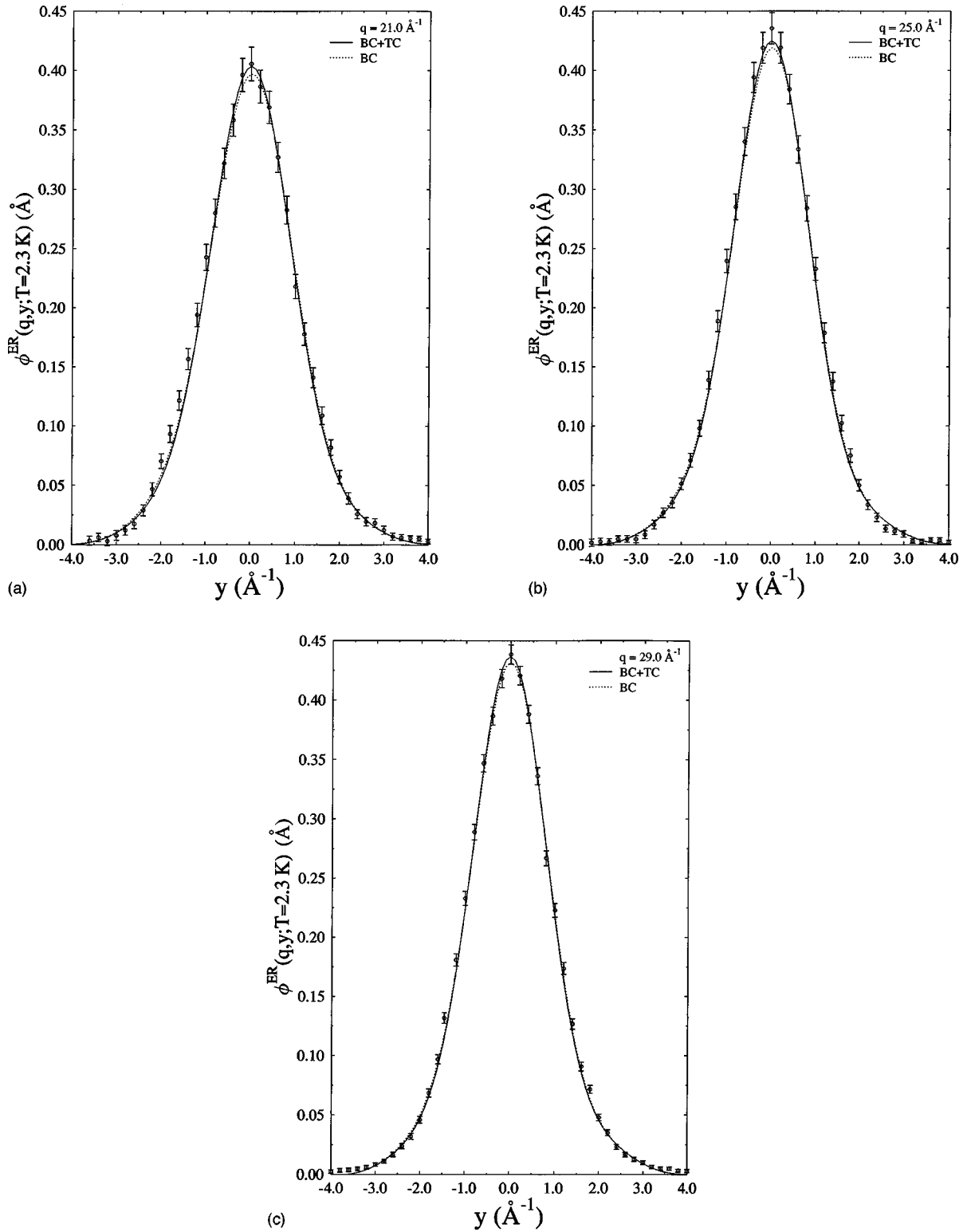


FIG. 3. (a) Calculated response and data (Refs. 3,14,16) for $q=21 \text{ \AA}^{-1}$, $T=2.5 \text{ K}$, including the effect of instrumental resolution. Dashed and drawn curves are without, respectively including TC contributions. (b) Same as (a) for $q=25 \text{ \AA}^{-1}$. (c) Same as (a) for $q=29 \text{ \AA}^{-1}$.

$$\bar{\beta}_4(q) = 24 \lim_{s \rightarrow 0} [\text{Re} \bar{\Omega}(q, s) / s^4]. \quad (34b)$$

The above FSI coefficient functions can only be calculated if a theory provides the FSI phase function $\bar{\Omega}(q, s)$. The GRS

theory is one such example. The dynamic calculation described in the previous sections, provides $\bar{\Omega}(q, s)$ for all s .

First we state that without truncations, the cumulant expansion and the GRS series ought to lead to the same response, and in particular to the same numerical values for the

cumulant coefficient functions $\bar{\beta}_m$. This is not self-evident since Eqs. (31a), (31b) and (34a), (34b) look quite dissimilar. The former are expectation values in terms of *diagonal* density matrices, whereas the $\bar{\Omega}$ underlying the GRS theory is an operator, averaged over a *non-diagonal* density matrix. Nevertheless the identity of the derived $\bar{\beta}_3(q)$ has been formally verified in the past (see for instance Ref. 9). In addition a numerical test has been performed using $\bar{\Omega} \rightarrow \bar{\Omega}^{BC}$, which suffices since $\bar{\beta}_3$ draws entirely on \bar{F}_1 or on $\bar{\Omega}^{BC}$. The calculated value and the one, extracted over a wide q range, indeed agree to high accuracy.¹¹

For a similar demonstration regarding $\bar{\beta}_4$ one uses Eqs. (22b), (14), (15) in (34a) and readily verifies that terms $\propto s^4$, needed in the threshold behavior (34b), originate exclusively from the TC terms $\bar{G}_2(s)$ [cf. Eqs. (19a), (19b)]. Observing that δV in Eqs. (13), (14) always appears quadratically, one has

$$\delta_s V(\mathbf{r}) = (1/2)s^2 \frac{\partial V(\mathbf{r})}{\partial z} + \mathcal{O}(s^3), \quad (35)$$

$$UU \propto s^4 (\hat{z} \cdot \mathcal{F}_1)^2 + \mathcal{O}(s^5),$$

and Eqs. (34a) and (34b) result.

We separately treat BC and TC contributions to $\bar{\beta}_4(q)$ and start with the above mentioned BC approximation for the regularized $\bar{F}_1(y, [t])$. One observes that even the BC FSI phase function $\bar{\Omega}^{BC}(q, s)$ contains terms $\propto s^4$, contributing to $\bar{\beta}_4$. Again, a remarkably stable, *negative* value could be extracted from calculated BC phases over a wide q -range¹¹ ($q^* = q/10$ in \AA^{-1})

$$q^{*2} \bar{\beta}_4^{(21)}(q) = (-2.27 \pm 0.02) \text{\AA}^{-4}. \quad (36)$$

One easily demonstrates that the same, *computed* from the first term in the brackets of Eq. (16a) is $q^{*2} \bar{\beta}_4^{(21)}(q) = -(M/10)^2 \sum_{j \neq 1} \langle \mathcal{F}_1(1, j)^2 \rangle = -2.19 \text{\AA}^{-4}$, again in close agreement with the *extracted* result (36). The negative outcome clearly contradicts the manifestly positive expression (31b) for the complete $\bar{\beta}_4$. The latter, however, draws also on additional TC contributions from $\bar{G}_2^{(2)}$ and $\bar{G}_2^{(3)}$, Eqs. (19a) and (19b), which we now address.

We start with the threshold value of the two-body part $\bar{G}_2^{(2)}$ of the TC contribution, which is readily shown to be exactly 4/3 times the first part and for the positive, complete two-body part one finds [cf. Eq. (33)]

$$\begin{aligned} q^{*2} \bar{\beta}_4^{(2)}(q) &= q^{*2} [\bar{\beta}_4^{(21)}(q) + \bar{\beta}_4^{(22)}(q)] \\ &= \frac{1}{3} (M/10)^2 \sum_{j \neq 1} \langle \mathcal{F}_1(1, j)^2 \rangle = 0.73 \text{\AA}^{-4}. \end{aligned} \quad (37)$$

Within $\approx 0.5\%$ the same value results when calculating the threshold value (36) and using for the FSI phase function $\bar{\Omega}(q, s)$ Eq. (22) with $\bar{G}_2^{(2)}$ as in Eqs. (18), (19a). As emphasized before, the close agreement evidences numerical accuracy and not consistency.

The genuine 3-body TC part, defined by Eqs. (33), (19b)

$$\bar{\beta}_4^{(3)}(q) = 24 \lim_{s \rightarrow 0} \left(\frac{1}{v_q} \right)^2 \text{Re} \left[\frac{\bar{G}_2^{(3)}(s)}{\bar{F}_0(s)} \right] \quad (38a)$$

$$= \frac{1}{3} \left(\frac{1}{v_q} \right)^2 (M/10)^2 \sum_{1 \neq k \neq j \neq 1} \langle \mathcal{F}_1(1, j) \cdot \mathcal{F}_1(1, k) \rangle \quad (38b)$$

involves the forces on ‘‘1’’ by two different medium particles. The expectation value in Eq. (38b) requires a diagonal 3-particle density matrix, and consistency requires it to be the non-diagonal (25), used in the calculation of $\bar{\Omega}$ in the limit $s=0$. Here too the 3-body part is negligible.

The remaining 2-body parts may be compared with previous results which have been calculated in different ways. Our result (37) lies in between (0.69, 0.86) \AA^{-4} , communicated by Polls as the outcome from various approximations to the pair-distribution functions $g(r)$.²⁹ Another stochastic calculation by Glyde and Boninsegni reported in Ref. 16, leads to $q^{*2} \bar{\beta}_4 = (98 \pm 10) \text{\AA}^{-4}$ which is about 25% in excess of our value. Previous experience has taught that averages, like the ones in Eqs. (31a) and (31b), are quite sensitive to the chosen, pair distribution. A spread of 10–15% may certainly be expected.

Finally, we compare the computed total $q^{*2} \bar{\beta}_4(q) = 0.73 \text{\AA}^{-4}$ with a few results, extracted from cumulant analyses of the data. For instance in Ref. 15 a value compatible with 0 is given, while an upper limit $q^{*2} \bar{\beta}_4(q) < 0.50 \text{\AA}^{-4}$ is cited in Ref. 16.

We close this section by comparing $\bar{F}_2(s)$, Eq. (14), and other published expressions for the same.^{4,30,10} Those are also quadratic in V , but contain in addition to ρ_2 , derivatives of ρ_2 and V . In contradistinction our result is quadratic in V and free of derivatives. We have shown above that each of its composing parts is $\propto [\mathcal{F}_1^2]$ with different co-factors. The alternative expressions provide directly one factor \mathcal{F}_1 and it is not at all evident that the other part can be cast in that form. The equations of motion for density matrices ultimately provide the evidence. The procedure followed in Eqs. (13)–(16) avoids those steps and leads directly to the desired result. This can be checked for the general response of a particle in a potential, Eq. (8c) of Ref. 30.

V. SUMMARY AND CONCLUSION

We have derived above an exact expression for the contribution of ternary collisions to the response of a nonrelativistic many-body system, where the struck constituent interacts with two other medium particles. Its numerical contribution has for the first time been evaluated for the response of liquid ${}^4\text{He}$, $T > T_c$ and momentum transfers in excess of 21\AA^{-1} . For those we know that the asymptotic limit and the dominant binary collision correction, accurately describe the response in a broad region around the quasi-elastic peak, but not necessarily at the peak itself (cf. for instance Ref. 11).

Our main interest was therefore focused on $y \approx 0$ and the region of the wings, where the intensity is only a fraction of that in the peak. Compromising only on the assumed 3-body density matrix, we computed the relative size of small TC

FSI effects and found those to discernibly improve the agreement with the data.

The above calculation completes a program to calculate the medium-to-large q response of liquid ${}^4\text{He}$. A number of conclusions are in order. Using exclusively the well-known atom-atom interaction, basic ground-state properties as are the single-atom momentum distribution, the pair-correlation function and nondiagonal, two-particle density distribution have been determined with great accuracy.

The above quantities are then basic input for the calculation of the linear response of the system. Only weak assumptions have been used for the required two- and three-particle density matrices, diagonal in all, except one coordinate. Excellent agreement has been obtained with data for a theory with demonstrated convergence.

Indeed, given the non-negligible scatter in the data and observing that one deals with atomic dynamics and not with QED, we feel that there is at present no incentive to study even finer theoretical details than discussed up to now.

Our final remark regards the response of liquid ${}^4\text{He}$ when compared with the responses of other systems, composed of atoms, molecules, atomic nuclei or sub-hadronic matter. We do not know of a system where the approach to the asymptotic limit has been measured and studied with an accuracy, possible for ${}^4\text{He}$.

ACKNOWLEDGMENTS

A.S.R. thanks A. Polls and H. Glyde for informative discussions.

-
- ¹T.R. Sosnick, W.M. Snow, and P.E. Sokol, *Phys. Rev. B* **41**, 11 185 (1990); T.R. Sosnick, W.M. Snow, R.N. Silver, and P.E. Sokol, *ibid.* **43**, 216 (1990).
- ²K.H. Andersen *et al.*, *Physica B* **180/181**, 865 (1992); **197**, 198 (1994).
- ³R.R. Azuah, Ph.D. thesis, Univ. of Keele, 1994.
- ⁴H.A. Gersch, L.J. Rodriguez, and Phil N. Smith, *Phys. Rev. A* **5**, 1547 (1973).
- ⁵R.N. Silver, *Phys. Rev. B* **37**, 3794 (1988); **38**, 2283 (1988); **39**, 4022 (1989).
- ⁶A.S. Rinat, *Phys. Rev. B* **40**, 6625 (1989).
- ⁷A.S. Rinat and M.F. Taragin, *Phys. Rev. B* **41**, 4247 (1990); A.S. Rinat, *ibid.* **42**, 9944 (1990).
- ⁸C. Carraro and S.E. Koonin, *Phys. Rev. B* **41**, 6741 (1990); *Phys. Rev. Lett.* **65**, 2792 (1990).
- ⁹F. Mazzanti, J. Boronat, and A. Polls, *Phys. Rev. B* **53**, 5661 (1996).
- ¹⁰J. Besprosvany, *Phys. Rev. B* **43**, 10 070 (1991).
- ¹¹A.S. Rinat, M.F. Taragin, F. Mazzanti, and A. Polls, *Phys. Rev. B* **57**, 5347 (1998).
- ¹²H.R. Glyde, *Phys. Rev. B* **50**, 6726 (1994).
- ¹³H.R. Glyde, R.T. Azuah, K.H. Anderson, and W.G. Stirling, *Condens. Matter Theor.* **10**, 27 (1995).
- ¹⁴R.T. Azuah, W.G. Stirling, H.R. Glyde, P.E. Sokol, and S.M. Bennington, *Phys. Rev. B* **51**, 605 (1995).
- ¹⁵K.H. Andersen, W.G. Stirling, and H.R. Glyde, *Phys. Rev. B* **56**, 8978 (1997).
- ¹⁶R.T. Azuah, W.G. Stirling, H.R. Glyde, M. Boninsegni, P.E. Sokol, and S.M. Bennington, *Phys. Rev. B* **56**, 14 620 (1995).
- ¹⁷G.B. West, *Phys. Rep.*, *Phys. Lett.* **18C**, 264 (1975).
- ¹⁸A. Rahman, K.S. Singwi, and A. Sjölander, *Phys. Rev.* **126**, 986 (1962).
- ¹⁹The GRS theory is not a perturbation series in V with $F_n \propto V^n$, which only holds for $n=1,2$.
- ²⁰H.A. Gersch and L.J. Rodriguez, *Phys. Rev. A* **8**, 905 (1973).
- ²¹R. Aziz, V.P.S. Nain, J.S. Carley, W.L. Taylor, and J.T. McConville, *J. Chem. Phys.* **70**, 4330 (1979).
- ²²P.A. Whitlock and R.M. Panoff, *Can. J. Phys.* **65**, 1409 (1987).
- ²³D.M. Ceperley and E.L. Pollock, *Can. J. Phys.* **65**, 1416 (1987).
- ²⁴D.M. Ceperley, in *Momentum Distributions*, edited by R.N. Silver and P.E. Sokol (Plenum, New York, 1989), p. 71; *Rev. Mod. Phys.* **67**, 279 (1995).
- ²⁵V.F. Sears, *Phys. Rev. B* **30**, 44 (1984).
- ²⁶G. Placek, *Phys. Rev.* **86**, 377 (1952); G.C. Wick, *ibid.* **94**, 1228 (1954).
- ²⁷Equation (31b) is the correct expression for $\bar{\beta}_4$. There are a number of publications (cf. Refs. 12,28) where $\mathcal{F}_1(i,j)$ appears replaced by its component $\hat{q} \cdot \mathcal{F}_1(1,j)$ in the \hat{q} direction. For isotropic media $\langle [\hat{q} \cdot \mathcal{F}_1(1,j)]^2 \rangle = \frac{1}{3} \langle [\mathcal{F}_1(1,j)]^2 \rangle$.
- ²⁸H.R. Glyde, *Excitations in Liquid and Solid He* (Oxford University Press, New York, 1994).
- ²⁹A. Polls (private communication).
- ³⁰S.A. Gurvitz and A.S. Rinat, *Phys. Rev. C* **47**, 2901 (1993).