Final State Effects in the high $q$ response of $^3$He–$^4$He mixtures

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Abstract

A modified Gersch–Rodriguez formalism describing the leading Final State Effects in the high momentum transfer response of low concentration $^3$He–$^4$He mixtures is presented and discussed. The leading corrections to the Impulse Approximation are expressed in terms of the interatomic potentials and the semidiagonal two–body density matrices of both the mixture and its boson–boson approximation, in which the $^3$He atoms are replaced by bosons of the same mass and at the same partial density. Numerical calculations of the Final State Effects functions of $^3$He and $^4$He are finally presented and discussed.

PACS: 67.60.-g, 61.12.Bt

KEYWORDS: dynamic structure function, FSE, mixtures
The dynamic structure function $S(q, \omega)$ is known to contain the maximum information a neutron scattering experiment can provide about the structure of a quantum fluid. Many theoretical and experimental work designed to study the Bose–Einstein condensate in superfluid $^{4}\text{He}$ has been done in the last thirty years, and much information regarding its quantum properties have been gathered so far. An alternative system in which Bose–Einstein condensation sets in is the isotopic $^{3}\text{He}–^{4}\text{He}$ mixture, stable at low temperatures and concentrations, and presenting much richer static and dynamic properties due to the strong interaction between bosons ($^{4}\text{He}$) and fermions ($^{3}\text{He}$). However, $^{3}\text{He}$ atoms are high neutron absorbers and the experimental measurement of the high $q$ dynamic structure function of systems containing $^{3}\text{He}$ is technically difficult. For this reason, only one measurement of the high $q$ response of the mixture has been reported up to the date, and the analysis of the data led to surprising conclusions such as a condensate fraction value $n_0 \approx 0.2$, in clear disagreement with almost all theoretical predictions which are usually close to $n_0 \approx 0.1^{1,2}$. However, and despite the existent discrepancies between theory and experiment, no new measurements of the high momentum transfer response of the mixture have been performed yet, and hence the question of what this value really is still remains open. Consequently, theoretical investigation of the dynamic structure function of the mixture and further analysis of the measured data is well justified.

The theoretical analysis of the $q \to \infty$ response of the mixture is however slightly more involved that in the pure $^{4}\text{He}$ case due to the presence of a fermionic component. In fact, most of the formalisms that have been used in the past to describe Final State Effects (FSE) in pure $^{4}\text{He}$ rely, in one way or another, on the presence of long–range order in the the one–body density matrix $\rho_1(r)$. Long range order makes $\rho_1(r)$ reach a finite $r \to \infty$ value without changing sign, and thus allowing a cumulant expansion of the Fourier transform of $S(q, \omega)$ around its high $q$ limit $\rho_1(tq/m)$. This is not the case when dealing with fermionic components, and therefore none of these formalisms can be directly applied to analyze the high $q$ response of $^{3}\text{He}$ without further modifications. In this work we address this problem and present a new formalism designed to describe FSE in the response of the $^{3}\text{He}–^{4}\text{He}$ mixture, where a $^{3}\text{He}$ component is present but dilute.

In the mixture and when the transferred momentum is high enough for the incoherent approximation to hold, the dynamic structure function becomes

$$S(q, \omega) = \sigma_4 (1 - x_3) S^{(4)}(q, \omega) + \sigma_3 x_3 S^{(3)}(q, \omega) ,$$

(1)

where $x_3$ is the $^{3}\text{He}$ concentration, and $\sigma_3$ and $\sigma_4$ are the cross sections of the separate scattering processes ($\sigma_3 = 5.61$ and $\sigma_4 = 1.34$ in units of barns). Each of the individual responses are the Fourier transform of their corresponding density–density correlation factor

$$S^{(\alpha)}(q, t) = \frac{1}{N_\alpha} \sum_{j=1}^{N_\alpha} \langle e^{-i \mathbf{q} \cdot \mathbf{r}_j} e^{i \mathbf{H} t} e^{i \mathbf{q} \cdot \mathbf{r}_j} e^{-i \mathbf{H} t} \rangle$$

(2)

where $\alpha = 3$ for $^{3}\text{He}$ and $\alpha = 4$ for $^{4}\text{He}$. In this expression, $\mathbf{H}$ stands form the Hamiltonian

$$H = -\frac{1}{2m_4} \sum_{j \in 4} \nabla_j^2 - \frac{1}{2m_3} \sum_{j \in 3} \nabla_j^2 + \frac{1}{2} \sum_{\alpha, \beta = 3, 4} \sum_{i \in \alpha} \sum_{j \in \beta} V^{(\alpha, \beta)}(r_{ij})$$

(3)
corresponding to a mixture in which a $^3$He and a $^4$He components coexists and interact through pairwise local and central potentials $V^{(\alpha,\beta)}(r)$.

Actually, $S^{(\alpha)}(q, t)$ is the starting point from where a high $q$ expansion of the response is performed, and this is done acting with the two translation operators $\exp(-i\mathbf{q} \cdot \mathbf{r}_j)$ and $\exp(i\mathbf{q} \cdot \mathbf{r}_j)$ on the time evolution operator $\exp(-i\mathcal{H}t)$ appearing in between. This leads to

$$S^{(\alpha)}(q, t) = \frac{1}{N_\alpha} e^{i\omega^{(\alpha)}_q t} \sum_{j=1}^{N_\alpha} \left\langle e^{i(t(H+L_j^{(\alpha)})} e^{-it\mathcal{H}} \right\rangle,$$

where $L_j^{(\alpha)} = \mathbf{v}^{(\alpha)} \cdot \mathbf{p}_j$, is the projection of the momentum of particle $j$ along the direction of the recoiling velocity $\mathbf{v}^{(\alpha)} = \mathbf{q}/m_\alpha$ and $\omega^{(\alpha)}_q = q^2/2m_\alpha$ may be understood as its kinetic energy when the momentum transferred to the system is high. Taking into account the symmetries of the ground state wavefunction, introducing an identity in the form $1 = \exp(-iL_j^{(\alpha)}t) \exp(iL_j^{(\alpha)}t)$ and moving the time evolution operator to the left, the density–density correlation factor becomes

$$S^{(\alpha)}(q, t) = e^{i\omega^{(\alpha)}_q t} \left\langle C^{(\alpha)}(t)e^{itL_1^{(\alpha)}} \right\rangle,$$

where $C^{(\alpha)}(s)$ is the operator carrying the effects of the FSE, and reads

$$C^{(\alpha)}(t) \equiv e^{-it\mathcal{H}} e^{it(H+L_1^{(\alpha)})} e^{-itL_1}.$$

In the high $q$ limit, $v^{(\alpha)}$ is large and $t$ is short while their product remains of order unity. Therefore, one is allowed to write the response as a function of $s = v^{(\alpha)}t$ instead of $t$, and expand it in inverse powers of the recoiling velocity $v^{(\alpha)}$. Defining a new Hamiltonian $\mathcal{H} = H/v^{(\alpha)}$, Eqs. (5) and (6) become

$$S^{(\alpha)}(q, s) = e^{i\omega^{(\alpha)}_q /v^{(\alpha)}} \left\langle C^{(\alpha)}(s)e^{is\mathbf{v}^{(\alpha)} \cdot \mathbf{p}_1} \right\rangle,$$

$$C^{(\alpha)}(s) = e^{-is\mathcal{H}} e^{is(\mathcal{H}+\mathbf{v}^{(\alpha)} \cdot \mathbf{p}_1)} e^{-is\mathbf{v}^{(\alpha)} \cdot \mathbf{p}_1},$$

where $\mathbf{v}^{(\alpha)}$ is the unit vector pointing in the direction of $\mathbf{v}^{(\alpha)}$. Direct differentiation of (7a) leads to the following first order differential equation satisfied by $C^{(\alpha)}(s)$

$$\frac{d}{ds}C^{(\alpha)}(s) \equiv \dot{C}^{(\alpha)}(s) = i \left[ \mathcal{H}(s) - \mathcal{H} \right] C^{(\alpha)}(s) \quad (8)$$

which must be solved together with the initial condition $C^{(\alpha)}(0) = 1$, the latter being implicit from the definition of $C^{(\alpha)}(s)$ in Eq. (7a). In Eq. (8), $\mathcal{H}(s)$ is an effective Hamiltonian that results from the action on $\mathcal{H}$ of the different exponential operators appearing in $C^{(\alpha)}(s)$

$$\mathcal{H}(s) \equiv e^{-is\mathcal{H}} e^{is(\mathcal{H}+\mathbf{v}^{(\alpha)} \cdot \mathbf{p}_1)} \mathcal{H} e^{-is(\mathcal{H}+\mathbf{v}^{(\alpha)} \cdot \mathbf{p}_1)} e^{is\mathcal{H}} \quad (9)$$

Different representations of the density-density correlation factor can be obtained from the different forms in which the solution of Eq. (8) can be organized. One form that has proved to be particularly useful in the past is the cumulant one, which captures the most salient features of the response and simplifies in the $q \to \infty$ limit.
\[ C^{(\alpha)}(s) \equiv e^{\epsilon_\alpha \Delta_0(s)} e^{\epsilon_\alpha^2 \Delta_1(s)} e^{\epsilon_\alpha^3 \Delta_2(s)} \cdots = \prod_{n=1}^{\infty} \exp \left[ \epsilon_\alpha^n \Delta_n(s) \right]. \]  

Assuming this analytical form, the first \( s \)-derivative of \( C^{(\alpha)}(s) \) can be easily calculated and plugged into Eq. (8). Then equating each order in \( \epsilon_\alpha \) in both sides of the equation one finds a hierarchy of coupled differential equations that can be solved for every \( \Delta_n \) once the previous \( \Delta, \Delta_1, \ldots, \Delta_{n-1} \) are known. The first terms in the chain can be readily obtained and lead to \( \epsilon_\alpha \)

\[ C^{(\alpha)}(s) = \exp \left[ i \epsilon_\alpha \int_0^s (\hat{H}_0(y) - H) \, dy \right] \exp \left[ i \epsilon_\alpha^2 \int_0^s \hat{H}_1(y) \, dy \right] \times \exp \left[ \epsilon_\alpha^3 \left( i \int_0^s \hat{H}_2(s') \, ds' - \int_0^s \int_0^{s'} \left[ \hat{H}_1(s'), \hat{H}_0(s'') - H \right] \, ds' \, ds'' \right) \right] \cdots, \]  

Alternatively, \( C(s) \) can be cast as an additive series setting

\[ e^{\epsilon_\alpha^2 \Delta_0(s)} \equiv 1 + \epsilon_\alpha^n \Gamma_n(s) \]  

where \( \Gamma_n(s) \) is the lowest order independent of \( \epsilon_\alpha \). In this case one finally arrives at the general solution

\[ C^{(\alpha)}(s) = [1 + \epsilon_\alpha \Gamma_1(s)] [1 + \epsilon_\alpha^2 \Gamma_2(s)] [1 + \epsilon_\alpha^3 \Gamma_3(s)] \cdots \equiv e^{i \epsilon_\alpha \int_0^s (\hat{H}_0(s') - H) \, ds'} + \left( e^{i \epsilon_\alpha^2 \int_0^s \hat{H}_1(s') \, ds'} - 1 \right) + \ldots. \]  

Equations (11) and (13) are different expressions of the same solution. Both of them can be used in Eq. (12a) to generate a representation of the density–density correlation factor in which each order in \( \epsilon_\alpha \) is separately displayed. As a matter of fact, both forms coincide in the \( \epsilon_\alpha \to 0 \) limit, where only the zero order term contributes. In this case \( C^{(\alpha)}(s) = 1 \) and \( S^{(\alpha)}(q, s) \) reduces to the Impulse Approximation

\[ S^{(\alpha)}_0(q, s) = e^{i \omega^{(\alpha)} / v^{(\alpha)} \int_0^s \hat{H}_0(s') \, ds'} e^{is \hat{y}^{(\alpha)} \cdot p_1} \equiv e^{i \omega^{(\alpha)} / v^{(\alpha)} \int_0^s (\hat{H}_0(s') - H) \, ds'} e^{is \hat{y} \cdot p_1}. \]  

which is known to dominate the \( q \to \infty \) behavior of the response. At high but finite \( q \), \( \epsilon_\alpha \) is small and thus the leading corrections to the IA are already captured by the first term in Eq. (13), and so all other terms may be discarded. This leads to the following approximation for the response

\[ S^{(\alpha)}_1(q, s) = e^{i \omega^{(\alpha)} / v^{(\alpha)} \int_0^s (\hat{H}_0(s') - H) \, ds'} e^{is \hat{y} \cdot p_1}. \]  

The difference \( \hat{H}_0(s') - H \) in the argument of the exponential can be written in terms of the interatomic potentials alone. In the general case considered here in which two different species coexist and interact through pairwise local and central forces, the argument of the exponential reduces to
\[
\hat{H}_0(s) - H = e^{is\hat{p}_1}He^{-is\hat{p}_1} - H \\
= H + \sum_{\beta=3,4} \sum_{j\in\beta} \left( e^{is\hat{p}_1}V^{(\alpha\beta)}(r_{1j})e^{-is\hat{p}_1} - V^{(\alpha\beta)}(r_{1j}) \right) - H \\
= \sum_{\beta=3,4} \sum_{j\in\beta} \left( V^{(\alpha\beta)}(r_{1j} + s) - V^{(\alpha\beta)}(r_{1j}) \right) \equiv \sum_{\beta=3,4} \sum_{j\in\beta} \Delta V^{(\alpha\beta)}(r_{1j}, s), \quad (16)
\]

where in the last line use has been made of the definition of the potential difference

\[
\Delta V^{(\alpha\beta)}(r_{ij}, r') \equiv V^{(\alpha\beta)}(r_{ij} + r') - V^{(\alpha\beta)}(r_{ij}). \quad (17)
\]

Moreover, the leftmost exponential operator inside the expectation value in Eq. (15) is diagonal in configuration space, and therefore \( S_1^{(\alpha)}(q, s) \) reduces to an integral over the semidiagonal \( N \)-body density matrix and the interatomic potentials

\[
S_1^{(\alpha)}(q, s) = \frac{1}{N_3!N_4!} e^{i\omega^{(\alpha)}/s^{(\alpha)}} \int dr^N \rho_N(r_1, r_2, \ldots, r_N; r_1 + s) \\
\times \exp \left[ \frac{i}{\nu^{(\alpha)}} \sum_{\beta=3,4} \sum_{j\in\beta} \int s^0 ds' \Delta V^{(\alpha\beta)}(r_{1j}, s') \right]. \quad (18)
\]

At zero temperature \( \rho_N \) is defined in terms of the ground state wavefunction \( \Psi_0 \)

\[
\rho_N(r_1, r_2, \ldots, r_N; r_1') \equiv N_3!N_4! \Psi_0^*(r_1, r_2, \ldots, r_N) \Psi(r_1', r_2, \ldots, r_N), \quad (19)
\]

where the \( N_3 \) coordinates corresponding to \( ^3\text{He} \) particles represent both position and spin coordinates.

Eq. (18) is simple compared to the expression of the exact response, but it is still very difficult to evaluate due to the \( N \)-body quantities entering on it. However, it is in the appropriate form for a Gersch–Rodriguez cumulant expansion. While the original Gersch–Rodriguez formalism deals with expectation values of time–ordered integrals of operators, the approximations made so far have brought the response to the Static Background Approximation. In this limit, the scattering time is assumed to be so short and the momentum transfer so high that in essence only the particle being struck by the incoming neutron moves in the process, and thus all other particles in the background are assumed to be frozen at their positions. Under these circumstances, the series simplifies and reduces to the general expansion rule

\[
\phi(r_1, r_1') + \int dr^N f(r_1, r_2, \ldots, r_N; r_1') \exp \left[ i \sum_m \int s^0 ds' \theta_m(s') \right] \equiv W_0 \exp \left[ \sum_{n=1}^{\infty} \omega_n \right], \quad (20)
\]

where \( \phi(r_1, r_1') \), \( f(r_1, \ldots, r_N; r_1') \) and \( \theta_m(s) \) are arbitrary functions, the latter also possibly depending on particle coordinates \( r_1, r_1', r_2, \ldots, r_N \). \( W_0 \) and \( \omega_n \) are the coefficients of the expansion and up to \( n = 1 \) read

\[
W_0 = \phi(r_1, r_1') + \int dr^N f(r_1, r_2, \ldots, r_N; r_1') \quad (21a)
\]

\[
\omega_1 = -\frac{1}{W_0} \sum_m \int dr^N f(r_1, \ldots, r_N; r_1') \left[ 1 - \exp \left[ i \int s^0 ds' \theta_m(s') \right] \right] \quad (21b)
\]
while expression for higher order terms can be derived following the steps described in the literature. Notice that due to the logarithmic nature of the expansion, this relation holds only if $W_0$ has no zeros. In the current case, $W_0$ is related to the one–body density matrix of the component whose density–density correlation factor is being analyzed, and whereas $\rho_1^{(4)}(s)$ is everywhere positive and fulfills the required condition, $\rho_1^{(3)}(s)$ presents a complex nodal structure that makes the applicability of the expansion rely on the appropriate choice of $\phi(r_1, r'_1)$.

When expressions (21), (21a) and (21b) are used to compute the density–density correlation factor of the $^4$He component of the mixture, one arrives at the natural extension of the original Gersch–Rodriguez result. Setting $\phi(r_1, r'_1) = 0$, one gets

$$W_0 = \frac{1}{N^3 N^4} \int dr^N \rho_N(r_1, r_2, \ldots, r_N; r_1 + s) = \frac{1}{\rho_4} \rho_1^{(4)}(s) \quad (22)$$

while $\omega_1$ reads

$$\omega_1 = -\frac{1}{N^3 N^4} \rho_4 \sum_{\beta=3,4, j \neq 1} \int dr^N \rho_N(r_1, \ldots, r_N; r_1 + s) \left[ 1 - \exp \left( \frac{i}{v^{(4)}} \int_0^s ds' \Delta V^{(43)}(r_{1j}, s') \right) \right]$$

$$= -\frac{1}{\rho_4} \int dr \rho_2^{(4,4)}(r, 0; r + s) \left[ 1 - \exp \left( \frac{i}{v^{(4)}} \int_0^s ds' \Delta V^{(44)}(r, s') \right) \right]$$

$$- \frac{1}{\rho_4} \int dr \rho_2^{(4,3)}(r, 0; r + s) \left[ 1 - \exp \left( \frac{i}{v^{(4)}} \int_0^s ds' \Delta V^{(43)}(r, s') \right) \right] \quad (23)$$

in terms of the $(4, 4)$ and $(4, 3)$ components of the semi–diagonal two–body density matrix of the mixture

$$\rho_2^{(\alpha, \beta)}(r_1, r_2; r'_1) = N_\alpha (N_\beta - \delta_{\alpha\beta}) \frac{\int dr_3 \ldots dr_N \Psi^*_0(r_1, r_2, \ldots, r_N) \Psi^{(4)}(r'_1, r_2, \ldots, r_N)}{\int dr^N |\Psi^*_0(r_1, r_2, \ldots, r_N)|^2}. \quad (24)$$

At this level, therefore, $S^{(4)}(q, s)$ is predicted to be the algebraic product of the IA and the FSE broadening function

$$S_1^{(4)}(q, s) = S^{(4)}_{1A}(q, s) R^{(4)}(q, s), \quad (25)$$

where

$$S^{(4)}_{1A}(q, s) = e^{i\omega_1^{(4)}/v^{(4)}} \frac{1}{\rho_4} \rho_1^{(4)}(s) \quad (26)$$

and

$$R^{(4)}(q, s) = \exp \left[ -\frac{1}{\rho_1^{(4)}(s)} \int dr \rho_2^{(4,4)}(r, 0; r + s) \left[ 1 - \exp \left( \frac{i}{v^{(4)}} \int_0^s ds' \Delta V^{(44)}(r, s') \right) \right] \right]$$

$$- \frac{1}{\rho_4} \int dr \rho_2^{(4,3)}(r, 0; r + s) \left[ 1 - \exp \left( \frac{i}{v^{(4)}} \int_0^s ds' \Delta V^{(43)}(r, s') \right) \right] \quad (27)$$
These results are formally equal to the Gersch–Rodriguez ones used to compute the high $q$ response of pure $^4\text{He}$, the only difference being the presence of $\rho_2^{(4,3)}$ which is the contribution coming from the interaction of the $^4\text{He}$ atoms with the $^3\text{He}$ atoms in the mixture. As a matter of fact, in the zero $^3\text{He}$ concentration limit this last term cancels and expression (27) coincides exactly with the one reported in ref. 16, thus stressing that the former is the natural extension of the latter to the mixture where two different isotopes coexist.

Unfortunately, no cumulant expansion of the $^3\text{He}$ density–density correlation factor can be performed as described above. This is because the zero order cumulant, which is proportional to the $^3\text{He}$ one–body density matrix, has infinitely many nodes. This problem can be bypassed recalling that in the high momentum transfer limit the most relevant processes in the scattering are those taking place at short distances, where dynamical correlations dominate over statistical ones. This means that in the $q \to \infty$ limit, and disregarding the effects on the Bose–Einstein condensate, FSE in boson and fermion systems should look like similar, and that therefore the contribution of the fermion statistics to the FSE can be introduced as a small correction to the effect produced by the dynamical correlations, which are entirely taken into account by a purely bosonic FSE function. But on the other hand, the IA is known to substantially depend on the statistics obeyed by the system. The $s$ representation of the IA is proportional to the one–body density matrix, so it seems that this is the only quantity that really requires a proper treatment of the statistics. One can consider, therefore, a factorization of the $N$–body density matrix of the mixture in the following form

$$\rho_N(r_1, r_2, \ldots, r_N; r'_1) = \rho_1^{(3)}(r_{11'}) \left[ \frac{1}{\rho_{1}^{B}(r_{11'})} \rho_N^{B}(r_1, r_2, \ldots, r_N; r'_1) \right]$$

$$+ \left[ \rho_N(r_1, r_2, \ldots, r_N; r'_1) - \rho_1^{(3)}(r_{11'}) \frac{1}{\rho_{1}^{B}(r_{11'})} \rho_N^{B}(r_1, r_2, \ldots, r_N; r'_1) \right], \quad (28)$$

where $\rho_1^{B}$ and $\rho_N^{B}$ are the one– and the $N$–body density matrices of a fictitious mixture (henceforth referred to as the boson–boson mixture) in which the $^3\text{He}$ atoms are replaced by bosons of the same mass and at the same partial density. Notice that this replacement does not introduce any singularity in $\rho_N$ because $\rho_N^{B}(r)$ corresponds to a bosonic phase and thus has no nodes.

With this prescription, the $^3\text{He}$ response of the mixture becomes the sum of two terms

$$S_1^{(3)}(q, s) \equiv S_B^{(3)}(q, s) + \Delta S^{(3)}(q, s), \quad (29)$$

where

$$S_B^{(3)}(q, s) = e^{i\omega q^{(3)}} / \omega^{(3)} \frac{1}{\rho_3} \rho_1^{(3)}(s)$$

$$\times \left[ \frac{\rho_3}{N_3!N_4!} \int d^N r \frac{1}{\rho_1^{B}(s)} \rho_N^{B}(r_1, r_2, \ldots, r_N; r_1 + s) \exp \left( \frac{i}{\omega^{(3)}} \sum_{\beta=3,4} \sum_{j \neq 1} \int_0^s ds' \Delta V^{(33)}(r_{1j}, s') \right) \right]$$

and
\[ \Delta S^{(3)}(q, s) = e^{i\omega_q^{(3)}/\omega^{(3)}} \frac{1}{N_3!N_4!} \int \! dr^N \left[ \rho_N(r_1, r_2, \ldots, r_N; r_1 + s) \right. \]
\[ \left. - \frac{\rho_1^{(3)}(s)}{\rho^B(s)} \rho_N^B(r_1, r_2, \ldots, r_N; r_1 + s) \right] \exp \left( \frac{i}{\omega^{(3)}} \sum_{\beta=3,4} \sum_{\beta' \neq 1} \int_0^s ds' \Delta V^{(3\beta)}(r_{1j}, s') \right) . \]

In this approximation, Eq. (30) describes part of the response that can be written as the product of the IA, which enters through \( \rho_1^{(3)}(s) \), with a bosonic FSE function, that is given by the term in square brackets. It is important to notice, however, that the IA and density matrices of the mixture and their boson–boson approximation as the product of the IA, which enters through \( \rho \rho^B \), is given by the term in square brackets. Note, however, that the IA and density matrices of the mixture and their boson–boson approximation.

This last term is expected to introduce small corrections to \( \Delta S^{(3)}(q, s) \) that only appear when the response is computed beyond the IA level.

As before, Eqs. (30) and (32) are difficult to handle due to the presence of \( \rho_N \) and \( \rho_N^B \). Nevertheless, the FSE function in (30) can be worked out just as in the \( ^4 \)He case due to the bosonic nature of the functions entering on it. Hence one finds

\[ S_B^{(3)}(q, s) = S_{IA}^{(3)}(q, s) R^{(3)}(q, s) , \]

where

\[ S_{IA}^{(3)}(q, s) = e^{i\omega_q^{(3)}/\omega^{(3)}} \frac{1}{\rho_3} \rho_1^{(3)}(s) \]

and

\[ R^{(3)}(q, s) = \exp \left[ -\frac{1}{\rho_1^{(3)}(s)} \int \! dr \rho_2^{(3,3)B}(r, 0; r + s) \left[ 1 - \exp \left( \frac{i}{\omega^{(3)}} \int_0^s ds' \Delta V^{(33)}(r, s') \right) \right] \right] \]
\[ - \frac{1}{\rho_1^{(3)}(s)} \int \! dr \rho_2^{(3,4)B}(r, 0; r + s) \left[ 1 - \exp \left( \frac{i}{\omega^{(3)}} \int_0^s ds' \Delta V^{(34)}(r, s') \right) \right] . \]

The \( ^3 \)He additive term \( \Delta S^{(3)}(q, s) \) can not be handled in the same way because in this case the zero order cumulant vanishes

\[ W_0 = \frac{1}{N_3!N_4!} \int \! dr^N \left[ \rho_N(r_1, r_2, \ldots, r_1 + s) - \frac{\rho_1^{(3)}(s)}{\rho_1^{(3)}(s)} \rho_N^B(r_1, r_2, \ldots, r_1 + s) \right] = 0 \]

thus violating the condition imposed on \( W_0 \).

The problem of finding a useful prescription for \( \Delta S^{(3)}(q, s) \) can be solved inspecting the structure of the two–body density matrices that would enter in the lowest order terms of a cumulant expansion, as they carry the leading contributions to the FSE in the \( q \to \infty \) limit. When Eq. (28) is integrated over all particle coordinates but \( r_1 \) and \( r_2 \), an equivalent factorization of \( \rho_2^{(3,\alpha)} \) is found. The difference between the \( ^3 \)He semidiagonal two–body density matrices of the mixture and their boson–boson approximation.

\[ 8 \]
\[ \Delta \rho_2^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') = \rho_2^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') - \frac{\rho_1^{(3)}(\mathbf{r}_1')}{\rho_1^{(3)}(\mathbf{r}_1)} \rho_2^{(3,\alpha)B}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') \]  

(36)

can be analyzed in the framework of the HNC/FHNC equations starting from a variational model of the ground state wave function. Careful inspection of the diagrams entering in \( (36) \) reveals that \( \Delta \rho_2^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') \) may be factorized as follows:

\[ \Delta \rho_2^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') = \rho_0 \rho_1^{(3)}(\mathbf{r}_1') G^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') - \rho_0 \rho_{1D}(\mathbf{r}_1') F^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') , \]  

(37)

where \( \rho_{1D}(\mathbf{r}_1') \) is an auxiliary function that adds the contribution of all those diagrams linking points 1 and 1' that are not connected to point 2 and with no statistical lines starting or ending at points 1 and 1'. Function \( G^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') \) and \( F^{(3,\alpha)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1') \) are the sum of all other diagrams not contributing to \( \rho_1^{(3)}(s) \) that contain dynamical and statistical lines linking the external points. Indeed, it can be seen from its diagrammatic structure that \( \rho_{1D}(\mathbf{r}_1') \) shares many common features with the one–body density matrix of a purely bosonic liquid, as for instance it is always positive and its large \( r \) value approaches a constant that would be ascribed to some sort of condensate fraction value, although it has no physical meaning in this case. As a matter of fact, numerical calculations show that at low \( ^3\text{He} \) concentrations \( \rho_{1D}(\mathbf{r}_1') \) and \( \rho_1^{(3)}(\mathbf{r}_1') \) are nearly identical, and so that both \( \rho_{1D}(\mathbf{r}_1') \) and \( \rho_1^{(3)}(\mathbf{r}_1') \) satisfy the expansion condition and that either of them can be used as the basic function \( \phi(\mathbf{r}_1, \mathbf{r}_1') \) upon which the cumulant expansion is being built. Choosing \( \rho_{1D}(\mathbf{r}_1') \) as the starting function, \( \Delta S^{(3)}(q, s) \) in Eq. \((31)\) can be brought to a form suitable for expansion purposes by adding and subtracting the former to the latter

\[ \Delta S^{(3)}(q, s) = e^{i\omega_3^{(3)} / v_3^{(3)}} \frac{1}{\rho_3} \left[ \rho_{1D}(s) + \frac{\rho_3}{N_3!N_4!} \int d\mathbf{r}^N \left( \rho_N(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{r}_1 + \mathbf{s}) - \frac{\rho_1^{(3)}(s)}{\rho_{1D}(s)} \rho_N^{(3,\alpha)B}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{r}_1 + \mathbf{s}) \right) \right] \]  

\[ - e^{i\omega_3^{(3)} / v_3^{(3)}} \frac{1}{\rho_3} \left[ \rho_{1D}(s) \right] , \]  

(38)

as now the term inside the square brackets admits a cumulant expansion. Up to the first order this leads to

\[ \Delta S^{(3)}(q, s) = e^{i\omega_3^{(3)} / v_3^{(3)}} \frac{1}{\rho_{1D}(s)} \rho_1^{(3)}(s) \]  

(39)

\[ \times \left[ \exp \left[ - \frac{1}{\rho_{1D}(s)} \int d\mathbf{r} \Delta \rho_2^{(3,\alpha)}(\mathbf{r}, 0; \mathbf{r} + \mathbf{s}) \left[ 1 - \exp \left( \frac{i}{v_3^{(3)}} \int_0^s ds' \Delta V^{(33)}(\mathbf{r}, \mathbf{s}) \right) \right] \right] \]  

\[ - \frac{1}{\rho_{1D}(s)} \int d\mathbf{r} \Delta \rho_2^{(3,\alpha)}(\mathbf{r}, 0; \mathbf{r} + \mathbf{s}) \left[ 1 - \exp \left( \frac{i}{v_3^{(3)}} \int_0^s ds' \Delta V^{(33)}(\mathbf{r}, \mathbf{s}) \right) \right] - 1 \]  

The results in Eqs. \((29), (32), (33), (34)\) and \((35)\) constitute the prediction of the \( ^3\text{He} \) response of the mixture in the present formalism. As before, the FSE functions are built upon the interatomic potentials and the semidiagonal two–body density matrices, even though
the latter must now be computed for both the real mixture and its boson–boson approximation. As in the $^4$He case, these results resemble the original ones derived by Gersch and Rodriguez and form in fact their extension to the mixture when the problem of finding a useful prescription for the $^3$He response is addressed.

The $^4$He and $^3$He FSE functions can be evaluated once one has a suitable description of the required ground state two–body density matrices. These can be computed starting from a variational Jastrow wavefunction in the framework of the HNC/FHNC equations for the mixture, generalizing the formalism developed in Refs.\textsuperscript{17,19}. In the simplest scheme one disregards the contribution of the Abe diagrams and works in the Average Correlation Approximation (ACA), in which the $(4,4)$, $(4,3)$ and $(3,3)$ correlation factors are assumed to be equal. In this limit, differences between the isotopes are left to the effects derived from their different mass and statistics. Despite the simplifications, the wavefunction generated in this way still captures the essential features of the mixture at $T=0$.

In the particular case of the $^3$He–$^4$He mixture, the interaction does not distinguish between isotopes and so all three potentials $V^{(\alpha,\beta)}(r)$ have been taken to be equal to the HFDHE2 Aziz potential\textsuperscript{20}. The computed FSE functions of the $x_3 = 0.095$ $^3$He concentration mixture at equilibrium density $\rho = 0.3554 \sigma^{-3}$ are shown in figure (1). The $^4$He ($^3$He) FSE function has been Fourier transformed from $s$ to the $Y_4$ ($Y_3$) West scaling, where $Y_\alpha = m_\alpha \omega/q - q/2$. The solid and dashed lines on the left show $R^{(4)}(q, Y_4)$ compared to the Gersch–Rodriguez FSE function of pure $^4$He at saturation density ($\rho = 0.365 \sigma^{-3}$). The solid, dashed and dotted lines on the right depict $R^{(3)}(q, Y_3)$, $\Delta S^{(3)}(q, Y_3)$ and the $^3$He Compton profile $J^{(3)}(Y_3) = (q/m_3)S^{(3)}(q, Y_3)$ in the IA. As it can be seen and despite the different densities, $R^{(4)}(q, Y_4)$ is quite similar to the pure $^4$He FSE function, the main differences being present at the tails. On the other hand, $R^{(3)}(q, Y_3)$ is close to both functions, even though the peak is slightly higher. This effect is mostly due to the low partial density of the $^3$He component at the mixture $\rho_3 = x_3 \rho = 0.0338 \sigma^{-3}$, compared with the partial density of the $^4$He component $\rho_4 = (1-x_3)\rho = 0.3216 \sigma^{-3}$ and the equilibrium density of pure $^4$He. Moreover, the $^3$He additive term is rather small compared with the IA prediction, thus indicating that at high $q$ statistical corrections to the purely bosonic FSE in the $^3$He peak are present but play a much less significant role compared to the effect produced by $R^{(3)}(q, Y_3)$.

In summary, we have presented a new formulation of FSE for $^3$He–$^4$He mixtures, where the presence of a fermionic component forbids a straightforward application of most of the existing FSE theories used in the analysis of the high momentum transfer response of pure $^4$He. The formalism is inspired in the theoretical analysis carried out by Gersch and Rodriguez, and actually reduces to it in the zero $^3$He concentration limit. The resulting expressions are expected to accurately describe the effect of FSE in the response of the mixture. Furthermore, numerical calculations reveal that the $^4$He FSE function is similar to the pure $^4$He one. In this way, FSE corrections to the $^4$He peak in the mixture and in the pure phase are expected to be similar. Statistical effects do not appreciably modify a picture in which the FSE of the $^3$He component are computed in the boson–boson approximation.

ACKNOWLEDGMENTS

The author would like to thank Prof.A.S.Rinat for valuable comments on the $1/v^{(\alpha)}$ expansion of the response. Profs.A.Polls and J.Boronat are also acknowledged for helpful
discussions on the diagrammatic expansion of the two-body density matrix of the mixture.
FIGURES

FIG. 1. Left: $R^{(4)}(q, Y_4)$ compared to the pure $^4\text{He}$ FSE function of Gersch and Rodriguez (solid and dashed lines). Right: $R^{(3)}(q, Y_3)$ and $\Delta S^{(3)}(q, Y_3)$ compared to the IA prediction for the $^3\text{He}$ peak in the mixture (solid, dashed and dotted lines, respectively).
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