A microscopic approach to the response of $^3$He-$^4$He mixtures

A. Fabrocini and L. Vichi

Department of Physics, University of Pisa, INFN Sezione di Pisa, I-56100 Pisa, Italy

F. Mazzanti and A. Polls

Departament d’Estructura i Constituents de la Matèria, Universitat de Barcelona,
Diagonal 647, E-08028 Barcelona, Spain

Abstract

Correlated Basis Function perturbation theory is used to evaluate the zero temperature response $S(q, \omega)$ of $^3$He-$^4$He mixtures for inelastic neutron scattering, at momentum transfers $q$ ranging from 1.1 to 1.7 Å$^{-1}$. We adopt a Jastrow correlated ground state and a basis of correlated particle-hole and phonon states. We insert correlated one particle-one hole and one-phonon states to compute the second order response. The decay of the one-phonon states into two-phonon states is accounted for in boson-boson approximation. The full response is splitted into three partial components $S_{\alpha\beta}(q, \omega)$, each of them showing a particle-hole bump and a one phonon, delta shaped peak, which stays separated from the multiphonon background. The cross term $S_{34}(q, \omega)$ results to be of comparable importance to $S_{33}(q, \omega)$ in the particle-hole sector and to $S_{44}(q, \omega)$ in the phonon one. Once the one-phonon peak has been convoluted with the experimental broadening, the computed scattering function is in semiquantitative agreement with recent experimental measurements.

67.55.Lf, 67.60.-g
1. INTRODUCTION

Isotopic atomic Helium mixtures are an intriguing case for many-body physicists. There exists a large body of experimental data, concerning mostly static properties (for instance, the chemical potentials and the maximum solubility\textsuperscript{1–3}). Excitation spectra and related quantities, as the zero concentration ($x_3 = 0$) $^3$He effective mass ($m_3^*$), have been also measured\textsuperscript{4}. Recently, inelastic neutron scattering experiments have been carried out both at low, or intermediate, and high momentum transfers\textsuperscript{6,7}. In both regions the measured response presents two generally distinguishable structures, to be ascribed to boson like collective excitations (phonons and rotons) and to Fermi particle-hole ones. However, this apparently simple picture hides a large interplay between the components of the mixtures, each of them probably contributing on comparable foot to both the branches of the response. The reason for this lies in the large correlation effects, which are present in the system because of the strong interatomic potential and of the large density. This are also the motivations why truly microscopic and ab initio studies of Helium mixtures are difficult, and, in the case of the response, practically absent in literature.

Qualitative studies of the response have been done in ref.\textsuperscript{8} (using a matrix dispersion-relation representation) and in ref.\textsuperscript{9} with a correlated RPA approach (very similar, in spirit, to the phenomenological Polarization Potential method used in ref.\textsuperscript{10}). Here we will employ the Correlated Basis Function (CBF) perturbation theory, to embody the above correlation effects directly into the basis functions. CBF has shown to be a powerful tool to succesfully study Helium at zero temperature: the energetics of both pure $^4$He and $^3$He are well described by sophisticated correlated ground state wave functions, containing explicit two-, three-body, back-flow and spin correlations\textsuperscript{11–13}; properties of one $^3$He impurity in $^4$He, such as chemical potential and effective mass are also quantitatively reproduced by such correlated wave functions\textsuperscript{14}. In particular, by using CBF based perturbation theory, with the insertion of up to two correlated independent phonon intermediate states, the impurity effective mass $m_3^*$ turns out to be $2.2m_3$, to be compared with the experimentally measured $2.3m_3$ value.

The behavior of the $^3$He effective mass with the concentration in dilute mixtures has
been recently object of some debate. Specific heat measurements\cite{15,16} at finite \(x_3\) do not show appreciable deviations from its \(x_3 = 0\) value. In ref.\cite{6} the Authors have to postulate a much larger value \((m_3^* \sim 2.95m_3\) at \(x_3 = 0.05)\) in order to reproduce the position of the particle–hole response with a Lindhard like function and using a simple Landau–Pomeranchuk (LP) quasiparticle spectrum\cite{3},

\[
\epsilon_k(LP) = \epsilon_0 + \frac{\hbar^2 k^2}{2m_3^*}.
\]  

(1)

This contradiction does not appear if one modifies the LP spectrum (LP modified, or LPM) as:

\[
\epsilon_k(LPM) = \epsilon_0 + \frac{\hbar^2 k^2}{2m_3^*} \frac{1}{1 + \gamma k^2}.
\]  

(2)

There are both experimental\cite{6,4} and theoretical\cite{5} indications of a deviation from the simple LP form.

In a CBF based approach, we assume to have an homogeneous mixture of \(N_3\) \(^3\)He atoms and \(N_4\) \(^4\)He atoms in a volume \(\Omega\), with partial densities \(\rho_{\alpha=3,4} = N_\alpha/\Omega\), total density \(\rho = \rho_3 + \rho_4\) and concentrations \(x_\alpha = \rho_\alpha/\rho\). We will keep constant densities, while letting \(N_\alpha\) and the volume going to infinity. The nonrelativistic Hamiltonian of the mixture is

\[
H = - \sum_{\alpha=3,4} \sum_{i=1}^{N_\alpha} \frac{\hbar^2}{2m_\alpha} \nabla_i^2 + \frac{1}{2} \sum_{\alpha,\beta=3,4} \sum_{i \neq j}^{N_\alpha,N_\beta} V(r_{ij}),
\]  

(3)

where the interaction is the same for all the different pairs of the mixture.

A realistic, correlated, variational ground state wave function \(\Psi_0\) is obtained by the Jastrow–Feenberg ansatz\cite{28}

\[
\Psi_0 = F_J F_T F_{BF} \phi_0(N_3),
\]  

(4)

where \(\phi_0(N_3)\) is the ground state Fermi gas wave function for the \(^3\)He component and \(F_J, F_T\) and \(F_{BF}\) are N–body correlation operators including explicit two–, three–body and back–flow dynamical correlations respectively. We will limit our analysis to the case of two–body, state independent (or Jastrow) correlations only \((F_T = F_{BF} = 1)\). \(F_J\) results to be
\[ F_J(N_4, N_3) = \prod_{i_4 < j_3}^{N_3} f^{(3,3)}(r_{i_4j_3}) \prod_{i_4 < j_4}^{N_4} f^{(4,4)}(r_{i_4j_4}) \prod_{i_3}^{N_4} \prod_{i_4}^{N_4} f^{(3,4)}(r_{i_3j_4}). \] 

where \( f^{(\alpha,\beta)}(r) \) are two–body correlation functions determined by minimizing the variational ground state energy.

It is possible to generate a correlated basis through the operator (5), to be used in a CBF perturbation theory (CBFPT). This theory has been successfully adopted for computing the inclusive response of nuclear matter and heavy nuclei to electron and hadron scattering, and has shown to be able to provide a semiquantitative agreement with experimental neutron inelastic scattering (nIS) data in pure, liquid atomic \(^4\)He. In this paper, we will apply CBFPT to compute the nIS response of the mixture, by considering as intermediate states the normalized, correlated \(^4\)He n–phonon states (nPH) \(|k_1, ..., k_n\rangle\), and \(^3\)He n–particle, m–hole states (np–mh) \(|p_1, ..., p_n, h_1, ..., h_m\rangle\).

The nPH states are given by

\[ |k_1, ..., k_n\rangle = \frac{\rho_4(k_1) ... \rho_4(k_n)|\Psi_0\rangle}{\langle \Psi_0|\rho_4^\dagger(k_n) ... \rho_4^\dagger(k_1)\rho_4(k_1) ... \rho_4(k_n)|\Psi_0\rangle^{1/2}}, \] 

where \( \rho_4(k) \) is the \(^4\)He density fluctuation operator

\[ \rho_4(k) = \sum_{i=1}^{N_4} e^{i k \cdot r_i}. \]

Correlated np–mh states are obtained in a similar way, by applying the correlation operator to the Fermi gas excited states \( \Phi_{np-mh}(N_3) \),

\[ |p_1, ..., p_n, h_1, ..., h_m\rangle = \frac{F_J|\Phi_{np-mh}\rangle}{\langle \Phi_{np-mh}|F_J^\dagger F_J|\Phi_{np-mh}\rangle^{1/2}}. \]

We will consider 1–phonon (1PH) and 1p–1h intermediate correlated states, which we will term as One Intermediate Excitation (OIE) states. The response computed at the OIE level will be called variational. In addition, we will also consider the possible decay of 1PH states into 2PH ones, which is essential in giving a physically meaningful \(^4\)He excitation spectrum and provides a quenching of the one–phonon peak. This term will be computed in a boson–boson approximation, i.e. neglecting the \(^3\)He antisymmetry. Such an approach may be justified on the basis of the low \(^3\)He concentration.
1p–1h states may also be coupled to 1PH and 2PH. Such a coupling may be taken into account by a corresponding self-energy insertion. Its analogous in the problem of the single $^3$He atom in $^4$He is responsible for the impurity large effective mass. To estimate the importance of this effect we will use the on–shell part of the impurity self–energy, again relying on the small value of $x_3$.

The plan of the paper is as follows. In section II we will briefly outline the CBFPT for the response of the mixture and the variational calculation will be described in some details. Section III is devoted to the description of the calculation of the coupling with the 2PH states and of the decays into 1PH and 2PH states. Section IV contains results for the response and the comparison with the experimental scattering functions. Moreover, the $^4$He and $^3$He excitation spectra are presented and discussed. Conclusions are drawn in section V.

2. CBFPT FOR THE RESPONSE

The Dynamical Structure Function (DSF) $S(q, \omega)$ of a $^3$He–$^4$He mixture at $T = 0$ is given by the imaginary part of the polarization propagator $D(q, \omega)$

$$S(q, \omega) = \frac{1}{\pi} \Im D(q, \omega),$$

where

$$D(q, \omega) = \frac{1}{N} \langle \tilde{\Psi}_0 | \rho^\dagger(q) \frac{1}{H - E_0 - \omega - i\eta} \rho(q) | \tilde{\Psi}_0 \rangle,$$

and

$$\rho(q) = \rho_3(q) + \rho_4(q),$$

$$\rho_\alpha(q) = \sum_{i=1,N_\alpha} e^{iq \cdot r_i},$$

and $N = N_3 + N_4$. In eq. the $\tilde{\Psi}_0$ is the exact ground state of $H$ with eigenvalue $E_0$.

The total DSF may be expressed in terms of partial $\alpha\beta$ DSF, $S_{\alpha\beta}(q, \omega)$, as

$$S(q, \omega) = \sum_{\alpha,\beta = 3,4} x_{\alpha\beta} S_{\alpha\beta}(q, \omega),$$

(13)
with $x_{\alpha\beta} = (x_{\alpha}x_{\beta})^{1/2}$ and
\[
S_{\alpha\beta}(q, \omega) = \frac{1}{\pi} \Im D_{\alpha\beta}(q, \omega) = \frac{1}{\pi} \frac{1}{\sqrt{N_\alpha N_\beta}} \langle \bar{\Psi}_0 | \rho^I_\alpha(q) \frac{1}{H - E_0 - \omega - i\eta} \rho_\beta(q) | \bar{\Psi}_0 \rangle.
\] (14)

The experimentally measured nIS double differential cross section for the mixture directly provides access to the total scattering function $\hat{S}(q, \omega)$, which is in turn related to the partial DSFs by the relation
\[
\hat{S}(q, \omega) = x_4^4 \sigma_4^4 S_{44}(q, \omega) + x_3^4 \sigma_3^4 S_{34}(q, \omega) + x_3^3 [\sigma_3^3 S_{33}(q, \omega) + \sigma_i^3 S_{3i}(q, \omega)]
\] (15)
\[x_4^4 \sigma_4^4 + x_3^3 (\sigma_3^3 + \sigma_i^3).
\]

The elementary cross sections, as given by Sears in units of barns, are $\sigma_4 = 1.34, \sigma_3 = 4.42, \sigma_i^3 = 1.19$ and $\sigma_3 = 4.70$. The incoherent DSF $S_{33}(q, \omega)$ also appears in the expression above, with the corresponding cross section $\sigma_i^3$. Because of the absence of spin correlations, it describes $^3$He spin fluctuations via the operator
\[
\rho^I_3(q) = \sum_{i=1,N_3} e^{iq \cdot r_i} I_i,
\] (16)
where $I_i$ is the spin of $^3$He i–nucleus.

We will focus, in the remainder, mainly on the calculation of $S_{\alpha\beta}$. To derive a perturbative expansion it is convenient to split $H$ into an unperturbed piece $H_0$ and an interaction term $H_1$, as follows
\[
\langle m | H_0 | n \rangle = \delta_{nm} \langle m | H | m \rangle = E_m^v,
\] (17)
and
\[
\langle m | H_1 | n \rangle = (1 - \delta_{nm}) \langle m | H | n \rangle = \bar{H}_{mn}.
\] (18)

Here $|m\rangle$ are correlated basis states, eigenstates of $H_0$. In particular, $|0\rangle = |\Psi_0\rangle$ is not an eigenstate of $H$ and its difference from $|\bar{\Psi}_0\rangle$ is treated perturbatively. The expansion is obtained by writing
\[
H - E_0 = H_0 - E_0^v + (H_1 - \Delta E_0),
\] (19)
where $\Delta E_0$ is the correction to the variational ground state energy $E^v_0$, and by developing the propagator $(H - E_0 - \omega - i\eta)^{-1}$ in powers of $(H_1 - \Delta E_0)$. A similar expansion is performed for the ground state $|\tilde{\Psi}_0\rangle$.

If the expansion is truncated at the zeroth order, the partial DSF are given by:

$$S_{\alpha\beta}(q, \omega) = \frac{1}{\sqrt{N_\alpha N_\beta}} \sum_n \langle \Psi_0|\rho_\alpha^+(q)|n\rangle\langle n|\rho_\beta(q)|\Psi_0\rangle \delta(\omega - \omega_n),$$

with $\omega_n = E^v_n - E^v_0$.

As stated in the introduction, we will first consider only OIE insertions, i.e. correlated 1PH and 1p–1h intermediate states, defined as:

$$|k\rangle = \frac{\rho_4(k)|\Psi_0\rangle}{\langle \Psi_0|\rho_4(k)\rho_4(k)|\Psi_0\rangle^{1/2}},$$

$$|p, h\rangle = \frac{F_f|\Phi_{1p-1h}\rangle}{\langle \Phi_{1p-1h}|F_fF_f|\Phi_{1p-1h}\rangle^{1/2}}.$$ 

### 2.1 THE VARIATIONAL RESPONSES

The variational response is given by the sum of two components,

$$S_{\alpha\beta}(q, \omega) = S^{1PH}_{\alpha\beta}(q, \omega) + S^{1p-1h}_{\alpha\beta}(q, \omega),$$

where $S^{1PH}_{\alpha\beta}(q, \omega)$ has a 1PH intermediate state

$$S^{1PH}_{\alpha\beta}(q, \omega) = \frac{1}{\sqrt{N_\alpha N_\beta}} \sum_k \langle \Psi_0|\rho_\alpha^+(q)|k\rangle\langle k|\rho_\beta(q)|\Psi_0\rangle \delta(\omega - \omega_k),$$

and $S^{1p-1h}_{\alpha\beta}(q, \omega)$ has a 1p–1h intermediate state

$$S^{1p-1h}_{\alpha\beta}(q, \omega) = \frac{1}{\sqrt{N_\alpha N_\beta}} \sum_{p, h} \langle \Psi_0|\rho_\alpha^+(q)|p, h\rangle\langle p, h|\rho_\beta(q)|\Psi_0\rangle \delta(\omega - \varepsilon_p + \varepsilon_h).$$

$\omega_k$ and $\varepsilon_p - \varepsilon_h$ are the variational energies of the OIE states considered.

$\omega_k$ is given by

$$\omega_k = \frac{1}{N_4} \frac{\langle k|H - E^v_0|k\rangle}{\langle k|k\rangle} = \frac{\hbar^2 k^2}{2m_4 S_{44}(k)},$$
and corresponds to the well known Feynman spectrum. In eq. (26), \( S_{44}(k) \) is the variational estimate of the 44 component of the Static Structure Function (SSF), \( S_{\alpha\beta}(k) \), given by:

\[
S_{\alpha \beta}(k) = \frac{1}{\sqrt{N_\alpha N_\beta}} \frac{\langle \Psi_0 | \rho_\alpha^\dagger(k) \rho_\beta(k) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}.
\]  

(27)

In a similar way, \( \epsilon_{x=p,h} \) is obtained by

\[
\epsilon_x = \frac{\langle x | H - E_0^x | x \rangle}{\langle x | x \rangle},
\]  

(28)

where \( |x\rangle \) is a particle or hole correlated state. We will discuss later the evaluation of \( \epsilon_x \).

By using the definition of the SSF given in eq. (27), \( \xi_\alpha(q; k) = \langle \Psi_0 | \rho_\alpha^\dagger(q) | k \rangle \) is readily obtained as

\[
\xi_\alpha(q; k) = \sqrt{N_\alpha} \frac{S_{44}(k)}{S_{44}(k)} \delta_{k-q},
\]  

(29)

giving, for \( S_{\alpha \beta}^{1PH}(q, \omega) \),

\[
S_{\alpha \beta}^{1PH}(q, \omega) = \sum_k \frac{S_{44}(k)S_{44}(k)}{S_{44}(k)} \delta_{k-q} \delta(\omega - \omega_k).
\]  

(30)

The one–phonon contribution to the variational \( \alpha–\beta \) responses shows a delta–like behavior, whose strength is \( Z_{\alpha \beta}^{1PH}(k) = S_{\alpha 4}(k)S_{4 \beta}(k)/S_{44}(k) \), and it is located at the Feynman phonon energy. We notice that (i) \( Z_{44}^{1PH}(k) = S_{44}(k) \) and that (ii) the 33 and 44 variational DSF are positive (\( S_{44}(k) \) being positive), whereas this may not be true for the 34 DSF.

The expression for the particle–hole response \( S_{\alpha \beta}^{1p-1h}(q, \omega) \) is more involved. A detailed description for a pure Fermi system (specifically, nuclear matter) can be found in and references therein. On the basis of that formalism, the extension to a boson–fermion mixture is straightforward.

In CBF theory, the non diagonal matrix elements \( \xi_\alpha(q; p, h) = \langle \Psi_0 | \rho_\alpha^\dagger(q) | p, h \rangle \) are computed by a cluster expansion in Mayer like diagrams, and by summing infinite classes of relevant terms. The \( \xi_\alpha \) are explicitly given by:

\[
\xi_\alpha(q; p, h) = \delta_{q-p+h} \frac{1}{\sqrt{D(p)D(h)}} (\tilde{h}_{dd,\alpha 3}(q) + \delta_{\alpha 3}[1 + \tilde{h}_{ed,33}(q)]),
\]  

(31)
where
\[ \tilde{h}_{xy,\alpha \beta}(q) = \rho_{\alpha} \int d^3 r e^{i q \cdot r} [g_{xy,\alpha \beta}(r) - \delta_{xy,dd}], \quad (32) \]
with \((x, y) = (d, e)\) and \(g_{xy,\alpha \beta}(r)\) are partial radial distribution functions (RDF). In fact, the total \(\alpha \beta\)-RDF, \(g_{\alpha \beta}(r)\), giving the probability of finding a \(\alpha\)-type particle \(1\) at a distance \(r_{12}\) from a \(\beta\)-type particle \(2\),
\[ g_{\alpha \beta}(r_{12}) = \frac{N_{\alpha}(N_{\beta} - \delta_{\alpha \beta})}{\rho_{\alpha} \rho_{\beta}} \int d^3 r_3 \ldots d^3 r_{N} |\Psi_0|^2 \int d^3 r_1 \ldots d^3 r_N |\Psi_0|^2, \quad (33) \]
is computed, in Fermi Hypernetted Chain (FHNC)\textsuperscript{25}, using the correlated g.s. \(\Psi_0\) and it turns out to be written as:
\[ g_{\alpha \beta}(r_{12}) = g_{dd,\alpha \beta}(r_{12}) + \delta_{\beta 3} g_{de,\alpha 3}(r_{12}) + \delta_{\alpha 3} g_{ed,3\beta}(r_{12}) + \delta_{\alpha 3} \delta_{\beta 3} g_{ee,33}(r_{12}). \quad (34) \]
The partial RDF are classified, in FHNC theory, according to whether the external particle (1 or 2) is reached by a statistical correlation (i.e. if the particle is involved in an exchange loop, \(e\)-vertex), or by a dynamical correlation, \((f^{(\alpha, \beta)})^2 - 1\), only (\(d\)-vertex).

The definitions of the partial RDF, together with the full set of the related FHNC equations, may be found in\textsuperscript{25}.

Actually, eq.(29) sums all cluster diagrams factorizable in products of dressed, two-body diagrams. They do not contain only two-body cluster terms, but include, in turn, an infinite number of particles, as they are written in terms of the RDFs, rather than the bare two-body correlations.

Three-body, non factorizable diagrams are also present in the cluster expansion of \(\xi_{\alpha}\), even if they do not appear in eq.(29). However, they have been inserted, following ref.\textsuperscript{19}.

The function \(D(x = p, h)\) is
\[ D(x) = 1 - \rho_3 \int d^3 r e^{i x \cdot r} (g_{dd,33}(r) - 1) L(k_F r), \quad (35) \]
where \(L(k_F r)\) is the FHNC generalization of the exchange Slater function \(l(k_F r) = 3 j_1(k_F r)/(k_F r)^3\), and \(k_F\) is the \(^3\)He Fermi momentum \((k_F^3 = 3\pi^2 \rho_3)\).
Again, as $D(x)$ turns out to be positive, $S_{33,44}^{1p-1h}(q, \omega)$ are positive, whereas $S_{44}^{1p-1h}(q, \omega)$ may be not.

Finally, the spin fluctuation matrix element, $\xi_3^I(q; p, h) = \langle \Psi_0 | \rho^I_3(q) | p, h \rangle$, is simply given by:

$$\xi_3^I(q; p, h) = \delta_{q-p+h} \frac{1}{\sqrt{D(p)D(h)}}. \quad (36)$$

3. CORRELATED ONE AND TWO PHONON INTERMEDIATE STATES

In this section we will first study the effect on the phonon responses of the insertion of orthogonal, correlated 2PH states:

$$|k_1k_2\rangle_o = (1 - |k\rangle\langle k|) |k_1k_2\rangle,$$

(37)

where the 2PH states of eq.(36) have been orthogonalized to the 1PH ones by a Gram-Schmidt procedure.

2PH states influence the partial polarization propagators $D_{\alpha\beta}(q, \omega)$ via the direct coupling to the ground state and via the decay of 1PH states into 2PH. The coupling to the g.s goes through the matrix element of the $^3$He fluctuation operator,

$$\xi_3(q; k_1, k_2) = \langle \Psi_0 | \rho^I_3(q) | k_1, k_2 \rangle_o, \quad (38)$$

( notice that $\xi_4(q; k_1, k_2)$ vanishes because of the Schmidt orthogonalization of the 2PH states), whereas the decay is driven by the non diagonal matrix element of the hamiltonian

$$a(k; k_1, k_2) = \langle k | H_1 | k_1, k_2 \rangle_o. \quad (39)$$

These CBF matrix elements have been computed in a boson–boson approximation (treating the $^3$He as a mass–3 boson) and by adopting the Convolution Approximation (CA) for the three–body distribution functions.

Their explicit expressions are:

$$\xi_3(q; k_1, k_2) = \frac{S_{34}(k_1)S_{44}(k_2)}{\sqrt{S_{44}(k_1)S_{44}(k_2)}} \left( S_{33}(q) - \frac{S_{34}^2(q) - S_{44}^2(q)}{S_{44}(q)} \right), \quad (40)$$
and

\[ a(k; k_1, k_2) = \frac{\hbar^2}{\sqrt{N_4^2 m_4}} \left( \frac{k \cdot k_1 S_{44}(k_2) + k \cdot k_2 S_{44}(k_1) - k^2 S_{44}(k_1) S_{44}(k_2)}{\sqrt{S_{44}(k_1) S_{44}(k_2)}} \right) \]

\[ \left( k^2 S_{34}(k) S_{34}(k_1) S_{34}(k_2) \right) \frac{x_4}{\sqrt{S_{44}(k) S_{44}(k_1) S_{44}(k_2)}} \right). \]

It is convenient, at this point, to introduce the correlated self-energy

\[ \Sigma_1(k, \omega) = \frac{1}{2} \sum_{k_1, k_2} \frac{|a(k; k_1, k_2)|^2}{\omega_{k_1} + \omega_{k_2} - \omega - i\eta}, \]

and the function \( \chi(q; k, \omega) \) given by:

\[ \chi(q; k, \omega) = \frac{1}{2} \sum_{k_1, k_2} a(k; k_1, k_2) \frac{1}{\omega_{k_1} + \omega_{k_2} - \omega - i\eta} \xi_3^\dagger(q; k_1, k_2). \]

If we define the dressed phonon propagator \( G^d(k, \omega) \) as

\[ G^d(k, \omega) = \frac{1}{\omega - \Sigma_1(k, \omega) - \omega - i\eta}, \]

then, the phonon contributions to the polarization propagators can be rearranged as:

\[ D_{44}^{PH}(q, \omega) = \frac{1}{N_4} \sum_k |\langle \Psi_0 | \rho_3^d(q) | k \rangle|^2 G^d(k, \omega), \]

\[ D_{34}^{PH}(q, \omega) = \frac{1}{\sqrt{N_3 N_4}} \sum_k \langle \Psi_0 | \rho_3^d(q) | k \rangle G^d(k, \omega) \langle k | \rho_3(q) | \Psi_0 \rangle + \frac{1}{\sqrt{N_4}} \chi(q; k, \omega), \]

and

\[ D_{33}^{PH}(q, \omega) = \frac{1}{N_3} \sum_k \langle \Psi_0 | \rho_3^d(q) | k \rangle G^d(k, \omega) \langle k | \rho_3(q) | \Psi_0 \rangle + \frac{2}{\sqrt{N_3}} \chi(q; k, \omega). \]

The DSF are then obtained by taking the imaginary parts of \( D_{\alpha\beta} \). Terms quadratic in \( \xi_3(q; k_1, k_2) \) have not been considered.

The relevant changes introduced by the insertion of the 2PH states in the phonon responses are:

1. the strengths of the delta–like 1PH peaks \( Z_{\alpha\beta} \) are generally quenched respect to \( Z_{w\alpha\beta} \).
\[ Z_{44}(k) = Z^\nu_{44}(k) \left( 1 + \frac{\partial \Re \Sigma_1(k, \omega)}{\partial \omega} \right)^{-1}_{\omega=\omega_k}. \] (48)

Analogous corrections occur for \( Z_{34}(k) \) and \( Z_{33}(k) \), which are also affected by those parts of the polarization propagators containing \( \xi_3(q; k_1, k_2) \);

2. the 1PH peaks are shifted by the real part of the on–shell self energy, since the \( ^4\text{He} \) spectrum is modified as

\[ \omega_k \longrightarrow \omega_k^{\text{CBF}} = \omega_k + \Re \Sigma_1(k, \omega_k^{\text{CBF}}); \] (49)

3. a multiphonon tail appears at large \( \omega \)–values, beyond the position of the 1PH peak, at the momentum transfers here considered.

4. CBF RESPONSES

In the class of the Jastrow correlated wave functions, the best variational choice is provided by the solution of the Euler equations

\[ 0 = \frac{\delta \langle \Psi_0 | H | \Psi_0 \rangle}{\delta f^{(\alpha \beta)}}. \] (50)

The resulting equations have been derived, within the FHNC framework, and solved for the \( ^3\text{He} \) impurity problem, for the boson–boson mixture and, lately, for the real fermion–boson case.

Another, often used approach consists in parametrizing the correlation functions and in minimizing the ground state energy with respect to the parameters. This is the choice we have adopted here. Besides that, some of the results we will present have been obtained within the Average Correlation Approximation (ACA). In ACA, the correlation functions are the same for all the types of pairs \( f^{(3,3)} = f^{(3,4)} = f^{(4,4)} \) and the differences in the distribution functions (or in the static structure functions) are due only to the different isotope densities and statistics. We will also show that going beyond the ACA does not affect our results.
We have used three types of correlation functions: the time honored, short ranged McMillan form (SR) and two long ranged functions a (LR and LR1).

The McMillan correlation, in ACA, is given by:

\[ f_{SR}(r) = \exp\left[ -\left(\frac{b\sigma}{r}\right)^5 \right], \]

where \( b = 1.18 \) and \( \sigma = 2.556 \text{Å} \). The SR correlation function gives a good description of the short range behavior of the pair wave function but fails to reproduce long range properties. For instance, it does not ensure the linear behavior of the \(^4\text{He}\) SSF at \( k \to 0 \) (the phonon dispersion). Such a dispersion reflects in a long range behavior of the correlation of the type \( f(r \to \infty) - 1 \propto -r^{-2} \). To this aim, we have also used a modified form, having the correct long range structure (LR), given by

\[ f_{LR}(r) = f_{SR}(r) \left[ A + B\exp\left( -\frac{(r-D)^2}{\tau r^4} \right) \right]. \]

The parameters of \( f_{LR}(r) \), giving the variational minimum of the \(^4\text{He}\) energy at the equilibrium density \( \rho_0 = 0.02185 \text{Å}^{-3} \), are \( b = 1.18, A = 0.85, B = 1 - A, D = 3.8 \text{Å} \) and \( \tau = 0.043 \text{Å}^{-2} \) (see Ref.\(^{23}\) for more details about the energetics of the mixture). The \( B \) and \( \tau \) parameters are related to the experimental pure \(^4\text{He}\) sound velocity \( c \) and to the low–\( k \) behavior of its SSF by the relations:

\[ \frac{B}{\tau} = \frac{m_4 c}{2\pi^2 \hbar \rho_0}; \quad S^{(4,4)}(k \to 0) = \frac{\hbar k}{2m_4 c}. \]

In order to check the accuracy of ACA, we have also used a LR correlation (LR1), formally identical to \( f_{LR} \), but with parameters depending on the type of the correlated pair. The 44 correlation function is the same as above, whereas the parameters of the 43 and 33 ones have been obtained by minimizing the energy of the pure \(^4\text{He}\) with one and two \(^3\text{He}\) impurities, respectively\(^{23}\).

Key ingredients in the CBF theory of the response in Helium mixtures are the radial distribution functions \( g_{\alpha\beta}(r) \) and the static structure functions \( S_{\alpha\beta}(k) \). Figs.(1) and (2) show these quantities in a 4.7% mixture, at a total density \( \rho = 0.02160 \text{Å}^{-3} \), for the \( f_{LR1}(r) \)
correlation, in FHNC/0 approximation (i.e. we have neglected the elementary diagrams\(^2\)). The results for the SSF, with the \(f_{SR}(r)\), differ mainly in the region of low–\(k\) values, in agreement with the previous discussion.

Table (1) shows the variational strenghts \(Z_{\alpha\beta}^v(k)\) of the one–phonon response for the same mixture and compares the results obtained with the SR and LR correlation functions at four momentum values, from \(q = 1.1\) to \(1.7\,\text{Å}^{-1}\). The positions of the variational delta peaks, \(\omega_k\), are also given. It has to be noticed that the Feynman spectrum overestimates the experimental data by at least \(10K\) both in the maxon and roton regions.

Table (2) provides the same quantities after the insertion of the 2PH states. Fig.(3) shows the \(^4\text{He}\) spectrum with the LR1 correlation. The figure also compares the spectrum with pure \(^4\text{He}\) at \(\rho_0\) and with the experimental results of ref.\(^6\) (circles) in a \(x_3 = 1.1\%\) mixture at SVP and of ref.\(^4\) (squares) for a \(x_3 = 6.0\%\) mixture.

The changes in going from pure \(^4\text{He}\) to the mixture are clearly visible. This is mainly a density effect. In fact, we obtain similar results if the LR–ACA correlation is used. CBF perturbative corrections appear to be large and bring the maxon energy close to the experiments. The roton is not well described, as it is too shallow respect to the data. This feature is also present in the \(^4\text{He}\) case. As for the \(^3\text{He}\) spectrum, we believe that most of the discrepancy in this part of the spectrum has to be ascribed to the use of CA in the calculation of the CBF matrix elements. Moreover, contributions from higher order CBF pertubative diagrams are known to be important to correctly reproduce the roton minimum in pure \(^4\text{He}\). However, the CA results show a change in the sign of the shift from mixture to pure system at \(q \simeq 1.8\,\text{Å}^{-1}\), in good agreement with the measured experimental value\(^6\) at constant pressure \((q \simeq 1.9\,\text{Å}^{-1})\). The boundaries of the \(1p–1h\) DSFs are related to the energies of the \(1p–1h\) state \(\epsilon_p – \epsilon_h\). \(\epsilon_{p(h)}\) has been computed by the procedure of ref.\(^6\). However, because of the low \(^3\text{He}\) density, it turns out to be extremely close to the free Fermi gas spectrum

\[
\epsilon_k^{FG} = \frac{\hbar^2 k^2}{2m_3},
\]

(54)
so, $\epsilon_k^{FG}$ has been used in all the calculations. Perturbative corrections to $\epsilon_k$ may be computed in CBF. In the case of the $^3$He impurity, CBFPT provides an accurate evaluation of its spectrum if the decay of the impurity excited state (given by a correlated plane wave) into correlated 1PH and 2PH states is considered. 1PH states account for $\sim 2/3$ of the difference between the experimental effective mass and the bare one, whereas 2PH states give the remainder. Because of the low density of the $^3$He component, it is reasonable to expect a similar behavior in the finite concentration mixture. It implies that we should insert in the CBFPT expansion the coupling between $1p - 1h$ states and 1PH and 2PH ones.

Work along this line is in progress. Here we have used for $\epsilon_k^{CBF}$ the CBFPT spectrum of the single impurity, obtained by extending to finite momenta the approach of ref.[14] for the effective mass. The involved matrix elements have been computed in CA for the three–body distribution functions. CA gives $m_3^*(CA) \sim 1.8 m_3$ for the impurity, whereas the more realistic Superposition Approximation (SA) gives $m_3^*(SA) \sim 2.2 m_3$. However, the SA $k \neq 0$ matrix elements are much more involved than their CA counterparts, and their evaluation, together with a description of the method, will be presented subsequently.[13]. Here, the effect of the missing effective mass has been estimated by simply scaling the CA spectrum as $\epsilon_k^{CBF} = [m_3^*(CA)/m_3^*(expt)]\epsilon_k^{CBF}(CA)$.

Fig.(4) shows the $^3$He spectra in different approximations, and compares them with the experimental data (circles from ref.[6] and squares from ref.[4]) and with the LP and LPM parametrizations given in the introduction, with parameters $m_3^* = 2.3 m_3$ and $\gamma = 0.132 \text{Å}^2$. Even from the CA calculation, a deviation from the LP behavior clearly appears. The estimated CBF value of $\gamma$ in CA turns out to be $\gamma(CA) = 0.052 \text{Å}^2$. We stress once more that we expect SA to provide a better description of the $^3$He spectrum behavior, as it correctly takes into account the core property of the system, requiring that the three–particle distribution functions vanish when any interparticle distance is lower than the radius of the repulsive core of the potential.

Fig.(5) gives the $1p - 1h$ DSF $S_{1p-1h}^{1p-1h}(q, \omega)$ at two momentum values ($q = 1.3$ and $1.7 \text{Å}^{-1}$), with the LR1 correlation and using the CBF $^3$He spectrum. The two 33 DSF are very close.
and dominant, becoming indistinguishable at higher momenta; the 44 component is always very small (notice that it has been amplified by a factor of 10 in the figure); the 34 part is negative and an order of magnitude larger than $S_{44}^{1p-1h}$ in absolute value, contributing to decrease the total response mainly at low momenta. The free Fermi Gas DSF would be located to a larger energy with a lower peak strength, compatible with the fact that the correlated system has a $^3$He effective mass 2.3 times larger than the bare mass (at $q = 1.3 \AA^{-1}$ the FG peak position is $\omega = 13.6K$ and the strength is $S_{33}^{1p-1h}(FG) = .115K^{-1}$). In addition, as for the phonon DSF, the use of the SR and LR correlations does not alter appreciably the results shown in the figure.

Table (3) shows the CBF values of the $m_{n,\alpha\beta}(q)$ sum rules of the DSF’s, for $n = 0, 1$, defined as:

$$m_{n,\alpha\beta}(q) = \int d\omega \ \omega^n \ S_{\alpha\beta}(q, \omega). \quad (55)$$

The exact DSF’s satisfy the $f-$sum rules

$$m_{1,\alpha\beta}(q) = \frac{\hbar^2 q^2}{2m_\alpha} \delta_{\alpha\beta}, \quad (56)$$

and for $n = 0$ one has $m_{0,\alpha\beta}(q) = S_{\alpha\beta}(q)$.

The table gives also the variational values of the SSF’s of eq.[27] and the $f-$sum rules. $m_0$ and the SSF’s, as well as $m_1$ and the $f-$sum rules are in good agreement for all $q$’s in the 44 case. For 33, $m_0$ is reasonably close to the variational SSF, whereas the $f-$sum rule is underestimated (we recall that the SSF’s have been computed with the variational ground states, not the exact one). The 34 $m_n$ are not satisfying, especially for $m_1$. In order to trace down the source of the differences we also show the contributions to the sums from the large–energy multiphonon tails of the DSF’s, $m_{1,0}(mPH)$. The tail provides a large part of the sum rules and, for $\alpha\beta = 34$, it is dominant. The effect is more clearly visible in $m_1$, where the tails of the DSF’s are multiplied by a large energy factor. As a consequence, a quantitatively correct estimate of $m_{1,\alpha\beta}$ would probably require a more accurate evaluation of the multiphonon contributions as well as the insertion of higher order perturbative diagrams.
To evaluate the total scattering function $\hat{S}(q, \omega)$, the DSF must be multiplied by the elementary cross sections and the concentrations of the species. In fig.s(6a,b) we give the partial CBF scattering functions (PSF):

\[
\hat{S}_{44}(q, \omega) = \frac{x_4 \sigma_4}{x_4 + x_3 (\sigma_3^c + \sigma_3^i)} S_{44}(q, \omega),
\]

\[
\hat{S}_{34}(q, \omega) = \frac{x_{34} \sigma_{34}}{x_4 + x_3 (\sigma_3^c + \sigma_3^i)} S_{34}(q, \omega)
\]

and

\[
\hat{S}_{33}(q, \omega) = \frac{x_3}{x_4 + x_3 (\sigma_3^c + \sigma_3^i)} [\sigma_3 S_{33}(q, \omega) + \sigma_3^i S_{33}^i(q, \omega)].
\]

The LR1 correlation has been used. The position and the strength of the phonon contribution to the PSF’s are explicitly given. In the $1p-1h$ sector, at the lower momentum, the $33$ PSF is strongly reduced by the $34$ PSF, which practically disappears at $q = 1.7\AA^{-1}$. The $44$ PSF is always negligible in this sector. In the phonon sector, the $44$ PSF is the dominant one. The $33$ component always results to be very small. The $34$ PSF at $q = 1.3\AA^{-1}$ slightly reduces the scattering function, while at $q = 1.7\AA^{-1}$ increases it.

In order to compare with the experimental scattering function, the theoretical PSF’s have to be convoluted with the experimental broadening functions. As at these momentum transfers the phonon peak is still delta shaped, because there is no overlap with the multiphonon background, we assume, in accordance with the authors of ref.6, that the width in energy of the low temperature results in that reference is entirely due to the instrumental resolution. For this reason we have convoluted the phonon peak with a gaussian having an average half maximum width of $1.3K$. A gaussian with a width of $1.2K$ has been used for the $1p-1h$ response.

The convoluted total scattering functions are compared with the experimental results of ref.6 in fig.s(7a,b,c) at $q = 1.1, 1.5$ and $1.7\AA^{-1}$, respectively, for the $4.7\%$ mixture we have considered so far.

At $q = 1.1\AA^{-1}$, both the position and the strength of the phonon branch are well described by our calculation. When approaching the roton minimum region, the agreement
worsens and we overestimate the experimental data. As discussed previously, we expect that the use of SA will improve the CBF description.

An analogous analysis can be performed for the $1p-1h$ sector. The use of the CBF–CA spectrum slightly misses the location of the bump, well described in turn by a LPM parametrization, which is essentially a fit to the experimental data. We recall that the relevant difference between the LPM and the CBF–CA energies lies in the $\gamma$-parameter value, smaller by a factor $\sim 0.4$ in the latter case. A simple, quadratic LP parametrization with $m_3^* = 2.3m_3$ seems to be ruled out.

The $^3$He scattering function $\hat{S}_3(q, \omega)$, defined as

$$\hat{S}_3(q, \omega) = \frac{x_3\sigma_4 + x_3(\sigma_3^c + \sigma_3^s)}{x_3(\sigma_3^c + \sigma_3^s)} \hat{S}(q, \omega),$$

and the function $\tilde{S}_3(q, \omega)$, given by

$$\tilde{S}_3(q, \omega) = \frac{\sigma_3 S_{33}(q, \omega) + \sigma_3^c S_{33}^{c}(q, \omega)}{\sigma_3^c + \sigma_3^s},$$

in the $1p-1h$ sector, are given in fig.(8). The figures contains also the convolution of $\hat{S}_3(q, \omega)$ with the experimental broadening function and the experimental results of ref.\[6\], at $q = 1.3\,\text{Å}^{-1}$. $\hat{S}_3$ and $\tilde{S}_3$ are identical if $S_{34}^{1p-1h} = S_{44}^{1p-1h} = 0$. So, their differences are basically a measure of the importance of the 34 contribution (the 44 one being negligible). Our results show a large suppression of $S_{33}^{1p-1h}$ due to $S_{34}^{1p-1h}$, which brings the CBF response much closer to the experiments.

5. CONCLUSIONS

Correlated Basis Perturbation Theory has been used to microscopically compute the scattering function in a $x_3 = 4.7\%$ $^3$He–$^4$He mixture at $T=0$. The theory has allowed for explicitely separating the different contributions to the response and for semiquantitatively assessing the relevance of the 34 component. In the $1p-1h$ region, the $S_{33}$ response is sizeably reduced by $S_{34}$ up to $q \simeq 1.5\,\text{Å}^{-1}$, whereas $S_{44}$ is always negligible. A similar effect, even if smaller in magnitude, is present in the phonon–roton sector, where the dominant $S_{44}$ is only slightly modified by $S_{34}$. 
The responses have been computed by inserting correlated \(1p-1h\) and \(1-\) and \(2-\)phonon intermediate states. Also the possible decay of \(1-\)phonon into \(2-\)phonon states has been estimated in boson–boson approximation and using the Convolution Approximation for the three–body distribution functions.

The microscopic quasiparticle \(^3\)He spectrum clearly shows a deviation from the simple LP form. The spectrum has been actually computed for the single impurity problem, but we do not believe that its evaluation in the low concentration mixture will dramatically change our findings. In particular, a deviation from LP was advocated in ref.\(^6\) to explain the experimental \(1p-1h\) response, in contrast with a possible large change of the \(^3\)He effective mass in mixture (from \(m_3^* = 2.3m_3\) at \(x_3 = 0\) to \(m_3^* = 2.9m_3\) at \(x_3 = 4.7\%\)). The CBF spectrum still does not reproduce fully quantitatively the data, and a more accurate calculation is needed.

The \(^4\)He excitation spectra in the phonon–roton branch of the pure system and the mixture at SVP have been compared. The shift between the two excitations appears to be due to the change in density. CBF gives a good description of the maxon region, but overestimates the roton, even if it gives an almost correct \(q\)-value for the change of sign of the shift.

The CBF scattering function at low momenta gives a reasonable description of the scattering data (both for the position and strength). The agreement worsens as \(q\) increases. The peaks are located at too a large energy and their strength is overestimated. We believe that the reason of this lies in the approximations made to compute the decay of \(1PH\) states into \(2PH\) and in the lack of higher intermediate states, which become more and more important as the momentum increases. In particular, the \(1p-1h\) sector does not include two probably relevant contributions: the decays of \(1p-1h\) states into (1) \(2p-2h\) and (2) \(1PH\) states. The former adds large energy tails to the \(1p-1h\) bump reducing its strength, and the latter is known to be responsible for a large part of the \(^3\)He effective mass. Our CBF calculation includes the real part of the \(1p-1h\) into \(1PH\) decay but does not consider its imaginary part.
The importance of the 34 contribution to the total scattering function is especially visible in the $^3\text{He}$ scattering function in the $1p - 1h$ region, where its introduction reduces the response by a factor $\sim 0.6$ at $q = 1.3\text{Å}^{-1}$.

More work is clearly needed in order to give a fully quantitative description of both the excitations and the responses of the Helium mixtures. However, from our results, we believe that CBF is a promising theory in view of achieving this goal.

**ACKNOWLEDGEMENTS**

The authors are grateful to Bjon Fåk for several fruitful exchanges. This research was supported in part by DGICYT (Spain) Grant Nos. PB92-0761, PB90-06131, PB90-0873 and the agreement DGICYT (Spain)--INFN (Italy).
REFERENCES

1 C.Ebner and D.O.Edwards, Phys.Rep. C 2, 77 (1970).

2 G.Baym and C.Phetick in The Properties of Liquid and Solid Helium, Vol.2, ed.K.H.Benneman and J.B.Ketterson (Wiley, NY 1978).

3 R.De Bruyn Ouboter and C.N.Yang, Physica B 144, 127 (1987).

4 P.A.Hilton, R.Scherm and W.G.Stirling, J.Low.Temp.Phys. 27, 851 (1978).

5 R.N.Bhatt, Phys.Rev. B 18, 2108 (1978).

6 B.Fäk, K.Guckelsberger, M.Korfer, R.Scherm and A.J.Dianoux, Phys.Rev. B 41, 8732 (1990).

7 Y.Wang and P.E.Sokol, Phys.Rev.Lett. 72, 1040 (1994).

8 A.Szprynger and M.Lucke, Phys.Rev. B 32, 4442 (1985).

9 E.Krotscheck and M.Saarela, Phys.Rep. 232, 1 (1993).

10 W.Hsu, D.Pines and C.H.Aldrich, Phys.Rev. B 32, 7179 (1985).

11 Q.N.Usmani, S. Fantoni and V.R. Pandharipande, Phys.Rev. B 26, 6123 (1982).

12 E. Manousakis, S. Fantoni, V.R. Pandharipande, and Q.N. Usmani, Phys.Rev. B 28, 3770 (1983).

13 M. Viviani, E. Buendía, S. Fantoni, and S. Rosati, Phys.Rev. B 38, 4523 (1988).

14 A. Fabrocini, S. Fantoni, S. Rosati, and A. Polls, Phys.Rev. B 33, 6057 (1986).

15 D.S.Greywall, Phys.Rev. B 20, 2643 (1979).

16 J.R.Owers-Bradley, P.C.Main. R.M.Browley, G.J.Batey and R.J.Church, J.Low Temp.Phys. 72, 201 (1988).

17 L.D.Landau and I.M.Khalatnikov, Zh.Eksp.Teor.Fiz. 19, 637 (1948).
18 E. Feenberg, *Theory of Quantum Fluids* (Academic Press, NY 1969).

19 A. Fabrocini and S. Fantoni, Nucl. Phys. A503, 375 (1989).

20 A. Fabrocini, Phys. Lett. B322, 171 (1994).

21 O. Benhar, A. Fabrocini, S. Fantoni and I. Sick, Nucl. Phys. A579, 493 (1994).

22 E. Manousakis and V.R. Pandharipande, Phys. Rev. B33, 150 (1986).

23 V. F. Sears in *Neutron Scattering*, Vol. 23A of *Methods of Experimental Physics*, ed. K. Skold and D. L. Price (Academic, NY 1986).

24 R. P. Feynman, Phys. Rev. 94, 262 (1954).

25 J. Boronat, A. Polls and A. Fabrocini, J. Low Temp. Phys. 91, 275 (1993).

26 J. C. Owen, Phys. Rev. B23, 5815 (1981).

27 A. Fabrocini and A. Polls, Phys. Rev. B30, 1200 (1984).

28 T. Chakraborty, A. Kallio, L. J. Lannto and P. Pietilainen, Phys. Rev. B27, 3061 (1983).

29 D. K. Lee and F. J. Lee, Phys. Rev. B11, 4318 (1975).

30 B. Friedman and V. R. Pandharipande, Phys. Lett. B100, 205 (1981).

31 A. Fabrocini, L. Vichi, F. Mazzanti and A. Polls, in preparation.

32 B. Fåk, private communication.
FIGURES

FIG. 1. Radial distribution functions for the mixture (see text). The solid line gives $g_{44}$, the
dashed line $g_{34}$ and the dotted one is $g_{33}$.

FIG. 2. Static structure functions for the mixture (see text). The solid line gives $S_{44}$, the
dashed line $S_{34}$ and the dotted one is $S_{33}$.

FIG. 3. $^4$He excitation spectrum in the mixture (crosses) and in the pure system (dashed line). The upper curves are the Feynam spectra. Squares and circles are mixture experimental data (See text).

FIG. 4. $^3$He excitation spectrum. The dashed line gives $\epsilon^C_{k}(CA)$, the solid line is $\epsilon^C_{k}$; also shown are the LP, LPM and free (F) spectra. Squares and circles are the experimental data (See text).

FIG. 5. $1p-1h$ DSF at $q = 1.3$ and $1.7\text{Å}^{-1}$. The continuous line gives $S_{33}$, the dot-dashed $S_{33}^i$, the dotted $10 \times S_{44}$ and the dashed $S_{34}$.

FIG. 6. CBF Partial scattering functions at $q = 1.3$ (6a) and $1.7\text{Å}^{-1}$ (6b). Continuous line $\hat{S}_{33}$, dashed line $\hat{S}_{34}^i$, dotted $\hat{S}_{44}$. The PH-$\alpha\beta$ numbers are the strengths of the phonon PSF, located at $\omega_q$.

FIG. 7. Total scattering functions at $q = 1.1$ (7a), $q = 1.5$ (7b) and $1.7\text{Å}^{-1}$ (7c) (solid lines). Also shown are the $1p-1h$ responses with the LP (dotted lines) and LPM (dashed lines) spectra and the experimental data (crosses).

FIG. 8. $1p-1h$ $^3$He scattering function at $q = 1.3\text{Å}^{-1}$. The solid line is $\hat{S}_3(q, \omega)$, the dashed line is $\hat{S}_3(q, \omega)$, the dotted line is the experimental convolution of $\hat{S}_3(q, \omega)$ and crosses are the experimental data.
TABLES

TABLE I. Variational strengths and positions of the one phonon DSF responses with different correlations (see text). \( q \) in Å\(^{-1} \) and \( \omega_q \) in \( K \)

|     | \( q \) | \( \omega_q \) | \( Z_{44}^v \) | \( Z_{34}^v \) | \( Z_{33}^v \) |
|-----|--------|----------------|----------------|----------------|----------------|
| \( SR \) | 1.1    | 20.44          | 0.356          | -0.146         | 0.060          |
| \( LR \) | 20.77  | 0.361          | -0.145         | 0.058          |
| \( LR1 \) | 20.75  | 0.362          | -0.147         | 0.060          |
| \( SR \) | 1.3    | 20.74          | 0.491          | -0.115         | 0.027          |
| \( LR \) | 21.68  | 0.461          | -0.122         | 0.032          |
| \( LR1 \) | 21.71  | 0.460          | -0.122         | 0.032          |
| \( SR \) | 1.5    | 19.91          | 0.681          | -0.072         | 0.008          |
| \( LR \) | 19.99  | 0.686          | -0.071         | 0.007          |
| \( LR1 \) | 20.02  | 0.685          | -0.069         | 0.007          |
| \( SR \) | 1.7    | 19.20          | 0.908          | -0.021         | 0.000          |
| \( LR \) | 19.24  | 0.899          | -0.023         | 0.001          |
| \( LR1 \) | 19.26  | 0.899          | -0.019         | 0.000          |
TABLE II. CBF strengths and positions of the one phonon DSF responses with different correlations (see text). $q$ in $\text{Å}^{-1}$ and $\omega_q$ in $K$.

|    | $q$ | $\omega_q$ | $Z_{44}$ | $Z_{34}$ | $Z_{33}$ |
|----|-----|-------------|----------|----------|----------|
| $SR$ | 1.1 | 13.73       | 0.275    | -0.066   | 0.016    |
| $LR$  | 13.69 | 0.272     | -0.068   | 0.017    |
| $LR1$ | 13.66 | 0.272     | -0.068   | 0.017    |
| $SR$ | 1.3 | 14.01       | 0.390    | -0.045   | 0.005    |
| $LR$  | 14.27 | 0.367     | -0.047   | 0.006    |
| $LR1$ | 14.25 | 0.366     | -0.044   | 0.005    |
| $SR$ | 1.5 | 13.84       | 0.559    | -0.014   | 0.000    |
| $LR$  | 13.79 | 0.558     | -0.014   | 0.000    |
| $LR1$ | 13.83 | 0.557     | -0.011   | 0.000    |
| $SR$ | 1.7 | 13.94       | 0.766    | 0.024    | 0.001    |
| $LR$  | 13.94 | 0.766     | 0.024    | 0.001    |
| $LR1$ | 13.96 | 0.765     | 0.027    | 0.001    |
TABLE III. CBF sum rules $m_0$ and $m_1$ with the LR1 correlation and CBF $^3$He spectrum, variational SSF's and $f$-sum rules. $q$ in Å$^{-1}$ and energies in $K$. In parentheses are shown the multiphonon tail contributions.

| $\alpha\beta$ | $q$  | $m_0(mPH)$   | $m_1(mPH)$   | $S_{\alpha\beta}$ | $f$–SR |
|--------------|------|--------------|--------------|-------------------|--------|
| 1.1          |      |              |              |                   |        |
| 44           | 0.37(0.08) | 7.38(3.58)  | 0.36        | 7.29              |        |
| 34           | -0.29(-0.08) | -4.80(-3.28) | -0.15       | 0.0               |        |
| 33           | 1.10(0.13)   | 8.88(4.67)  | 0.98        | 9.73              |        |
| 1.3          |      |              |              |                   |        |
| 44           | 0.49(0.10)   | 10.27(4.97) | 0.46        | 10.19             |        |
| 34           | -0.24(-0.08) | -4.53(-3.22) | -0.12       | 0.0               |        |
| 33           | 1.05(0.09)   | 8.97(3.47)  | 0.98        | 13.59             |        |
| 1.5          |      |              |              |                   |        |
| 44           | 0.68(0.12)   | 13.59(5.86) | 0.68        | 13.56             |        |
| 34           | -0.14(-0.06) | -3.18(-2.53) | -0.07       | 0.0               |        |
| 33           | 1.00(0.05)   | 9.15(2.14)  | 0.99        | 18.09             |        |
| 1.7          |      |              |              |                   |        |
| 44           | 0.91(0.14)   | 17.40(6.72) | 0.90        | 17.42             |        |
| 34           | -0.04(-0.04) | -1.66(-1.86) | -0.02       | 0.0               |        |
| 33           | 0.96(0.03)   | 9.93(1.25)  | 1.00        | 23.24             |        |