A MICROSCOPIC LOOK AT LIQUID HELIUM: THE $^3$HE IMPURITY CASE

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The description of the properties of liquid Helium is a challenge for any microscopic
many–body theory. In this context, we study the ground state and the excitation
spectrum of one $^3$He impurity in liquid $^4$He at $T = 0$ with the aim of illustrating
the power of the correlated basis function formalism in describing heavily corre-
lated systems. The strong interatomic interaction and the large density require
the theory to be pushed to a high degree of sophistication. A many–body corre-
lation operator containing explicit two– and three–particle correlation functions
is needed to obtain a realistic ground state wave function, whereas a perturbative
expansion including up to two phonon correlated states must be enforced to study
the impurity excitation energies. The theory describes accurately the experimen-
tal spectrum along all the available momentum range. As empirically shown by
the experiments, a marked deviation from the quadratic Landau-Pomeranchuck
behavior is found and the momentum dependent effective mass of the impurity
increases of $\sim 50\%$ at $q \sim 1.7\, \text{Å}^{-1}$ with respect to its $q = 0$ value. Although
the main emphasis is given to the Correlated Basis Function theory, we present
also comparisons with other methods, as diffusion Monte Carlo, variational Monte
Carlo with shadow wave functions and time dependent correlations.

1 Introduction

Atomic Helium fluids are an endless source of physical motivations for both theo-
rists and experimentalists. We have so far accumulated a huge amount of experi-
mental information and the activity is continuously pushed further to explore new
situations. An example is the physical realization of almost two–$^1$ (films) and
one–dimensional$^2$ (nanotubes) systems and the consequent possibility to study the
dependence on dimensionality of correlation effects. Helium clusters are another
extremely promising field and the present experimental capabilities make possible
to investigate the minimum number of atoms needed to have superfluidity$^3$. For
theoricians, Helium liquids can be considered as excellent laboratories to test
many-body theories. In fact, the interaction is simple and depends only on the dis-
tance between the atoms. In addition, the effects of having different kinds of quan-
tum statistics may be studied, since here the quantum behaviour has macroscopic
manifestations. Actually, the fact that Helium remains liquid at zero temperature
is a consequence of the large zero point motion of the atoms in the fluid and can
be considered as a macroscopic quantum effect.

In spite of the enormous progress in the last two decades we have not yet
achieved a completely satisfying explanation of some experimental facts. Let’s just
mention that a full microscopic description of superfluidity in liquid $^3$He is still missing. It is not possible, in a single presentation, to summarize the present status of the whole Helium physics field, so we will exploit the fact that in the last two years several microscopic many-body theories have been used to study the ground and excited states of one $^3$He impurity in liquid $^4$He at zero temperature and use this system to illustrate the power and peculiarities of these techniques. The main emphasis will be given to Correlated Basis Function (CBF) but comparisons with the results obtained with Shadow Wave Function (SWF), Time Dependent Correlations (TDC) or Diffusion Monte Carlo (DMC) will be given.

The theoretical study of one $^3$He impurity in atomic liquid $^4$He is very helpful in understanding the properties of $^3$He-$^4$He mixtures. $^3$He and $^4$He are isotopes which follow Fermi and Bose statistics, respectively. They can form a liquid mixture which remains stable at zero temperature, with a maximum solubility of the $^3$He component at zero pressure of $\sim 6.6\%$. Both types of statistics coexist in the mixture with the consequence that the excitation spectrum is particularly rich. There are two types of excitations, whose lowest energy one corresponds to a particle-hole band associated to $^3$He quasi-particles. The quasi-particles have a single particle spectrum characterized by an effective mass, $m_3^*$, mainly due to the interaction with the $^4$He atoms. A little higher in energy lies the collective phonon-roton branch, associated to $^4$He and little affected by the presence of the $^3$He component. There is a marginal low momentum admixture between the two branches and they have been clearly separated in recent inelastic neutron scattering experiments at low momentum transfer.

As the $^3$He concentration, $x_3$, in the mixture is small, it is justified to study the $x_3 \to 0$ limit, or the impurity problem. The analysis of the impurity behavior not only provides clues to understand the mixture itself but also gives useful information on pure $^4$He liquid. As we will see, the impurity can be used as a theoretical probe to examine the kinetic and potential energies of the bulk system.

The bulk properties of helium liquid are well measured and a complete thermodynamic information is also available for $^3$He-$^4$He mixtures. In particular, the chemical potential of the $^3$He impurity at $^4$He saturation density ($\rho_0(^4He) = 0.02186\text{A}^{-3}$) and zero temperature is $\mu_3 = -2.78$ K, to be compared with the chemical potential of pure $^4$He, $\mu_4 = -7.17$ K, and with the one of liquid $^3$He, $\mu_3 = -2.5$ K at its own saturation density, $\rho_0(^3He) = 0.0163\text{A}^{-3}$.

The recent inelastic neutron scattering experiments at low momenta and low concentrations have given access to the impurity excitation spectrum. The experiments show a significant deviation from the quadratic Landau-Pomeranchuck (LP) spectrum, $\epsilon_{LP}(q) = \hbar^2 q^2 / 2m_3^*$. The measured spectrum is well described in a modified LP (MLP) form

$$\epsilon_{MLP}(q) = \frac{\hbar^2 q^2}{2m_3^*} \frac{1}{1 + \gamma q^2}. \quad (1)$$

Although there are still some uncertainties in the analysis of the data, the estimated values of the MLP parameters, at $P = 1.6$ bar and $x_3 \sim 0.05$ are $m_3^* \approx 2.2 m_3$ and $\gamma \approx 0.13 \text{ A}^2$. A recent analysis of specific heat measurements gives a slightly different zero momentum effective mass of $m_3^* = 2.18 m_3$, taking into
account the corrections due to the $^3$He finite concentration in the mixture.

The purpose of this contribution is to report the recent progress in the microscopic description of the impurity system. This will give us the opportunity to comment also on the present status of the description of the $^4$He liquid and enlight some aspects of the dynamics of $^3$He-$^4$He mixtures.

2 Static properties

For a quantum microscopic description we start from an empirical Hamiltonian, defined in terms of the masses of the atoms and of their mutual interactions. In the case of one impurity, the Hamiltonian reads

$$H = -\sum_{i=1}^{N_4} \frac{\hbar^2}{2m_4} \nabla_4^2 + \sum_{i,j} V(|r_i(4) - r_j(4)|) - \frac{\hbar^2}{2m_3} \nabla_3^2 + \sum_{i=1}^{N_4} V(|r_i(3) - r_i(4)|).$$

(2)

Due to the isotopic character of the mixture, the interaction is the same between the different pairs of atoms. A simple representation of the potential is the Lennard-Jones interaction

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - 2 \left( \frac{\sigma}{r} \right)^{6} \right],$$

(3)

where $\epsilon = 10.22$ K gives the depth of the potential and $\sigma = 2.556$ Å defines the length scale. Nowadays, the more accurate Aziz potential and its revised version HFD-B(HE) are used in realistic calculations. The He–He potential is characterized by a strong short range repulsion (such that the atoms, at a first approximation, can be considered as hard–spheres of diameter $\sim 2.6$ Å) and a weak attraction at medium and large distances. An important feature to keep in mind is that the ionization energy of the atoms and the first excitation energy are large (of the order of the eV) when compared with the energies which play a role in the physics of Helium liquids and that are of the order of the Kelvin ($1$ eV $\sim 11000$ K). Therefore, the Helium atoms are truly the elementary constituents of the system.

The chemical potential of the $^3$He impurity is defined by

$$\mu_3 = \frac{\langle \Psi(3; N_4) | H(3; N_4) | \Psi(3; N_4) \rangle - \langle \Psi(N_4) | H(N_4) | \Psi(N_4) \rangle}{\langle \Psi(N_4) | \Psi(N_4) \rangle},$$

(4)

i.e. as the energy difference when one $^3$He atom is added to $N_4$ $^4$He atoms at constant volume. The quantities to be subtracted are of order $N_4$ while the result of order of unity. Therefore, one must explicitly take into account these cancellations between large quantities to have a good estimate of $\mu_3$.

In a variational approach the next step consists in choosing a suitable trial function ($\Psi_0 = \Psi_0(3; N_4)$) for the ground state of $N_4$ $^4$He atoms plus one $^3$He in a volume $\Omega$, taken in the $N_4$, $\Omega \to \infty$ limit, at constant $^4$He density, $\rho_4 = N_4/\Omega$. The background wave function is simply obtained by omitting the impurity in the wave function. The extended Jastrow–Feenberg correlated wave function

$$\Psi_0(3; N_4) = F_2(3; N_4) F_3(3; N_4),$$

(5)
represents a realistic choice for \( \Psi_0(3; N_4) \). \( F_{2,3} \) are \( N \)-body correlation operators including explicit two- and three-body dynamical correlations. \( F_2 \) is written as a product of two body Jastrow, \( ^3\text{He} - ^4\text{He} \) and \( ^4\text{He} - ^4\text{He} \) correlation functions,

\[
F_2(3; N_4) = \prod_{i=1,N_4} f^{(3,4)}(r_{3i}) \prod_{m>i=1,N_4} f^{(4,4)}(r_{lm}),
\]
and \( F_3 \) is given by a corresponding product of triplet correlations, \( f^{(\alpha,\beta,\gamma)}(r_\alpha, r_\beta, r_\gamma) \).

The minimization of the ground state energy gives, in principle, the correlation functions via the solution of the Euler equations, \( \delta E / \delta f^{(\alpha,\beta)} = 0 \) and \( \delta E / \delta f^{(\alpha,\beta,\gamma)} = 0 \). Most of the results presented in this paper have been obtained by using an analytical form for the three-body correlation and solving the Euler equations for the Jastrow factor within the Hypernetted Chain (HNC) integral equations technique for the distribution functions.

The parametrized triplet correlations have the Feynman form,

\[
f^{(\alpha,\beta,\gamma)}(r_\alpha, r_\beta, r_\gamma) = \exp \left[ -\frac{1}{2} \sum_{\text{cyc}} \xi(r_\alpha r_\beta) \xi(r_\alpha r_\gamma) \hat{r}_{\alpha \beta} \cdot \hat{r}_{\alpha \gamma} \right]
\]

\( \xi(r) \) being a parametrized variational function. An optimization of the triplet correlations in a larger functional space shows that the Feynman form is nearly optimal. Optimal three body correlations for the impurity in the bulk, solving the Euler equation for \( f^{(\alpha,\beta,\gamma)} \), have been recently obtained and used.

For the sake of illustration we give the energy equations with two body correlations only. The cancellations occurring in the calculation of \( \mu_3 \) may be effectively dealt with by writing the expectation value of \( H(3; N_4) \) as \( E_0^v(3; N_4) = E_4^v + \mu_3^v \),

where \( E_4^v \) is the energy of the medium (proportional to \( N_4 \)) and \( \mu_3^v \) is the chemical potential of the \( ^3\text{He} \) atom (of the order of unity). In fact, the background energy, \( E_4^v \), cancels in the difference. The background energy, obtained within the Jackson-Feenberg prescription for the kinetic energy, is given by

\[
\frac{E_4^v}{N_4} = \frac{\rho_4}{2} \int dr g^{(4,4)}(r) \left[ V(r) - \frac{\hbar^2}{2m_4} \nabla^2 \ln f^{(4,4)}(r) \right],
\]

\( \mu_3^v = \mu_{\text{int}} + \mu_{\text{rea}} \) is decomposed into the interaction term \( \mu_{\text{int}} \),

\[
\mu_{\text{int}} = \rho_4 \int dr g^{(3,4)}(r) \left[ V(r) - \frac{\hbar^2}{4m_{\text{red}}} \nabla^2 \ln f^{(3,4)}(r) \right],
\]

\( m_{\text{red}} \) being the reduced mass \( m_{\text{red}} = m_3m_4/(m_3 + m_4) \), and \( \mu_{\text{rea}} \), due to the medium rearrangement,

\[
\mu_{\text{rea}} = \frac{1}{2} \rho_4 \int dr g^{(4,4)}_\text{rea}(r) \left[ V(r) - \frac{\hbar^2}{2m_4} \nabla^2 \ln f^{(4,4)}(r) \right].
\]

The distribution functions are defined by

\[
g^{(4,4)}(r_{12}) + \frac{1}{\Omega_{\text{rea}}^{(4,4)}(r_{12})} = \frac{N_4(N_4 - 1)}{\rho_4^2} \int dx_3 \ldots \frac{| \Psi(3; N_4) |^2}{\int d\Omega \ | \Psi(3; N_4) |^2},
\]
\[ g^{(3,4)}(r_{31}) = \frac{\Omega N_4}{\rho_4} \int \frac{d \mathbf{r}_2 d \mathbf{r}_3 \ldots}{d \Omega} |\Psi(3; N_4)|^2. \]  

(12)

One can also introduce the corresponding static structure functions, via the Fourier transforms:

\[ S(k) \equiv S^{(4,4)}(k) = 1 + \rho_4 \int d \mathbf{r} e^{i \mathbf{k} \cdot \mathbf{r}} \left[ g^{(4,4)}(r) - 1 \right]. \]  

(13)

and

\[ S^{(3)}(k) \equiv S^{(3,4)}(k) = \rho_4 \int d \mathbf{r} e^{i \mathbf{k} \cdot \mathbf{r}} \left[ g^{(3,4)}(r) - 1 \right]. \]  

(14)

In the \( k \to 0 \) limit

\[ \lim_{k \to 0} S^{(3)}(k) = -(1 + \alpha) \]  

(15)

where \( \alpha \) is the excess volume parameter, i.e. the relative increment in the molar volume when the impurity is added to the system, keeping the pressure constant. The mobility of the lighter mass \(^3\)He is larger and its presence tends to increase the pressure. As a consequence, the volume must be enlarged to keep the pressure constant. The experimental value of \( \alpha \) at the \(^4\)He saturation density is 0.284.

The problem of calculating the expectation values has so been translated into that of the evaluation of the distribution functions. Cluster expansion and integral equations provide a viable and effective tool to perform this task. To this aim, one introduces the function \( \hbar = f^2 - 1 \) and expands the distribution functions in powers of \( \hbar \). The terms of the expansions are diagrammatically classified and summed up to infinite orders by Hypernetted Chain integral equations, whose properties have been pedagogically reviewed by Fabrocini and Fantoni, for both Bose and Fermi systems.

The impurity problem has been often analyzed within the Average Correlation Approximation (ACA). ACA is obtained by taking the same dynamical correlation functions for the impurity and for the medium. In this case, \( g^{(3,4)} = g^{(4,4)} \) and

\[ g^{(4,4)}_{rea}(r_{12}) = \frac{\partial g^{(4,4)}(r_{12})}{\partial \rho_4}, \]  

(16)

therefore

\[ \mu_{\text{int}}^{\text{ACA}} = 2 e(\rho_4) + \left( \frac{m_4}{m_3} - 1 \right) t^{(4)}(\rho_4) \]  

(17)

where \( e(\rho_4) \) and \( t^{(4)}(\rho_4) \) are the total and the kinetic \(^4\)He energies per particle, respectively. \( \mu_{\text{rea}}^{\text{ACA}} \) is then given in ACA by

\[ \mu_{\text{rea}}^{\text{ACA}} = \frac{P(\rho_4)}{\rho_4} - e(\rho_4) \]  

(18)

\( P(\rho_4) \) being the thermodynamical pressure. In this way the chemical potential is expressed as

\[ \mu_{\text{ACA}} = e(\rho_4) + \frac{P(\rho_4)}{\rho_4} + \left( \frac{m_4}{m_3} - 1 \right) t^{(4)}(\rho_4) = \mu_4(\rho_4) + \left( \frac{m_4}{m_3} - 1 \right) t^{(4)}(\rho_4). \]  

(19)
The chemical potential of the impurity in ACA is the chemical potential of pure $^4$He corrected by a kinetic energy term properly scaled to take into account the different mass of the impurity. Actually this formula can be easily generalized to wave functions containing also n-body correlations. A recent diffusion Monte Carlo calculation, which contains optimized n-body correlations, has given $t_4 = 14.32$ K and $\mu_4 = -7.27$ K at saturation density. Employing these values, one gets $\mu_4^{ACA} = -2.58$ K. If the optimization of the correlations affecting the impurity is performed, the chemical potential value is closer to the experimental one.

An alternative trial wave function for Bose systems has been recently proposed: the so called Shadow wave function method. It has been successfully used for microscopic calculations on liquid and solid $^4$He at zero temperature and has been generalized to the impurity system. In the SWF approach the wave function is given by

$$\Phi_{SWF}(R) = \int dS \ F_{SWF}(R, S)$$

where $R = (\vec{r}_3, \vec{r}_1, ..., \vec{r}_N)$ are the coordinates of the particles and $S = (\vec{s}_3, \vec{s}_1, ... \vec{s}_N)$ is a set of auxiliary variables, representing centers of motion of the particles and integrated over the whole space. The interparticle correlations are embedded in

$$F_{SWF} = \varphi_p(R) \times f_{p3}(|\vec{r}_3 - \vec{s}_3|) \times \prod_{i=1}^{N_4} f_{ps}(|\vec{r}_i - \vec{s}_i|) \times \varphi_s(S).$$

$\varphi_p(R)$ is a Jastrow factor, as well as $\varphi_s(S)$, which includes correlations at all orders (pair, triplet, ...) through the shadow correlations, after integrating over $S$. One of the main features of $\Phi_{SWF}$ is the possibility to describe both liquid and crystalline phases within the same functional form, respecting Bose symmetry and translational invariance. The expectation values between these trial wave functions are usually calculated by Monte Carlo techniques. The extension of ACA to the shadow variables approach, i.e. by taking the correlation factors $f_p$, $f_s$ and $f_{ps}$ as recently optimized for pure $^4$He also for the impurity correlations, gives $\mu_3 = -2.43$ K at saturation density, close to the ACA value obtained with the DMC results as input. In the case of the SWF the three-, four- and n-body correlations are generated through the correlations with the shadow variables, while in the correlated basis theory they are explicitly introduced in the variational wave function and in the DMC method they are incorporated and/or optimized in the DMC algorithm for solving the many-body Schrödinger equation.

The density dependence of the pure $^4$He energy and of the $^3$He impurity chemical potential is reasonably well described by CBF if the correlations are properly optimized and the cluster expansion diagrams are fully summed, with the inclusion of the elementary ones. CBF shows a good agreement with the results obtained within the two other approaches briefly discussed above. Even if the finite size of the simulation box introduces some uncertainties in the Monte Carlo methods and some limitations in the study the long range behavior of the distribution functions, DMC provides in principle the most accurate results. In fact, by using the HFD-B(HE) Aziz potential it reproduces the $^4$He experimental saturation
density \( \rho_0 \), as already mentioned it gives \( \mu_4^{(DMC)}(\rho_0) = -7.27(1) \) K and provides \( \mu_3^{(DMC)}(\rho_0) = -2.79(25) \) K and \( \alpha = 0.284(10) \). The kinetic and potential energies of the pure liquid \(^4\)He at \( \rho_0 \) are \( t(\rho_0) = 14.32(5) \) K and \( v(\rho_0) = -21.59(5) \) K, respectively.

Before leaving this subsection, we show in Figure 1 the static-structure functions \( S(k) \) and \( S^{(3)}(k) \). They are the main inputs in the calculation of the excitation spectrum and have been obtained at the experimental saturation density with the Aziz potential and solving the Euler-Lagrange equations for the two-body correlation functions, keeping the triplet correlations fixed. \( S^{(3)}(k) \) has the proper behavior at \( k \to 0 \) (15). The ACA cannot reproduce this limit because \( S_{ACA}(k) = S(k) - 1 \).

2.1 The \(^3\)He impurity as a probe in liquid \(^4\)He

The difference of expectations values in Eq.(4) shows that \( \mu_3 \), as given by the equation, is not necessarily an upper bound to the true chemical potential. However, if we assume that the trial wave function is the exact wave function of liquid \(^4\)He, then \( \mu_3^{ACA} \) provides an exact upper bound to \( \mu_3^{expt} \),

\[
\mu_3^{expt}(\rho_4) \leq \mu_3^{expt}(\rho_4) + \left( \frac{m_4}{m_3} - 1 \right) t(\rho_4). \tag{22}
\]

Since \( \mu_4^{expt}(\rho_4) \) and \( \mu_3^{expt}(\rho_4) \) are experimentally known, the previous inequality can be used to establish a model independent lower bound to the kinetic energy of liquid \(^4\)He,

\[
t(\rho_4) \geq t^{LB}(\rho_4) = \left[ \frac{m_3}{m_4 - m_3} \right] \left[ \mu_3^{expt}(\rho_4) - \mu_4^{expt}(\rho_4) \right]. \tag{23}
\]
At the same time, an upper bound to the potential energy per particle can be determined by
\[ v(\rho_4) \leq v^{UB}(\rho_4) \equiv e^{exp}(\rho_4) - t^{LB}(\rho_4) \] (24)
where \( e^{exp}(\rho_4) \) is the \(^4\)He energy per particle. At the experimental saturation density, \( \mu_4^{exp}(\rho_0) = -7.17 \) K and \( \mu_3^{exp}(\rho_0) = -2.78 \) K, therefore \( t_4^{LB}(\rho_0) = 13.4 \) K and \( t^{UB}(\rho_0) = -20.6 \) K. These bounds are basically respected by all the theoretical calculations performed with the Aziz potential. Also the extraction of the kinetic energy from the most recent inelastic neutron scattering data is consistent with the kinetic energy lower-bound \[ (25) \]

3 The excitation spectrum of the \(^3\)He impurity

3.1 Variational calculation

Let us focus now on the variational description of the impurity excited states. For pure \(^4\)He, a simple trial wave function for an excited state characterized by a momentum \( \vec{q} \) may be built in terms of Feynman phonons
\[ \Psi_q(N_4) = \rho_4(\vec{q})\Psi_0(N_4), \] (25)
where \( \Psi_0(N_4) \) is the \(^4\)He ground state and
\[ \rho_4(\vec{q}) = \sum_{i=1,N_4} e^{i\vec{q}\cdot\vec{r}_i} \] (26)
is the \(^4\)He density fluctuation operator. The excitation energy, \( \omega(q) \), of \( \Psi_q(N_4) \) is
\[ \omega(q) = \frac{\langle \Psi_q(N_4) | H - E_0 | \Psi_q(N_4) \rangle}{\langle \Psi_q(N_4) | \Psi_q(N_4) \rangle} = \frac{\langle \Psi_0(N_4) | \rho_q^\dagger \rho_q (H - E_0) | \Psi_0(N_4) \rangle}{\langle \Psi_q(N_4) | \Psi_q(N_4) \rangle} + \frac{\langle \Psi_0(N_4) | \rho_q^\dagger [H - E_0, \rho_q] | \Psi_0(N_4) \rangle}{\langle \Psi_q(N_4) | \Psi_q(N_4) \rangle} \] (27)
The first term of the right hand side vanishes when \( \Psi_0(N_4) \) is the exact ground state or contains optimal two-body correlations. The second term leads to the well known Feynmann dispersion relation:
\[ \omega(q) = \omega_F(q) = \frac{\hbar^2 q^2}{2mS(q)}, \] (28)
where \( S(q) \) is the static structure function defined in Eq.\[ (13) \]. This relation gives the correct low momentum \( (q \leq 0.4 \text{Å}^{-1}) \) linear behavior of the phonon-roton spectrum, \( \omega(q) = \hbar q v_s \), where \( v_s \) is the speed of sound in liquid \(^4\)He \( (v_s(\rho_0) \sim 238 m/s) \), provided that
\[ \lim_{q \to 0} S(q) = \frac{\hbar q}{2m_4 v_s}. \] (29)
In an analogous way, the impurity excited state is given by
\[ \Psi_q(3; N_4) = \rho_3(q)\Psi_0(3; N_4), \] (30)
where \( \rho_3(q) = e^{iq \cdot r_3} \) is the impurity excitation operator. The excitation energy is

\[
e_0(q) = \frac{\langle \Psi_q(3; N_4) | H(3; N_4) - E_0(3; N_4) | \Psi_q(3; N_4) \rangle}{\langle \Psi_q(3; N_4) | \Psi_q(3; N_4) \rangle} = \frac{\hbar q^2}{2m_3},
\]

(31)

and one obtains a dispersion relation corresponding to the free particle, with \( m_3^* = m_3 \).

A better ansatz, which takes into account the backflow of \(^4\text{He} \) atoms around \(^3\text{He} \), is provided by

\[
\Psi_{BF}^q(3; N_4) = \rho_3(q)F_B(q; 3; N_4)\Psi_0(3; N_4)
\]

(32)

with

\[
F_B(q; 3; N_4) = \prod_{i=1}^{N_4} \exp \left[ iq \cdot (r_i - r_3)\eta(r_3i) \right].
\]

(33)

Backflow correlations do not change the binding energy of the impurity and only affect the excitation spectrum, which, however, remains parabolic:

\[
e_{BF}(q) = \frac{\hbar^2 q^2}{2m_3} \left[ 1 + a_1 + a_2 + a_3 \right],
\]

(34)

where

\[
a_1 = \rho_4 \int d\mathbf{r} \varrho^{(3,4)}(\mathbf{r}) \left( 2\eta(\mathbf{r}) + \frac{2}{3}r\eta'(\mathbf{r}) \right),
\]

(35)

\[
a_2 = \frac{m_3}{\mu_{\text{red}}} \rho_4 \int d\mathbf{r} \varrho^{(3,4)}(\mathbf{r}) \left( \eta(\mathbf{r})^2 + \frac{1}{3} \left[ r^2(\eta'(\mathbf{r}))^2 + 2\eta(\mathbf{r})r\eta'(\mathbf{r}) \right] \right),
\]

(36)

\[
a_3 = \rho_4^2 \int d\mathbf{r}_{31} d\mathbf{r}_{32} g^{(3,4,1,2)} \left( \eta_{31}\eta_{32} + \frac{1}{3} \left[ \mathbf{r}_{31}\eta'_{31}\eta'_{32}\mathbf{r}_{32} + 2\eta_{31}\eta_{32}\mathbf{r}_{32}^2 \right] \right),
\]

(37)

where \( g^{(3,1,2)} \) is a three body distribution function. A good choice for the variational function \( \eta(r_{3i}) \) has been found to be

\[
\eta(r) = A_0 \exp \left( -\frac{(r-r_0)^2}{\omega_0} \right),
\]

(38)

and the parameters \( r_0, \omega_0 \) and \( A_0 \) are varied to find the minimum. With this variational ansatz, one gets a \( q \)-independent effective mass of \( m_3^*/m_3 \sim 1.7 \). A minimization through a full functional variation with respect to \( \eta(r_{3i}) \) does not change this result.

### 3.2 Correlated perturbative approach

A systematic way to incorporate effects more complicated than the two-body backflow is provided by the Correlated Basis Function perturbation theory. In such an approach, CBF is used to build richer excitations on top of \( \Psi_q \) by allowing the total momentum to be shared between the impurity and the phonons in the medium. The underlying idea consists in incorporating the non-perturbative correlations directly.
into the basis functions and then developing a perturbative expansion in this basis. Usually, since the correlated states are a good approximation to the eigenstates of the hamiltonian, the first low orders of the perturbation theory are sufficient for getting reliable and realistic results.

In the case of the impurity, the correlated basis is classified according to the number of Feynman phonons in each intermediate state,

\[ \Psi_{q, q_1 \ldots q_n}(3; N_4) = \rho_3(q - q_1 - \ldots - q_n)\rho_4(q_1)\ldots \rho_4(q_n)\Psi_0(3; N_4). \] (39)

The multiphonon states will mix in the perturbative process with the unperturbed state \( \Psi_q = \rho_3(q)\Psi_0 \). The states (39) are not orthogonal among each other and either they must be properly normalized following the procedure described in Ref.(34) or the perturbative expansion must be carried on in a non orthogonal basis.

The results presented in this work have been obtained including one phonon (OP) and two independent phonon (TIP) intermediate states and all the perturbative diagrams corresponding to successive rescatterings of the one phonon states (OPR). While the correlation factors are intended to care for the short range modifications of the ground state wave function due to the strongly repulsive interatomic potential, the basic physical effect induced by the perturbative corrections may be traced back to different types of backflow around both the impurity and the \(^4\)He atoms.

In order to construct the CBF perturbative series, the unperturbed and the interaction Hamiltonians are defined via their matrix elements:

\[ H_{0, ij} = \delta_{ij} \frac{\langle \Psi_i | H | \Psi_j \rangle}{\langle \Psi_i | \Psi_i \rangle} = \delta_{ij} E_i^n, \] (40)

\[ H_{I, ij} = (1 - \delta_{ij}) \frac{\langle \Psi_i | H - E_q N_{ij} | \Psi_j \rangle}{((\langle \Psi_i | \Psi_i \rangle(\langle \Psi_j | \Psi_j \rangle))^{1/2}} = (1 - \delta_{ij})(H_{ij} - E_q N_{ij}), \] (41)

where \( E_q = E_0(3; N_4) + \epsilon_0(q) + \delta \epsilon(q) \) is the eigenvalue of \( H \) for the state with momentum \( q \). The diagonal matrix elements of \( H_I \) are zero by construction and, therefore, there are no first order perturbative corrections.

The Brillouin-Wigner series for the perturbative correction \( \Delta E_q \) to \( E_q^n \), appropriate for non-orthogonal states, is given by:

\[ \Delta E_q = \sum_{j \neq q} \frac{(H_{qj} - E_p N_{qj})(H_{jq} - E_p N_{jq})}{E_q - E_j^n} + \ldots, \] (42)

where \( E_q \) is the final energy and the overlap matrix elements, \( N_{qj} = \langle \Psi_q | \Psi_j \rangle \), take care of the non-orthogonalization. The series is first expanded around the correction to the medium energy, \( \Delta E_0 = E_4 - E_4^n \), and then resummed in such a way to cancel all the terms diverging in the \( N_4 \to \infty \) limit and originating from both the cluster expansion of the matrix elements and the perturbative expansion itself. This procedure has been devised for the ground-state energy of an infinite Fermi system and then generalized to the case of the impurity.

The difficulties related to the divergencies can be avoided by working in the orthogonalized scheme, in fact the \( n \)-phonon states may be Schmidt-orthogonalized.
to states with a lower number of phonons. For instance, the orthogonalized OP state reads as:

$$|\mathbf{q}; \mathbf{q}_1\rangle = \frac{|\Psi_{\mathbf{q};\mathbf{q}_1}\rangle - |\Psi_{\mathbf{q}_1}\rangle \langle \Psi_{\mathbf{q}}|\Psi_{\mathbf{q};\mathbf{q}_1}\rangle}{\langle \Psi_{\mathbf{q};\mathbf{q}_1}|\Psi_{\mathbf{q};\mathbf{q}_1}\rangle^{1/2}}, \quad (43)$$

while the two-phonon state, $\Psi_{\mathbf{q};\mathbf{q}_1+\mathbf{q}_2}$, may be orthogonalized in a similar way to $\Psi_{\mathbf{q}}$, $\Psi_{\mathbf{q};\mathbf{q}_1+\mathbf{q}_2}$, and $\Psi_{\mathbf{q};\mathbf{q}_1,2}$. The orthogonalization makes the convergence of the series faster as the non orthogonalized states have large mutual overlaps.

The different terms in (46) represent contributions from the corresponding inter-

$$\langle \mathbf{q}|H|\mathbf{q}; \mathbf{q}_1\rangle = -[N_4 S(q_1)]^{-1/2} \frac{\hbar^2}{2m_3} \mathbf{q} \cdot \mathbf{q}_1 S^{(3)}(q_1), \quad (44)$$

where $S(q)$ and $S^{(3)}(q)$ are the two-body structure functions of eqs. (13) and (14).

The diagonal matrix elements have the particularly simple form:

$$\langle \mathbf{q}; \mathbf{q}_1..\mathbf{q}_n|H|\mathbf{q}; \mathbf{q}_1..\mathbf{q}_n\rangle = E_0^n + \epsilon_0(q) + \sum_{i=1,n} w_F(q_i) \quad (45)$$

with $E_0^n = \langle \Psi_0|H|\Psi_0\rangle/\langle \Psi_0|\Psi_0\rangle$.

Finally, the impurity excitation energy is $\epsilon(q) = \epsilon_0(q) + \Delta \epsilon(q)$, where, within the truncation we have used,

$$\Delta \epsilon(q) \sim \Delta \epsilon_{OP}(q) + \Delta \epsilon_{TIP}(q) + \Delta \epsilon_{OPR}(q). \quad (46)$$

The different terms in (46) represent contributions from the corresponding inter-

The OP and TIP contributions to $\Delta \epsilon(q)$ are shown in Figure 5 of Ref. (5). We stress that the CBF based perturbative approach requires the evaluation of two levels of diagrams, the perturbative and the cluster ones. We use Brillouin-Wigner perturbation theory, so the correction itself depends on $\epsilon(q)$ and the series must be summed self-consistently. For instance, the OP contribution is solution of

$$\Delta \epsilon_{OP}(q) = \sum_{\mathbf{q}_1} \frac{|\langle \mathbf{q}|H - E_0 - \epsilon(q)|\mathbf{q}; \mathbf{q}_1\rangle|^2}{\epsilon(q) - \epsilon_0(|\mathbf{q} - \mathbf{q}_1|) - w_F(q_1)}$$

$$= \frac{\Omega}{(2\pi)^3} \left( \frac{\hbar^2}{2m_3} \right)^2 \int d^3q_1 \frac{1}{N_4 S(q_1)} \frac{|S^{(3)}(q_1)|^2}{\epsilon(q) - \epsilon_0(|\mathbf{q} - \mathbf{q}_1|) - w_F(q_1)}, \quad (47)$$

and the OP effective mass, at $q = 0$, is

$$m_\pi^2 = \left[ 1 - \frac{\hbar^2}{4\pi^2 \rho_4 2m_3^3} \int dq \frac{q^2 S^{(3)}(q)}{2m_3} \right]^{-1}. \quad (48)$$

The spectrum obtained by taking only OP states is very close to the LP one with an effective mass similar to that given by the variational calculation with backflow.
correlations. Actually, in several papers it has been pointed out that second order perturbative expansion with OP states introduces two–body backflow correlations into the wave function. We find $m_3^*(QP) = 1.8 \, m_3$, in good agreement with an analogous CBF treatment by Saarela (m_3^* \sim 1.9 \, m_3) and with the backflow variational calculations.

The matrix elements involving TIP states (whose lengthy expressions are given in Ref.(5)), involve, as already anticipated, the two– and three–body structure functions, i.e. the Fourier transforms of the two– and three–body distribution functions, $g^{(2)}(r_{12})$ and $g^{(3)}(r_1, r_2, r_3)$. $g^{(3)}$ may be evaluated within several approximations, the most common of which are the convolution (CA) and the superposition (KSA) ones. The CA correctly accounts for the sequential relation between $g^{(3)}$ and $g^{(2)}$ and factorizes in momentum space, $S_{CA}^{(3)}(q_1, q_2, q_3) = S(q_1)S(q_2)S(q_3)$. The SA factorizes in $r$–space, $g_{KSA}^{(3)}(r_1, r_2, r_3) = g^{(2)}(r_{12})g^{(2)}(r_{13})g^{(2)}(r_{23})$, and adequately describes the short range region. The momentum space factorization property makes the CA more suited to our perturbative study.

The two approximations give $m_3^*(CA) = 1.6 \, m_3$ and $m_3^*(KSA) = 2.1 \, m_3$ at $q = 0$, with OP and TIP states. A calculation including a four–body correction (the Abe term) in the three–body distribution function and the OPR contribution provides $m_3^* = 2.2 \, m_3$ at saturation density. Moreover, a key ingredient for a correct behavior of $\epsilon(q)$ in the large $q$ sector is a good description of the $^4$He roton. This requires the use of the superposition approximation that, on the other hand, is not correct in the $^4$He phonon region. The inclusion of backflow correlations in the correlated intermediate states gave an overall agreement with the experimental $^4$He spectrum but largely increased both the difficulty of the evaluation of the matrix elements and the uncertainty related to the use of high order distribution functions. In the impurity case a good compromise (termed CA1), which does not require a big computational effort, was found by using the CA and the experimental values of the $^4$He spectrum, $\omega_{expt}(q)$, in the energy denominators.

In Figure 2, we show the impurity spectrum in CA1, together with the experimental $^3$He and $^4$He curves. The OPR terms are included and the LP and MLP fits to $\epsilon_{expt}(q)$ are shown. Since the branch of the dynamical response due to the excitations of the low concentration $^3$He component in the Helium mixtures overlaps the collective $^4$He excitation at $q > 1.7 \, \AA^{-1}$, $\epsilon_{expt}(q)$ is not known in that region.

The CBF spectrum is very close to $\epsilon_{expt}(q)$ up to its merging into the $^4$He dispersion relation. For the $\gamma$ parameter in the MLP parametrization, the theory gives $\gamma(CBF) \sim 0.19 \, \AA^2$ and $m_3^*(CBF) = 2.1 \, m_3$. If the spectrum is parametrized in terms of a momentum dependent effective mass, $\epsilon(q) = \hbar^2 q^2 / 2m_3^*(q)$, then we find $m_3^*(q = 1.7 \, \AA^{-1}) = 3.2 \, m_3$, with an increase of $\sim 50\%$ respect to the $q = 0$ value.

Beyond $q \sim 1.9 \, \AA^{-1}$, the impurity quasiparticle is no longer an excitation with a well defined energy and it can decay into $^4$He excitations and acquire a finite lifetime, $\tau$. A finite $\tau$–value reflects a non zero imaginary part of the $^3$He complex on–shell self–energy, $W(q) = \Im \Sigma(q, \epsilon(q))$. $W(q)$, amplified by a factor 4 and computed with only OP intermediate states, is shown in Figure 2. Our $W(q)$ is close to the one found in Refs. A numerical extrapolation of the computed
\( \epsilon_{CBF}(q) \) into the roton region does not show any evidences of a \(^3\)He roton-like structure.

Shadow wave functions have been used also for studying the excited states of the impurity. In this case, an excited state of momentum \( q \) is constructed by associating the momentum to the impurity shadow variables,

\[
\Psi^3_q(R) = \int dSF(R, S) \tilde{\delta}_q.
\]  

(49)

Similarly, a \(^4\)He excited states is built as:

\[
\Psi^B_q(R) = \int dSF(R, S) \tilde{\sigma}_q.
\]  

(50)

The momentum is carried on by the shadow variables with

\[
\tilde{\delta}_q = e^{i\mathbf{q} \cdot \mathbf{s}_3}, \quad \tilde{\sigma}_q = \sum_{j=1}^{N_4} e^{i\mathbf{q} \cdot \tilde{s}_j}.
\]  

(51)

where \( \tilde{s}_{j,3} \) are shadow variables modified by an explicit back-flow correlation

\[
\tilde{s}_j = s_j + \sum_{l \neq j} (s_j - s_l) \lambda(s_{jl}).
\]  

(52)

The two shadow wave functions are eigenstates of the momentum operator, both with momentum \( q \), and are therefore orthogonal to the ground state. However, they are not orthogonal between them. They must be orthogonalized and a 2 \( \times \) 2 Hamiltonian must be diagonalized for each momentum in order to properly consider the collective and the single-particle impurity branches. This procedure has been
followed by Galli et al. by a Monte Carlo algorithm and the final spectrum is compatible with a MLP spectrum with parameters $m_3^* = 2.06 m_3$ and $\gamma = 0.0314 \, \text{Å}^2$. The spectrum is close to the LP form and $m_3^* = 1.74 m_3$ when there is no back-flow term in the shadow variables ($\lambda(r_{ij}) \equiv 0$).

Other methods have confronted themselves with the impurity problem in the many–body arena. We first mention diffusion Monte Carlo, who has recently given an effective mass of $m_3^*/m_3 = 2.29$ at saturation density, at zero momentum. Another one is based on a dynamic theory that allows for time dependent correlations, whose equations of motion are determined through a minimum action principle. This theory has been successfully applied to study the excitation spectrum of pure $^4$He \cite{diffusion_monte_carlo}. The method is very closely related to CBF and, in a simplifying hypothesis known as ”uniform limit approximation”, one recovers the second order expression in the OP space. The resulting spectrum is well adjusted to the MLP form with $m_3^* = 2.09 m_3$ and $\gamma = 0.114 \, \text{Å}^2$ at saturation density \cite{time_dependent_correlations}.

4 Conclusions

We have shown in this contribution that a variational theory employing correlated wave functions is able to provide a good description of the ground state of one $^3$He impurity in liquid $^4$He. In addition, a perturbative expansion in a correlated basis may give a quantitative picture of the impurity excitation spectrum, provided the basis considers correlated states with two independent phonons and one phonon rescattering diagrams, which play a non marginal role at large momenta. The agreement with other many–body methodologies, as shadow wave functions, diffusion Monte Carlo and time dependent correlations, is quite good. This gives confidence in the possibility of extending the CBF theory to other, less studied, aspects of the physics of liquid Helium. To stay in the field of the mixtures, first CBF analyses of the inelastic neutron scattering cross sections, both at low and high momentum transfers \cite{CBF_inelastic_neutron_scattering}, have revealed an encouraging semiquantitative agreement with the available experimental results \cite{CBF_inelastic_neutron_scattering}. This topic needs to be more carefully investigated, also within a close interaction with the experimental teams working, or willing to work, in this subject.

Finally, to conclude this presentation, we rest our case.

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References

1. *Excitations in Two-Dimensional and Three-Dimensional Quantum Fluids*, Vol. 257 of NATO Advanced Study Institute, Series B: Physics, A.F.G. Wyatt and H.J. Lauter, eds. (Plenum, New York, 1991).
2. W. Teizer, R. B. Hallock, E. Dujardin, and T. W. Ebbesen, Phys. Rev. Lett. 82, 5305 (1999)
3. S. Grebenev, J. P. Toennies and A. Vilesov, Science 279, 2083 (1998)
4. Microscopic Quantum Many-Body Theories and Their Applications, J. Navarro and A. Polls eds., Lecture Notes in Physics, Vol. 510, (Springer-Verlag, Heidelberg, 1998)
5. A. Fabrocini, S. Fantoni, S. Rosati and A. Polls, Phys. Rev. B 33, 6057 (1986)
6. A. Fabrocini and A. Polls, Phys. Rev. B 58, 5209 (1998)
7. D. E. Galli, G.L. Masserini and L. Reatto, Phys. Rev. B 60, 3476 (1999)
8. E. Krotscheck, J. Paaso, M. Saarela, K. Schookhuber and R. Zillich Phys. Rev. B 58, 12282 (1998)
9. J. Boronat and J. Casulleras, Phys. Rev. B 59, 8844 (1999)
10. B. Fäk, K. Guckelsberger, M. Korfer, R. Scherm and A. J. Dianoux, Phys. Rev. B 41, 8732 (1990).
11. J. Boronat, A. Fabrocini and A. Polls, Phys. Rev. B 39, 2700 (1989)
12. J. Wilks in The properties of Liquid and Solid Helium (Clarendon Press, Oxford, 1967)
13. C. Ebner and D. O. Edwards, Phys. Rep. 2, 77 (1970).
14. L. D. Landau and I. M. Khalatnikov, Zh. Eksp. Teor. Fiz. 2, 637 (1948)
15. E. Krotscheck, M. Saarela, K. Schörkhuber, and R. Zillich, Phys. Rev. Lett. 80, 4709 (1998)
16. S. Yorozu, H. Fukuyama, and H. Ishimoto, Phys. Rev. B 48, 9660 (1993)
17. R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G.T. McConville, J. Chem. Phys. 70, 4330 (1979)
18. R. A. Aziz, F. R. W. McCourt, and C. C. K. Wong, Mol. Phys. 61, 1487 (1987)
19. E. Feenberg, Theory of Quantum Liquids, Academic, New York, 1969.
20. S. Moroni, S. Fantoni, and G. Senatore, Phys. Rev. B 52, 13547 (1995)
21. A. Fabrocini and A. Polls, Phys. Rev. B 30, 1200 (1984)
22. K. Schmidt, M.H. Kalos, M.A. Lee, and G.V. Chester, Phys. Rev. Lett. 45, 573 (1980)
23. Q.N. Usmani, S. Fantoni, and V.R. Pandharipande, Phys. Rev. B 26, 6123 (1982)
24. M. Saarela and E. Krotscheck, J. Low Temp. Phys. 90, 415 (1993)
25. E. Krotscheck and M. Saarela, Phys. Rep. 232, 1 (1993)
26. A. Fabrocini and S. Fantoni in Advances in Quantum Many-Body Theories, Vol. 2, R.F. Bishop and N.R. Wilet eds., (World Scientific, Singapore, 1998)
27. J. Boronat, A. Fabrocini, and A. Polls, J. Low Temp. Phys. 74, 347 (1989)
28. G. Baym, Phys. Rev. Lett. 17, 952 (1966)
29. S. A. Vitiello, K. Runge, and M. H. Kalos, Phys. Rev. Lett. 60, 1970 (1988)
30. S. Moroni, D. E. Galli, S. Fantoni, and L. Reatto, Phys. Rev. B 58, 909 (1998)
31. R.T. Azuah, W.G. Stirling, H.R. Glyde, M. Bonisegni, P.E. Sokol, and S.M. Bennington, Phys. Rev. B 56, 14620 (1997)
32. R. P. Feynman, Phys. Rev. 94, 262 (1954)
33. J. C. Owen, Phys. Rev. B 23, 5815 (1981)
34. S. Fantoni and V. R. Pandharipande, Phys. Rev. C 37, 1697 (1988)
35. P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, (McGraw-Hill, New York), 1953.
36. S. Fantoni, *Phys. Rev.* B 29, 2544 (1984)
37. T. B. Davison and E. Feenberg, *Phys. Rev.* 178, 306 (1969)
38. M. Saarela, *Recent Progress in Many Body Theories*, ed. Y. Avishai (Plenum, New York, 1990), Vol. 3, p. 337.
39. R. Abe, *Prog. Theor. Phys.* 21, 421 (1959)
40. E. Manousakis and V. R. Pandharipande, *Phys. Rev.* B 33, 150 (1986)
41. M. Saarela, *Phys. Rev.* B 33, 4596 (1986)
42. J. Boronat, F. Dalfovo, F. Mazzanti and A. Polls, *Phys. Rev.* B 48, 7409 (1993)
43. A. Fabrocini, L. Vichi, F. Mazzanti, and A. Polls, *Phys. Rev.* B 54, 10035 (1996)
44. Y. Wang and P. E. Sokol, *Phys. Rev. Lett.* 72, 1040 (1994)