Effective mass of one $^4\text{He}$ atom in liquid $^3\text{He}$

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A microscopic calculation of the effective mass of one $^4\text{He}$ impurity in homogeneous liquid $^3\text{He}$ at zero temperature is performed for an extended Jastrow–Slater wave function, including two- and three-body dynamical correlations and also backflow correlations between the $^4\text{He}$ atom and the particles in the medium. The effective mass at saturation density, $m_4^*/m_4 = 1.21$, is in very good agreement with the recent experimental determination by Edwards et al. The three-particle correlations appear to give a small contribution to the effective mass and different approximations for the three-particle distribution function give almost identical results for $m_4^*/m_4$.

Recently, Edwards et al. have used the Zharkov–Silin Fermi liquid theory of dilute solutions of $^4\text{He}$ in normal liquid $^3\text{He}$ to determine the chemical potential ($\mu_4$) and the effective mass ($m_4^*$) for the limiting case of one $^4\text{He}$ impurity. The experimental input data for this analysis were the recent low temperature measurements of the phase separation by Nakamura et al. The same theory was previously applied to older experimental data by Laheurte and Saam, and their predictions for $\mu_4$ and $m_4^*$ differ notably from those of Ref. At zero pressure, Edwards et al. report $\mu_4 = -6.95$ K and $m_4^*/m_4 = 1.1$, whereas $\mu_4 = -6.60$ K and $m_4^*/m_4 = 4.5$ in Refs. The disagreement was attributed to the fact that the validity of the Fermi liquid theory is ensured at temperatures below 0.1 K while the results of Ref. were obtained from experimental data at $T \geq 0.5$ K. Although the difference between the two experimental values of $\mu_4$ is rather small, our recent microscopic calculations seem to support the more bounded result of Edwards et al. On the other hand, the experimental determinations of the impurity effective mass are appreciably different. At this point, it is clear that a fully microscopic calculation of $m_4^*$ would be very enlightening.

In the present work, we evaluate the excitation spectrum and the effective mass of a $^4\text{He}$ impurity in liquid $^3\text{He}$ using a trial wave function of the type

$$\Psi_v(k) = \rho_B(k) \Psi_0,\quad (1)$$

where $\Psi_0$ is the ground–state wave function of the $^3\text{He}$ medium plus one $^4\text{He}$ atom and $\rho_B(k)$ is an excitation operator defined as:

$$\rho_B(k) = \rho_I(k) F_B,\quad (2)$$

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$$\rho_B(k) = \rho_I(k) F_B,\quad (2)$$
where $\rho_I(k) = \exp(ik \cdot r_I)$ describes the impurity traveling through the medium as a plane wave of momentum $k$ and the correlation operator

$$F_B = \prod_{i=1}^{A} f_B(k, r_{II})$$

incorporates backflow correlations between the impurity $I$ ($^4$He atom) and the $A$ $^3$He atoms of the bulk. Backflow correlations have proved to be relevant for a realistic study of the effective mass of one $^3$He impurity in liquid $^4$He. They play also an important role in the evaluation of the binding energy of pure $^3$He.

The Hamiltonian of the system is written as

$$H(A + 1) = H(A) + H_I(A + 1),$$

where

$$H(A) = -\hbar^2 \sum_{i=1}^{A} \nabla_i^2 + \sum_{i<j}^{A} V(r_{ij})$$

is the Hamiltonian of the pure $^3$He background, and

$$H_I(A + 1) = -\hbar^2 \frac{1}{2m_4} \nabla_I^2 + \sum_{i=1}^{A} V(r_{II})$$

are additional terms related to the impurity.

The variational approach starts with the choice of the trial wave function $\Psi_0$. As in our previous paper, we take an extended Jastrow–Slater wave function for the $A + 1$ particles:

$$\Psi_0 = F_J F_T \phi(1, ..., A),$$

where $\phi(1, ..., A)$ is the Fermi gas wave function for the $A$ $^3$He atoms, $F_J$ is a Jastrow correlation operator embodying two–body dynamical correlations

$$F_J = \prod_{i<j}^{A} f^{(3,3)}(r_{ij}) \prod_{i=1}^{A} f^{(3,1)}(r_{II}),$$

and the triplet correlation operator $F_T$ is written as:

$$F_T = \prod_{i<j<k}^{A} e^{-q_{ijk}/2} \prod_{i<j}^{A} e^{-q_{iij}/2},$$

with

$$q_{\alpha jk} = \sum_{cyc} \xi(r_{\alpha j}) \xi(r_{\alpha k}) r_{\alpha j} \cdot r_{\alpha k}.$$
To calculate the chemical potential of the $^4$He impurity, the expectation value of the Hamiltonian with respect to $\Psi_v(k)$ is given by

$$E^v(k) = E_0^v + \frac{\langle \Psi_0 | \rho_B [H, \rho_B] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (11)$$

where $E_0^v = \langle \Psi_0 | H | \Psi_0 \rangle$. In this case, the $^4$He effective mass is equal to the bare mass, pointing to an excessively simple choice for the excitation operator.

A better ansatz is given by $\Psi_v(k)$ of Eq. (1) which explicitly contains backflow correlations between the impurity and the $^3$He atoms. In particular, the backflow correlation operator has been taken of the form

$$F_B = \prod_i \exp \left[ i k \cdot r_I \eta(r_{Ii}) \right] \quad (13)$$

As the interatomic potential depends only on the relative distance between the atoms, it commutes with $\rho_B(k)$. Therefore, in Eq. (11) it is only necessary to consider the commutator with the kinetic energy operator. After some integration by parts, a generic contribution of the kinetic energy operator to Eq. (11) may be expressed through the following relation:

$$X_\alpha = \frac{\langle \Psi_0 | \rho_B [\nabla_\alpha, \rho_B] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = X_\alpha^\rho + X_\alpha^\phi \quad (14)$$

with

$$X_\alpha^\rho = -\frac{\langle \Psi_0 | \left( \nabla_\alpha \rho_B \right) \left( \nabla_\alpha \rho_B \right) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (15)$$

and

$$X_\alpha^\phi = \frac{\langle \phi | (F_J F_T)^2 \rho_B \left( \nabla_\alpha \rho_B \right) | \phi \rangle}{\langle \Psi_0 | \Psi_0 \rangle} - \frac{\langle \phi | \nabla_\alpha \rho_B \left( \nabla_\alpha \rho_B \right) \left( F_J F_T \right)^2 | \phi \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad (16)$$

where the subscript $\alpha$ labels the generic particle. The arrows indicate in which direction (right or left) the derivatives are acting.

The first term $X_\alpha^\rho$ is analogous to the expression obtained in the case of the $^3$He impurity in liquid...
The second one $X_α^φ$ directly originates from the Fermi character of the $^3$He medium, as it comes from the kinetic energy operator acting on the Slater determinant $φ$. Clearly, $α = I$ does not contribute to $X_α^φ$. Moreover, by inspecting the cluster expansion of $X_α^φ$, it results to be strictly zero. In fact, for direct cluster terms, where the $α$–particle is not exchanged, each of the two pieces of $X_α^φ$ is zero, after summing over the momentum carried by $α$. Terms in which $α$ is exchanged cancel because each of them gives the same contribution in both pieces.

The explicit expression for the impurity single–particle excitation energy, measured with respect to the $^4$He chemical potential, is then

$$\varepsilon_k = E^v(k) - E_0^v = \frac{\hbar^2 k^2}{2m_4} \left[1 + e_2 + \frac{m_4}{\mu} e_m + e_3\right], \quad (17)$$

where

$$e_2 = \rho \int d\mathbf{r}_{ij} g_{ij}^{(2)} \left(2\eta_{ij} + \frac{2}{3} r_{ij}\eta_{ij}'\right), \quad (18)$$

$$e_m = \rho \int d\mathbf{r}_{ij} g_{ij}^{(2)} \left[\eta_{ij}^2 + \frac{1}{3} (r_{ij}(\eta_{ij}')^2 + 2\eta_{ij} r_{ij}\eta_{ij}')\right], \quad (19)$$

and

$$e_3 = \rho^2 \int d\mathbf{r}_{ij} d\mathbf{r}_{ik} g_{ijk}^{(3)} \left[\eta_{ij}\eta_{ik}\right.$$

$$+ \frac{1}{3} (r_{ij}\eta_{ij}'\eta_{ik}' r_{ik} (\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{r}}_{ik})^2 + 2\eta_{ij} \eta_{ik}' r_{ik})\left] \right. \quad (20)$$

$\mu$ is the reduced mass ($\mu^{-1} = m_3^{-1} + m_4^{-1}$) and $g_{ij}^{(2)}$ and $g_{ijk}^{(3)}$ are the two– and three–body distribution functions between the impurity and the $^3$He atoms of the medium. They are the only quantities carrying information about the antisymmetry of the $^3$He bulk. It is worthwhile to remind that, by changing $m_4$ with $m_3$ in Eq. (17), one recovers the expression for the reverse problem of one $^3$He impurity in liquid $^4$He (Eq. 2.26 of Ref. 8), with the obvious substitution of the appropriate distribution functions.

All the calculations presented in this paper have been performed in the framework of the so called Average Correlation Approximation (ACA). In this approximation one considers the same dynamical correlation functions for all the pairs and triplets in the system, not distinguishing between the two isotopes. This assumption relies on the fact that the interatomic potential is the same for all the pairs. The drawbacks of the ACA in the evaluation of the chemical potential of the $^4$He impurity have been extensively discussed in Ref. 5.

We have used the interatomic Aziz potentials and the two–body correlation factor $f(r)$ has been taken of the McMillan type.

$^4$He. $^3$He
The variational parameter $b$ has been fixed by means of a numerical minimization of the energy of pure liquid $^3$He. The value $b = 1.15 \sigma$ ($\sigma = 2.556$ Å), determined at the $^3$He experimental equilibrium density ($\rho_{0}^{\exp} = 0.277$ $\sigma^{-3}$), has been used for all the densities. The function $\xi(r)$ of the triplet correlation (10) has the same parametrized form used in pure phase calculations:

$$\xi(r) = \sqrt{\lambda_t} \exp \left[ -\left( \frac{r - r_t}{\omega_t} \right)^2 \right].$$  \hspace{1cm} (22)

The density dependence of the triplet variational parameters is neglected and the optimum values at $\rho_{0}^{\exp}$ have been used everywhere. These values are $\lambda_t = -0.75 \sigma^{-2}$, $r_t = 0.85 \sigma$ and $\omega_t = 0.45 \sigma$.

The distribution functions have been computed by using the Fermi HyperNetted Chain (FHNC) technique, in the so called FHNC/S(T) approximation ( and triplet) contributions. As reported in Ref. 5, the chemical potential provided by the variational wave function $\Psi_0$, at the FHNC/ST saturation density ($\rho = 0.252$ $\sigma^{-3}$), is $-6.60$ K.

The function $\eta(r)$ (13), adopted for the backflow correlation, is of the form:

$$\eta(r) = A_0 \exp \left[ -\left( \frac{r - r_0}{\omega_0} \right)^2 \right].$$  \hspace{1cm} (23)

In our case, the backflow parameters $A_0 = 0.2$, $r_0 = 0.8 \sigma$ and $\omega_0 = 0.375 \sigma$, taken from Ref. 13, are used at all the densities.

As the single–particle spectrum (17) is quadratic in $k$, the effective mass is given by

$$\left( \frac{m^*_4}{m_4} \right)^{[\beta]} = \frac{1}{1 + e_2 + (m_4/\mu) e_m + e_3^3},$$ \hspace{1cm} (24)

where $\beta$ labels the approximation used in evaluating the three–body distribution function.

Table I reports the effective mass obtained at the experimental equilibrium density $\rho_{0}^{\exp}$ in different approximations. Also given is the value of the two–body contribution ($m_4^*/m_4$)$^{[2]}$, i.e. taking $e_3^3 = 0$ in Eq. (24).

The Jastrow (FHNC/S) and the Jastrow plus Triplet correlation (FHNC/ST) models give nearly the same results. The three-body distribution function has been evaluated in the Kirkwood superposition approximation (KSA), in the convolution approximation (CA) and including the Abe terms (KSA+ABE). As shown in the Table, the three different approximations to $g_{1jk}^{(3)}$ give very close results.

The effective mass at $\rho_{0}^{\exp}$ in FHNC/ST, with the inclusion of the Abe diagrams, turns out to be 1.21. This
result is in very good agreement with the most recent experimental determination $m_4^*/m_4 = (1.1 + 0.4/ - 0.1)$.

As it has been pointed out by Leggett, the effective mass of one impurity in a Fermi liquid is always larger than the bare mass. In FHNC/ST, $e_2 = -0.37$, $e_m = 0.08$ and the three–body term (20), in all approximations, is very small, $e_3 \simeq 0.01$. Therefore, the denominator of Eq. (24) is smaller than unity, providing an effective mass larger than one.

The HNC/S results have been obtained by setting $\phi_0 = 1$ in the wave function, i.e. by treating the $^3$He as a bosonic fluid. The comparison with the FHNC/S results indicates that, at this density, the influence of the Fermi character of the medium on the calculation of the effective mass of the impurity is nearly negligible.

The density dependence of the calculated effective mass is reported in Table II and it is also shown in Fig. 1 (full triangles). As one can see, the effective mass increases linearly with density.

It is also interesting to compare our results for $m_4^*/m_4$ with the effective mass of one $^3$He impurity in liquid $^4$He. As there are not exchange or spin correlations between the two isotopes, one expects the effective mass to be driven mainly by the density. To deeper explore this hypothesis we have plotted in Fig. 1 the density dependence of the effective mass of a $^3$He impurity in liquid $^4$He, for both the experimental data (full circles) and the theoretical estimates, obtained by using backflow correlations (empty circles). The density dependence is in both cases approximately linear. Although the slopes are different, the extrapolated values of $m_3^*/m_3$, at the $^3$He saturation density, are similar and close to the present evaluation of $m_4^*/m_4$. As it has been mentioned before, by taking the proper mass factor $m_3/\mu$ in front of $e_m$, Eq. (17) is approximately valid for one $^3$He impurity in liquid $^4$He, since the differences in the distribution functions in the two cases are small. In fact, if one performs a calculation at $\rho_0^{exp}$ using the mass factor $m_3/\mu$, then the HNC/ST result (shown by an open diamond in Fig. 1) coincides with the backflow extrapolated value. The small difference between this value and the proper result (full triangle) of $m_4^*/m_4$ arises almost completely from the different mass factors in front of $e_m$. The difference practically coincides with the estimate

$$\Delta \left( \frac{m_4^*}{m_4} \right) = \frac{1}{1 + e_2 + (m_3/\mu) e_m + e_3} - \frac{1}{1 + e_2 + (m_4/\mu) e_m + e_3} = 0.073,$$

obtained by considering the same distribution functions in the two systems. Assuming a linear extrapolation, the experimental value for $m_3^*/m_3$ (solid line) is close to the backflow extrapolation (long–dashed line) at $\rho_0^{exp}$, pointing out that possible perturbative corrections, beyond the backflow terms, are small at this low density. These corrections have been evaluated in Correlated Basis Function theory (CBF) for $m_4^*/m_3$ in $^4$He. They result to be
about 0.5 at the $^4$He saturation density ($\rho = 0.365 \sigma^{-3}$) and rapidly decreasing with the density. It is worthwhile to notice that the effective mass of a $^3$He atom at the Fermi surface of pure $^3$He ($m^*/m = 2.8$) is much larger than the effective mass of the $^4$He impurity. The statistics and the spin effects, which are suppressed in the case of the $^4$He impurity, appear to be the main responsible for this difference.

To briefly summarize, we have calculated the effective mass of one $^4$He impurity in liquid $^3$He by using backflow correlations. These correlations provide for an accurate description of the $^4$He impurity spectrum at low momenta. Our results support the new experimental determination of Edwards et al.\textsuperscript{1} and are far from the previous result of Laheurte and Saam.\textsuperscript{3,4}

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FIG. 1. Density dependence of the impurity effective mass. Full and open circles are respectively the experimental data and the backflow results for \( m_3^*/m_3 \). The open diamond is the backflow result for \( m_3^*/m_3 \) at \( \rho_0^{exp} \), indicated by an arrow. The full triangles are the backflow results for \( m_4^*/m_4 \). The experimental result is plotted as a full diamond with its error bar. The lines are linear fits to the corresponding points.

**TABLE I.** \(^4\)He effective mass at \( \rho_0^{exp} = 0.277 \) \( \sigma^{-3} \) in different approximations.

| \( m_i^*/m_i \) | HNC/S | FHNC/S | FHNC/ST |
|-----------------|-------|--------|---------|
| \([m_3^*/m_3]^{[2]}\) | 1.209 | 1.221  | 1.225   |
| \([m_3^*/m_3]^{[KS\,A]}\) | 1.197 | 1.208  | 1.213   |
| \([m_3^*/m_3]^{[CA]}\) | 1.187 | 1.196  | 1.200   |
| \([m_3^*/m_3]^{[KS\,A\,+\,ABE]}\) | 1.197 | 1.206  | 1.210   |

**TABLE II.** \(^4\)He effective mass as a function of density in FHNC/ST approximation.

| \( \rho(\sigma^{-3}) \) | 0.253 | 0.277 | 0.300 | 0.330 |
|------------------------|-------|-------|-------|-------|
| \( m_i^*/m_i \) | 1.20  | 1.22  | 1.25  | 1.28  |
| \([m_3^*/m_3]^{[KS\,A\,+\,ABE]}\) | 1.19  | 1.21  | 1.23  | 1.26  |