

Effective mass of one ^4He atom in liquid ^3He

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A microscopic calculation of the effective mass of one ^4He impurity in homogeneous liquid ^3He 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 ^4He atom and the particles in the medium. The effective mass at equilibrium 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, Petersen, and Culman¹ have used the Zharkov-Silin Fermi liquid theory of dilute solutions of ^4He in normal liquid ^3He to determine the chemical potential (μ_4) and the effective mass (m_4^*) for the limiting case of one ^4He impurity. The experimental input data for this analysis were the recent low-temperature measurements of the phase separation by Nakamura *et al.*² The same theory was previously applied to older experimental data by Laheurte and Saam,^{3,4} and their predictions for μ_4 and m_4^* differ notably from those of Ref. 1. At zero pressure, Edwards, Petersen, and Culman report $\mu_4=-6.95$ K and $m_4^*/m_4=1.1$,¹ whereas $\mu_4=-6.60$ K and $m_4^*/m_4=4.5$ in Refs. 3 and 4. The disagreement was attributed to the fact that the validity of the Fermi liquid theory is ensured at temperatures below 0.1 K,¹ while the results of Refs. 3 and 4 were obtained from experimental data at $T\geq 0.5$ K. Although the difference between the two experimental values of μ_4 is rather small, our recent microscopic calculations⁵ seem to support the more strongly bound result of Edwards, Petersen, and Culman. 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 ^4He impurity in liquid ^3He using a trial wave function of the type

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

where Ψ_0 is the ground-state wave function of the ^3He medium plus one ^4He atom and $\rho_B(\mathbf{k})$ is an excitation operator defined as

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

where $\rho_I(\mathbf{k}) = \exp(i\mathbf{k}\cdot\mathbf{r}_I)$ describes the impurity travelling through the medium as a plane wave of momentum \mathbf{k} and the correlation operator

$$F_B = \prod_{i=1}^A f_B(\mathbf{k}, \mathbf{r}_{iI}) \quad (3)$$

incorporates backflow correlations between the impurity I (^4He atom) and the A ^3He atoms of the bulk. Backflow correlations have proved to be relevant for a realistic study of the effective mass of one ^3He impurity in liquid ^4He .⁶⁻⁸ They play also an important role in the evaluation of the binding energy of pure ^3He .^{9,10}

The Hamiltonian of the system is written as

$$H(A+1) = H(A) + H_I(A+1), \quad (4)$$

where

$$H(A) = -\frac{\hbar^2}{2m_3} \sum_{i=1}^A \nabla_i^2 + \sum_{i<j} V(r_{ij}) \quad (5)$$

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

$$H_I(A+1) = -\frac{\hbar^2}{2m_4} \nabla_I^2 + \sum_{i=1}^A V(r_{iI}) \quad (6)$$

are additional terms related to the impurity.

The variational approach starts with the choice of the trial wave function Ψ_0 . As in our previous paper,⁵ we take an extended Jastrow-Slater wave function for the $A+1$ particles:

$$\Psi_0 = F_J F_T \phi(1, \dots, A), \quad (7)$$

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

$$F_J = \prod_{i < j}^A f^{(3,3)}(r_{ij}) \prod_{i=1}^A f^{(3,I)}(r_{iI}), \quad (8)$$

and the triplet correlation operator F_T is written as

$$F_T = \prod_{i < j < k}^A \exp[-q_{ijk}^{(3,3,3)}/2] \prod_{i < j}^A \exp[-q_{ijk}^{(I,3,3)}/2], \quad (9)$$

with

$$q_{\alpha jk}^{(\alpha,3,3)} = \sum_{\text{cyc}} \xi^{(\alpha,3)}(r_{\alpha j}) \xi^{(\alpha,3)}(r_{\alpha k}) \mathbf{r}_{\alpha j} \cdot \mathbf{r}_{\alpha k}. \quad (10)$$

Here, \sum_{cyc} denotes a summation on the cyclic permutations of the indices α, j, k , where the index α may either represent a ^3He atom or the ^4He impurity. The triplet correlations have been found to be very important to properly describe the equation of state of the pure phase⁹⁻¹¹ and to calculate the chemical potential of the ^4He impurity.⁵

The expectation value of the Hamiltonian with respect to $\Psi_v(\mathbf{k})$ is given by

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

where we have taken advantage of the unitary character of the excitation operator $\rho_B(\mathbf{k})$. If one ignores backflow correlations between the impurity and the medium, by assuming $\rho_B(\mathbf{k}) = \rho_I(\mathbf{k})$, a simple parabolic spectrum for $E^v(k)$ is obtained:

$$E^v(k) = E_0^v + \frac{\hbar^2 k^2}{2m_4}, \quad (12)$$

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

A better ansatz is given by $\Psi_v(\mathbf{k})$ of Eq. (1) which explicitly contains backflow correlations between the impurity and the ^3He atoms. In particular, the backflow correlation operator has been taken of the form^{7,8}

$$F_B = \prod_{i=1}^A \exp[i\mathbf{k} \cdot \mathbf{r}_{Ii} \eta(r_{Ii})]. \quad (13)$$

As the interatomic potential depends only on the relative distance between the atoms, it commutes with $\rho_B(\mathbf{k})$. 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:

$$X_\alpha = \frac{\langle \Psi_0 | \rho_B^\dagger [\nabla_\alpha^2, \rho_B] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = X_\alpha^\rho + X_\alpha^\phi, \quad (14)$$

with

$$X_\alpha^\rho = - \frac{\langle \Psi_0 | (\vec{\nabla}_\alpha \rho_B^\dagger) (\vec{\nabla}_\alpha \rho_B) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (15)$$

and

$$X_\alpha^\phi = \frac{\langle \phi | (F_J F_T)^2 \rho_B^\dagger (\vec{\nabla}_\alpha \rho_B) \vec{\nabla}_\alpha | \phi \rangle}{\langle \Psi_0 | \Psi_0 \rangle} - \frac{\langle \phi | \vec{\nabla}_\alpha \rho_B^\dagger (\vec{\nabla}_\alpha \rho_B) (F_J F_T)^2 | \phi \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (16)$$

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

The term X_α^ρ (15) is analogous to the expression obtained in the case of the ^3He impurity in liquid ^4He .^{7,8} The second one directly originates from the Fermi character of the ^3He medium, as it comes from the kinetic energy operator acting on the Slater determinant ϕ . Clearly, $\alpha = I$ 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 ^4He 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

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

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

and

$$e_3 = \rho^2 \int d\mathbf{r}_{Ij} d\mathbf{r}_{Ik} g_{Ijk}^{(3)} \{ \eta_{Ij} \eta_{Ik} + \frac{1}{3} [r_{Ij} \eta'_{Ij} \eta'_{Ik} r_{Ik} (\hat{\mathbf{r}}_{Ij} \cdot \hat{\mathbf{r}}_{Ik})^2 + 2\eta_{Ij} \eta'_{Ik} r_{Ik}] \}. \quad (20)$$

μ 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 ^3He atoms of the medium. They are the only quantities carrying information about the antisymmetry of the ^3He 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 ^3He impurity in liquid ^4He [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 inter-

atomic potential is the same for all the pairs. The slight drawbacks of the ACA in the evaluation of the chemical potential of the ^4He impurity have been extensively discussed in Ref. 5. In the present problem, corrections to the ACA are expected to be even lower than in the calculation of the chemical potential because their influence is reduced to small changes in the distribution functions [Eqs. (17)–(20)].

We have used the interatomic Aziz potential¹² and the two-body correlation factor $f(r)$ has been taken of the McMillan type:

$$f(r) = \exp\left[-\frac{1}{2}\left(\frac{b}{r}\right)^5\right]. \quad (21)$$

The variational parameter b has been fixed by means of a numerical minimization of the energy of pure ^3He liquid. The value $b=1.15\sigma$ ($\sigma=2.556\text{ \AA}$), determined at the ^3He experimental equilibrium density ($\rho_0^{\text{expt}}=0.277\sigma^{-3}$), 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:^{9–11}

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

The density dependence of the triplet variational parameters is neglected and the optimum values at ρ_0^{expt} have been used everywhere. These values are $\lambda_t=-0.75\sigma^{-2}$, $r_t=0.85\sigma$ and $\omega_t=0.45\sigma$.¹³

The distribution functions have been computed by using the Fermi hypernetted chain (FHNC) technique, in the so-called FHNC/S(T) approximation⁹ to take into account the elementary diagram (and triplet) contributions. As reported in Ref. 5, the chemical potential provided by the variational wave function Ψ_0 , at the FHNC/ST equilibrium density ($\rho_0=0.252\sigma^{-3}$), is -6.60 K .

The function $\eta(r)$ (13), adopted for the backflow correlation, is of the form^{7–10,13}

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

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

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

where β labels the approximation used in evaluating the three-body distribution function.

Table I reports the effective mass obtained at the experimental equilibrium density ρ_0^{expt} in different approximations. Also given is the value of the two-body contribution $(m_4^*/m_4)^{[2]}$, i.e., taking $e_3^\beta=0$ 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

TABLE I. ^4He effective mass at $\rho_0^{\text{expt}}=0.277\sigma^{-3}$ in different approximations.

	HNC/S	FHNC/S	FHNC/ST
$(m_4^*/m_4)^{[2]}$	1.209	1.221	1.225
$(m_4^*/m_4)^{[\text{KSA}]}$	1.197	1.208	1.213
$(m_4^*/m_4)^{[\text{CA}]}$	1.187	1.196	1.200
$(m_4^*/m_4)^{[\text{KSA+ABE}]}$	1.197	1.206	1.210

terms (KSA+ABE).⁹ As shown in the table, the three different approximations to $g_{ijk}^{(3)}$ give very close results.

The effective mass at ρ_0^{expt} 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 $m_4^*/m_4=(1.1+0.4/-0.1)$.¹ As it has been pointed out by Leggett,¹⁴ 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, $e_3^\beta\approx 0.01$. 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 $\phi=1$ in the wave function, i.e., by treating the ^3He 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 ^3He impurity in liquid ^4He . As there are no 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 ^3He impurity in liquid ^4He , for both the experimental data (full circles)¹⁵ and the theoretical estimates, obtained by using backflow correlations (empty circles).⁸ The density dependence is in both cases approximately linear. Although the slopes are different, the extrapolated values of m_3^*/m_3 , at the ^3He equilibrium 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/μ in front of e_m , Eq. (17) is approximately valid for one ^3He impurity in liquid ^4He , since the differences in the distribution functions in the two cases are small.¹⁶ In fact, if one performs a calculation at ρ_0^{expt} using the mass factor m_3/μ , then the HNC/ST result (shown by an open diamond in Fig. 1) coincides with the backflow extrapolated value. The small differ-

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

$\rho(\sigma^{-3})$	0.253	0.277	0.300	0.330
$(m_4^*/m_4)^{[2]}$	1.20	1.22	1.25	1.28
$(m_4^*/m_4)^{[\text{KSA+ABE}]}$	1.19	1.21	1.23	1.26

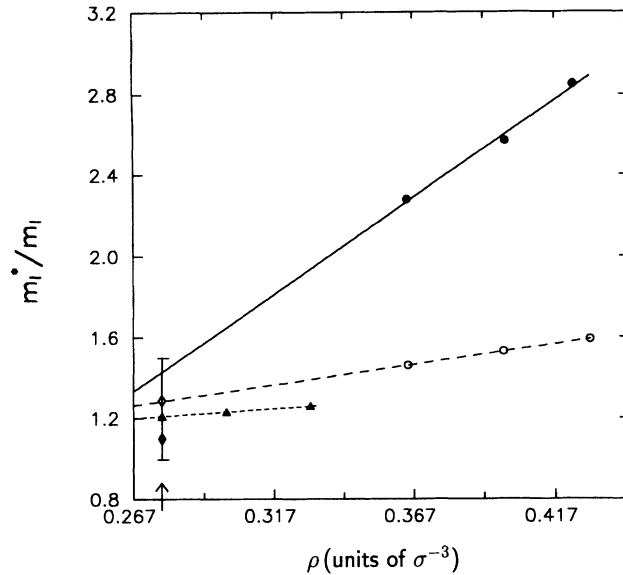


FIG. 1. Density dependence of the impurity effective mass. Full and open circles are, respectively, the experimental data and the backflow results for m_3^*/m_3 . The open diamond is the backflow result for m_3^*/m_3 at ρ_0^{expt} , indicated by an arrow. The full triangles are the backflow results for 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.

ence 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

$$\Delta\left(\frac{m_4^*}{m_4}\right) = \frac{1}{1 + e_2 + (m_3/\mu) e_m + e_3} - \frac{1}{1 + e_2 + (m_4/\mu) e_m + e_3} = 0.073, \quad (25)$$

obtained by assuming 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 ρ_0^{expt} , pointing out that possible perturbative corrections, beyond the backflow terms, are small at this low density. These corrections have been evaluated⁸ in correlated basis function theory (CBF) for m_3^*/m_3 in ^4He . They result to be about 0.5 at the ^4He equilibrium density ($\rho=0.365 \sigma^{-3}$) and they rapidly decrease with the density.

It is worthwhile to notice that the effective mass of a ^3He atom at the Fermi surface of pure ^3He ($m^*/m=2.8$) (Ref. 17) is much larger than the effective mass of the ^4He impurity. The statistics and the spin effects, which are suppressed in the case of the ^4He impurity, appear to be mainly responsible for this difference.

To briefly summarize, we have calculated the effective mass of one ^4He impurity in liquid ^3He by using backflow correlations. These correlations provide for an accurate description of the ^4He impurity spectrum at low momenta. Our results support the experimental determination of Edwards, Petersen, and Culman¹ and are far from the previous result of Laheurte and Saam.^{3,4}

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