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# Effective Mass of $^3$He in Liquid $^4$He†

V. R. Pandharipande* and Naoki Itoh
*Department of Physics, University of Illinois, Urbana, Illinois 61801*
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The Jastrow wave function with relative angular-momentum-dependent correlation functions, is shown to give the back flow of $^4$He around the $^3$He impurity. Variational calculations with these wave functions and the Lennard-Jones (6, 12), and Bruch-McGee-2 potentials respectively give $m^* = 2.1 m_3$ and $2.25 m_3$. A simple density dependence of $m^*$ is discussed.

## I. INTRODUCTION

Within the Jastrow approximation "that correlations between more than two particles can be represented by a product of two-particle correlation functions," the wave function

$$\Psi(k_j) = \prod_m f_{jm} \prod_{m<n} f_{mn} e^{i\vec{k}_j \cdot \vec{r}_j} \tag{1.1}$$

describes the state of one $^3$He quasiparticle (denoted by $j$) in liquid $^4$He. The effective mass of $^3$He is then given by

$$\frac{\partial}{\partial k_j} \left( \frac{\langle \Psi(k_j)|H|\Psi(k_j)\rangle}{\langle \Psi(k_j)|\Psi(k_j)\rangle} \right) = \frac{\hbar^2 k_j}{m^*}, \tag{1.2}$$

where

$$H = \sum_\alpha \frac{-\hbar^2}{2m_\alpha} \nabla_\alpha^2 + \frac{1}{2} \sum_{\alpha,\beta} v_{\alpha\beta} \tag{1.3}$$

(subscripts $\alpha$, $\beta$ refer to all particles).

Previous calculations[1,2] of $m^*$ initially assume that $f_{jm}$ is real, spherically symmetric, and independent of $k_j$. In this case the $\nabla_j \phi_j \cdot \nabla_j f_{jm}$ term,

$$\phi_j = e^{i\vec{k}_j \cdot \vec{r}_j}, \tag{1.4}$$

is zero, and $k_j^2 \hbar^2 / 2m_3$ is the only term in energy expectation value that depends on $k_j$. This term is obtained by operating $\nabla_j^2$ on $\phi_j$, and gives $m^* = m_3$. It was then argued that (1.1) is too simple, and does not incorporate the backflow of $^4$He; the authors[1,2] improved upon it by perturbative methods in first order.

Pandharipande[3] has calculated the $f_{jm}$ variationally, including the $\nabla_j \phi_j \cdot \nabla_j f_{jm}$ term. These $f_{jm}$ are complex and $k$ dependent. In Sec. II we show that (i) they incorporate the backflow of $^4$He, and (ii) at small $k_j$ the $\nabla_j \phi_j \cdot \nabla_j f_{jm}$ term gives an attractive contribution proportional to $k_j^2$. Section III reports a calculation of $m^*$ with the methods developed by Pandharipande and Bethe[4] (PB) to calculate the expectation values in (1.2).

## II. PROPERTIES OF $f$

The $f$ are calculated with the constraint $f = 1$ for $r > d$ and $\nabla f(d) = 0$, by minimizing the two-body term in the cluster expansion of (1.2). The healing distance $d$ is subsequently taken to be so large that the effects of the constraint are negligible. PB have shown that with these $f$ the two-body term dominates. Its contribution from the correlation volume ($r < d$) is

$$\frac{1}{\Omega} \int_0^d \psi^* \left( v - \frac{\hbar^2}{m} (k^2 + \nabla^2) \right) \psi \, d^3 r, \tag{2.1}$$

where

$$k = k_j m_4 / (m_3 + m_4), \tag{2.2}$$

$$m = m_3 m_4 / (m_3 + m_4), \tag{2.3}$$

and formally

$$\psi = f\phi = f e^{i\vec{k}\cdot\vec{r}}. \tag{2.4}$$

The $\psi$ is decomposed into partial waves,

$$\psi = \sum_{l=0}^{\infty} i^l (2l+1) U_l(r) P_l(\cos\theta), \tag{2.5}$$

where $\theta$ is the angle between $\vec{r}$ and $\vec{k}$. The contribution of each partial wave is minimized separately to obtain the "Schrődinger equation"

$$-\frac{\hbar^2}{m} \left( \frac{\partial^2 u_l}{\partial r^2} + \frac{l(l+1)}{r^2} u_l \right) + v u_l = \left( \frac{\hbar^2}{m} k^2 + \lambda^l(k) \right) u_l, \tag{2.6}$$

with

$$u_l = U_l(r) r.$$

The $\lambda^l(k)$ are determined from the boundary conditions on $f$.

It is convenient here to define $l$-dependent correlation functions $f_l$:

$$f_l = U_l / J_l, \tag{2.7}$$

where $J_l$ are spherical Bessel functions in the expansion of $\phi$,

$$\phi = \sum_{l=0}^{\infty} i^l (2l+1) J_l(kr) P_l(\cos\theta). \tag{2.8}$$

The $f$ is complex:

$$f = f_r + i f_i \tag{2.9}$$

(we use subscripts $r$ and $i$ to denote the real and imaginary parts) and

$$f_r = \psi_i \phi_i + \psi_r \phi_r ,\quad f_i = \psi_i \phi_r - \phi_i \psi_r . \tag{2.10}$$

The $\phi_i$ and $\psi_i$ have odd parity, while that of $\phi_r$ and $\psi_r$ is even. Thus we obtain

$$f_r(\vec{r}) = f_r(-\vec{r}) \quad \text{and} \quad f_i(\vec{r}) = -f_i(-\vec{r}). \tag{2.11}$$

In the limit of small $k$ the $J_l$ can be expanded in powers of $kr$, and only $l=0$ and 1 need be considered. This gives

$$f_r = f_0(r) + \text{ terms involving } k^2$$

and

$$f_i = kr \cos\theta[f_1(r) - f_0(r)] + \cdots . \tag{2.12}$$

The $f_0$ and $f_1 - f_0$ at small $k$ are shown in Fig. 1.

The wave function (1.1) is now

$$\Psi(k_j) = e^{i\vec{k}_j\cdot\vec{r}_j} \prod_m \left(f_0(r_{jm}) + i\vec{k}_j\cdot\vec{r}_{jm}[f_1(r_{jm}) - f_0(r_{jm})]\frac{m_4}{m_3+m_4}\right) \prod_{m<n} f_{mn} , \tag{2.13}$$

and it resembles the Feynman-Cohen[5] wave function

$$\Psi_{\rm FC}(k_j) = \exp\left(i\vec{k}_j\cdot\vec{r}_j + i\sum_m \vec{k}_j\cdot\vec{r}_j\,\chi(r_{jm})\right)\Psi_0, \tag{2.14}$$

provided that

$$\Psi_0 \simeq \prod_{\alpha<\beta} f_{\alpha\beta} \tag{2.15}$$

and the exponential in (2.14) is expanded using the smallness of $k_j$. The imaginary part of $f_{jm}$ gives a current corresponding to the backflow of $^4$He atoms around the $^3$He impurity with a velocity proportional to $k_j$.

The first term of

$$-(\hbar^2/m)\phi^* f^* \nabla\phi\cdot\nabla f = (\hbar^2/m)[-i\vec{k}\cdot(f_r\nabla f_r + f_i\nabla f_i) + \vec{k}\cdot(f_r\nabla f_i - f_i\nabla f_r)] \tag{2.16}$$

gives zero contribution, while that of the second is attractive and proportional to $k^2$. Thus this term increases the effective mass of the $^3$He impurity.

The effect of the mass difference in $^3$He and $^4$He is automatically included in these $f$. The $f_{mn}$ ($^4$He-$^4$He correlation functions) are calculated with reduced mass $\frac{1}{2}m_4$ instead of that given by (2.3).

## III. CALCULATIONS AND RESULTS

PB write the energy expectation value in (1.1) as

$$E(k_j) = W + U + (\hbar^2/2m_3)k_j^2 , \tag{3.1}$$

$$W = \frac{1}{2\Omega}\sum_{\alpha<\beta}\int V_{\alpha\beta}g_{\alpha\beta}\,d^3r , \tag{3.2}$$

and

$$U = -\frac{1}{\Omega^2}\sum_{\alpha\beta\gamma}\frac{\hbar^2}{2m_\alpha}\int g_3(\vec{r}_{\alpha\beta}, \vec{r}_{\alpha\gamma}) \times \frac{\nabla_\alpha f_{\alpha\beta}\cdot\nabla_\alpha f_{\alpha\gamma}}{f_{\alpha\beta}f_{\alpha\gamma}}\,d^3r_{\alpha\beta}\,d^3r_{\alpha\gamma} . \tag{3.3}$$

The notation here is identical to that in PB, $g_{\alpha\beta}$ being the pair-correlation function and $\Omega$ the normalization volume. The $g$ is calculated by a hypernetted-chain equation which is shown to be fairly accurate when used with the present correlation functions and the energy expression (3.1). It is noted that the angle average of $f^2_{mj}(k, r)$ is relatively insensitive to $k$, and hence to the contribution of the chains, and the $U$ can be calculated from $f_0(r)$. This corresponds to neglecting terms with $(f_1 - f_0)^2$ in many-body ($\geq 3$) clusters. In this approximation the only terms depending on $k_j$ are

$$E(k_j) = (\hbar^2/2m_3)k_j^2 + \rho\int V_{jm}g_{jm}\,d^3r_{jm} + \text{const}, \tag{3.4}$$

where $\rho$ is the $^4$He density,

$$V_{jm}(r<d) = \lambda^l(k)P^l ,\quad V_{jm}(r>d) = v(r), \tag{3.5}$$

and

$$g_{jm}(r) = h\, f_l^2(k, r)P^l . \tag{3.6}$$

The $P^l$ are angular-momentum projection operators, and $(h-1)$ is the contribution of the chains. The integral in (3.4) can be expanded in powers of $k$:

$$\int V_{jm}g_{jm}\,d^3r_{jm} = a + bk^2 + \cdots \tag{3.7}$$

(note that there is no term linear in $k$), and

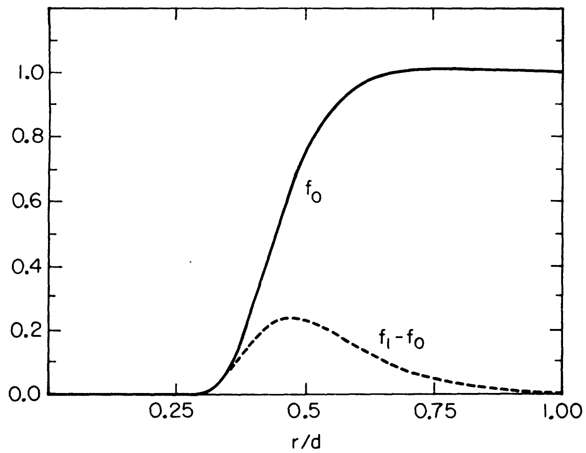


FIG. 1. $f_0$ and $f_1-f_0$ at $d=2.6\ r_0$.

$$\frac{m^*}{m_3}=\frac{\hbar^2/2m_3}{(\hbar^2/2m_3)+[bm_4^2\rho/(m_3+m_4)^2]}\ . \tag{3.8}$$

The $m^*$ is calculated at various values of $d$ ranging from $2r_0$ to $3r_0$, where $r_0$ is the unit radius,

$$\tfrac{4}{3}\pi\rho r_0^3=1\ . \tag{3.9}$$

It is very insensitive to $d$ for $d>2.4\ r_0$, and increases by a few percent as $d$ is increased from 2 to $2.4\ r_0$.

The dominant contribution to $m^*$ comes from the lowest-order two-body clusters ($g_{jm}=f_{jm}^2$). The chains reduce $m^*$ by only $\simeq$10%, and hence they are calculated by neglecting the difference in $f_0(r)$ between $^3$He-$^4$He and $^4$He-$^4$He pairs.

If the effect of the chains is neglected the $b$ is independent of $\rho$, and the $m^*$ obeys the approximate relation

$$m^*/m_3 \simeq 1/(1+c\rho)\ , \tag{3.10}$$

where $c$ is a negative constant. Such a relation could also be suggested from the observed rapid increase of the effective mass of $^3$He in liquid $^3$He from $3.1m_3$ to $5.8m_3$ with a density change from 0.27 to $0.38/\sigma^3$. However, there are exchange contributions in $^3$He (also, the relative $k$ are not small due to Fermi momentum), and hence Eq. (3.7) is not justified.

The $m^*$ values obtained for the Lennard-Jones (6, 12), and Bruch-McGee-2 (BM2) potentials[4] are, respectively, $2.1m_3$ and $2.25m_3$. These should be compared with the experimental value of $2.34m_3$.[6] The perturbative calculations give 2.37,[1] and 2.8,[2] while Feynman and Cohen[5] obtain $1.67m_3$ with classical backflow.

PB have already shown that the liquid-$^3$He energy can be lowered by ~0.6°K over that obtained with real spherically symmetric $f$, by using the state-dependent $f$. We hope that these correlation functions can also be used to calculate the Landau parameters in $^3$He liquid and dense neutron matter.

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