Concentration Dependence of the Effective Mass of ^{3}He Atoms in ^{3}He-^{4}He Mixtures

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Recent measurements by Yorozu *et al.* [S. Yorozu, H. Fukuyama, and H. Ishimoto, Phys. Rev. B **48**, 9660 (1993)] as well as by Simons and Mueller [R. Simons and R. M. Mueller, Czech. J. Phys. Suppl. **46**, 201 (1996)] have determined the effective mass of ^{3}He atoms in a ^{3}He-^{4}He mixture with great accuracy. We here report theoretical calculations for the dependence of that effective mass on the ^{3}He concentration. Using correlated basis function perturbation theory to infinite order to compute effective interactions in the appropriate channels, we obtain good agreement between theory and experiment. [S0031-9007(98)06235-8]

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The effective mass of a ^{3}He atom in liquid ^{4}He is due to two effects. The dominant one is hydrodynamic backflow of the ^{4}He liquid around the impurity [1,2]. This effect is largely independent of the ^{3}He concentration. The second effect is the dynamics imposed on the ^{3}He component by the Pauli principle [3]. This effect causes a noticeable concentration dependence which has recently been measured with high accuracy by Yorozu *et al.* [4] and by Simons *et al.* [5]; it is the subject of this paper.

Ground state properties of ^{3}He-^{4}He mixtures like the energetics of the system and its local structure are today quite well understood from a microscopic point of view [6]. For a microscopic understanding of the *hydrodynamic* effective mass, rather advanced methods are needed [7] due to the high density of the ^{4}He background. On the other hand, the ^{3}He component in the mixture is dilute, and the interaction between individual ^{3}He atoms is dominated by phonon exchange. Therefore, much simpler methods than those necessary [8] for obtaining reliable results in pure ^{3}He are adequate for calculating ground state properties of dilute mixtures [6].

Microscopic many-body theory postulates an empirical Hamiltonian

$$H = -\sum_\alpha \sum_{i=1}^{N_\alpha} \frac{\hbar^2}{2m_\alpha}\nabla^2_{i,\alpha} + \frac{1}{2}\sum_{\alpha\beta}\sideset{}{'}\sum_{i,j}^{N_\alpha,N_\beta} V(|\mathbf{r}_i^{(\alpha)} - \mathbf{r}_j^{(\beta)}|) \tag{1}$$

that contains only a two-body interaction [9] and the masses of the two types of particles. One then uses the Feenberg form [10,11] for the ground state wave function,

$$\begin{aligned}\Psi_0(\{\mathbf{r}_i^{(\alpha)}\}) &= e^{\frac{1}{2}U(\{\mathbf{r}_i^{(\alpha)}\})}\Phi_0(\{\mathbf{r}_i^{(3)}\}),\\ U(\{\mathbf{r}_i^{(\alpha)}\}) &= \frac{1}{2!}\sum_{\alpha\beta}\sideset{}{'}\sum_{i,j}^{N_\alpha,N_\beta} u^{\alpha\beta}(\mathbf{r}_i,\mathbf{r}_j)\\ &\quad + \frac{1}{3!}\sum_{\alpha\beta\gamma}\sideset{}{'}\sum_{i,j,k}^{N_\alpha,N_\beta,N_\gamma} u^{\alpha\beta\gamma}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k),\end{aligned} \tag{2}$$

where $\Phi_0(\{\mathbf{r}_i^{(3)}\})$ is a Slater determinant of plane waves ensuring the antisymmetry of the fermion component of the mixture. The superscripts $\alpha, \beta, \ldots$ refer to the type of correlated particles; the prime on the summation symbol in Eqs. (1) and (2) indicates that no two pairs (i,α), (j,β) can be the same. The correlation functions $u^{\alpha\beta}(\mathbf{r}_i,\mathbf{r}_j)$ and $u^{\alpha\beta\gamma}(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)$ are determined by the functional minimization of the ground state energy

$$E_0 = \langle\Psi_0|H|\Psi_0\rangle/\langle\Psi_0 \mid \Psi_0\rangle \tag{3}$$

with respect to the correlation functions [12–14]. Details of the procedure have been described in Ref. [6].

Within the above variational theory, the single particle excitation spectrum is calculated by allowing for an occupation of single particle orbitals n_k in the Slater function that is different from the fermion ground state $n_k^{(0)} = \theta(k_F - k)$, where k_F is the Fermi momentum of the ^{3}He component. The single particle spectrum can then be calculated, using the diagrammatic techniques of the (Fermi)-hypernetted chain [(F)HNC] theory [6], by

$$\epsilon^{(3)}(k) = \frac{\delta E_0}{\delta n_k} = t_3(k) + u(k) + U_0, \tag{4}$$

where we use $t_\alpha(k) = \hbar^2k^2/2m_\alpha$ for the kinetic energy of a free particle of species α. U_0 is a constant related to the chemical potential, and $u(k)$ a momentum dependent average field. The general graphical analysis of the variational single-particle field $u(k)$ has been carried out in Ref. [15]; if the ^{3}He component is dilute, the average field can be written in the form of a Hartree-Fock field in terms of a local, effective interaction $\tilde{W}_{\rm eff}(q)$

$$u(k) = -\int \frac{d^3q}{(2\pi)^3\rho_3}\, n_q^{(0)}\tilde{W}_{\rm eff}(|\mathbf{k} - \mathbf{q}|). \tag{5}$$

It is known [8] that the naive use of a variational wave function of the type (2) leads to an effective mass of *pure* ^{3}He that is—in sharp contrast to experiments [16,17]—less than one [18]. The cause of this deficiency is that the wave function (2) describes the *average* correlations between particles, but it is not sensitive to the *specifics* of the correlations in the vicinity of the Fermi surface. The cure for the problem is correlated-basis functions (CBF) theory [10] to infinite order [19]. The theory can be mapped on a Green's function approach in terms of effective interactions [20] that are provided by the variational theory. The single particle properties are described by a complex *self-energy* $\Sigma(k,E)$; the single particle spectrum $\epsilon^{(3)}(k)$ is obtained from the solution of equation

$$\epsilon^{(3)}(k) = t_3(k) + \Sigma(k, \epsilon^{(3)}(k)). \tag{6}$$

If only one-phonon coupling processes are considered, the self-energy $\Sigma(k,E)$ is given by the so-called $G0W$ approximation [21,22]

$$\Sigma(k,E) = i\int \frac{d^3q\,d(\hbar\omega)}{(2\pi)^4\rho_3}\, G^{(0)}\left(|\mathbf{k}-\mathbf{q}|, \frac{E}{\hbar}-\omega\right) \times \tilde{V}_{\mathrm{eff}}(q,\omega). \tag{7}$$

$$G^{(0)}(k,\omega) = \frac{1-n_k^{(0)}}{\hbar\omega - t_3(k) + i\eta} + \frac{n_k^{(0)}}{\hbar\omega - t_3(k) - i\eta} \tag{8}$$

is the free single-particle Green's function and

$$\tilde{V}_{\mathrm{eff}}(q,\omega) = \tilde{V}^{33}_{\text{p-h}}(q) + \sum_{\alpha\beta} \tilde{V}^{3\alpha}_{\text{p-h}}(q)\chi_{\alpha\beta}(q,\omega)\tilde{V}^{3\beta}_{\text{p-h}}(q) \tag{9}$$

is the effective, *energy dependent* ^{3}He-^{3}He interaction. In Eq. (9), $\tilde{V}^{\alpha\beta}_{\text{p-h}}(q)$ is the local, *particle-hole irreducible* interaction matrix [6], and $\chi_{\alpha\beta}(q,\omega)$ is the density-density response matrix. The particle-hole irreducible interactions, which are in conventional Green's functions theories the most significant source of uncertainty, are provided by the variational ground state theory.

To separate the "hydrodynamic" and the "fermionic" component of the self-energy, we rewrite the single-particle Green's function as

$$\begin{aligned} G^{(0)}(k,\omega) = {} & \frac{1}{\hbar\omega - t_3(k) + i\eta} \\ & + n_k^{(0)}\left[\frac{1}{t_3(k) - \hbar\omega - i\eta} - \frac{1}{t_3(k) - \hbar\omega + i\eta}\right] \\ \equiv {} & G_H^{(0)}(k,\omega) + G_F^{(0)}(k,\omega) \end{aligned} \tag{10}$$

and, correspondingly, the self-energy as

$$\Sigma(k,E) = \Sigma_H(k,E) + \Sigma_F(k,E). \tag{11}$$

The hydrodynamic part $\Sigma_H(k,E)$ of the self-energy is, in the limit $\rho_3 \rightarrow 0$, identical to the self-energy of a single ^{3}He impurity in the ^{4}He host liquid [cf. Eq. (3.30) of Ref. [7]]; since we have found in Ref. [6] that the concentration dependence is generally weak it is appropriate to identify $\Sigma_H(k,E)$ with the self-energy of a single ^{3}He atom also at finite concentrations; we will return to this quantity later.

Let us first focus on the *second* term in Eq. (11). The energy integration yields the compact form

$$\Sigma_F(k,E) = -\int \frac{d^3q}{(2\pi)^3\rho_3}\, n_q^{(0)}\tilde{V}_{\mathrm{eff}}[\mathbf{k}-\mathbf{q}, E - t_3(q)]. \tag{12}$$

The relationship to Eq. (5) is apparent: If $\tilde{V}_{\mathrm{eff}}(q,\omega)$ were energy independent, $\Sigma_F(k,\omega)$ would be just a Hartree-Fock average field of the form (5). Indeed, the expression (5) can be derived from Eq. (12) using the same "average-energy" procedure that has been employed to establish the connection between the parquet-diagram theory and the optimized HNC theory [23], namely, to identify

$$\tilde{W}_{\mathrm{eff}}(q) = \tilde{V}_{\mathrm{eff}}(q, \omega(q)), \tag{13}$$

where the average energy $\hbar\omega(q)$ is chosen such that both the energy dependent and the energy independent interactions produce the same static structure function. We stress that this result is only an *observation* on how the static approximation and the $G0W$ approximation are related. It does *not* imply that this approximation is also *adequate* for the single-particle properties.

With the relationship between theories established, we now turn to the numerical application. The ingredients of the theory—the effective interactions $\tilde{V}^{\alpha\beta}_{\text{p-h}}(q)$ and $\tilde{W}_{\mathrm{eff}}(q)$ as well as the Feynman spectrum $\epsilon^{(4)}(k)$ have been obtained in Ref. [6]. The first important quantity is the *hydrodynamic effective mass*. Because of the high density of the background more elaborate methods than the $G0W$ approximation must be used for a quantitative prediction [7]. To identify the Fermi-liquid effects we are interested in here, we have, however, not used these results, but rather let the hydrodynamic mass be a free parameter. After the concentration dependence was calculated from the Fermi-liquid contributions we made a single parameter fit to the experiments of Refs. [4,5] to optimize the *overall* agreement. That way, we arrived at the following interpolation formulas for the hydrodynamic mass:

$$\left.\frac{m_H}{m_3}\right|_{\mathrm{expt}} = 2.18 + 2.43r + 2.67r^2 - 1.17r^3 \tag{14}$$

for the data of Ref. [4] and

$$\left.\frac{m_H}{m_3}\right|_{\mathrm{expt}} = 2.15 + 2.16r + 4.47r^2 \tag{15}$$

from those of Ref. [5]. Here, $r = \rho_4/\rho_0 - 1$, ρ_4 is the ^{4}He density and $\rho_0 = 0.02\,183$ Å^{-3} is its value at the saturation vapor pressure. Typically, the discrepancy between the two different extrapolations is 0.03 these values are throughout the full density regime about 0.1 above our theoretical calculation of Ref. [7].

A possible complication to be considered is the momentum dependence of the hydrodynamic effective mass since the particles at the Fermi surface have a finite momentum.

For that purpose, we have calculated the single-impurity spectrum,

$$\hbar\omega_H(k) = t_3(k) + \Sigma_H(k, \hbar\omega_H(k)), \qquad (16)$$

and have determined the momentum dependence of the hydrodynamic mass by writing, in a momentum regime $0 \leq k \leq 0.4$ Å^{-1} (chosen such that the upper boundary is comparable to the Fermi momentum at the highest pressure and concentration) the spectrum in the form

$$\hbar\omega_H(k) \approx \frac{\hbar^2 k^2}{2m_H(1 + bk^2)}. \qquad (17)$$

We have verified that this form is adequate at small momenta and has a weak density dependence in agreement with experiments [24,25]. We have used the value $b = 0.114$ at all densities.

Three calculations have been carried out to determine the Fermi-liquid contributions to the effective mass of the ^{3}He component as a function of concentration and density. The transformation from the density and concentration dependence to the pressure and concentration is done using experimental results given in Ref. [26]. The first is the simple approximation (5). To account for the hydrodynamic backflow, one must supplement the Fermion contribution (4) by the hydrodynamic contribution; the spectrum has the form

$$\epsilon^{(3)}(k) = \hbar\omega_H(k) + u(k) + U_0, \qquad (18)$$

where the Fermi correction $u(k)$ is given in Eq. (5). The effective masses derived from this spectrum are significantly above the experimental one; cf. Fig. 1.

In the next step, we use the full self-energy in an "on-shell" approximation

$$\epsilon^{(3)}_{\mathrm{OS}}(k) = \hbar\omega_H(k) + \Sigma_F(k, t_3(k)). \qquad (19)$$

This form of the self-energy relaxes the approximations made by the variational theory. We see in Fig. 1 that the agreement with the experiment is no better than in the FHNC approximation, the effective mass now being significantly *below* the experimental value.

Finally, we carry out a self-consistent calculation of the effective mass. Because of the low concentrations, we may assume a single-particle spectrum of the form $t_3(k) = \hbar\omega_H(k)$ in the Green's function (8) and, consequently, in Eq. (12); note that the hydrodynamic mass is included in the Green's function. This effective mass is then calculated self-consistently by requiring that the spectrum $\epsilon^{(3)}(k)$ determined by

$$\epsilon^{(3)}(k) = \hbar\omega_H(k) + \Sigma_F(k, \hbar\omega_H(k)) \qquad (20)$$

can be fitted by the same effective mass that has been used in the self-energy. This theoretical calculation produces, especially at lower densities, a slightly stronger concentration dependence than seen experimentally. Compared with both the FHNC and the on-shell approximation, the self-consistent result shown in Fig. 1 appears quite satisfactory.

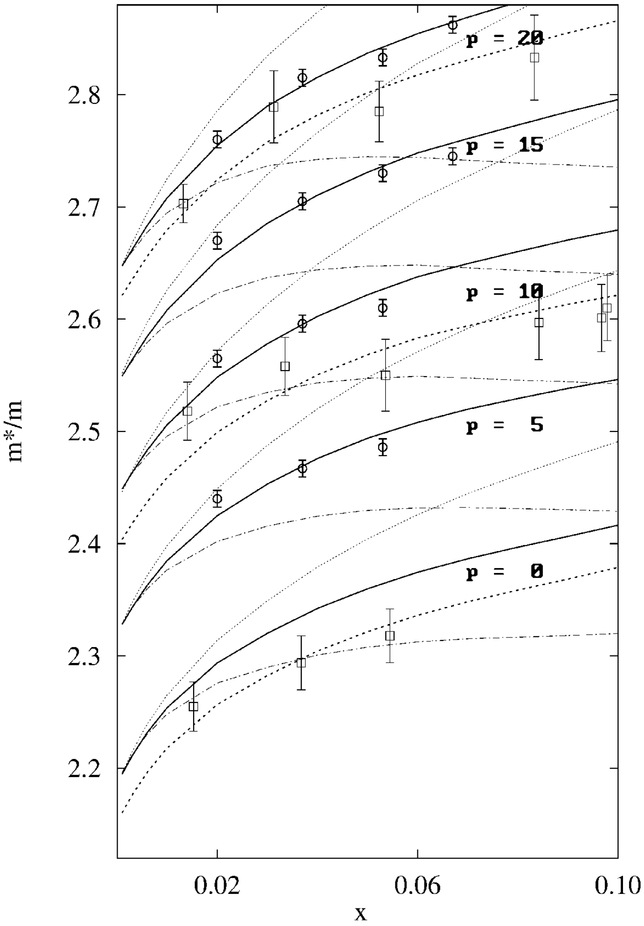

FIG. 1. Theoretical and experimental effective mass ratio $m^*(P,x)/m$ as a function of pressure P and concentration x. The thick full curve is the fully self-consistent result with the hydrodynamics mass fitted to the experiments of Ref. [4] (circles with error bars). The thin, dash-dotted curve is the on-shell approximation and the thin, short dashed curve the static approximation using the same hydrodynamic mass. The thick dashed curve is the fully self-consistent result using the hydrodynamic mass fitted to the results of Ref. [5] (boxes with error bars).

The essential difference between the on-shell and the self-consistent calculation is that information about the hydrodynamic backflow has gone into $G^{(0)}_F(k, \omega)$. Note that hydrodynamic backflow is—as a feature of excitations—generically *not* included in the approximation (5). Indeed, generalizing the variational theory to dynamic correlations *without* introducing the coupling to the background would lead to an effective mass close to the on-shell mass, which is notably too low.

To produce Fig. 1 we have used—as stated before—the hydrodynamic mass given in Eqs. (14) and (15), respectively. Our calculations predict a curvature of the effective mass as a function of concentration x, leading to a hydrodynamic effective mass slightly lower than the one predicted by linear extrapolation; cf. Table I. Such a curvature is caused by the Fermi functions; already the

TABLE I. Pressure dependence of the hydrodynamic effective mass and the coefficients of the expansion (21) as obtained from the present calculation and fitted to the data of Ref. [4]. Also shown are the linear extrapolation of Ref. [5] as well as our fit to these data.

P (atm)	m_H/m_3 (this work)	a	b	c	d	m_H/m_3 (Ref. [5])	m_H/m_3 (fitted to Ref. [5] data)
0	2.18	1.49	1.39	−18.2	36.7	2.23 ± 0.02	2.15
5	2.31	1.07	3.00	−22.6	40.2		
10	2.44	0.789	4.48	−28.2	50.4	2.52 ± 0.02	2.39
15	2.54	0.501	6.17	−36.1	66.8		
20	2.64	0.310	7.41	−42.1	80.1	2.70 ± 0.03	2.62

simple approximation (18) predicts a behavior

$$m^*(x)/m_3 = m_H/m_3 + ax^{2/3} + bx + cx^{5/3} + dx^{7/3}. \qquad (21)$$

The precise values of these coefficients are a matter of a microscopic calculation. In Table I we list the values of a, b, c, and d for different pressures as obtained from the least squares fit to the self-consistent solution of Eq. (20).

In summary, we have demonstrated that the concentration dependence of the effective mass is essentially a Fermi-liquid effect, enhanced by the renormalization of the single particle propagator through hydrodynamic backflow. The technical simplifications caused by the relatively low density of the fermion component has allowed us to highlight the relevant physical mechanisms quite clearly. The data of Ref. [5] are consistently below those of Ref. [4]; the difference of 0.03 might be attributable to the different pressure gauge. This difference might appear negligible, but we need to point out that it produces uncomfortably large uncertainties in predictions for the first antisymmetric Landau Fermi liquid parameter F_0^a from magnetic susceptibility measurements [27].

On the other hand, we find that the concentration dependence of the effective mass—in other words the generic Fermi-liquid effect—is consistent between both sets of experiments and theory. Extrapolations to zero concentration also appear to be consistent.

Besides providing an accurate microscopic calculation of the concentration dependence of the ^{3}He effective mass in ^{4}He, we have analyzed various procedures for calculating the effective mass. By comparing the static calculation with the dynamic CBF calculation, we have discussed an instructive example for the delicate interplay between single-particle and Fermi-liquid effects in ^{3}He-^{4}He mixtures.

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