Microscopic Calculation of the Low-Temperature Properties of ^{3}He-^{4}He Mixtures

J. C. Owen

Department of Theoretical Physics, The University, Manchester M13 9PL, United Kingdom

The effective interaction between two ^{3}He atoms in ^{4}He is obtained by assuming the ground-state wave function to be a product of pair correlations. It is used to evaluate some of the low-temperature properties of mixtures.

The phenomenological theories of Bardeen, Baym, and Pines[1] (BBP) and of Emery[2] give a consistent description of the low-temperature properties of dilute solutions of ^{3}He in ^{4}He in terms of a weak effective interaction between the ^{3}He atoms. In this Letter I will show that a wave function constructed from the product of pair correlations leads to the microscopic calculation of an effective interaction and hence to the evaluation of Landau parameters and transport properties.

Let us assume a ground-state wave function for two antiparallel-spin ^{3}He atoms in ^{4}He of the form

$$\psi = f_{33}(r_{i_3 j_3}) \prod_{i_3, i_4} f_{34}(r_{i_3 i_4}) \prod_{i_4 < j_4} f_{44}(r_{i_4 j_4}), \tag{1}$$

where $f_{ab}(r)$ is a pair-correlation function between helium atoms of masses a and b. Following the theory for a one-component liquid,[3] the minimization of the energy with respect to each of the $f_{ab}(r)$ gives three Euler-Lagrange equations in the following form:

$$- m_{ab}^{-1} \hbar^2 \nabla^2 g_{ab}^{1/2}(r) + [V(r) + W_{ab}(r)] g_{ab}^{1/2}(r) = 0, \tag{2}$$

where $g_{ab}(r)$ is the distribution function between atoms of type a and b,

$$g_{ab}(r_{12}) = \langle \psi_0 | \sum_{(i,j) \in (a,b)} \delta(\vec{r}_i - \vec{r}_1) \delta(\vec{r}_j - \vec{r}_2) | \psi_0 \rangle.$$

$m_{ab}^{-1} = 0.5(m_a^{-1} + m_b^{-1})$ are the reduced masses and $V(r)$ is the bare Lennard-Jones potential which is the same between all pairs of atoms. The induced potentials involve an infinite series of many-body integrals which can be expressed in terms of the distribution functions g_{ab}. Using the hypernetted chain (HNC) approximation[3] to this series and keeping only leading-order terms in the ^{3}He density gives the following expressions for the Fourier transforms of the induced potentials:

$$\tilde{W}_{ab}(k) = -\hbar^2 k^2 [4 m_4 \rho_4 S_{44}^2(k)]^{-1} [S_{a4}(k) - 1][S_{b4}(k) - 1][2 m_{ab}^{-1} m_4 S_{44}(k) + 1]. \tag{3}$$

ρ_4 is the ^{4}He density and $S_{ab}(k)$ are liquid structure functions [unity plus ρ_4 multiplied by the Fourier transform of $g_{ab}(r) - 1$]. The HNC approximation will be used from here on because of the simple form of Eqs. (3). It does not affect the formal discussion below, but might affect the numerical results by perhaps (10–15)%.

The first equation ($a = 4$, $b = 4$) describes the ^{4}He background and has been obtained before.[3,4] It is found that the solution $g_{44}(r)$ behaves as $1 + O(r^{-4})$ for large r and that $S_{44}(k) \to 0$ for $k \to 0$ in agreement with the properties predicted for the true ground-state wave function. The second equation ($a = 4$, $b = 3$) involves one ^{3}He atom and describes its interaction with the ^{4}He background. Its solution $g_{34}(r)$ also behaves as $1 + O(r^{-4})$ and its Fourier transform $S_{34}(k)$ tends to a finite constant as $k \to 0$. The constant gives the fractional difference between the volumes occupied by ^{4}He and ^{3}He atoms and is the negative of the param-

eter called α by BBP.

The third equation describes an effective interaction $V(r) + W_{33}(r)$ between two ^{3}He atoms which is determined by the structure functions S_{34} and S_{44}. The small-k limit of $\tilde{W}_{33}(k)$ allows us to make contact with BBP. In this limit $S_{44} \to 0$ and hence

$$\tilde{W}_{33}(0) = -(1 + \alpha)^2 m_4 s^2 \rho_4^{-1}, \tag{4}$$

where $\alpha = -S_{34}(0)$ and $s = \lim[k S_{44}^{-1}(k) \hbar / 2 m_4]$ which would be the speed of sound in ^{4}He if the product wave function were the true ground-state function.[5] The same result is obtained by BBP from thermodynamic arguments about phonon exchange in the ^{4}He background.

BBP then show that this induced interaction is largely canceled by the bare interaction and that the net effective interaction is proportional to α^2. We can show the corresponding result that the

scattering length of the effective interaction is quadratically small in the mass difference between ^{3}He and ^{4}He atoms. The reason is that the scattering length for the effective interaction between two ^{4}He atoms is exactly zero as a result of the screening of the interaction by the background. The only way in which an ^{3}He atom is distinguished from an ^{4}He atom is by the difference in their masses. Thus, the difference between the scattering lengths for a pair of ^{3}He atoms and a pair of ^{4}He atoms should be quadratically small in this mass difference. This result can be proved from Eqs. (2) and (3) by showing that $g_{33}^{1/2}(r)$ is equal to $2g_{34}^{1/2}(r) - g_{44}^{1/2}(r)$ plus corrections of order of the square of the mass difference. The functions $g_{44}^{1/2}$ and $g_{34}^{1/2}$ both approach unity as r^{-4} for large r and so the r^{-1} term in $g_{33}^{1/2}$, which gives the scattering length, is quadratically small in the mass difference.

The nonlinear equations (2) and (3) for $g_{44}^{1/2}$ and $g_{34}^{1/2}$ are solved numerically. The calculated structure functions are shown in Fig. 1 for a background ^{4}He density of 0.0219 Å^{-3}, which is the experimental density of zero pressure. The figure also shows an experimental determination of $S_{44}(k)$ by x-ray scattering.[6] For dilute mixtures the relative momentum of ^{3}He atoms on the Fermi surface is less than 1 Å^{-1} and so the detailed behavior of the structure functions for small k should be the most important. The calculated value of $-S_{34}(0)$ is 0.32 as compared with the measured value of 0.29.[7]

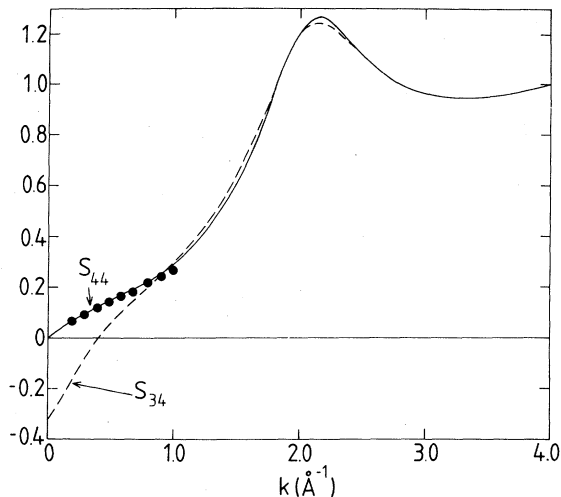Figure 2 shows the induced potentials $W_{33}(r)$

and $W_{44}(r)$ and the effective ^{3}He-^{3}He potential together with the bare Lennard-Jones potential. The structure of $W_{44}(r)$ can be understood by noting that it is equal to $m_4^{-1}\hbar^2 g_{44}^{-1/2}(r)\nabla^2 g_{44}^{1/2}(r) - V(r)$ and that $g_{44}(r)$ is zero inside the repulsive core of $V(r)$, rises to a nearest-neighbor peak at about the mean interparticle spacing, and then oscillates around unity. W_{33} is very similar because the bare interaction is the same and the mass difference is small.

In order to describe the properties of moving ^{3}He atoms, we consider the scattering of two ^{3}He atoms with momenta $\vec{k}_1$ and $\vec{k}_2$. The atoms have an associated cloud of ^{4}He atoms backflowing around them and they acquire an effective mass, m_3^*. The interaction between the two ^{3}He atoms will then consist of two parts—a part which is the same as for ground-state atoms, which is $V(r) + W_{33}(r)$, and a part which comes from the interactions of the velocities of the two backflow clouds. This second part will depend on the momenta of the ^{3}He atoms with respect to the ^{4}He background and so it cannot be included in an effective interaction which depends on the relative separation (or momentum) of the ^{3}He atoms. It is therefore neglected for now to obtain a wave function $\varphi(\vec{r})$ for the two ^{3}He atoms which depends only on their relative separation and energy and satisfies the scattering equation

$$m_3^{-1}\hbar^2\nabla^2\varphi(\vec{r}) + [V(r) + W_{33}(r) - E]\varphi(\vec{r}) = 0, \qquad (5)$$

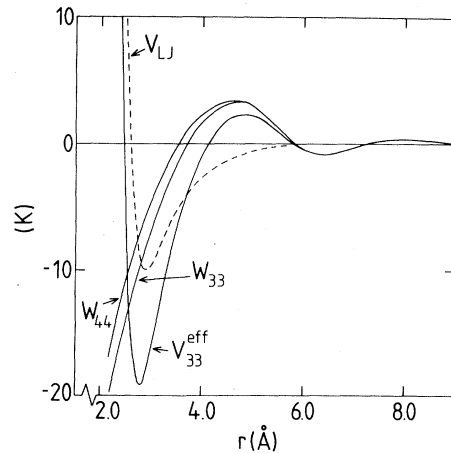where $W_{33}(r)$ is the induced interaction given in Eq. (2) and the center-of-mass energy is related

FIG. 1. The calculated structure functions and (Ref. 6) the x-ray measurements (dots) of $S_{44}(k)$.

FIG. 2. The induced potentials W_{33} and W_{44}, the effective interaction $V_{33}^{eff} = V_{LJ} + W_{33}$, and the bare Lennard-Jones interaction (V_{LJ}).

to the relative momentum by $E = \hbar^2(\vec{k}_1 - \vec{k}_2)^2/4m_3{}^*$.

Although the effective mass $m_3{}^*$ for one ^{3}He atom could in principle be calculated microscopically with use of a wave function containing a backflow component as suggested by Feynman,[5] a rather difficult calculation involving at least three-particle correlations is necessary in order to get reasonable results.[8] In the numerical results given below, therefore, the value for the effective mass is taken from experiment. Notice, however, that it is the bare mass which multiplies the kinetic-energy operator in Eq. (5) because in the zero-momentum limit the full induced interaction between the ^{3}He atoms is already included in $W_{33}(r)$.

The scattering equation is solved for the phase shifts as a function of energy in each relative partial wave and the scattering amplitudes, or T matrix, evaluated as
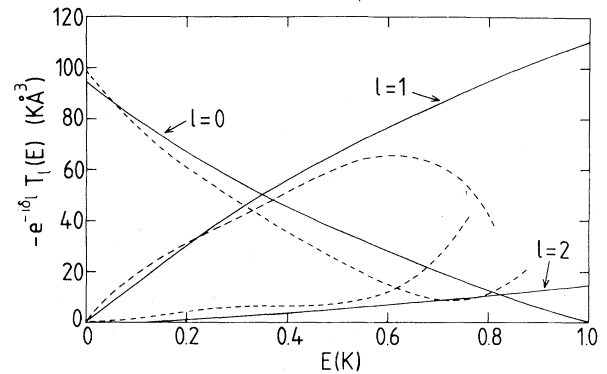

FIG. 3. The partial wave components of the T matrix as a function of energy from this calculation (solid lines) and from Ebner's fit (Ref. 9) (dotted lines).

$$T_l(E) = - 4\pi\hbar^2 m_3{}^{-1}\{\exp[2iS_l(E)] - 1\}(- 4E\hbar^2 m_3)^{-1/2}. \qquad (6)$$

Figure 3 shows the calculated values of the real quantity $- \exp(i\delta_l)T_l$ as a function of energy. They are compared with the same quantities calculated in the Born approximation from the effective interaction of Ebner[9] which is fitted to the transport properties of 1.3% and 5% solutions. For a 5% solution, two atoms on the Fermi surface have a maximum energy in their center-of-mass frame of about 0.7 K and so the fitted T matrix is not significant for larger energies. The phase shifts are all small (less than 0.05 rad) and only about one-tenth those for the bare Lennard-Jones potential. The T matrix is almost real and only weakly attractive.

With a T matrix for two antiparallel-spin ^{3}He atoms, the calculation of Landau parameters and transport properties to leading order in the ^{3}He concentration follows the standard formulas of dilute–Fermi-liquid theory.[2,7] Although the pre-

ceding discussion is for antiparallel-spin atoms, spin-symmetric quantities can also be evaluated because, to leading order in the concentration, exchanging the ^{3}He atoms simply removes the even-l components of the T matrix.

Table I gives the calculated properties for 1.3% and 5% concentrations of ^{3}He compared with the experimental measurements. The spin-diffusion and thermal-diffusion coefficients were calculated with use of the exact solutions to the transport equations. The effective masses for 1.3% and 5% solutions were taken from experiment as 2.38 and 2.46 bare masses, respectively.[10]

The agreement between theory and experiment is good for the 1.3% solution and gets worse for the 5.0% solution. The weak link in the present calculation is probably the neglect of backflow-backflow interaction. This interaction must cer-

TABLE I. Landau parameters, spin diffusion [σT^2 (cm^2 K^2 sec^{-1})], and heat diffusion [κT (erg cm^{-1} sec^{-1})] for 1.3% and 5.0% concentrations of He^3.

	1.3% of ^{3}He		5.0% of ^{4}He	
	Expt.	Calc.	Expt.	Calc.
$F_0{}^{(s)}$		− 0.21		− 0.48
$F_0{}^{(a)}$	0.09 ± 0.03	0.08	0.08 ± 0.03	0.03
$F_1{}^{(s)}$	0.05 ± 0.02	0.07	0.15 ± 0.02	0.23
$F_1{}^{(a)}$		0.06		0.17
σT^2	17×10^{-6}	14×10^{-6}	90×10^{-6}	46×10^{-6}
κT	11	7.5	24	16.5

tainly be repulsive because neglecting it amounts to assuming that each ^{3}He atom can always generate its own optimum flow pattern in the ^{4}He independently of the other ^{3}He atoms. BBP show that it will have a dipole-dipole form, $(\vec{k}_1 \cdot \hat{r})(\vec{k}_2 \cdot \hat{r})$. For zero center-of-mass motion of the two interacting ^{3}He atoms this gives an extra repulsion in s and d waves but zero repulsion in relative p waves. Thus, after averaging over the center-of-mass momentum it would make the effective interaction more repulsive with energy and more so in s waves than in p waves. Figure 3 shows that this would bring the calculated T matrix closer to Ebner's, which is fitted to reproduce the transport properties shown in Table I.

These calculations used the Lennard-Jones potential for the bare He-He interaction. We have found that use of the more recent HEDHE2 potential[11] changes the structure functions and T matrix by about 10% and gives slightly better agreement with experiment. It does not, however, account for the differences between theory and experiment shown in Table I.

Finally, we note that the calculation of the effective interaction allows us to estimate the transition temperature T_c for the onset of Cooper pairing in the ^{3}He. In weak-coupling theory[1] T_c is $T_F \exp[1/N(0)T_l(2E_F)]$, where $N(0)$ is the density of states and E_F the energy at the Fermi surface. For s-wave pairing T_c never exceeds a few microkelvin. For p-wave pairing T_c increases

rapidly with concentration but is still less than 1 μK for a 5% solution. The theory is easily extended to higher background pressures and for a 9.5% solution at 10 atm we find a T_c for p-wave pairing of 0.15–0.3 mK, depending on the value used for m_3^*. This may be an upper bound, however, since for pure ^{3}He the weak-coupling formula must be reduced by a factor of 0.05 in order to fit experiment.[12]

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