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SURFACE TENSION AND DENSITY PROFILE OF LIQUID ^3He ⁺

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Résumé.— On calcule par une nouvelle technique variationnelle la tension superficielle et le profil de densité au voisinage de la surface. On tient compte des effets dus à la structure du liquide en utilisant la fonction de distribution radiale expérimentale de ^3He . Le calcul donne une tension superficielle égale à $0.134 \text{ K/\AA}^2$, en bon accord avec la valeur expérimentale extrapolée. On prédit un domaine de surface ayant à peu près l'épaisseur de deux couches atomiques. Mais, contrairement au calcul récent de Mackie et Woo/3/, nous ne trouvons pas de région de haute densité bien que nous utilisions la même fonction de distribution radiale.

Abstract.— The surface tension and density profile of liquid ^3He at zero temperature are calculated by a new variational technique. Liquid-structure effects are included by using the measured radial distribution function of bulk ^3He as input. The calculation yields a surface tension of $0.134 \text{ K/\AA}^2$ which compares well with the extrapolated experimental result. We predict a surface region that is about two atomic layers in thickness. But in contrast to the recent calculation of Mackie and Woo/3/, no high-density region results even though we use the same radial distribution function as input.

The surface tension of liquid ^3He has been measured over a range of temperatures/1/. But experiment on the density profile and the thickness of the surface layer is lacking. On the theoretical side there have been some recent microscopic calculations/2-3/ with some surprising predictions/3/ on the density profile. We present here a new approach based on variations on an assumed effective surface potential to get more insight about the surface properties of liquid ^3He .

Consider N ^3He atoms in box $0 \leq x \leq L_x, 0 \leq y \leq L_y$ and $-L_z \leq z \leq L_z$ with a free surface in the neighbourhood of $z=0$. We assume the Hamiltonian of the system to be

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i < j=1}^N v(r_{ij}) \quad (1)$$

where $v(r)$ denotes the ^3He - ^3He potential (customarily Lennard-Jones 6-12 with deBoer-Michels/4/ parameters).

We take the trial ground state many-body wave function in the form

$$\psi = F D_s, \text{ where } F = \prod_{i,j} \exp\left[-\frac{1}{2} u(r_{ij})\right] \quad (2)$$

and D_s is a Slater determinant model function. The single particle orbitals $\{\phi_{k_x, k_y, k_z}(\vec{r})\}$ that form the determinant are chosen to satisfy the symmetry and boundary conditions of the problem. This is accomplished in this work by assuming a model surface potential of the form

$$v_s(z) = \frac{1}{2} v_0 \left[1 + \tanh\left(\frac{z-Z_0}{2a}\right) \right] \quad (3)$$

and solving the Schrödinger equation with this potential for $\phi_{k_x, k_y, k_z}(\vec{r})$, in terms of hypergeometric functions. The energy expectation value E can then be expressed in terms of $u(r_{ij})$, $v_s(z)$, and the one-, two- and three-particle density functions/8/ defined by

$$P^{(n)}(\vec{r}_1, \dots, \vec{r}_n) = \frac{N!}{(N-n)!} \frac{\int |\psi|^2 d\vec{r}_{n+1} \dots d\vec{r}_N}{\int |\psi|^2 d\vec{r}_1 \dots d\vec{r}_N}, \quad (4)$$

$n = 1, 2, 3, \dots$

In particular $P^{(1)}(\vec{r}) = P^{(1)}(z) = \rho(z)$ the density of the system.

The surface energy E_s is obtained by removing from E the bulk energy E_B and can be written as

$$E_s = \int dx dy \int_{-\infty}^{\infty} dz \left[\varepsilon(z) - \frac{\varepsilon_B}{\rho_B} \rho(z) \right] \quad (5)$$

In deriving Equation (5) we have used the particle number conservation condition

$$\int dx dy \int_{-\infty}^{\infty} \left[\rho(z) - \rho_B \theta(z-Z_0) \right] dz = 0 \quad (6)$$

where $\theta(x) = \begin{cases} 0 & x > 0, \\ 1 & x < 0, \end{cases}$ and Z_0 is the position of the Gibb's surface. $\varepsilon(z)$ and ε_B are energy densities and ρ_B is the equilibrium bulk number density.

Assuming that we have solved the bulk uniform liquid problem, equation(5) indicates we need $\rho(z)$ and $\varepsilon(z)$ to get the surface tension. To make the computation of $\rho(z)$ and $\varepsilon(z)$ easier it was found necessary to make some approximations :

i) We use the experimental/5/ pair correla-

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tion function $g_B(r|\rho_B)$.

ii) We take $u(r) = - (b\sigma/r)^5$ with $\sigma = 2.556$ Å and $b = 1.138$, from variational calculations performed for bulk ^3He .

iii) We make use of the Kirkwood superposition approximation/6/.

With these approximations $\varepsilon(z)$ becomes a unique functional of $\rho(z)$ only.

To obtain $\rho(z)$ we solve a non-linear integral equation derived with the method of reference/7/ and given by

$$\begin{aligned} \ln P^{(1)}(z_1|\lambda) = \ln P^{(1)}(z_1|0) + 2\pi \int d\lambda' \int_{-\infty}^{\infty} P^{(1)}(z_2|\lambda') \\ f(|z_{12}|) dz_2 + (2\pi)^2 \int_0^\lambda d\lambda' \int_{-\infty}^{\infty} dz_2 dz_3 P^{(1)} \\ (z_2|\lambda') P^{(1)}(z_3|\lambda') f(|z_{23}|) [\bar{G}_1(|z_{12}|) \\ + G_2(|z_{12}|)/2] \end{aligned} \quad (7)$$

where

$$f(x) = \int_x^\infty ru(r)g_B(r|\rho_B)dr \quad (8)$$

$$G_1(x) = \int_x^\infty r[\bar{g}_B(r|\rho_B) - 1]dr \quad (9)$$

and

$$G_2(x) = \int_x^\infty r[\bar{g}_B(r|\rho_B) - 1]^2 dr \quad (10)$$

The coupling parameter λ has values $0 \leq \lambda \leq 1$ and $P^{(1)}(z|1) = \rho(z)$, while

$$P^{(1)}(z|0) = 2 \sum_{\substack{k_x, k_y, k_z \\ \text{(occ.)}}} |\phi(\vec{r})|_{k_x, k_y, k_z}^2 \quad (11)$$

is the density of the non-interacting system. The sum in equation (11) is over occupied states up to the highest level characterized by $k_N = (k_x^2 + k_y^2 + k_z^2)^{1/2}$, which is determined by requiring that the solution $P^{(1)}(z|1)$ of equation (7) be equal to ρ_B for $z \ll 0$.

Since the parameter Z_0 is determined by equation (6), v_0 and a are the only variational parameters. The physical surface energy is then determined by finding the absolute minimum with respect to both v_0 and a , and is done in two stages as table I indicates.

Thus we obtained the surface tension to be 0.134 K/Å^2 , which compares reasonably well with experiment. The corresponding values of the parameters are $v_0 = 6.90 \text{ K}$, $a = 1.722 \text{ Å}$, $Z_0 = 2.31$ and $k_N = 0.9134 \text{ Å}^{-1}$. Using v_0 and k_N we estimate a "work function" of about 0.20 K per atom . This study predicts a density profile with no high-density region, in contrast to the prediction of /3/. If the prediction of the latter is verified experimentally, the present result implies that the form of the

v_0 (K)	Z_0/a	a (Å)	k_N (Å ⁻¹)	Surface Tension(KÅ ⁻²)
6.70	1.23	1.747	0.9035	0.155
	<u>1.24</u>	<u>1.751</u>	<u>0.9030</u>	<u>0.1535</u>
	1.23	1.753	0.9027	0.154
6.90	1.31	1.718	0.9140	0.139
	<u>1.34</u>	<u>1.722</u>	<u>0.9134</u>	<u>0.134</u>
	1.30	1.725	0.9130	0.139
7.10	1.20	1.685	0.9250	0.149
	<u>1.22</u>	<u>1.689</u>	<u>0.9245</u>	<u>0.148</u>
	1.20	1.696	0.9234	0.152

Table I : Values of parameters : The underlined values are these for which the surface energy is a minimum for the respective v_0 .

effective surface potential chosen here is not sufficiently general. It should not be a smooth function of z .

A detailed discussion of the method and results will be reported elsewhere/8/.

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