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SURFACE TENSION AND DENSITY PROFILE OF LIQUID $^3$He

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Abstract.—The surface tension and density profile of liquid $^3$He at zero temperature are calculated by a new variational technique. Liquid-structure effects are included by using the measured radial distribution function of bulk $^3$He as input. The calculation yields a surface tension of $0.134 \text{ K}\cdot\text{Å}^2$ 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 $^3$He 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 $^3$He.

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

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

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

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

$$\psi = D_s \phi$$

where $D_s$ 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

$$v_s(z) = \frac{1}{2} v_0 \tanh \left( \frac{z - Z_0}{2a} \right)$$

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 $u(r_{ij})$, $v_0(z)$, and the one-, two- and three-particle density functions/8/ defined by

$$p(n) = \frac{N!}{(N-n)!} \int \left( \frac{v_0^2}{2m} \right)^{n+1} \left( \frac{v_0^2}{2m} \right)^{N-n} \prod_{j=1}^{n} d^3r_j$$

with $n=1,2,3,...$

In particular $p^{(1)}(z) = p^{(1)}(z) = \rho(z)$ 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

$$E_s = \int dx \int dy \int dz \left[ \rho(z) - \frac{B}{\rho_B} \rho(z) \right]$$

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

$$\int dx \int dz \left[ \rho(z) - \frac{B}{\rho_B} \rho(z) \right] = 0$$

where $\theta(z) = \int_0^z \rho(z') dz'$ and $Z_0$ is the position of the Gibb's surface. $c(z)$ and $c_B$ are energy densities and $\rho_B$ is the equilibrium bulk number density.

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

1) We use the experimental/5/ pair correle-
ii) We take \( u(r) = -(\text{balr})' \) with \( U = 2.556 \) Å and \( b = 1.138 \), from variational calculations performed for bulk \( ^3\text{He} \).

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

With these approximations \( \zeta(z) \) becomes a unique functional of \( p(z) \) only.

To obtain \( p(z) \) we solve a non-linear integral equation derived with the method of reference\( ^171 \) and given by

\[
\ln F(1)(z_1|\lambda) = \ln F(1)(z_1|0) + 2\pi \int_0^\infty d\lambda \lambda \sum_{z_2} \int_0^\infty d\lambda' F(1)(z_2|\lambda') \zeta(z_1z_2) + G_1(z_1|\lambda)F(1)(z_1|\lambda) + G_2(z_1|\lambda)^2 \tag{7}
\]

where

\[
f(x) = \frac{e}{\pi} r u(r) g_\beta(r | \rho_\beta) \, dr \tag{8}
\]

\[
G_1(x) = \frac{e}{\pi} \int g_\beta(r | \rho_\beta) - 1 \, dr \tag{9}
\]

and

\[
G_2(x) = \frac{e}{\pi} \int g_\beta(r | \rho_\beta) - 1 \, 2 \, dr \tag{10}
\]

The coupling parameter \( \lambda \) has values \( 0 < \lambda < 1 \) and \( F(1)(z_1|0) = \tilde{\rho}(z) \), while

\[
f(1)(z|0) = 2 \sum k_{x'} k_{y'} k_{z'} \zeta^{(1)}(z_{x' y' z'})^2 \tag{11}
\]

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 \( \tilde{p}(1)(z|0) \) of equation (7) be equal to \( \rho_\beta \) for \( z = \infty \).

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 kJ/m², which compares reasonably well with experiment. The corresponding values of the parameters are \( v_0 = 6.90 \) K, \( a = 2.722 \) Å, \( Z_0 = 2.31 \) Å and \( k_N = 0.9137 \) 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

<table>
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<th>( v_0 ) (K)</th>
<th>( Z_0/a )</th>
<th>( n ) (Å)</th>
<th>( v_N ) (kJ/m²)</th>
<th>Surface Tension(KJ/m²)</th>
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Table I: Values of parameters: The underlined values are these for which the surface energy is a minimum for the respective \( v_0 \).

The 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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