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On the Wave Function of a Quantum Fluid in a Force Field

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The wave function of a Bose or Fermi liquid in a potential v *(e.g., the van der Waals potential of a metallic boundary wall, or the polarization potential of an ion in the liquid) is taken to be* $\Pi s(i)\Phi$, *where* Φ *is the wave function in the absence of* v. *The function* s *is determined by a many-body variational calculation. For a weak potential,* s *and the density are explicitly determined up to a quadrature.*

1. INTRODUCTION

Knowledge of the wave function of a quantum fluid in an external field is necessary for the understanding of several phenomena in which liquid helium adheres to or is bounded by solids. We have in mind the properties of helium films,[1] and heat transfer between solids and liquid helium.[2] In both cases, the attractive van der Waals forces[3] between the solid and the helium liquid play the dominant role. A related problem is the distortion of the wave function of helium by the polarization force between an ion in the liquid and each helium atom. Such distortion may have important effects on the mobility of ions in helium.[4]

In this paper we shall derive equations determining the wave function and the density of a quantum fluid subject to such forces. The techniques used are those developed in the study of the surface structure of helium,[5] and of vortex lines in helium.[6] The discussion will correspondingly be abbreviated. We begin by considering the effect of a potential $v(z)$ on a fluid bounded by a plane solid surface at $z = 0$.

2. WAVE FUNCTION AND ENERGY

Consider a system of N atoms of mass m, held in a box of side L at absolute zero. The Hamiltonian of the system is taken to be

$$H_0 = -(\hbar^2/2m)\sum_i \nabla_i^2 + \sum_{i<j}\sum u(r_{ij}) + \sum_i w(\mathbf{r}_i) + \sum_i mgz_i \tag{1}$$

The third term is the short-range potential of the (impenetrable) walls. It may, for example, be an infinite step function, which can equivalently be replaced by the boundary condition that the wave function be zero at the walls. The last term is the gravitational potential, which has negligible effect apart from imposing a preferred direction on the system. We assume that the system is in the liquid phase, and has a free surface at $z \simeq D < L$. The ground state $\Phi(\mathbf{r}_1 \cdots \mathbf{r}_N)$ of H_0, with eigenvalue E_0, is assumed known. For most of the space occupied by the liquid, Φ is very well approximated by the wave function of bulk liquid at some number density $\bar{n}_0$.

We now let some external field $v(z)$ be switched on at the $z = 0$ wall. The potential v is assumed to be of substantially longer range than w—i.e., extending over at least several atomic diameters. The Hamiltonian becomes

$$H = H_0 + \sum_i v(z_i) \tag{2}$$

and we shall variationally optimize the wave function

$$\Psi = S\Phi \qquad S = \Pi s(z_i) \tag{3}$$

by minimizing the expectation value of H. We have

$$H_0\Psi = E_0\Psi - (\hbar^2/2m)\Phi^{-1}\sum_i \nabla_i \cdot (\Phi^2 \nabla_i S) \tag{4}$$

so that

$$\int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi H \Psi \bigg/ \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi^2 - E_0$$

$$= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \left[(\hbar^2/2m)\sum_i (\nabla_i S)^2 + S^2 \sum_i v(z_i)\right]\Phi^2 \bigg/ \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi^2$$

$$= N\int d\mathbf{r}_1 \cdots d\mathbf{r}_N \{(\hbar^2/2m)[s'(z_1)/s(z_1)]^2 + v(z_1)\}\Psi^2 \bigg/ \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi^2 \tag{5}$$

(H_0 and H are real linear operators, so that Φ and Ψ can be taken real). We define a number density $n(\mathbf{r})$ by

$$n(\mathbf{r}_1) = N\int d\mathbf{r}_2 \cdots d\mathbf{r}_N \Psi^2 \bigg/ \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi^2 \tag{6}$$

For the problem defined above, n is a function of z only, and the expectation value $\langle H - E_0 \rangle$ can be written as

$$\int d\mathbf{r}\, n(z)\{(\hbar^2/2m)[s'(z)/s(z)]^2 + v(z)\}$$

$$= L^2 \int dz\, n(z)\{(\hbar^2/2m)[s'(z)/s(z)]^2 + v(z)\} \qquad (7)$$

We have assumed that L is large relative to the atomic diameter, so that edge effects can be neglected.

3. VARIATIONAL CALCULATION

To determine the best wave function of the form (3), we take variations δs in s; the best s is to satisfy the equation

$$\delta\langle H - E_0\rangle = 0 \qquad (8)$$

From (7) we have

$$\int d\mathbf{r}\{\delta n[(s'/s)^2 + (2mv/\hbar^2)] + 2n(s'/s)[(\delta s'/s) - (s'\delta s/s^2)]\} = 0 \qquad (9)$$

The variation δn in the number density is given by[5]

$$\delta n(z_1) = 2[\delta s(z_1)/s(z_1)]n(z_1) + 2\int d\mathbf{r}_2[\delta s(z_2)/s(z_2)]\,[n_2(\mathbf{r}_1, \mathbf{r}_2) - n(z_1)n(z_2)] \quad (10)$$

where the pair density function n_2 is defined by

$$n_2(\mathbf{r}_1, \mathbf{r}_2) = N(N-1)\int d\mathbf{r}_3 \cdots d\mathbf{r}_N \Psi^2 \Big/ \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi^2 \qquad (11)$$

Substituting (10) into (9), and using the symmetry

$$n_2(\mathbf{r}_2, \mathbf{r}_1) = n_2(\mathbf{r}_1, \mathbf{r}_2) \qquad (12)$$

we find the following equation for s:

$$[s(z_1)/n(z_1)]\,[n(z_1)s'(z_1)/s^2(z_1)]' = [2mv(z_1)/\hbar^2] + [1/L^2 n(z_1)]$$

$$\times \int dx_1\, dy_1 \int d\mathbf{r}_2\{[s'(z_2)/s(z_2)]^2 + [2mv(z_2)/\hbar^2]\}[n_2(\mathbf{r}_1, \mathbf{r}_2) - n(z_1)n(z_2)] \qquad (13)$$

As in Ref. 5 we define a generalized pair correlation function g and a kernel G:

$$n_2(\mathbf{r}_1, \mathbf{r}_2) = n(z_1)n(z_2)g(\mathbf{r}_1, \mathbf{r}_2) \qquad (14)$$

$$G(z_1, z_2) = \lim_{L\to\infty} L^{-2} \int dx_1\, dy_1 \int dx_2\, dy_2 [g(\mathbf{r}_1, \mathbf{r}_2) - 1] \tag{15}$$

Then the function s is determined, in the limit of large L, by the nonlinear integrodifferential equation [cf. Eq. (20) of Ref. 5]

$$\begin{aligned}[s(z_1)/n(z_1)]\,[n(z_1)s'(z_1)/s^2(z_1)]' &= [2mv(z_1)/\hbar^2] \\ &\quad + \int dz_2 n(z_2) G(z_1, z_2)\{[s'(z_2)/s(z_2)]^2 + [2mv(z_2)/\hbar^2]\}\end{aligned} \tag{16}$$

The limit in Eq. (15) is shown in Ref. 5 to exist subject to a rather weak condition on g. Further, since $g(\mathbf{r}_1, \mathbf{r}_2)$ is a function of z_1, z_2 and of

$$\rho_{12} = [(x_1 - x_2)^2 + (y_1 - y_2)^2]^{1/2} \tag{17}$$

in all regions of the box except near the x and y boundary walls, we have

$$\begin{aligned} G(z_1, z_2) &= \int_{-\infty}^{\infty} dx\, dy [g(z_1, z_2, [x^2 + y^2]^{1/2}) - 1] \\ &= 2\pi \int_0^{\infty} d\rho\, \rho [g(z_1, z_2, \rho) - 1] \\ &= 2\pi \int_{|z_1 - z_2|}^{\infty} dr\, r [g(z_1, z_2, r) - 1] \end{aligned} \tag{18}$$

where $r^2 = \rho^2 + (z_1 - z_2)^2$.

Equations (16) and (18) give an exact formal solution to the problem of finding the best wave function of the type (3) for a Bose or Fermi fluid in the field $v(z)$. Before going on to an approximate evaluation of the functions n and g, we will discuss the related problem of a quantum fluid in a central field $v(r)$.

4. CENTRAL FIELD

We consider a large system with Hamiltonian

$$H = H_0 + \sum_i v(r_i) \tag{19}$$

where now

$$H_0 = (-\hbar^2/2m) \sum_i \nabla_i^2 + \sum_i \sum_j u(r_{ij}) + \sum_i w(r_i) \tag{20}$$

with $w(r)$ representing the short-range part of the potential due to an impurity in the fluid, and $v(r)$ representing the long-range part. For example, w could be an effective potential which keeps atoms out of a sphere of radius R

in the case of an electron bubble in liquid helium, and the corresponding $v(r)$ would then be the attractive polarization potential between the electron and the helium atoms. We again assume that we know Φ, the ground-state wave function of H_0 with eigenvalue E_0.

The appropriate trial wave function is

$$\Psi = S\Phi \qquad S = \prod_i s(r_i) \tag{21}$$

and the expectation value in the state Ψ of $H - E_0$ is

$$\int d\mathbf{r}\, n(r)\{(\hbar^2/2m)[s'(r)/s(r)]^2 + v(r)\} \tag{22}$$

Equations (9) and (10) are modified simply by replacing z by r. The equation corresponding to (13) is, with $d\Omega = \sin\theta\, d\theta\, d\phi$,

$$\begin{aligned}[s(r_1)/r_1^2 n(r_1)]\,[r_1^2 n(r_1) s'(r_1)/s^2(r_1)]' &= [2mv(r_1)/\hbar^2] + [1/4\pi n(r_1)] \\ &\times \int d\Omega_1 \int d\mathbf{r}_2\{[s'(r_2)/s(r_2)]^2 + [2mv(r_2)/\hbar^2]\}[n_2(\mathbf{r}_1, \mathbf{r}_2) - n(r_1)n(r_2)]\end{aligned} \tag{23}$$

and the corresponding generalized pair correlation function g and kernel G are defined by

$$n_2(\mathbf{r}_1, \mathbf{r}_2) = n(r_1)n(r_2)g(\mathbf{r}_1, \mathbf{r}_2) \tag{24}$$

$$G(r_1, r_2) = (1/4\pi)\int d\Omega_1 \int d\Omega_2[g(\mathbf{r}_1, \mathbf{r}_2) - 1] \tag{25}$$

The function s is thus determined by the integrodifferential equation

$$\begin{aligned}[s(r_1)/r_1^2 n(r_1)]\,[r_1^2 n(r_1) s'(r_1)/s^2(r_1)]' &= [2mv(r_1)/\hbar^2] \\ &+ \int_0^\infty dr_2 r_2^2 n(r_2) G(r_1, r_2)\{[s'(r_2)/s(r_2)]^2 + [2mv(r_2)/\hbar^2]\}\end{aligned} \tag{26}$$

Since g is a function of the three variables r_1, r_2, and r_{12}, where

$$r_{12}^2 = r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_{12} \tag{27}$$

the expression for the kernel G simplifies to

$$G(r_1, r_2) = 2\pi \int_{-1}^{1} d\mu[g(r_1, r_2, [r_1^2 + r_2^2 - 2r_1 r_2 \mu]^{1/2}) - 1] \tag{28}$$

5. APPROXIMATIONS FOR *n* AND *g*

It remains to evaluate the functions n and g which are both functionals of s. As regards g, an argument was given in Ref. 6 to justify the approximation

$$g\begin{pmatrix} z_1 & z_2 \\ r_1 ,& r_2 ,& r \end{pmatrix} \simeq g_0\begin{pmatrix} z_1 & z_2 \\ r_1 ,& r_2 ,& r \end{pmatrix} \tag{29}$$

where g_0 is the pair correlation function of the fluid with wave function Φ. We shall make the same approximation here. At a distance of a few atomic diameters from the wall or the ion, g_0 becomes $g_0(r)$, the pair correlation function of the bulk fluid. Then G may be expressed in terms of the experimentally known liquid-structure factor

$$F(k) = 1 + \bar{n}_0 \int d\mathbf{r} \exp(i\mathbf{k}\cdot\mathbf{r})[g_0(r) - 1] \tag{30}$$

From Ref. 5 we have

$$G_0(z_1, z_2) = (1/\pi\bar{n}_0) \int_0^\infty dk[F(k) - 1] \cos k(z_1 - z_2) \tag{31}$$

The corresponding expression for spherical symmetry may be obtained from Eq. (28), the Fourier inverse of Eq. (30), and the expansion[7]

$$(\sin kr_{12}/kr_{12}) = \sum_{l=0}^{\infty} (2l + 1)P_l(\cos\theta_{12})j_l(kr_1)j_l(kr_2) \tag{32}$$

We get [cf. Eq. (40) of Ref. 6]

$$G_0(r_1, r_2) = (2/\pi\bar{n}_0) \int_0^\infty dk\, k^2[F(k) - 1]j_0(kr_1)j_0(kr_2) \tag{33}$$

To obtain a relation between n and s, we also proceed in a similar way to Refs. 5 and 6. Equation (10) suggests the functional form

$$n(z) = n_0(z)s^2(z) \exp\tau(z) \tag{34}$$

where $n_0(z)$ is the single-particle density corresponding to Φ (and is thus independent of s). Taking variations in s and using (10) and (14) gives

$$\delta\tau(z_1) = 2 \int d\mathbf{r}_2[\delta s(z_2)/s(z_2)]n(z_2)[g(\mathbf{r}_1, \mathbf{r}_2) - 1] \tag{35}$$

which has the approximate solution

$$\tau(z_1) = \int d\mathbf{r}_2\, n(z_2)[g(\mathbf{r}_1, \mathbf{r}_2) - 1] \tag{36}$$

plus a function independent of s.

When v is switched off, $n(z) = n_0(z)$. Thus we can write

$$\begin{aligned}\tau(z_1) &= \int d\mathbf{r}_2[n(z_2) - n_0(z_2)][g(\mathbf{r}_1, \mathbf{r}_2) - 1] \\ &= \int_0^\infty dz_2[n(z_2) - n_0(z_2)]G(z_1, z_2]\end{aligned} \tag{37}$$

The corresponding relation for spherical symmetry is

$$\begin{aligned}\tau(r_1) &= \int d\mathbf{r}_2[n(r_2) - n_0(r_2)][g(\mathbf{r}_1, \mathbf{r}_2) - 1] \\ &= \int_0^\infty dr_2 r_2^2[n(r_2) - n_0(r_2)]G(r_1, r_2)\end{aligned} \tag{38}$$

The Percus–Yevick and the convolution–hypernetted chain equations of classical statistical mechanics have similar form,[8,6] and all three are equivalent in the lowest order in the density.

6. WEAK FIELDS

Finally, we shall given an approximate solution to the general equations valid in regions where v can be taken to be "weak." We expect these regions to be those where v is small compared to a typical internal or zero-point energy, for example, mc^2, where c is the speed of sound. This energy is 2.36 meV for liquid ^{4}He. The polarization potential between an ion of charge e and atoms of polarizability α is $-\alpha e^2/2r^4$. This is approximately -0.3 meV at the surface of an electron bubble in helium, and we may thus expect the expressions for s and n derived below to be good approximations for all r where $n_0(r)$ is constant. The range in which the potential can be considered to be weak is more precisely determined in each case by the criterion

$$|s - 1| \ll 1 \tag{39}$$

We write $s = \exp\sigma$ in the general equations (16) and (26), and expand in powers of σ. At the same time we approximate n_0 by $\bar{n}_0$, g by $g_0(r_{12})$, and make the lowest order approximations for τ:

$$\begin{aligned}\tau(z_1) &\simeq 2\bar{n}_0 \int_0^D dz_2 \sigma(z_2) G_0(z_1, z_2) \\ \tau(r_1) &\simeq 2\bar{n}_0 \int_R^\infty dr_2 r_2^2 \sigma(r_2) G_0(r_1, r_2)\end{aligned} \tag{40}$$

Keeping only linear terms, we obtain the equations

$$\sigma''(z_1) = (2m/\hbar^2)\left[v(z_1) + \bar{n}_0 \int_0^D dz_2 v(z_2) G_0(z_1, z_2) \right]$$

$$[r_1\sigma(r_1)]'' = (2m/\hbar^2) r_1 \left[v(r_1) + \bar{n}_0 \int_R^\infty dr_2 r_2^2 v(r_2) G_0(r_1, r_2) \right] \tag{41}$$

so that

$$\sigma(z) = (2m/\hbar^2) \int_z^\infty dz_1 (z_1 - z) \left[v(z_1) + \bar{n}_0 \int_0^D dz_2 v(z_2) G_0(z_1, z_2) \right]$$

$$r\sigma(r) = (2m/\hbar^2) \int_r^\infty dr_1 (r_1 - r) r_1 \left[v(r_1) + \bar{n}_0 \int_R^\infty dr_2 r_2 v(r_2) G_0(r_1, r_2) \right] \tag{42}$$

In this approximation, the densities are given by

$$\begin{aligned}[n(z) - \bar{n}_0]/\bar{n}_0 &= 2\sigma(z) + \tau(z) \\ &= 2\left[\sigma(z) + \bar{n}_0 \int_0^D dz_1 \sigma(z_1) G_0(z_1, z) \right] \end{aligned} \tag{43}$$

and

$$[n(r) - \bar{n}_0]/\bar{n}_0 = 2\left[\sigma(r) + \bar{n}_0 \int_R^\infty dr_1 r_1^2 \sigma(r_1) G_0(r_1, r) \right] \tag{44}$$

Thus the wave function and the density of a quantum fluid in a weak field are explicitly determined in terms of the pair correlation function of the bulk fluid. It is, however, clear that the approximations made cannot be accurate very close to the boundaries $z = 0$ or $r = R$.

There the wave function is determined mainly by the short-range potential w. In principle it may be calculated by the methods of this paper, using Eq. (16) or (26) with v replaced by w and with the appropriate correlation functions. But the potential w (which excludes the fluid from some region) cannot be regarded as weak, and the equations cannot be linearized.

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