

## Microscopic theory of surface excitations in superfluid He<sup>4</sup>†

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A many-body wave function, similar to the Feynman wave function for bulk excitations in liquid helium, is proposed for the surface excitations. A discrete surface excitation is found to exist for  $k < 2.0 \text{ \AA}^{-1}$ ; its energy is calculated both variationally and by solution of an effective one-body Schrödinger equation. The latter also permits calculation of the effect of the surface on the bulk excitations. The absence of backflow in the wave function is a serious defect for  $k \gtrsim 0.8 \text{ \AA}^{-1}$ .

### I. INTRODUCTION

The temperature dependence of the surface tension of liquid helium is due principally to the presence of quantized surface waves. Atkins<sup>1</sup> used the classical dispersion relation for surface waves in an incompressible nonviscous fluid

$$\omega^2 = (\sigma_0/\mu_0) k^3, \quad (1)$$

where  $\sigma_0$  is the surface tension at zero temperature and  $\mu_0$  is the mass density at zero pressure, to calculate the temperature dependence of the surface tension, and obtain fair agreement with experiment<sup>2</sup> for  $T < 1 \text{ K}$ . Edwards, Eckardt, and Gasparini<sup>3</sup> have recently extended Atkins's analysis, including the effects of compressibility, phonon dispersion, and Gibbs's "surface mass." Their analysis is essentially hydrodynamic, but includes some quantum effects through the use of an energy functional which is designed to yield the correct empirical dispersion relation for bulk phonons and through a phenomenological modification of the hydrodynamic boundary conditions to take account of the fact that the surface is not sharp. With appropriate choice of their phenomenological parameters, Edwards, Eckardt, and Gasparini are able to fit recent measurements<sup>3</sup> of the temperature dependence of the surface entropy in the temperature regime  $T < 1 \text{ K}$ .

Our purpose here is to calculate the dispersion relation for the surface excitations directly from a many-body wave function. This approach, though somewhat laborious, eliminates the question of how the classical hydrodynamics should be modified to take account of quantum effects. The numerical accuracy of our dispersion relation is not very great, for reasons which will be discussed. Nevertheless, the calculation is of interest for two reasons: (a) It employs the simplest possible wave function, which permits obvious generalizations (which lead, unfortunately, to very difficult calculations); and (b) a unified theory of surface and bulk excitations is obtained, both arising from the same equation. This equation also yields the scat-

tering phase shifts of bulk excitations scattered from the surface, and hence the contribution of the bulk excitations to the surface tension.

### II. WAVE FUNCTION FOR EXCITATIONS

We consider a liquid which is infinite in the  $x$  and  $y$  directions, with a free surface parallel to a plane of constant  $z$ . The number density approaches 0 as  $z \rightarrow \infty$ , and approaches the bulk density  $\rho_0$  as  $z \rightarrow -\infty$ . In analogy with the Feynman<sup>4</sup> theory of the elementary excitations in the bulk fluid, we use as a trial function for the excited states of the semi-infinite fluid

$$\psi = \psi_0 \sum F(\vec{r}_i), \quad (2)$$

where  $\psi_0$  is the ground-state wave function of the semi-infinite fluid. Translational invariance in the  $x$  and  $y$  directions allows  $\psi$  to be taken as an eigenfunction of the momentum operators in these directions, so that

$$F(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} f(z), \quad (3)$$

where  $\vec{k}$  is a vector in the  $x$ - $y$  plane, and thus

$$\psi = \psi_0 \sum e^{i\vec{k}\cdot\vec{r}_i} f(z_i). \quad (4)$$

If we believe that classical hydrodynamics provides an adequate description of the system for sufficiently small  $\vec{k}$ , then we can infer the limiting form of  $f(z)$  for small  $\vec{k}$ . Classically, the velocity potential for a surface wave of small amplitude and long wavelength is

$$\epsilon e^{i\vec{k}\cdot\vec{r}} e^{kz}, \quad (5)$$

where  $\epsilon$  is proportional to the amplitude. The quantum-mechanical wave function describing a state in which a large-scale hydrodynamic motion is superimposed on the ground state of a Bose fluid is<sup>4</sup>

$$\psi_0 \exp\left(i \sum \chi(\vec{r}_i)\right), \quad (6)$$

where  $\chi(\vec{r})$  is the velocity potential, i. e.,

$$\vec{v}(\vec{r}) = (\hbar/m) \nabla \chi(\vec{r}). \quad (7)$$

Using the form (5) for  $\chi$  and expanding the wave function (6) through the linear term in  $\epsilon$ , we obtain a superposition of the ground state  $\psi_0$  and the state

$$\psi_0 \sum e^{i\vec{k}\cdot\vec{r}_i} e^{kz_i}, \quad (8)$$

the latter being orthogonal to the ground state since it belongs to a different eigenvalue of the momentum parallel to the surface. We identify this latter state as the state with a single surface excitation, and thus find that  $f(z) \sim e^{kz}$  for small  $\vec{k}$ . The terms in  $\epsilon^2$ ,  $\epsilon^3$ , etc., in the expansion of (6) belong to momentum eigenvalues  $2\vec{k}$ ,  $3\vec{k}$ , ..., and represent states with multiple excitations.

Using the fact that  $H\psi_0 = E_0\psi_0$ , we can calculate the expectation value of  $H - E_0$  on the state (4), obtaining

$$\begin{aligned} \epsilon(k) = & \frac{\hbar^2}{2m} \int dz \left( \frac{df}{dz} \frac{df^*}{dz} + k^2 f f^* \right) \rho(z) \times \left( \int f f^* \rho(z) dz \right. \\ & \left. + \int \int B(z_1, z_2, k) f(z_1) f^*(z_2) \rho(z_1) \rho(z_2) dz_1 dz_2 \right)^{-1}, \end{aligned} \quad (9)$$

where

$$B(z_1, z_2, k) = \int \int g(\vec{r}_1, \vec{r}_2) e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)} dx_1 dy_1. \quad (10)$$

In Eq. (9)  $\rho(z)$  is the number density in the ground state and  $g$  is related to the two-particle distribution function in the ground state by the equation

$$\rho^{(2)}(\vec{r}_1, \vec{r}_2) = \rho(z_1) \rho(z_2) g(\vec{r}_1, \vec{r}_2). \quad (11)$$

The condition that  $\epsilon(k)$  be stationary with respect to variation of the function  $f^*$  leads to the equation

$$\begin{aligned} \frac{\hbar^2}{2m} \left( \frac{d^2 f}{dz^2} + \frac{d \ln \rho}{dz} \frac{df}{dz} - k^2 f \right) \\ + \lambda \left( f + \int B(z, z', k) \rho(z') f(z') dz' \right) = 0, \end{aligned} \quad (12)$$

where  $\lambda$  is the stationary value of  $\epsilon(k)$ .

We have calculated  $\epsilon(k)$  variationally, using Eq. (9) with an exponential trial function, and also by solving Eq. (12). Before presenting the numerical results, we discuss some general properties of Eq. (12).

### III. CONTINUUM SOLUTIONS

We consider Eq. (12) for a fixed value of the parallel momentum  $\vec{k}$ . The spectrum of eigenvalues  $\lambda$  will consist of a continuum and possibly also some discrete eigenvalues. Deep in the interior, where  $\rho = \rho_0$ , Eq. (12) is translationally invariant and thus has solutions of the form  $f = e^{iqz}$ . Inserting this form into (12), we find

$$\lambda = \frac{\hbar^2}{2m} \frac{k^2 + q^2}{S((k^2 + q^2)^{1/2})}, \quad (13)$$

where  $S$  is the liquid structure factor in the bulk fluid, i. e.,

$$S(p) = 1 + \rho_0 \int [g(r) - 1] e^{i\vec{p}\cdot\vec{r}} d\vec{r}. \quad (14)$$

Equation (13) is, of course, the well-known Feynman<sup>4</sup> dispersion relation for a bulk excitation of momentum  $\vec{k} + \vec{q}$ , where  $\vec{k}$  is parallel to the surface and  $\vec{q}$  is perpendicular to the surface.

For large positive  $z$ , the density falls off exponentially, the asymptotic form<sup>5</sup> being

$$\rho(z) \sim \exp[-(-8m\epsilon_B/\hbar^2)^{1/2} z], \quad (15)$$

where  $\epsilon_B$  is the energy per atom of the liquid in its ground state ( $\epsilon_B \sim -7.2$  K/atom). In this region we can omit the integral in Eq. (12), which contains an extra power of  $\rho$ , and obtain the asymptotic differential equation

$$f'' - Cf' + (2m\lambda/\hbar^2 - k^2)f = 0, \quad (16)$$

where  $C = (-8m\epsilon_B/\hbar^2)^{1/2}$ . The solution is  $f = e^{\gamma z}$ , where

$$\gamma = \frac{1}{2} [C \pm (C^2 + 4k^2 - 8m\lambda/\hbar^2)^{1/2}]. \quad (17)$$

The quantity raised to the  $\frac{1}{2}$  power, which we call  $\Delta$ , is

$$\Delta \equiv C^2 + 4k^2 - \frac{8m\lambda}{\hbar^2} = \frac{8m}{\hbar^2} \left( -\epsilon_B + \frac{\hbar^2 k^2}{2m} - \lambda \right). \quad (18)$$

Since  $-\epsilon_B + \hbar^2 k^2/2m$  is the energy necessary to remove an atom from the liquid in its ground state and put it into a state of momentum  $\vec{k}$  in the space outside, we see that  $\Delta$  is positive unless the energy  $\lambda$  of the excitation is large enough to evaporate an atom from the liquid while conserving momentum parallel to the surface. At temperatures below 1.5 K, we can assume  $\Delta > 0$  for the thermodynamically important excitations. The case  $\Delta < 0$  describes a state in which an atom has been evaporated from the fluid, and will not concern us here (though it is relevant to the calculation of the surface term in the free energy of the vapor). The normalizability of the wave function requires that  $\rho f f^*$  remain finite (in the case  $\Delta > 0$  we require  $\rho f f^* \rightarrow 0$  for large  $z$ ). If  $\Delta > 0$ , we have  $\rho f f^* \sim e^{\pm \Delta^{1/2} z}$ . In order that only the decreasing exponential be present for large positive  $z$ , the solution for large negative  $z$  must be the correct linear combination of  $e^{iqz}$  and  $e^{-iqz}$ , both of which belong to the same eigenvalue  $\lambda$ . Since  $f$  may be taken as real [all coefficients in (12) are real], its asymptotic form must be  $\cos(qz + \delta)$ . We shall see that the contribution of the bulk excitations to the surface

tension can be expressed in terms of the phase shift  $\delta(k, q)$ .

#### IV. SURFACE STATES

A surface state corresponds to a solution of (12) for which  $f \rightarrow 0$  as  $z \rightarrow -\infty$  and  $\rho f^2 \rightarrow 0$  as  $z \rightarrow \infty$ . For a given  $\vec{k}$ , we can show that the eigenvalues (if any) associated with surface states form a discrete set; numerically, we find only one surface state for each  $\vec{k}$ . Although we do not fully understand the mathematical properties of Eq. (12), we assume that the eigenvalues for surface states are below the continuum. The numerical calculations confirm this. The Feynman dispersion relation (13) implies that for  $k \lesssim 0.75 \text{ \AA}^{-1}$ ; the lower limit of the continuum occurs when  $q=0$ , corresponding to  $\lambda = \hbar^2 k^2 / 2mS(k)$ . For  $0.75 \lesssim k \lesssim 1.8 \text{ \AA}^{-1}$ , the lower limit of the continuum occurs when  $q^2 = k_0^2 - k^2$  (where  $k_0$  is the wave number of the minimum-energy roton), corresponding to  $\lambda = \hbar^2 k_0^2 / 2mS(k_0)$ .

At the outset, it was not obvious to us that (12) has any discrete eigenvalues. We investigated this question variationally, using the trial function  $f(z) = e^{\alpha z}$  in the variational principle (9). In the limit  $\alpha \rightarrow 0$ , the wave function is identical with the Feynman wave function for a bulk excitation of momentum  $\vec{k}$ . In this case the surface region makes a negligible contribution to the numerator and denominator of (9), and we obtain

$$\epsilon(k; \alpha=0) = \hbar^2 k^2 / 2mS(k). \quad (19)$$

The maximum permissible value of  $\alpha$ , such that  $\rho f^2 \rightarrow 0$  as  $z \rightarrow \infty$ , is  $\alpha = \frac{1}{2}C = 1.085 \text{ \AA}^{-1}$ . The corresponding wave function describes a situation in which it is overwhelmingly likely that one atom is

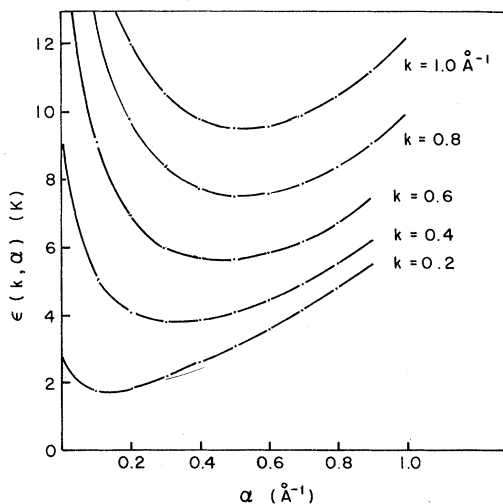


FIG. 1. Variational calculation of energy of surface excitation for  $k \leq 1.0 \text{ \AA}^{-1}$  with trial function  $f(z) = e^{\alpha z}$ .

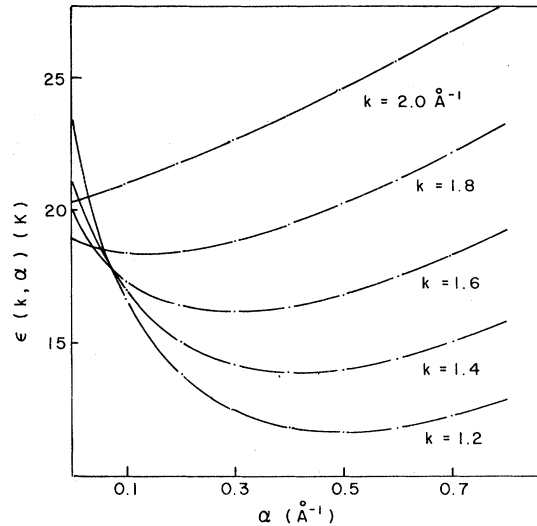


FIG. 2. Variational calculation of energy of surface excitation for  $1.2 \leq k \leq 2.0 \text{ \AA}^{-1}$ . The disappearance of the surface state for  $k \geq 2.0 \text{ \AA}^{-1}$  is a consequence of the fact that a slight decrease in the density raises the energy of bulk excitations for  $k \geq 2.0 \text{ \AA}^{-1}$ .

far outside the liquid, moving with momentum  $\vec{k}$  parallel to the surface. We expect the energy of this state to be

$$\epsilon(k; \alpha = 1.085) = -\epsilon_B + \hbar^2 k^2 / 2m, \quad (20)$$

and readily obtain this result from (9), recognizing that numerator and denominator are dominated by the region of large positive  $z$ , and that the second term in the denominator is negligible compared with the first.

The results of some of the variational calculations are shown in Fig. 1. We see that  $\epsilon(k; \alpha)$  has a minimum for some value of  $\alpha$  between 0 and  $\frac{1}{2}C$ , corresponding to a true surface excitation (i. e.,  $\rho f^2 \rightarrow 0$  as  $z \rightarrow \pm\infty$ ). The decrease in energy as  $\alpha$  is lowered slightly below the critical value  $\frac{1}{2}C$  is expected, because the almost-free atom now spends some time within range of the attraction of other atoms. For small  $\alpha$ , the wave function may be thought of as describing a bulk excitation of momentum  $\vec{k}$ , but in a fluid of slightly lower density than the bulk. Thus, the negative value of  $\partial\epsilon/\partial\alpha$  at  $\alpha=0$  corresponds to the fact that for given  $\vec{k}$  the energy of the bulk excitations decreases with decreasing bulk density.

Figure 2 exhibits the results of variational calculations for larger values of  $k$ . The most interesting feature is the disappearance of the surface state when  $k=2.0 \text{ \AA}^{-1}$ , corresponding to the change in sign of  $\partial\epsilon/\partial\alpha$  at  $\alpha=0$ . The bulk liquid structure factor  $S(k; \rho)$  used in the present calculations has the property

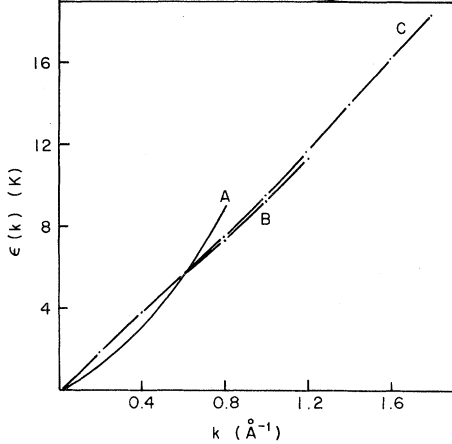


FIG. 3. Comparison of (A) classical dispersion relation for surface tension waves with (C) results of variational calculation and (B) numerical solution of Eq. (12). Inclusion of backflow would lower (B) and (C) considerably for  $k \geq 0.8 \text{ \AA}^{-1}$ .

$$\left. \frac{\partial S}{\partial \rho} \right|_{\rho=\rho_0} < 0 \text{ for } k \leq 1.9 \text{ \AA}^{-1},$$

$$\left. \frac{\partial S}{\partial \rho} \right|_{\rho=\rho_0} > 0 \text{ for } k \geq 2.0 \text{ \AA}^{-1}$$

(we have calculated  $S$  at intervals  $\Delta k = 0.1 \text{ \AA}^{-1}$ ). Thus the energy (19) of the bulk excitations ceases to decrease with decreasing density for  $k \geq 2.0 \text{ \AA}^{-1}$ , which is exactly the  $k$  value for which the surface excitation disappears.

The calculations require, of course, a knowledge of  $\rho(z)$  and  $g(\vec{r}_1, \vec{r}_2)$  in the ground state. For this purpose we rely on our previous work,<sup>6,7</sup> in which the ground-state wave function of the semi-infinite fluid with a free surface was taken to be a product of two-body and one-body factors. The two-body factor is given by Eq. (12) of Ref. 7. A "local-density" approximation [Eq. (10) of Ref. 7] is used to evaluate the correlation function  $g(\vec{r}_1, \vec{r}_2)$  in the inhomogeneous fluid. Evaluation of the function  $B(z_1, z_2, k)$  is then straightforward but somewhat expensive, since a double integral must be done numerically for each value of  $(z_1, z_2, k)$ . A small modification was made in the density profile [Eq. (8) of Ref. 7] in order to give it the correct asymptotic form (15) at large  $z$ . The asymptotic region is unimportant in the ground-state calculations, but more important in evaluating (9). A differential equation satisfied by  $\rho(z)$  for large  $z$  may be obtained by varying the surface energy [Eq. (7) of Ref. 6] with respect to the function  $\psi(z) = \rho^{1/2}(z)$ . In the asymptotic region the variation of  $g$  with respect to  $\psi(z)$  may be neglected, and  $g$  is a function

only of  $|\vec{r}_1 - \vec{r}_2|$ . The resulting differential equation is

$$\frac{\hbar^2}{2m} \frac{d^2 \psi}{dz^2} + [2 \mathcal{E}(z) - \epsilon_B] \psi = 0, \quad (21)$$

where  $\mathcal{E}(z)$  is given by Eq. (8) of Ref. 6. We integrated (21) numerically, starting at large positive  $z$  where the solution is  $\psi = e^{-Cz/2}$ , with  $\mathcal{E}(z)$  evaluated numerically from our previous work.<sup>8</sup> The solution of (21) was joined to our previous  $\rho(z)$  at the point  $z_0$ , where the logarithmic derivatives of the two functions are equal. This point is quite far out in the tail of the surface; we find  $\rho(z_0) = 0.03\rho_0$ .

The optimal values of  $\alpha$  are 0.12, 0.32, 0.46, 0.52, and  $0.54 \text{ \AA}^{-1}$  for  $k = 0.2, 0.4, 0.6, 0.8,$  and  $1.0 \text{ \AA}^{-1}$ . In Sec. II we argued that  $f(z) \sim e^{kz}$  for small  $k$ , which implies that the optimal  $\alpha$  should be equal to  $k$  when  $k$  is small. Our numbers do not appear to have this limiting property, though Fig. 1 shows that the choice  $\alpha = k$  would change the energy negligibly for  $k = 0.2, 0.4,$  and  $0.6$ . The energy  $\epsilon(k)$  is fitted much better by a straight line than by the classical  $k^{3/2}$  behavior at small  $k$  (see Fig. 3). We ascribe the incorrect limiting behavior of  $\epsilon(k)$  and  $\alpha$  to shortcomings of our approximate ground-state wave function, which will be discussed below.

We have also obtained an accurate numerical solution of (12) for  $k = 0.2, 0.4, 0.6, 0.8, 1.0,$  and  $1.2 \text{ \AA}^{-1}$ . The resulting energy eigenvalues are given in Table I, and differ very little from those found variationally. The form of (12) makes numerical solution difficult, since  $B$  does not vanish for either order of the variables, and we therefore cannot integrate in from either end. Our procedure was to approximate the integral operator by a second-order differential operator. In the integral we wrote

$$f(z') = f(z) + (z' - z)f'(z) + \frac{1}{2}(z' - z)^2 f''(z) \quad (22)$$

TABLE I. Energy of surface excitation calculated variationally with exponential trial function and by numerical solution of Eq. (12).

$k \text{ (\AA}^{-1}\text{)}$	Solving Eq. (12) $\hbar \omega(k) \text{ (K)}$	Variational $\hbar \omega(k) \text{ (K)}$
0.2	1.72	1.71
0.4	3.78	3.79
0.6	5.55	5.60
0.8	7.33	7.47
1.0	9.27	9.51
1.2	11.34	11.67
1.4		13.92
1.6		16.18
1.8		18.38

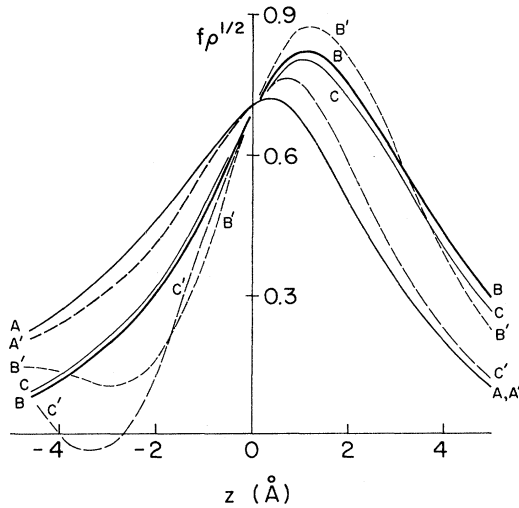


FIG. 4. Comparison of variational (exponential) wave function for surface excitation with numerical solution of Eq. (12). A, B, and C are variational wave functions; A', B', and C' are numerical wave functions for  $k = 0.4, 0.8,$  and  $1.2 \text{ \AA}^{-1}$ . Positive  $z$  is the exterior, negative  $z$  the interior of the fluid. All curves are normalized to 0.707 at  $z = 0$ , the point where the density is half the bulk density. Curves A and A' are indistinguishable for  $z > 0$ .

and calculated the moments

$$\begin{aligned} I_0(z, k) &= \int B(z, z', k) \rho(z') dz', \\ I_1(z, k) &= \int B(z, z', k) \rho(z') (z' - z) dz', \\ I_2(z, k) &= \frac{1}{2} \int B(z, z', k) \rho(z') (z' - z)^2 dz'. \end{aligned} \quad (23)$$

Equation (12) then becomes

$$\frac{\hbar^2}{2m} \left( \frac{d^2 f}{dz^2} + \frac{d \ln \rho}{dz} \frac{df}{dz} - k^2 f \right) + \lambda (f + I_0 f + I_1 f' + I_2 f'') = 0. \quad (24)$$

We integrated (24) numerically for different values of  $\lambda$ , starting at large positive  $z$  with the asymptotic form  $e^{\gamma z}$  [where  $\gamma$  is the negative root in (17)], until a value of  $\lambda$  was found for which  $f \rightarrow 0$  as  $z \rightarrow -\infty$ . The integral in (12) was then evaluated with this  $f$ , and the resulting differential equation

$$\frac{\hbar^2}{2m} \left( \frac{d^2 f}{dz^2} + \frac{d \ln \rho}{dz} \frac{df}{dz} - k^2 f \right) + \lambda [f + G(z)] = 0 \quad (25)$$

[where  $G(z)$  is the integral] was numerically integrated starting with the asymptotic form  $e^{\gamma z}$  at large positive  $z$ , until a new value of  $\lambda$  was found for which  $f \rightarrow 0$  as  $z \rightarrow -\infty$ . In principle,  $G(z)$  could then be reevaluated and the procedure repeated, but in practice we attained self-consistency without further iterations. The success of the proce-

sure is undoubtedly due to the fairly short-range character of the function  $B$ .

A careful numerical search was made for additional discrete eigenvalues, and none were found. Reut and Fisher<sup>9</sup> have suggested that the dispersion relation for surface excitations has a second branch, with a minimum  $\epsilon \sim 2 \text{ K}$  occurring at  $k \sim 0.5 \text{ \AA}^{-1}$ . We see no sign of a second branch, and Edwards, Eckardt, and Gasparini do not require it to fit the thermodynamic data.

The function  $f(z)$  obtained from solution of (12) is compared with the variational  $f(z)$  in Fig. 4. The two functions are in close agreement for small  $k$ , but for  $k \gtrsim 1.2 \text{ \AA}^{-1}$  the solution of (12) oscillates in the interior. Numerical solution of (12) becomes much more difficult as  $k$  increases, since the oscillations of  $f$  extend deeper and deeper into the interior (the precursor of the eventual merging of the surface and bulk states), necessitating the use of an increasingly large interior cutoff value of  $z$ . The considerable labor involved in extending the solution beyond  $k = 1.2 \text{ \AA}^{-1}$  seemed unjustified for several reasons: (i) The excitation energy  $\epsilon(k)$  is too large to be of thermodynamic importance; (ii) the absence of backflow in the wave function (see Sec. V) makes the calculation increasingly inaccurate for larger  $k$ ; and (iii) the decay of one surface excitation into two, which is energetically possible, becomes very important for  $k \gtrsim 1.0 \text{ \AA}^{-1}$ , as Saam<sup>10</sup> has pointed out. Thus the excitations probably lose their identity as long-lived objects.

Even without solving (12) for large  $k$ , we can see that the eventual disappearance of the surface state is a feature of (12) and not merely an artifact of the variational ansatz. For large  $k$  the function  $B(z_1, z_2, k)$  becomes negligible, so that the nonlocal term in (12) may be omitted, resulting in the differential equation

$$\frac{\hbar^2}{2m} \left( \frac{d^2 f}{dz^2} + \frac{d \ln \rho}{dz} \frac{df}{dz} - k^2 f \right) + \lambda f = 0,$$

which is associated with a variational principle similar to (9), but without the second term in the denominator. The variational principle trivially implies  $\lambda > \hbar^2 k^2 / 2m$ , while the asymptotic form of the differential equation in the interior,

$$\frac{\hbar^2}{2m} \left( \frac{d^2 f}{dz^2} - k^2 f \right) + \lambda f = 0,$$

allows an exponentially decreasing solution only if  $\lambda < \hbar^2 k^2 / 2m$ . Hence there is no surface state for sufficiently large  $k$ .

#### V. LIMITING BEHAVIOR FOR SMALL AND LARGE $k$

We have used an approximate ground-state wave function  $\psi_0$  to calculate the correlation function

$B(z_1, z_2, k)$  which occurs in (9) and (12). In order to obtain the correct limiting behavior of  $f$  and  $\lambda$  for small  $k$ , it is necessary that  $\psi_0$  contain the correct surface correlations; i. e.,  $\psi_0$  must contain the zero-point fluctuations of the surface excitations of small  $k$ . The  $\psi_0$  of Refs. 6 and 7 does not contain these fluctuations correctly, but can be patched up to contain them. The procedure is quite circular, and is really no better than modifying curves B and C of Fig. 3 by hand so as to join the  $k^{3/2}$  curve at small  $k$ .

A similar situation exists in regard to the bulk excitations. We expect a long-wavelength phonon of wave number  $p$  to have an energy  $\epsilon(p) = \hbar cp$ , where  $c$  is the speed of sound. The Feynman wave function (2), with  $F(\vec{r}) = e^{i\vec{p}\cdot\vec{r}}$  as required by translational invariance, yields  $\epsilon(p) = \hbar^2 p^2 / 2mS(p)$ . Thus we need  $S(p) = \hbar p / 2mc$  for small  $p$  in order to obtain the correct limit. A Jastrow wave function, for example, which is a product of short-range two-body factors, will not lead to this asymptotic form of  $S(p)$ . Suppose one believes, however, that the Hamiltonian can be separated into two parts, of which one describes a compressible medium and is equivalent to a set of oscillators in the normal coordinates  $\rho_{\vec{p}} = \sum e^{i\vec{p}\cdot\vec{r}_i}$  with frequencies  $\omega(p) = cp$ , and the other describes motions on a smaller scale of wavelengths. Then the wave function will be Gaussian in the oscillator normal coordinates, the coefficients being known. Reatto and Chester<sup>11</sup> have pointed out that this Gaussian factor is also of the Jastrow form, but with a long-range rather than a short-range two-body factor. This procedure builds the desired limiting behavior of  $S(p)$  into a Jastrow wave function, but the procedure is at most self-consistent and not really derived from first principles.

Similarly, Eq. (12) will yield the desired limiting behavior of  $f(z)$  and  $\epsilon(k)$  if we modify  $\psi_0$  by including a factor which is Gaussian in the normal coordinates describing the surface excitations. The normal coordinate (for small  $k$ ) is

$$C_{\vec{k}} = \sum e^{i\vec{k}\cdot\vec{r}_i} e^{kz_i} \quad (26)$$

and the correct Gaussian factor is

$$\exp\left(-\frac{\sigma_0}{2A\rho_0^2} \sum_{k < k_c} \frac{k^2 C_{\vec{k}} C_{-\vec{k}}}{\hbar\omega_k}\right), \quad (27)$$

corresponding to the ground state of the Hamiltonian for a collection of noninteracting classical surface waves, with wave vectors  $k < k_c$ . The classical frequency  $\omega_k$  is given by Eq. (1), and  $A$  is the area of the surface. If the factor (27) is included in the ground-state wave function, then for small  $k$  the solution of (12) will be  $f(z) = e^{kz}$ ,  $\lambda = \hbar\omega_k$ . We note that the exponent in (27) is a sum of one- and

two-body terms, the latter depending on more than the scalar distance.

The wave function (4) does not incorporate backflow, i. e., the dipolelike hydrodynamic motion of atoms in the vicinity of a moving atom. Inclusion of this effect requires two-body terms as well as one-body terms in the factor multiplying  $\psi_0$ . Calculations of the bulk excitation spectrum<sup>12</sup> show that the inclusion of backflow is important in the roton region ( $k \sim 2 \text{ \AA}^{-1}$ ) and still significant (lowering the energy by about 35%) when  $k \sim 1 \text{ \AA}^{-1}$ . The effect of backflow on the energy of a surface excitation of momentum  $\vec{k}$  will be less than its effect on the energy of a bulk excitation of the same  $\vec{k}$ , since the surface excitation lives in a region of lower density. Nevertheless, the inclusion of backflow in (4) would undoubtedly produce substantial lowering of the energy of the surface excitations for  $k \geq 0.8 \text{ \AA}^{-1}$ . The difficulties in computing with such a wave function seem excessive. Thus the accuracy of our work is limited at large  $k$  by the absence of backflow and at small  $k$  by the absence of correct long-wavelength correlations in our ground-state wave function.

#### VI. CONTRIBUTION OF BULK EXCITATIONS TO SURFACE TENSION

The Helmholtz free energy of the liquid consists of a term proportional to the volume plus a term proportional to the surface area. The surface tension is the surface free energy per unit area. This arises principally from the surface excitations, but also from the effect of the free surface on the bulk excitations. Edwards, Eckardt, and Gasparini find that this effect gives rise to a (10–20)% lowering of the surface entropy in the range  $1 < T < 1.5 \text{ K}$ . In this section we analyze the effect in terms of the phase shifts associated with the continuum solutions of Eq. (12).

As we have discussed in Sec. III, a bulk excitation with wave number  $k$  parallel to the surface and wave number  $q$  perpendicular to the surface is represented by a solution of (12) which has the asymptotic form  $\cos(qz + \delta)$  for large negative  $z$ . The surface  $z = 0$ , which we call the "center" of the surface, is defined by the equation

$$\int_0^\infty \rho(z) dz = \int_{-\infty}^0 [\rho_0 - \rho(z)] dz, \quad (28)$$

which states that the mass outside the surface  $z = 0$  is equal to the missing mass inside the surface  $z = 0$ . Suppose that the liquid has two free surfaces, centered at  $z = 0$  and  $z = -D$  (where  $D$  is much larger than the thickness of the surface). The solution of (12) in the vicinity of  $z = -D$  is obtained from the solution in the vicinity of  $z = 0$  by the substitution  $z \rightarrow -z - D$ . The allowed values of  $q$  are

determined by the requirement that the two solutions agree in the interior, i. e.,

$$\cos(qz + \delta) = \pm \cos(-qz - qD + \delta), \quad (29)$$

which implies

$$q = (n\pi/D) + (2\delta/D), \quad n = 0, 1, 2, \dots \quad (30)$$

The free energy of the bulk excitations, neglecting interactions among the excitations, is thus

$$F = \frac{A}{2\pi\beta} \int_0^\infty k dk \sum_q \ln(1 - e^{-\beta\hbar\omega(k,q)}), \quad (31)$$

where  $A$  is the surface area,  $\beta = 1/k_B T$ , and  $\omega(k, q) = \omega((q^2 + k^2)^{1/2})$  is the dispersion relation for bulk excitations. Converting the  $q$  sum to an integral and making a Taylor expansion of  $\omega(k, q)$  around  $q = n\pi/D$ , we obtain a volume and a surface term in the free energy, the latter being

$$\frac{F_{\text{surf}}}{A} = \frac{\hbar}{\pi^2} \int_0^\infty k dk \int_0^\infty dq \frac{\delta(k, q)}{e^{\beta\hbar\omega(k,q)} - 1} \frac{\partial \omega}{\partial q}. \quad (32)$$

Numerical evaluation of this formula requires the solution of (12) for many different  $(k, q)$ , and seems hardly worthwhile in view of the inaccuracy of our

calculation of the dispersion relation of surface excitations.

## VII. DISCUSSION

In the range  $0.4 < k < 1 \text{ \AA}^{-1}$ , our dispersion relation for the bulk excitations is close to that calculated by Edwards, Eckardt, and Gasparini for values of their phenomenological parameters  $a \sim 1.0 \text{ \AA}^2$ ,  $\delta \sim 0 \text{ \AA}$ . They obtain a good fit to the data with  $a \sim 1.5 \text{ \AA}^2$ ,  $\delta \sim 0 \text{ \AA}$ , corresponding to a somewhat lower curve than ours. Inclusion of backflow in our wave function would, of course, lower our curve.

The absence of backflow and the previously discussed difficulties at small  $k$  limit the numerical accuracy of the present calculations. Nevertheless, the numbers are at least reasonable and are obtained fairly directly from Schrödinger's equation. The fact that Eq. (12) has an eigenvalue (surface state) below the continuum indicates that the wave function (4) is at least a good first approximation. The absence of a second discrete eigenvalue is interesting, but subject to possible revision if a better wave function were used.

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<sup>8</sup>This procedure is not perfectly self-consistent, since  $\mathcal{G}(z)$  depends on the function  $\rho(z)$ . An additional iteration, in which  $\mathcal{G}(z)$  is recomputed with the new  $\rho(z)$ , would produce negligible change.

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