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On the Theory of Quantized Vortices *

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Model many-body wave functions are constructed for a quantized vortex line and ring. The corresponding variational energies are calculated using an approximate integral equation derived by Percus and Yevick for classical fluids. The energy of the line is close to that found in the Hartree theory. However, the density distribution in the core region is markedly different, and the core size is somewhat smaller, being of the order of 1 Å. The velocity of translation of the vortex ring is calculated by a new method, and excellent agreement is obtained with the experimental results of Rayfield and Reif. The condensed-state wave function is computed numerically, and it is found that in the core of the vortex there are about 20% fewer particles in the condensed state than in the zero-momentum state when the system is in equilibrium.

I. INTRODUCTION

It is now well established that quantized vortex lines and rings can be excited in superfluid helium.[1,2] These vortices are quantized in the sense that the circulation associated with the superfluid flow is an integral multiple of h/m, where m is the mass of a helium atom. There is a variety of experimental evidence[1] which shows that, apart from the vortex core, the flow field associated with such a vortex is very similar to that of a classical vortex, namely irrotational and incompressible. The most striking evidence for this is the remarkable accuracy with which the experimental data[2] on the energy and velocity of large quantized vortex rings can be fitted to the standard classical formulae.[3] However the classical theory of vortices contains no unique theory of the core, which indeed can in this theory be taken to be any one of a number of different models. Nearly all the data that is available suggest that the core of a quantum vortex in helium has a spatial scale of a few interatomic spacings[1] and may indeed be very much smaller. If this is accepted, then clearly a quantum description of the core is mandatory; and it is equally important to construct a theory which takes into account the strong short-range interatomic correlations that are present in the fluid.

The purpose of this paper is to construct a model wave function for a vortex line and ring, and to calculate the energy of each.

The only theory of quantized vortices that we have at present is the well-known Hartree or order-parameter theory developed by Gross,[4] Pitaevskii,[5] and Fetter.[6] The obvious objection to this kind of theory is that by its very nature it is unlikely to give an accurate description of phenomena which take place in spatial regions of the order of a few interatomic spacings. Consequently it is probably unreliable in its description of the core of a quantum vortex. On the other hand, there is little reason to doubt that it gives a satisfactory description of the large scale potential flow outside the core region. Until we have data from experiments that are sensitive to the core structure we shall be unable to distinguish the predictions of this theory from any other that is proposed. We hope that some of the results presented in this paper will stimulate such experiments.

In Sec. II we present the model wave function for a vortex line, and in Sec. III we present the results of an approximate calculation of the energy per unit length of such a line. Section IV is devoted to the energy and velocity of a vortex ring. Very close agreement is obtained with the experimental data.[2] Our model wave leads to a macroscopically occupied state of the single-particle density matrix, and in Sec. V we show how the amplitude and phase of this state can be calculated. Our conclusions are presented in Sec. VI, where we outline further possible developments of our model and calculations.

II. THE MODEL WAVE FUNCTION

There are two requirements that our trial wave function must satisfy. First it should, except perhaps in the region of the core, lead to the same velocity field as a classical vortex line. There is very strong evidence to support this requirement from Rayfield and Reif's measurements[2] of the energy and velocity of quantized vortex rings. In the core region we have no strong grounds for this requirement, and we therefore leave the question open for the moment. Our second requirement is that the model wave function take into account the strong interatomic correlations that are present in liquid helium. This latter requirement follows from the fact[1,2] that the core region has a spatial scale of at most a few interatomic distances.

It is well known[7] how to construct a wave function that meets these two requirements. For simplicity, we assume that we have a cylindrical container of volume V of liquid helium with mean density $\bar{n}=N/V$. Then if Φ_0 is the exact ground state for this system, then a suitable model wave function is

$$\Phi_{\mathrm{TL}}=e^{iS}\Phi_0(r_1\cdots r_n)\,, \tag{2.1}$$

where $S=\sum_\alpha \psi(r_\alpha)\,.$ (2.2)

Here r_α denotes the position of the αth particle,

and $\psi(r)$ is the velocity potential for the classical irrotational flow we wish to reproduce. For a vortex line on the axis of the cylinder

$$\psi = \gamma\theta , \tag{2.3}$$

where θ is the cylindrical angle about the axes and γ is for the moment an arbitrary real constant. With Φ_{TL} given by (2.1) and (2.2), we find that current density $j(\vec{r})$ and number density $n(\vec{r})$ are given by

$$\vec{j}(\vec{r}) = -\hbar/m(\nabla\psi)\overline{n} , \tag{2.4}$$

and $$n(\vec{r}) = \overline{n} = N/V. \tag{2.5}$$

Consequently if the velocity field $\vec{v}(\vec{r})$ is defined by the equation

$$\vec{v}(\vec{r}) = \vec{j}(\vec{r})/n(\vec{r}) , \tag{2.6}$$

then we find that with (2.3)

$$\vec{v}(\vec{r}) = (v_r, v_\theta, v_z) = (0, \gamma\hbar/mr, 0). \tag{2.7}$$

Here we have used cylindrical polar coordinates (r, θ, z). This flow field is easily seen to be irrotational and incompressible everywhere. How, ever, this model wave function leads to an infinite flow energy because the velocity field diverges as $r \to 0$. Feynman[7] has suggested a modification of the model that removes this difficulty. Namely,

$$\Phi_{TL} = \prod_{\alpha=1}^{N} f(r_\alpha) e^{is}\Phi_0 , \tag{2.8}$$

where $f(\vec{r})$ is chosen to be a function of r alone that vanishes as $r \to 0$ tends to unity as r becomes large. With this function,

$$\vec{j}(\vec{r}) = \hbar/m(\nabla\psi)n(\vec{r}) \tag{2.9}$$

and

$$n(\vec{r}_1) = N\int d2\cdots dN \prod_{\alpha=1}^{N} f^2(r_\alpha)\Phi_0^2 / \int d1\cdots dN \times \prod_{\alpha=1}^{N} f^2(r_\alpha)\Phi_0^2 . \tag{2.10}$$

The velocity field $\vec{v}(\vec{r})$ is therefore the same as before, and the expectation value of the Hamiltonian H is given by

$$\langle H\rangle = E_0 + \frac{\hbar^2}{2m}\int[|\nabla\psi|^2 + (\nabla\ln f)^2]n(\vec{r})d^3r , \tag{2.11}$$

where E_0 is the exact ground-state energy. The integral in (2.11) will converge as long as $n(\vec{r})$ vanishes sufficiently fast as $r \to 0$, and this can be assured as long as $f(\vec{r})$ vanishes sufficiently fast $r \to 0$.

The trial function given by (2.8) is an eigenfunction of the z component of the total angular momentum with eigenvalue $N\hbar$. We may therefore use it to calculate the energy variationally, and our task then reduces to finding that function $f(\vec{r})$ which minimizes the expectation value of H.

There is still however one undetermined parameter in Φ_{TL}, namely γ in Eq. (2.3). This is directly related to the circulation in the system for

$$\int_C \vec{v}\cdot d\vec{l} = \gamma h/m, \tag{2.12}$$

where the integral is evaluated around any closed path C enclosing the z axis. The quantization of circulation is usually derived by demanding that the trial function be a single-valued function of its arguments, from which it follows that $\gamma = n$ with n an integer. We find this procedure unsatisfactory because there are no general grounds for demanding that a wave function be single valued, and indeed there are known counterexamples.[8] However, we show in Appendix A that if we *assume* that our system possesses one or more single-valued states, then all possible states of the system must be single valued. We believe that it is perfectly reasonable to assure that the ground state of liquid helium is single valued; and consequently we can conclude that Φ_{TL} must also be single valued, and thus $\gamma/2\pi$ must be an integer. The quantization of circulation in units of h/m then follows at once.

For convenience, we rewrite (2.11) in a slightly different form. We set $f(r) = \exp[-1/2h(r)$ with $h(r)$ real; then

$$\langle H\rangle = E_0 + \frac{\pi\hbar^2}{m}\int\left[\frac{1}{r^2} + \tfrac{1}{4}\left(\frac{dh}{dr}\right)^2\right]n(r)rdr , \tag{2.13}$$

where E is the energy per unit length of line and E_0 the exact ground-state energy per unit length of cylinder.

III. THE ENERGY OF A VORTEX LINE

To calculate the energy of a line, we have to compute the density $n(r)$ corresponding to the trial function ϕ_{TL}, with $f(r) = \exp[-\frac{1}{2}h(r)]$. We first note that the density, defined by Eq. (2.10) is formally identical with the density of a classical system with an equilibrium probability distribution Φ_0^2 in the presence of an external potential $\sum_i V(r_i) = kT_{\text{eff}}\sum_i h(\vec{r}_i)$, where T_{eff} is some arbitrary effective temperature and k is Boltzmann's constant. Our problem is therefore exactly equivalent to the problem of calculating the density in this equivalent classical system. There are several methods by which this might be done. We have chosen to use the Percus-Yevick (PY) and convoluted-hypernetted-chain (CHNC) approximate integral equations[9]: first, because these equations are known to be reasonable accurate at liquid helium densites[10] and second, because they are relatively simple to solve and consequently we can carry our a wide search to determine the best trial function $h(r)$. We hope at a later date to check the calculations presented in this paper by means of a Monte Carlo calculation. From the information that is available from exact variational calculations[10] of the radial distribution functions and ground-state energy for liquid helium, we estimate that the PY and CHNC equations should

yield energy values for the vortex line that are accurate to 10-15%.

The PY equation for $n(\vec{r})$ is[9]

$$n(\vec{r})e^{h(\vec{r})} = \bar{n}[1 + \int C_0(\vec{r}-\vec{r}')(n(\vec{r}')-\bar{n})d^3r'] , \quad (3.1)$$

while the CHNC equation is[9]

$$n(\vec{r})e^{h(\vec{r})} = \bar{n}\exp[\int C_0(\vec{r}-\vec{r}')(n(\vec{r}')-\bar{n})d^3\vec{r}'] .$$

These equations are derived in Appendix B. The only reference to the ground state is $C_0(\vec{r}-\vec{r}')$, the direct correlation function corresponding to the probability distribution Φ_0^2. This is related to the liquid-structure factor $S_0(\vec{k})$ by the equation

$$S_0(\vec{k}) = [1 - \bar{n}C_0(\vec{k})]^{-1} , \quad (3.3)$$

where $C_0(\vec{k})$ is the Fourier transform of $C_0(\vec{r})$ and $\bar{n}$ is the mean density. The structure factor $S_0(\vec{k})$ cannot, of course, be measured directly. However, apart from its behavior for small k, its measured values at finite temperature should be little different from those at absolute zero. Feynman[7] has argued convincingly that the zero point motion of the phonons dominates the behavior of $S_0(k)$ for small k; namely that its form for small k is $\hbar k/2mc$. A model wave function that leads to this result has been constructed by Reatto and Chester.[15] We show in Appendix C that the linear behavior of $S(k)$ for small wave numbers is a necessary condition for the existence of an absolute minimum in the energy and a function of a. If $S_0(k)$ tends to a constant as $k \to 0$ then only a local minimum exists. We also give a physical argument in Appendix C which leads to the same conclusion. We have consequently taken the measured values of $S(\vec{k})$ for $|\vec{k}| > 0.6$ Å, and below this value of $|\vec{k}|$ we have assumed a linear form for $S_0(\vec{k})$ with slope $\hbar k/2mc$. We tried three different forms for $f(r)$ $= \exp[-h(r)]$,

$$\text{I.}\quad f(r) = e^{-(a/r)^m} ,$$

$$\text{II.}\quad f(r) = r^m/(r^m + a^m) ,$$

$$\text{III.}\quad f(r) = 1 - e^{-(r/a)^m} . \quad (3.4)$$

The first of these leads to an $f(r)$ that tends to zero, as $r \to 0$, faster than any power of r; the second leads to an $f(r)$ which tends to unity, as $r \to \infty$, faster than any inverse power of r; while the last form tends to zero as r^m and to unity as r^{-m}. We feel that these classes of function cover a sufficiently wide range for our purposes.

The PY and CHNC equations were solved by the standard iteration method.[11] Most of this work was done after the equations had been Fourier-transformed. However, some solutions were found directly in coordinate space, and the two methods produced identical results. In Appendix D we set down some of the details of the techniques.

The flow term in the energy diverges logarithmically at large r. Consequently we have to choose a definite radius in order to present our results. We have chosen it to be 6 Å; outside of this region the fluid density is accurately uniform, and therefore plays no part in the variational calculation.

We found that the functions II and III, both with $m=2$, $a \simeq 1$ Å, lead to very similar energies for the vortex line; these results are shown in Fig. 1. In Fig. 2 we show the corresponding density profiles. These profiles show that a reasonable estimate for the radius of the core of the vortex is 1 Å. This is, at first sight, remarkably small compared with the typical correlation length of 3 Å as revealed by the the radial distribution function. This later function also drops much more rapidly to zero than our density profile. Indeed, our votex core is roughly speaking "half full of fluid."

The following points are interesting. First, the CHNC equation usually gave steeper minima than the PY equation, even though the absolute values at the minima were almost identical. The reason for this is discussed in Appendix C. Second, we feel that the fact that these two different approximate equations lead to the same energies at the minimum confirms our belief that the equations are quite accurate at helium densities. Third, the value of the energy at the minimum values of a and m are not sensitive to the detailed shape of $C_0(k)$, for k greater than about 0.6 Å. Finally we compare our results with those obtained by Amit and Gross using the Hartree theory. The density profile.

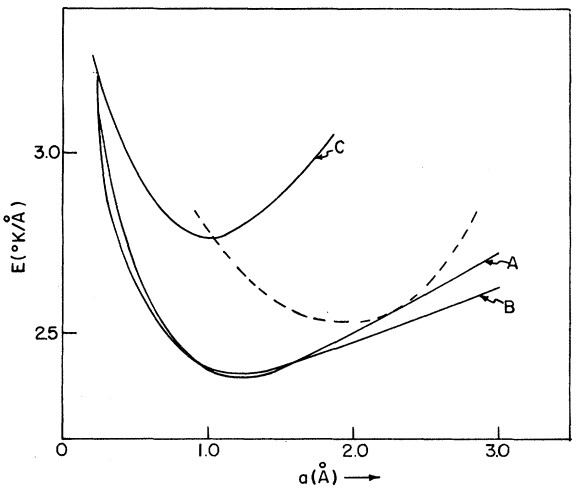

FIG. 1. The energy of a vortex line as a function of the variational parameter a. Curve A corresponds to the trial function $f(r) = 1 - \exp[-(r/a)^2]$, curve B corresponds to a trial function $f(r) = r^2/(r^2 + a^2)$, curve C corresponds to a trial function $f(r) = 1 - \exp[-(r/a)^4]$, and the dashed curve corresponds to the Hartree theory. The energies are calculated per angstrom of vortex line contained in a cylindrical bucket of 6 Å radius.

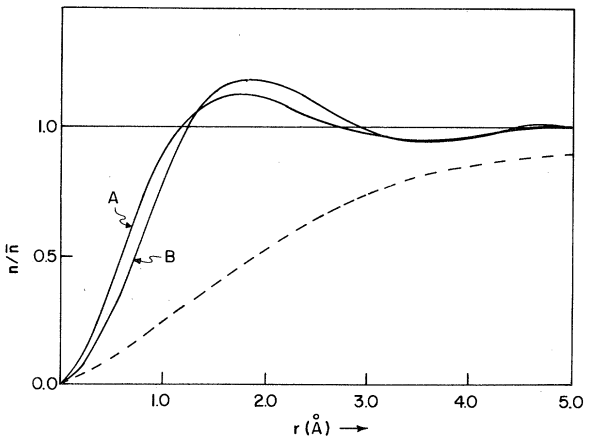

FIG. 2. The reduced total fluid density $n(r)/\bar{n}$ as a function of distance from the vortex line. Curve A corresponds to the trial function $f(r) = 1 - \exp[-(r/a)^2]$, curve B to the function $f(r) = r^2/r^2 + a^2$, and the dashed curve to the Hartree theory.

they obtained is shown in Fig. 2, and we see that their core size is much larger although the shape of the core is considerably smoother. The energies they obtained variationally are shown in Fig. 1, and we see that at the minimum they are very close to our own. The single adjustable parameter in the Hartree theory was chosen by these authors to fit the velocity of sound. The philosophy behind the two methods is of course very different. It is nevertheless interesting that they lead to nearly the same results for the energy of the core of the line.

IV. THE ENERGY AND VELOCITY OF A VORTEX RING

Our wave function for a vortex line can be used to estimate the energy of a large vortex ring. Figure 3 shows a cross section of such a ring together with the coordinates used in our calculation. Now if $R >> a$, we expect that the energy of such a ring will be the sum of the kinetic energy of the incompressible flow outside the core and the energy of the core. This latter energy can be accurately approximated by $2\pi R\epsilon$, where ϵ is the energy per unit length of a straight vortex line. This approximation can be described by a trial wave function,

$$\phi_{TR} = \exp[i\textstyle\sum_\alpha \psi_R(\vec{r}_\alpha)] \exp[-\textstyle\sum_\alpha h(\xi_\alpha)]\Phi_0 \ , \quad (4.1)$$

where ψ_R is the classical velocity potential for a vortex ring and $h(\xi)$ is the same function we used for the straight vortex line. This model function will clearly give an upper bound to energy of a ring because we have constrained the flow to be that of a classical vortex ring and the core to have a circular cross section. These should be excellent approximations as long as $R/a >> 1$. The expectation value of the Hamiltonian is now given by

$$\langle H \rangle = E_0 + \frac{\kappa^2 m}{8\pi^2} \int_{\text{inner}} (|\nabla\psi_R|^2 + \tfrac{1}{4}|\nabla h|^2) n(\vec{r}) d^3r$$

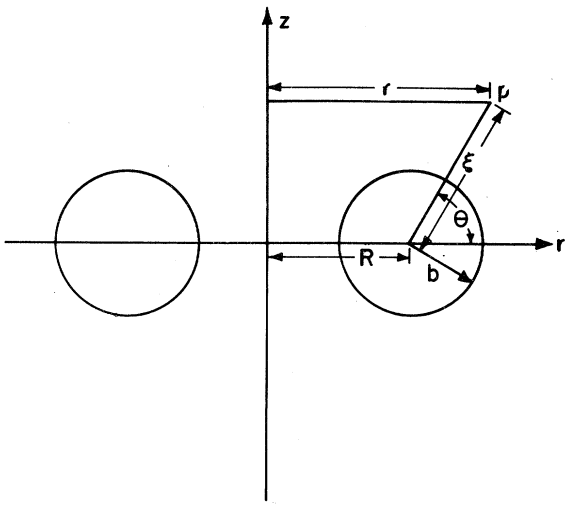

FIG. 3. The coordinates used for the vortex ring. The ring is symmetrically placed on the z axis and has radius R. A general point in the flow field has coordinates (r, ξ, θ).

$$+\frac{\kappa^2 \bar{n} m}{8\pi^2} \int_{\text{outer}} |\nabla\psi_R|^2 d^3r \ , \quad (4.2)$$

where $\kappa = h/m$. We have broken up the integral over the whole fluid into two parts. The first is over an inner region where the density $n(\vec{r})$ is nonuniform. We take this region to be a torid with a cross section of radius b. If $b \sim (4-5)$ Å, then with the density $n(\xi)$ will be equal to $\bar{n}$ on the surface of the toroid. Inside the toroid we can accurately approximate $\vec{v}$ by a single component $v_\theta = h/m\xi$, and $n(\xi)$ will, by our assumption, have the same form as the density $n(r)$ for the straight vortex line. The integral over the inner region is thus equal to $2\pi R\epsilon(b)$, where $\epsilon(b)$ is the energy per unit length of a line vortex in a cylinder of radius b. The second integral is over the remainder of the fluid where $n(\xi)$ is a constant. This contribution to the energy is therefore equal to the energy of a classical hollow vortex ring of radius R and with a cross section of radius b.

For completeness we write down the velocity potential[3] $\psi(r)$

$$\psi_R(r, z, \xi) = (\kappa/2\pi)(Rr)^{1/2} k^3 C(k) \ , \quad (4.3)$$

$$\text{where} \quad k^2 = 4\pi Rr/(z^2 + \xi^2 + 4Rr) \quad (4.4)$$

$$\text{and} \quad C(k) = \int_0^{\pi/2} \frac{\sin^2\theta \cos^2\theta}{(1 - k^2 \sin^2\theta)} \ . \quad (4.5)$$

From these equations we find that if $\xi << R$, then

$$v = (0, v_\theta, 0); \quad \text{where} \quad v_\theta = \kappa/2\pi\xi \ . \quad (4.6)$$

Our final result for the energy is thus

$$E = E_0 + \tfrac{1}{2}\kappa^2 m\bar{n} R[\ln(8R/b) - \alpha] \ , \quad (4.7)$$

$$\text{where} \quad \alpha = 2 - (4\pi/\kappa^2\bar{n})\epsilon(b) \ . \quad (4.8)$$

This expression for the energy is accurate to order $(b/R)^2$ and is, of course, independent of the value chosen for b as long as b is large compared with the core radius and small compared with R. When a and R become comparable, an entirely different calculation has to be made; nevertheless our wave function will still give an upper bound to the energy of such a ring.

To compare the energy of our model wave function with the experimental data, we have to estimate the velocity of translation of the ring. The quantities measured by Rayfield and Reif are the energy and velocity, and very little experimental information is available about the size of the rings. However, as we have already remarked, the data can be fitted quite accurately with the formulas for the energy and velocity of a classical vortex ring. This fit determines the circulation κ and the radius of the core a. The circulation is accurately given by h/m while a is close to 1 Å. From this fit we can draw two conclusions. First, the rings are undoubtedly large, between 500–5000 Å, and secondly, the major portion of the energy of the rings is the kinetic energy of flow outside the core region. A reasonable estimate of the core energy is that it amounts to at most 5% of the entire energy of the smaller rings. Our theory is a theory of the core of the vortex. Since only 5% of the energy of these rings resides in the core, only differences between theory and experiment of this magnitude are significant.

We first note that because our model wave functions, either for a line or a ring, are not solutions of Schrödinger's equation, they will decay in time into other excitations of the system – presumably phonons and rotons. Consequently, we cannot expect our model of a vortex ring to propagate indefinitely with a uniform velocity. However we may reasonably hope that initially the ring will start to move as a whole and then somewhat later it will decay into other excitations. We shall therefore calculate the initial velocity of translation and use this to make a comparison with the experimental data. At this point, it is interesting to make a comparison with the Hartree theory. In that theory one could, in principle, make an exact calculation of the wave function for a large vortex ring, and this would then be expected to have permanent velocity of translation. Indeed it has been shown by Fetter[12] that an accurate solution for a pair of vortex lines leads to a permanent velocity of translation of the pair through the fluid. However, no accurate solution for the ring is known in this theory, and consequently the question of translational velocity has been usually handled by *ad hoc* methods.[13] In a recent paper,[12] Fetter has proposed a method of calculating the velocity of translation which is very similar to that outlined below.

The position of the ring at any time may be defined by the position of its core, that is the region of the fluid where $[n(r)-\bar{n}]$ is different from zero. We therefore define a mean density coordinate $\bar{z}$ for the ring by the equation

$$\bar{z}_1 = \int z[n(\vec{r})-\bar{n}]d^3r / \int [n(\vec{r})-\bar{n}]d^3r \,, \qquad (4.9)$$

and identify $d\bar{z}_1/dt$ with the velocity of translation of the ring. This velocity is independent of the origin of coordinates. The definition we have just proposed has to be modified slightly since the denominator in Eq. (4.9) vanishes because our calculation preserves the total number of particles in the system. It can be shown that, as $r \to \infty$, $n(r) \to \bar{n}$ exactly, even to order $1/N$, as long as the ground-state wave function contains the long range correlations which produce the linear behavior of $S_0(k)$ for small k. This difficulty is easily overcome if we generalize Eq. (4.9) to

$$\bar{z}_p = \int z[n(\vec{r})-\bar{n}]^p d^3r / \int [n(\vec{r})-\bar{n}]^p d^3r \,, \qquad (4.10)$$

and confine ourselves to integer values of $p > 1$. We shall see that $d\bar{z}_p/dt$ is quite insensitive to the value chosen for p.

If we apply this definition of the translational velocity to a pair of vortex lines, we find that we recover exactly the classical answer to order a/R, where a is the core radius and R is the distance apart of the lines. To this accuracy the initial velocity of translation is independent of the value chosen for p and independent of the quantum structure of the core. These results provide us with some degree of confidence that our definition is reasonable.

For a vortex ring we find that

$$\frac{d\bar{z}_p}{dt} = \frac{\kappa}{4\pi R}\left[\ln\frac{8R}{b} - 2 - \ln\left(\frac{1+\sqrt{2}}{2}\right) - \int_0^b f_p(\xi)\ln(\xi/b)\,\xi d\xi \Big/ \int_0^b f_p(\xi)\xi d\xi\right], \qquad (4.11)$$

where $f_p(\xi) = [n(\xi)-\bar{n}]^p$.

In Fig. 4, we have plotted the product of the energy and velocity from our theory and from the experimental data. This product is a slowly varying function of R, and thus the comparison with

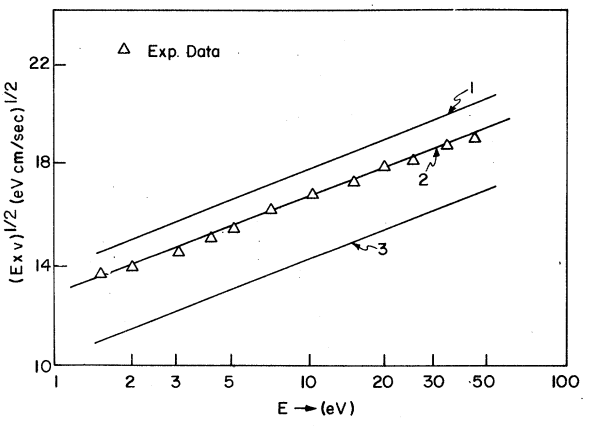

FIG. 4. The product $(E\times V)^{1/2}$ as a function of E for a vortex ring. Curve 1 corresponds to $p=4$; curve 2 to $p=2$ in Eq. (4.11) for the velocity of translation. Curve 3 corresponds to the impulse value of $\partial E/\partial P$, where P is the impulse necessary to generate a ring of radius R.

experiment is more easily made. We see that with $p=2$ excellent agreement is obtained; $p=4$ yields somewhat less satisfactory values. On this figure we have also plotted the results using the impulse definition of the translational velocity,[13] and we see that this also leads to less satisfactory agreement. We must emphasize that these comparisons merely tell us (a) that our model of the core is reasonably accurate, and (b) that our method of computing the velocity of translation is also reasonable. To make an accurate comparison with experiment we need data on rings one order of magnitude smaller in radius and, hopefully, measurements of their size as well. If this latter information is not available, then a direct comparison is impossible and only indirect comparisons can be made via some identification of the translational velocity. Since this identification at the moment is somewhat uncertain, it obscures the comparison with experiment.

V. THE CONDENSED-STATE WAVE FUNCTION

It has never been rigorously established that the ground state of liquid helium leads to a macroscopic occupation of the zero-momentum state of the single-particle density matrix. There are, of course, good reasons to support the belief that this kind of macroscopic occupation does occur for both the ground state and the low lying excited states. Since we cannot establish this property for Φ_0, we equally cannot establish it for our model states given by Eqs. (2.8) and (4.1). There are, however, model states for which we can establish that Bose-Einstein condensation occurs, and for which we can also calculate the amplitude and phase of the condensed state. These trial functions can be obtained by replacing Φ_0 by a Jastrow function Φ_J in Eqs. (2.8) and (4.1), where

$$\Phi_J = \prod_{\alpha\neq\beta} F(|r_\alpha - r_\beta|) \quad \text{with} F(|r|) = e^{-u(r)}. \tag{5.1}$$

The function $F(r)$ is chosen so that Φ_J yields the best variational estimate for the ground-state energy.[10] This trial function for the ground state yields excellent values for the energy, and moreover leads to a structure factor $S_J(\vec{k})$ which is also in good agreement with experiment.[10]

With this trial function, the expectation value of the Hamiltonian is given by

$$\langle H\rangle = E_J + \frac{\hbar^2}{2m}\int(|\nabla\psi|^2 + \tfrac{1}{4}|\nabla h|^2) n_{JV}^{(1)}(\vec{r})d^3r + \tfrac{1}{2}\int[T(\vec{r}) + V(\vec{r})][n_{JV}^{(2)}(\vec{r},\vec{r}') - n_J^{(2)}(\vec{r}'-\vec{r}')]d^3rd^3r, \tag{5.2}$$

where E_J is the variational energy corresponding to Φ_J, the second term has the same form as in our previous calculation, and the third term arises because Φ_J is not an eigenfunction of H. The function $n_{JV}^{(1)}(\vec{r})$ is the single-particle density constructed from $\exp[-\sum_\alpha h(\chi\alpha)]\Phi_J{}^2$, and $n_{JV}^{(2)}(\vec{r},\vec{r}')$ is the corresponding two-particle distribution function, while $n_J^{(2)}$ is the two-particle distribution function corresponding to $\Phi_J{}^2$. The interaction potential is $V(\vec{r})$ while $T(\vec{r}) = \hbar^2/2m\nabla^2 u(\vec{r})$. The function $n_{JV}^{(2)}$ would be extremely difficult to calculate; and we have therefore replaced it by the approximate form

$$n_{JV}^{(2)}(\vec{r},\vec{r}') = n_{JV}^{(1)}(\vec{r})n_{JV}^{(1)}(\vec{r}')g_J(\vec{r}-\vec{r}'), \tag{5.3}$$

where $g_J(\vec{r}-\vec{r}')$ is the pair correlation function corresponding to $\Phi_J{}^2$. This is a super-position approximation for $n_{JV}^{(2)}$, which has all the qualitative features we desire and should, we feel be sufficiently accurate to allow us to make a reliable estimate of the last term in Eq. (5.2). With this approximation and using the best known Φ_J, we found that the value of $\langle H\rangle - E_J$ was, at the minimum, within a few percent of the value of $\langle H\rangle - E_0$ which we calculated in Sec. III. The density $n_{JV}^{(1)}$ also differs from $n(\vec{r})$ by only a few percent at most. We therefore conclude that this type of model state leads to essentially the same results as before.

We now demonstrate that this kind of trial function does lead to Bose-Einstein condensation. The single-particle density matrix $\sigma(1,1')$ is defined by the equation

$$\sigma(1,1') = N\int\Psi(1,2\cdots N)\Psi^*(1',2,\ldots N)d2d3\cdots dN, \tag{5.4}$$

where Ψ is a normalized wave function. With our trial function (4.1), this can be written as

$$\sigma(1,1') = \exp\{i[\psi(1)-\psi(1')]\}\hat{\sigma}(1,1'), \tag{5.5}$$

where $\hat{\sigma}(1,1') = N/Q_N\int f(1)f(1')\times\prod_{\alpha>2} f^2(\alpha)\Phi_J(1,2\cdots N)\Phi_J(1',2\cdots N)d2\cdots dN$, (5.6)

and $Q_N{}^{1/2}$ is the normalization constant for ϕ_{TP}. The eigenfunctions of $\sigma(1,1')$ have the form $\exp[i\psi(1)]\times\chi(1)$, where χ is an eigenfunction of $\hat{\sigma}(1,1')$. If our model state has a macroscopically occupied state χ_M, then

$$\hat{\sigma}(1,1') \to \chi_M(1)\chi_M{}^*(1') \tag{5.7}$$

as the separation of 1 and 1′ increases indefinitely. Now it follows at once from Eq. (5.6) that

$$\hat{\sigma}(1,1') = C\exp[\tfrac{1}{2}h(1) + \tfrac{1}{2}h(1') + \tfrac{1}{4}u(1,1')]g(1,1'). \tag{5.8}$$

Where C is a constant and $g(1,1')$ is the pair distribution function for an equivalent classical system in which $N-1$ particles are coupled with full strength $u(\vec{r})$ and are acted upon by an external potential to $h(\vec{r})$, while 1 and 1′ are coupled with strength $\frac{1}{2}u(\vec{r})$ to the remaining $N-1$ and are also acted upon by an external potential $h(\vec{r})$. For reasons of symmetry, we have also coupled 1 to 1′ with a potential $\frac{1}{4}u(\vec{r})$. We now evaluate the constant C. If we consider a region of the fluid far from the vortex core, then the fluid will be

quite uniform and unaffected by the presence of the vortex. Consequently we conclude that if 1 and 1′ are both far from the core and also far apart from one another, then

$$\hat{\sigma}(1,1') = n_0 , \tag{5.9}$$

where n_0 is the fraction of particles in the zero-momentum state in the system when it is in equilibrium with no vortex present. For any Φ_J with $u(\vec{r})$ of finite range, n_0 exists. If we compare Eq. (5.7) with Eq. (5.8) then we see that $C = n_0$, because $h, u \to 0$ and $g \to 1$ as 1 and 1′ become far apart.

Now consider 1 and 1′ to be far apart but both still in the region of the core, e.g., far apart vertically above one another; then

$$g \to [\hat{n}(1)/\bar{n}][\hat{n}(1')/\bar{n}] \tag{5.10}$$

and $u \to 0$, hence

$$\hat{\sigma}(1,1') \to n_0 \frac{\hat{n}(1)}{\bar{n}} \frac{\hat{n}(1')}{\bar{n}} \exp[\tfrac{1}{2}h(1) + \tfrac{1}{2}h(1')]. \tag{5.11}$$

Where $\hat{n}$ is the single-particle density for one of the half-coupled particles in our effective classical system, and $\bar{n}$ is the mean density. Comparing this result with Eq. (5.7), we see that

$$\chi_M = \sqrt{n_0}[\hat{n}(1)/\bar{n}] \exp[\tfrac{1}{2}h(1)] . \tag{5.12}$$

Thus to calculate χ_M we have to compute $\hat{n}(\vec{r})$. This can be done in a manner very similar to the way in which we computed $n(\vec{r})$ in Sec. III. The PY equation for $\hat{n}(\vec{r})$ is

$$\hat{n}(\vec{r}) e^{h(\vec{r})} = \bar{n} + \int \tilde{C}_0(\vec{r} - \vec{r}')[n(\vec{r}') - \bar{n}]d^3\vec{r}' , \tag{5.13}$$

while the CHNC equation is

$$\hat{n}(\vec{r}) e^{h(\vec{r})} = \exp\{\int [n(\vec{r}') - \bar{n}]\, \tilde{C}_0(\vec{r} - \vec{r}')d^3\vec{r}'\} . \tag{5.14}$$

In both these equations $\tilde{C}_0(\vec{r} - \vec{r}')$ is the direct correlation function in which the particle with coordinate $\vec{r}$ is half coupled to the remainder while the particle with coordinate $\vec{r}'$ is fully coupled to the remainder. This correlation function can be readily calculated using the PY equations for a mixture.[14] Once $\tilde{C}_0$ has been calculated, Eqs. (5.12) and (5.13) yield $\hat{n}(\vec{r})$ at once. We found little difference in $\hat{n}(\vec{r})$ from these equations; in Fig. 5 we plot $|\chi_M|^2/n_0$ and compare it with the total reduced density $n_1/\bar{n}$. We see that they are very similar in form. The physical significance of the differences is not known to us. We have also calculated the ratio of the number of particles in the condensate with and without a vortex present. Since most of the fluid in the system is quite unaffected by the presence of the vortex, the calculation is only meaningful if we confine our attention to the vortex core. Defining this to be a region of radius 6 Å, we then find that in this region the ratio is about 0.8. That is to say, the presence of the vortex has removed about 20% of the particles from the condensate. It would be interesting to know what this ratio is for a vortex with two or more units of circulation.

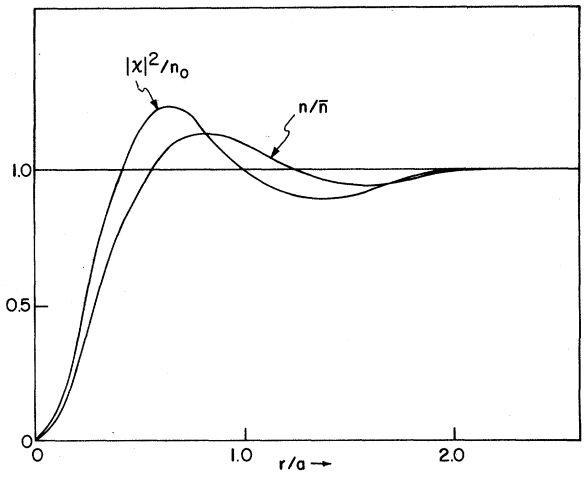

FIG. 5. The square of the amplitude of the condensed-state wave function χ_M as a function of r.

We plan to perform this calculation when our techniques have improved.

VI. CONCLUSIONS

The calculations we have presented in this paper, both for the vortex line and ring seem to us to lead to very reasonable values for the energies concerned. The radius of the core region is, however, quite small ~1 Å. Nevertheless we seriously doubt that any more sophisticated wave function or more accurate calculation will substantially change this number. The reason why the radius turns out to be so small is simply that the centrifugal barrier is really quite small and consequently produces little distortion in the fluid. The repulsive potential barrier between two helium atoms is enormous in comparison and thus produces a very much larger local distortion in the fluid. For example, this repulsive barrier reaches a height of 12°K, the mean kinetic energy of a helium atom, at about 2.5 Å, while the cen trifugal barrier of a singly quantized line reaches the same height at 1 Å, the core radius. This, we feel, is the essential reason why the core is so small. This simple estimate would lead to a core diameter of 2 Å for a doubly quantized line

Our numerical values for the energy are quite close to those obtained from the Hartree theory, but our density profile is, of course, much more realistic.

One of the most interesting extensions of our theory would be to calculate the core size at higher pressures. Preliminary calculations shows that the core radius decreases as the pressure is increased. However, the approximate integral equations we have used become less reliable at these higher densities and we feel that further investigation of this effect should be delayed until we have developed the requisite Monte Carlo techniques to evaluate the density profile accurately. This method will also of course provide a check on our calculations at zero pressure.

We plan to extend the work presented in this paper in two directions. First, we shall construct, using the generalized Hartree theory as a guide, more sophisticated wave functions. These will undoubtedly lead to a nonzero density of "normal" fluid and a non-curl-free flow field in the core. This should result in an appreciable lowering of the energy of the line. Secondly, we hope to apply our methods to small vortex rings. These are of interest because they open the possibility of a much more sensitive test of the theory, since a much larger fraction of the energy resides in the core.

APPENDIX A: ON THE SINGLE-VALUEDNESS OF WAVE FUNCTIONS

In this Appendix we shall show that if a system has one or more single-valued states, then all the acceptable states of the system must be single valued. We note in passing that the single valuedness of states in quantum mechanics receives little serious consideration in texts on the subject; the only really pertinent remarks we have been able to find are those in the article by Pauli.[8] The theorem we have stated does not in any way rule out the possibility that all the states of a system are multivalued. It therefore does not conflict with the example of the three-dimensional rigid rotator.[8]

Let ψ_S be a single-valued state of a system and ψ_M a multivalued one. Then, by the superposition principle,

$$\psi = a\psi_S + b\psi_M \tag{A.1}$$

is an acceptable state if ψ_S and ψ_M are, with a and b, two arbitrary constants. We now postulate that the probability amplitude of any acceptable state should be single-valued. This postulate seems to be a necessity on purely physical grounds. The probability amplitude corresponding to (A.1) is

$$|\psi|^2 = |a|^2 |\psi_S|^2 + |b|^2 |\psi_M|^2 + ba^* \psi_S \psi_M + b^* a \psi_S \psi_M^* . \tag{A.2}$$

Now it is quite possible – and indeed often the case – that $|\psi_M|^2$ is single-valued even though ψ_M itself is not. For example, if for a single degree of freedom ϕ, $\psi_M = \exp(i\alpha\phi)$ with α different from an integer, then ψ_M is multivalued while $|\psi_M|^2$ is not. Consequently the first two terms in Eq. (A.1) may well be single-valued. However, the second two terms obviously cannot be single-valued individually; and since a and b are arbitrary constants, the sum of them cannot be either. We thus conclude that $|\psi|^2$ is not single-valued. This conflicts with our postulate that probability amplitudes should be single-valued, and we therefore conclude that ψ_M is not an acceptable state. Hence all states must be single-valued if one is. Notice that we could still have $|\psi|^2$ single-valued if all the states are suitably multivalued.

APPENDIX B: DERIVATION OF THE PY AND CHNC EQUATIONS FOR $n(\vec{r})$

The s-particle quantum distribution function for the trial function is

$$n_s(1\cdots s) = \frac{V^s \int \phi_0^2 \exp[-\sum_\alpha h(\vec{r}_\alpha)]\, d(s+1)\cdots dN}{\int \phi_0^2 \exp[-\sum_\alpha h(r_\alpha)]\, d1\cdots dN} , \tag{B.1}$$

which is exactly analogous to the classical, dimensionless s-particle distribution function in a canonical ensemble, at an effective temperature T_{eff} given by $h(\vec{r}) = kT_{\text{eff}}\, v(\vec{r})$ where v is an external potential. Classically, of course $\phi_0^2 = \exp(-kT_{\text{eff}}/V_N)$, where V_N is the potential energy of the system, but it will be seen that one need not specify the detailed form of ϕ_0^2 to derive the equations we are interested in. One can pursue this analogy further by defining the grand distribution function in the classical grand canonical ensemble at the same effective temperature. If Ξ is the grand partition function, then

$$\Xi = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int \phi_0^2 \exp\left[-\sum_\alpha h(r_\alpha)\right] d1\cdots dN , \tag{B.2}$$

where z is the fugacity; and then the s-particle distribution function having dimensions of $1/V^s$ is

$$n_s(1\cdots s/h) = \frac{1}{\Xi} \sum_{n=s}^{\infty} \frac{z^n}{(n-s)!} \times \int \phi_0^2 \exp\left[-\sum_\alpha h(\vec{r}_\alpha)\right] d(s+1)\cdots dN . \tag{B.3}$$

Here the h is written explicitly to show that the system is in an external potential.

First it can easily be shown that

$$\delta n_1(\vec{r}|h)/\delta h(\vec{r}\,') = n_1(\vec{r}|h) n_1(\vec{r}\,'|h) - n_1(\vec{r}|h)\delta(\vec{r}-\vec{r}\,') - n_2(\vec{r},\vec{r}\,'|h). \tag{B.4}$$

Next the direct correlation function in the presence of an external potential may be defined by

$$C(\vec{r},\vec{r}\,'|h) = \delta\{\ln[n_1(\vec{r}|h)e^{h(\vec{r})}]\}/\delta n_1(\vec{r}\,'|h), \tag{B.5}$$

which obviously gives

$$\frac{\delta h(\vec{r})}{\delta n_1(\vec{r}\,'|h)} = \frac{1}{n_1(\vec{r}\,'|h)}\delta(\vec{r}-\vec{r}\,') + C(\vec{r},\vec{r}\,') . \tag{B.6}$$

Now $\delta n(\vec{r}\,')/\delta h(\vec{r}\,'')$ and $\delta h(\vec{r})/\delta n(\vec{r}\,')$ are matrix inverses of each other

$$\int \frac{\delta h(\vec{r})}{\delta n_1(\vec{r}\,'|h)} \frac{\delta n_1(\vec{r}|h)}{\delta h(\vec{r}\,'')} d^3r' = \delta(\vec{r}-\vec{r}\,'') . \tag{B.7}$$

Then substituting (B.6) and (B.4) into this expression gives directly

$$g(\vec{r},\vec{r}\,''|h) - 1 = C(\vec{r},\vec{r}\,''|h) + \int d^3r' C(\vec{r},\vec{r}\,'|h) n_1(\vec{r}\,'|h)[g(\vec{r}\,',\vec{r}\,''|h) - 1] , \tag{B.8}$$

which is the basic relation between C and the pair

correlation function g.

Now consider a function F which is a functional of n_1 and h. It can be expanded in a functional expansion in n_1.

$$F[n_1,h]=F(\bar{n},0)+\int d^3r_1\left.\frac{\delta F}{\delta n_1(\vec{r}_1\,|\,h)}\right|_{h=0}\times[n_1(\vec{r}\,|\,h)-\bar{n}]+\cdots . \quad (B.9)$$

To obtain the PY equation for n_1, we choose $F=n_1(\vec{r}\,|\,h)\exp h(\vec{r})$. Then Eq. (B.5) gives

$$\left.\frac{\delta F}{\delta n_1(\vec{r}\,'|\,h)}\right|_{h=0}=n_1(\vec{r}\,|\,h)\,e^{h(\vec{r})}C(\vec{r},\vec{r}\,'|\,h)\Big|_{h=0}=\bar{n}C_0(\vec{r}-\vec{r}\,') \quad (B.10)$$

where $C_0(\vec{r}-\vec{r}\,')$ is the direct correlation function for the system in the absence of the external potential, that is, for the ground-state system described by $\phi_0{}^2$. Taking the first two terms of Eq. (B.9), we find

$$n_1(\vec{r}\,|\,h)\,e^{h(\vec{r})}=n+\int d^3r'\bar{n}C_0(\vec{r}-\vec{r}\,')\times[n_1(\vec{r}\,'|\,h)-\bar{n}]\ , \quad (B.11)$$

which is the desired PY equation.

To obtain the CHNC equation, we choose

$$\exp F=n_1(\vec{r}\,|\,h)e^{h(\vec{r})}.$$

Then Eqs. (B.5) and (B.9) give

$$\ln[n_1(\vec{r}\,|\,h)\,e^{h}]=\ln\bar{n}+\int d^3r'C_0(\vec{r}-\vec{r}\,')\times[n_1(\vec{r}\,'|\,h)-\bar{n}] \quad (B.12)$$

and thus

$$n_1(\vec{r}\,|\,h)\,e^{h}=\bar{n}\exp\{\int d^3r'C_0(\vec{r}-\vec{r}\,')\times[n_1(\vec{r}\,|\,h)-\bar{n}]\}\ .$$

The entire analysis above has been done without specifying the form of $\phi_0{}^2$.

APPENDIX C: THE BEHAVIOR OF THE ENERGY AS A FUNCTION OF THE CORE RADIUS

The energy E per unit length of a single vortex line is given by Eq. (2.13) as

$$\langle H\rangle=E=E_0+\frac{\pi\hbar^2}{m}\int[\,|\nabla\psi|^2+\tfrac{1}{4}(\nabla h)^2]n(r)d^3r. \quad (C.1)$$

In this Appendix we shall show that E increases indefinitely as the core radius a increases without limit. Since E also tends to infinity as $a\to 0$, we are assured that E has a minimum for some finite value of a.

For our trial functions, $h(r)$ depends on r/a alone and we can therefore write (C.1) in the form

$$E=E_0+\frac{\pi\hbar^2}{m}\int\left[\frac{1}{x^2}+\frac{1}{4}\frac{dh(x)}{dx}\right]^2 n(x)xdx, \quad (C.2)$$

where $x=r/a$. Now $n(x)$ will *not* be a function of x alone and our task is to determine how it depends on a for large values of a. The function $n(x)$ is determined by the approximate integral equations (B.11) and (B.12), and these show that apart from $h(x)$ the only other function that enters is the direct correlation function $C_0(\vec{r})$. This function has the form[15]

$$\bar{n}C_0(\vec{r})=-(r_0/r)^2+C_{\rm sr}(\vec{r}/l)\ , \quad (C.3)$$

where the first term comes from the long-range correlations introduced by the zero-point motion of the phonons, and the second is a short-range function that arises from the short-range correlations introduced by the strong repulsive and weak attractive forces between the helium atoms. We expect this function to be characterized by a single correlation length l of the order of 2-3 Å. Since $C_0(\vec{r})$ contains both a long-range and short-range part, we must expect that $n(x)$ will depend on the two ratios r_0/a and l/a. We therefore rewrite Eq. (C.2) in the form

$$E=E_0+\frac{\pi\hbar^2}{m}\int\left[\frac{1}{x^2}+\frac{1}{4}h'(x)^2\right]n\left(x,\frac{r_0}{a},\frac{l}{a}\right)xdx\ . \quad (C.4)$$

The first term in the integral in Eq. (C.4) is very long-range, and will therefore be dominated by values of $x>>1$ for which values $n\to\bar{n}$. We therefore expect that this term is largely independent of a-except for very small values of a when it will increase indefinitely. This behavior is completely confirmed by our calculation. On the other hand, the term containing $h'(x)^2$ is a very short-range term, falling off at least as fast as x^{-6} in all our calculations. We therefore expect that its behavior as a function of a will be dominated by the behavior of $n(x)$ for small x. We shall now show that $n(x)$ for small x increases indefinitely with a for $a\gg l$, where l is the characteristic correlation length in the fluid.

We do this first for $n(x)$ determined by the PY equation. This equation can be written, for sufficiently small r, in the form

$$n(r)e^{h(r)}=\bar{n}+\bar{n}\int\bar{C}_0(\mathbf{r}')[n(r')-\bar{n}]r'dr'\ , \quad (C.5)$$

where $\bar{C}_0(r')=\int dz'\int d\varphi' C_0(\vec{r}\,')$

$$=\int C_0(k)J_0(kr')kdk\ . \quad (C.6)$$

This last equation follows from Eq. (D.3). Now from Eq. (C.3) we see that

$$C_0(k)=r_0{}^2/k+C_{\rm sr}(kl)\ . \quad (C.7)$$

Here $C_{\rm sr}(kl)$ is a well-behaved short-range func-

tion of kl. Combining (C. 7) and (C. 6), we find that

$$\bar{C}_0(r') = \bar{C}_0(r'/a, l/a, r_0/a)$$
$$= (r_0/a)^2(a/r')a + \bar{C}_{sr}(r'/a, l/a)a^{-2} . \quad (C.8)$$

The factors a and a^{-2} in the two terms in (C. 8) arise when we express $\bar{C}_0$ in terms of r'/a and l/a. When we substitute (C. 8) in (C. 5), we find that

$$n(r'/a, l/a, r_0/a)e^{h(r'/a)}$$
$$= \bar{n} + a^3(r_0/a)^2 \int [n - \bar{n}]dx + \int C_{sr}(x, l/a)[n - \bar{n}]x dx . \quad (C.9)$$

Now the first integral on the right-hand side is dominated by values of $x \sim 1$ and will consequently be largely independent of a for large a. It is, however, multiplied by a factor $a^3(r_0/a)^2 = ar_0^2$, and so this term will increase linearly with a for large a. The second integral will for the same reasons be independent of a for large a, and this term will therefore be independent of a for large a. We therefore conclude that $n(r)\exp[h(r)]$ will increase linearly with a for large a and small r. This behavior was completely confirmed by our numerical computations. A very similar analysis can be applied to the CHNC equation for $n(r)$ and leads to the conclusion that $n(r)\exp[h(r)]$ as determined by that equation will increase as $\exp a$ for large a and small r.

We have, of course, only established that $n(r)\exp[h(r)]$ behaves in this manner in the limit as $r \to 0$. However, we can reasonably expect this behavior to persist as long as r is smaller than the smallest length in the theory which is l, when $a \gg l$. This in turn implies that we shall expect the second integral in Eq. (C. 2) to be an increasing function of a for large a. This result was also confirmed by our calculations. We therefore reach the interesting conclusion that it is the long-range correlations introduced by the zero-point motion of the phonons that in our model stabilizes the radius of the vortex core. A more physical argument for the effect of phonons on the core diameter may be made in the following way: if only short range correlations are present and $a \gg l$, then the density profile can be determined from the condition

$$\mu_0(n(r)) + h(r) = \text{const} \quad (C.10)$$

when $\mu_0(n(r))$ is the chemical potential of the equivalent classical fluid. This means that $n(r)$ scales exactly with a and the deficit of particles is easily absorbed (as long as a is much less than the size of the container) in the far region due to the finite "compressibility" of the system. It then follows from the form of $\langle H \rangle$ that the energy is independent of a for large a.

In presence of long range correlations the "compressibility" is infinite, that is the rigidity of the wave function does not allow the absorption of any deficit. Then $n(r)$ cannot be determined from (C. 10) and it does not scale with a. In fact, when a increases to compensate for the "hole" so produced, there must be a *local* region in which $n(r)$ increases. This reacts back on the "hole" making it difficult to have a large hole. This corresponds to the fact that $n(r)\, e^{h(r)}$ is an increasing function of a for small r and produces an increase of $\langle H \rangle$ with a.

APPENDIX D: THE METHOD OF SOLUTION OF THE INTEGRAL EQUATIONS

We outline here the method of solution of the PY and CHNC equation for $n(\vec{r})$.

The PY equation for $n(\vec{r})$ is

$$n(\vec{r})e^{h(\vec{r})} = \bar{n} + \bar{n} \int C_0(\vec{r} - \vec{r}')[n(\vec{r}') - \bar{n}]d^3r' . \quad (D.1)$$

Since C_0 is spherically symmetric and $h(\vec{r})$ has cylindrical symmetry, $n(\vec{r})$ will also have cylindrical symmetry. We can use this result to reduce the equation to the form

$$n(r)e^{h(r)} = \bar{n} + \bar{n} \int_0^\infty dr' r' Z(r, r')[n(r') - \bar{n}], \quad (D.2)$$

where

$$Z(r, r') = \int_0^\infty k dk\, C_0(k) J_0(kr) J_0(kr') . \quad (D.3)$$

Once $C_0(k)$ has been given in terms of $S_0(k)$, the kernel $Z(r, r')$ can easily be constructed and Eq. (D. 2) solved by iteration. This method proved lengthy, particularly as we wished to vary $C_0(k)$ to determine how sensitive our energy values were to this function. A more convenient form of the equation can be obtained by Fourier-transforming Eq. (D. 1). The result is

$$G(k) = C_0(k)\Delta n(k) , \quad (D.4)$$

where $C_0(k)$ is in the three-dimensional Fourier transform of $C_0(r)$, and $G(k)$ and $\Delta n(k)$ are the zero-order Bessel transforms of $n(r)\exp[h(r)] - \bar{n}$ and $n(r) - \bar{n}$, respectively. For example,

$$\Delta n(k) = \int_0^\infty r dr\, J_0(kr)[n(r) - \bar{n}] . \quad (D.5)$$

The function $C_0(k)$ now stands as a multiplicative factor in the equation, and can therefore be easily varied. The iterative method used to solve (D. 4) is very simple. One starts with an assumed form for $n(r)$, substitutes it into the right-hand side of either Eq. (D. 1) or (D. 4), and thus calculates a new $n(r)$ from the equation. This process is repeated until the input and output differ by no more than a prescribed amount. If this method is naively followed, the iterations are invariably unstable and diverging functions are obtained. This phenomenon can easily be cured if at any step we mix the *two previous* functions together to form an input function. Thus

$$n_{in}^{\,p} = \alpha n_{out}^{\,p} + (1 - \alpha) n_{out}^{\,p-1} , \quad (D.6)$$

where $n_{in}^{\,p}$ is the input function for the pth step, $n_{out}^{\,p-1}$ is that obtained at the $(p-1)$th iteration. The constant α is chosen to secure convergence with the minimum number of iterations. With a convergence criteria of 1% everywhere in the range, the energies were found to be at least this accurate. Several check runs were made with a

convergence criterion of 0.1%. The range of integration was varied according to the type of function $h(r)$ that was under investigation, the value of m, and the value of a. A variable integration grid was used to distribute the points as economically as possible in the range. Typical α values ranged from 0.2 to 0.02, and the number of iterations required ranged from 50 to 100. The starting function was usually chosen to be $\exp[-h(r)]$.

A very similar reduction can be made for the CHNC equation. The iterative procedure was, however, much more troublesome if the iteration was started from $\exp[-h(r)]$. This difficulty was overcome by taking the solution of the PY equation as the starting function. A convergent solution was then found with only 20–50 further iterations.

The solution we obtained by these iterative techniques in k space were checked in several cases by a direct iteration in r space using Eqs. (D.2) and (D.3). The results obtained by the two methods always agreed to within the convergence criterion.[16]

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[1]H. E. Hall, Advan. Phys. 9, 89–146 (1960).

[2]G. W. Rayfield and F. Reif, Phys. Rev. 136, A1194 (1964).

[3]H. Lamb, Hydrodynamics (Dover Publications, Inc., New York, 1945), p. 237.

[4]E. P. Gross, Nuovo Cimento 20, 454 (1961).

[5]L. P. Pitaevski, Zh. Eksperim. i Teor. Fiz. 40, 646 (1961) [English transl.: Soviet Phys. – JETP 13, 451 (1961)].

[6]A. L. Fetter, Phys. Rev. 138, A429 (1965).

[7]R. P. Feynman, Progress in Low Temperature Physics (North-Holland Publishing Co., Amsterdam, 1955), Vol. 1, Chap. 2.

[8]W. Pauli, in Handbuch der Physik, edited by S. Flügge (Springer-Verlag, Berlin, 1958), Vol. I.

[9]H. L. Frisch and J. L. Lebowitz, The Equilibrium Theory of Classical Fluids (W. A. Benjamin, Inc., New York, 1964).

[10]D. Schiff and L. Verlet, Phys. Rev. 160, 208 (1967); more detailed and relevant information is contained in a 1965 preprint of this paper by D. L. Levesque, D. Schiff, T. Khiet, and L. Verlet.

[11]D. Levesque, Physica 32, 1985 (1966).

[12]A. L. Fetter, Phys. Rev. 151, 100 (1966).

[13]E. P. Gross and D. Amit, Phys. Rev. 145, 130 (1966).

[14]J. L. Lebowitz, Phys. Rev. 133, A895 (1964).

[15]G. V. Chester and L. Reatto, Phys. Rev. 155, 88 (1967)

[16]R. N. Metz, Ph.D thesis, Cornell University, 1967 (unpublished).