

## Persistent Currents in Many-Boson Systems\*

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A theoretical study of persistent currents in liquid He<sup>4</sup> is given, in which a system of  $N$  interacting bosons confined to a cylindrical container is chosen as a model. It is argued that these currents are metastable and a general model-independent stability criterion valid for all temperatures is derived. In this formulation it is essential that there is a single-particle state  $\varphi_c$  with nonzero angular momentum  $l_c$  which is occupied by a macroscopic number [ $O(N)$ ] of particles. The stability criterion is applied to the study of two soluble models, one, an independent-particle model studied for all temperatures, the other a quasiparticle model studied for  $T=0^\circ\text{K}$ . For both models persistent currents are possible at  $T=0$  provided that the interactions between particles are sufficiently strong and  $l_c$  does not exceed a characteristic critical value  $l_M$ . The quantity  $l_M$  is calculated for different choices of single-particle functions, and in particular for the solutions of a Hartree equation, which is relevant to a description of line vortices with quantized circulation. The density  $\rho_c(T)$  of particles macroscopically occupying  $\varphi_c$  at a temperature  $T$ , as well as the critical temperature  $T^*$  above which no persistent currents are possible, are calculated for the independent-particle model.

### I. INTRODUCTION

THE varieties of thermal and hydrodynamic phenomena which strikingly differentiate He II from other substances are familiar to even the beginning student of physics. Recent experiments<sup>1-3</sup> have revealed an additional unique phenomenon, the existence of persistent macroscopic circulating currents analogous to persistent electric currents in ring-shaped superconductors. On the basis of these experiments considerable quantitative information concerning these persistent currents is available at present.

The purpose of this paper is twofold: The first is to obtain a completely general criterion, valid for all temperatures, for the existence of a persistent current in a system of interacting bosons confined to a cylindrical geometry. The second purpose is to illustrate the use of this criterion by studying two interesting tractable microscopic models of a many-boson system.

Concerning the format of this paper, Sec. II begins with a brief critical review of some of the main highlights of the Reppy-Depatie experiment.<sup>1</sup> In the course of this review we argue that "persistent" currents must be interpreted as a metastable phenomenon. This discussion is followed by the formulation of a general criterion for the metastability of these currents at  $T=0^\circ\text{K}$ , which is based on the assumed existence of a type of Bose-Einstein condensation. Sections III and IV are devoted to a study limited to zero temperature of

the two models presented in this paper. In the simpler of these models many-body eigenfunctions are restricted to the form of symmetrized products of single-particle wave functions, the latter being chosen as free-particle eigenfunctions as well as the approximate solutions of a Hartree equation. For computational simplicity we assume that the particles are hard spheres described in the approximation of the Fermi pseudopotential, and we find that the system can, in fact, support metastable persistent currents. The second of these models provides a more realistic description of a many-boson system, whereby Bogoliubov-like terms are retained in the Hamiltonian. In this model the stability criterion expresses itself as the positive-definiteness of the excitation spectrum, and again the system is found capable in certain circumstances of supporting persistent currents. In Sec. V we obtain the generalization of the metastability criterion appropriate to a system in thermal contact with a heat reservoir. This criterion is used to study the first model for nonzero temperatures in Sec. VI. Finally, in Sec. VII we summarize the main conclusions of this work and discuss several questions which remain to be studied theoretically.

### II. METASTABILITY OF PERSISTENT CURRENTS

#### A. Reppy-Depatie Experiment

##### 1. Description of Experiment

We devote the first part of this section to a brief review of the Reppy-Depatie experiment<sup>1</sup> and its interpretation in order to provide the necessary background and to set the stage for the development in the main body of the paper. In the experiment a sealed cylindrical container of liquid He<sup>4</sup> at a temperature  $T_1$  below the lambda point ( $T_\lambda=2.18^\circ\text{K}$ ) was made to

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<sup>1</sup> J. D. Reppy and D. Depatie, Phys. Rev. Letters **12**, 187 (1964). This article also contains references to earlier experimental work on the subject.

<sup>2</sup> J. D. Reppy, Phys. Rev. Letters **14**, 733 (1965).

<sup>3</sup> J. B. Mehl and W. Zimmermann, Jr., Phys. Rev. Letters **14**, 815 (1965).

rotate about its axis at a speed in excess of the superfluid critical velocity for a period of time so as to ensure that the container and the entire liquid rotated together as a single unit. The container was then gradually braked to rest. After waiting periods of up to twelve hours the brake was released so that the container hung free. When the system was warmed from  $T_1$  to above  $T_\lambda$ , the container began to rotate. Since warming the system to above  $T_\lambda$  enables the liquid to interact with the container, the observed rotation implies that just prior to heating there was a circulating current in the liquid. Of key interest is the result that the measured angular velocities of the container were found to be independent of the length of the waiting period preceding these measurements thereby demonstrating the "persistence" of these currents. The experiment was then repeated for a series of temperatures  $T_1$  between 1.2°K and  $T_\lambda$ . The measured values  $L_p(T)$  of the angular momentum  $L$  of the persistent current at the temperature  $T$  are compatible with the relation  $L_p(T) = K\rho_s(T)$ , where  $\rho_s(T)$  is the superfluid density of stationary He II and  $K$  is a temperature-independent constant.<sup>4</sup> In a variation of the experiment a persistent current was first prepared at a temperature  $T_1 (\lesssim T_\lambda)$  and then, while the container was kept from rotating, the system was slowly cooled to a lower temperature  $T_2$ . The measured value of  $L$  at this lower temperature was found to be  $L_p(T_2)$ , not  $L_p(T_1)$ .

## 2. Analysis of Experiment

These results, first the persistence of the circulating current and second the apparent dependence of its angular momentum upon temperature alone, would suggest that a persistent current is a thermal *equilibrium* phenomenon and thus, for example, that  $L_p(T)$  is a parameter characterizing the equilibrium state. On closer inspection, however, several aspects of the experiment dictate against such a conclusion. The measured value of  $L$  at the lower temperature  $T_2$  was  $L_p(T_2)$  rather than  $L_p(T_1)$  only if (1)  $T_1$  was below  $T_\lambda$  and if (2) the temperature was lowered to  $T_2$  at an extremely slow rate. The value of  $L$  for the system at  $T_2$  is therefore not entirely independent of the previous history of the system, and thus a persistent current cannot be a thermal equilibrium phenomenon.

The apparently contradictory ideas of the previous paragraph suggest that with careful preparation the system can be in a state of *metastable* equilibrium of very long lifetime. When subjected to a rapid temperature decrease from  $T_1$  to  $T_2$  the system is dislodged from the metastable state so that the measured value of  $L$  at  $T_2$  is not found to be  $L_p(T_2)$ . The same explanation can be given for the finding by Reppy and Depatie that solid-body rotation of the container and liquid could be precipitated not only if the system was

<sup>4</sup> Recent work by Reppy (see Ref. 2) suggests that this result holds for temperatures up to within  $10^{-5}$ °K of the lambda point.

warmed to above  $T_\lambda$  but also if it was subjected to a brief heat pulse which hardly raised the temperature from its original value.

Theoretical support for the notion that the persistent current is a metastable phenomenon comes from the following easily proved lemma: The thermal equilibrium value  $\langle \mathbf{L}(0) \rangle$  of the angular momentum of a system of particles interacting via velocity-independent forces and confined to a nonrotating container in an inertial frame is zero.<sup>5</sup> If one then assumes that  $\langle \mathbf{L}(\omega) \rangle$ , the thermal equilibrium value of  $\mathbf{L}$  when the container rotates at constant angular velocity  $\omega$ , is a *continuous* function for small  $\omega$ , it follows that the Reppy-Depatie finding of a measurable circulating current for  $\omega=0$  relates to a metastable phenomenon.<sup>6</sup>

An important clue to the origin of the metastability of the persistent current is provided by the fact that such currents could not be prepared at temperatures above the lambda point. If we adopt London's ideas that the superfluid properties of liquid helium are manifestations of a macroscopic occupation of a particular single-particle state then a persistent current might be described in terms of a macroscopic occupation of a current-carrying single-particle state. Of course, we realize that other explanations for the existence of persistent currents, which do not depend upon the assumption of macroscopic occupation of a single-quantum state, may be possible.

<sup>5</sup> Denote the total angular momentum (vector) operator and its thermal equilibrium value for the conditions stated in the text by  $\mathbf{L}$  and  $\langle \mathbf{L}(0) \rangle$ , respectively, so that  $\langle \mathbf{L}(0) \rangle = Q^{-1} \text{Tr}(\epsilon^{-\beta H} \mathbf{L})$ , where  $H$  is the Hamiltonian of the system,  $\text{Tr}(\dots)$  denotes the trace operation,  $1/\beta$  is the product of Boltzmann's constant and the absolute temperature, and  $Q = \text{Tr} \epsilon^{-\beta H}$  is the partition function. It is sufficient to assume that the force between a pair of particles is dependent only upon the distance between them so that  $H$  is time-reversal invariant. Thus if  $T$  denotes the time-reversal operator, because  $\text{Tr}(\dots)$  is invariant under a cyclic interchange of factors

$$\langle \mathbf{L}(0) \rangle = Q^{-1} \text{Tr}[(T \epsilon^{-\beta H} T^{-1})(T \mathbf{L} T^{-1})] = -Q^{-1} \text{Tr}(\epsilon^{-\beta H} \mathbf{L}) = 0.$$

<sup>6</sup> The generally accepted idea is that  $\langle \mathbf{L}(\omega) \rangle$  is a linear function  $\langle \mathbf{L}(\omega) \rangle = I_0 \omega$  for small  $\omega$ , where the moment of inertia of the liquid  $I_0$  is reduced below its classical solid-body value for temperatures below the lambda point. To speculate that in place of the above linear relation one has instead  $\lim_{\omega \rightarrow 0} \langle \mathbf{L}(\omega) \rangle \neq \langle \mathbf{L}(0) \rangle = 0$  seems to us ill-advised. For the isotropic Heisenberg ferromagnet below the Curie point the thermal-equilibrium magnetization  $\langle \mathbf{M}(\mathbf{H}) \rangle$  is a discontinuous function of the external magnetic field  $\mathbf{H}$ :  $\lim_{\mathbf{H} \rightarrow 0} \langle \mathbf{M}(\mathbf{H}) \rangle \neq \langle \mathbf{M}(0) \rangle = 0$ . The origin of this discontinuity is of course well known; the ferromagnetic coupling between spins  $s(\neq 0)$  results in a ground state which, in the absence of an external magnetic field, is infinitely degenerate corresponding to the equal probability for the magnetization to point in all directions in space. The application of even an arbitrarily weak uniform external magnetic field lifts the degeneracy of the system singling out the particular ground state for which the magnetization points in the direction of the external field. For liquid helium the totally different character of the particles (no intrinsic spin) and of their mutual interaction to our mind rules out any such analogy to the ferromagnet.

Finally, we should mention that for linear flow of a system of particles interacting via velocity independent forces, because of Galilean invariance, one can easily show that the system has higher energy when its center of mass is in motion than when it is at rest (Bloch's theorem). For rotational flow the analogous derivation cannot be given.

### B. Stability Criterion ( $T=0^\circ\text{K}$ )

In order to develop this idea and in particular to formulate a quantitative stability criterion for a persistent current at  $T=0^\circ\text{K}$ , we first enumerate a suitable set of wave functions for the system. We consider a large box of volume  $\Omega$  containing  $N$  identical bosons which are described by a Hamiltonian  $H$ . Let  $\{\varphi_s(\mathbf{r})\}$  denote a complete orthonormal set of single-particle wave functions which satisfy prescribed boundary conditions with respect to  $\Omega$ . The precise nature of this set is of little interest to us at this point. Boson creation and destruction operators for the state  $\varphi_s$  will be denoted by  $a_s^\dagger$  and  $a_s$ , respectively. We now introduce the orthonormal set of state vectors

$$| \{N_s\} \rangle = \prod_s [(N_s!)^{-1/2} (a_s^\dagger)^{N_s}] | 0 \rangle \quad (2.1)$$

for which

$$\sum_s N_s = N. \quad (2.2)$$

The vector  $|0\rangle$  is normalized to unity, and it is characterized by

$$a_s | 0 \rangle = 0 \quad (\text{all } s). \quad (2.3)$$

It will be recalled that  $| \{N_s\} \rangle$  is the second quantized representative of the  $N$ -particle configuration space wave function which is a symmetrized product of single-particle functions, whereby  $N_s$  particles occupy the state  $\varphi_s$ . The set of vectors (2.1) comprise an orthonormal basis for the Hilbert space appropriate to the  $N$ -particle system.

Consider now the set of eigenvectors  $|\alpha\rangle$  and eigenvalues  $E_\alpha$  of  $H$  or, as is more reasonable to expect, a suitably truncated form of  $H$ . In particular, consider an eigenvector  $|\bar{\alpha}, N_c\rangle$  of this set of energy  $E_{\bar{\alpha}}(N_c)$  for which the occupation number  $N_c$  of particles in the current-carrying single-particle state  $\varphi_c$  is macroscopic<sup>7</sup>:

$$\langle \bar{\alpha}, N_c | a_c^\dagger a_c | \bar{\alpha}, N_c \rangle = N_c = O(N). \quad (2.4)$$

For example if the container is a cylinder symmetric about the  $z$  axis and if  $l_z$  denotes the  $z$  component of the single-particle angular momentum operator  $\mathbf{l}$  then a possible choice of  $\varphi_c$  is one for which  $\langle \varphi_c | l_z | \varphi_c \rangle$  is nonzero. Now imagine that the system is prepared so that at some chosen instant of time it is in the macroscopic current-carrying state corresponding to the eigenvector  $|\bar{\alpha}, N_c\rangle$ . The question is, will the system remain in this state or, because of small stray external perturbations, will it undergo rapid transitions to other eigenstates of  $H$  of diminished total current?

To answer this question consider those eigenvectors of  $H$  which differ from  $|\bar{\alpha}, N_c\rangle$  in that  $o(N)$  particles are redistributed into other single-particle states. We label

<sup>7</sup> A number  $N_1$  will be called macroscopic or of order  $N$ , written  $N_1 = O(N)$ , if in the usual limit that  $N, \Omega \rightarrow \infty$  with  $N/\Omega$  held constant ("volume limit") the quantity  $N_1/N$  is nonzero. If in the volume limit  $N_1/N$  is zero we write  $N_1 = o(N)$ . Finally, two macroscopic numbers  $N_1$  and  $N_2$  will be said to be "equal to order  $N$ " if in the volume limit  $(N_1 - N_2)/N$  is zero.

these eigenvectors by  $|\bar{\alpha} + \delta\alpha, N_c \pm o(N)\rangle$ , or, since  $N_c = O(N)$ , simply as  $|\bar{\alpha} + \delta\alpha, N_c\rangle$ , and their eigenvalues by  $E_{\bar{\alpha} + \delta\alpha}(N_c)$ . More precisely, if  $\delta N_s$  denotes the difference in occupation number of the state  $\varphi_s$  for the vectors  $|\bar{\alpha} + \delta\alpha, N_c\rangle$  and  $|\bar{\alpha}, N_c\rangle$ , i.e.,

$$\delta N_s = \langle \bar{\alpha} + \delta\alpha, N_c | a_s^\dagger a_s | \bar{\alpha} + \delta\alpha, N_c \rangle - \langle \bar{\alpha}, N_c | a_s^\dagger a_s | \bar{\alpha}, N_c \rangle, \quad (2.5)$$

then

$$\lim_{N, \Omega \rightarrow \infty} N^{-1} \sum_s |\delta N_s| = 0. \quad (2.6)$$

Now if the system were inclined to make a transition because of an external perturbation from the state corresponding to  $|\bar{\alpha}, N_c\rangle$  to a state corresponding to an eigenvector  $|\alpha\rangle$  even of lower energy featuring either a different value (to order  $N$ ) of  $\langle \alpha | a_c^\dagger a_c | \alpha \rangle$  or macroscopic occupation of  $\varphi_{s(\neq c)}$ , the system would, in general, first have to pass through a succession of vectors of the type  $|\bar{\alpha} + \delta\alpha, N_c\rangle$ .<sup>8</sup> Therefore, if for all vectors  $|\bar{\alpha} + \delta\alpha\rangle$ ,

$$E_{\bar{\alpha}}(N_c) < E_{\bar{\alpha} + \delta\alpha}(N_c), \quad (2.7)$$

the system will remain in the state corresponding to the eigenvector  $|\bar{\alpha}, N_c\rangle$  even though there surely exist other eigenvectors  $|\alpha\rangle$  (not of the form  $|\bar{\alpha} + \delta\alpha, N_c\rangle$ ) featuring still lower energy.<sup>9</sup> That is, if (2.7) is satisfied, then a metastable persistent current occurs in the system initially placed in the physical state corresponding to the eigenvector  $|\bar{\alpha}, N_c\rangle$ . If, however, there exists even one state  $|\bar{\alpha} + \delta\alpha, N_c\rangle$  for which (2.7) fails to hold, the system will make a transition from  $|\bar{\alpha}, N_c\rangle$  to  $|\bar{\alpha} + \delta\alpha, N_c\rangle$  and the prepared current will be rapidly dissipated.

The metastability criterion (2.7) has been stated in general terms without reference to any given model.<sup>10</sup> In the following two sections we shall apply this criterion to the system of particles when described by two different truncated versions of  $H$ . Our immediate goal will be to obtain quantitative conditions on the class of acceptable current-carrying single-particle states  $\varphi_c$  for which the system will support a metastable persistent current.

### III. INDEPENDENT-PARTICLE MODEL

( $T=0^\circ\text{K}$ )

Assume that the system of  $N$  bosons is confined to a cylinder of volume  $\Omega$  with radius  $R$  and height  $L$  and

<sup>8</sup> Exceptions to this could occur for large coherent perturbations capable of effecting a simultaneous evacuation of  $O(N)$  particles from the current-carrying state  $\varphi_c$ . Such perturbations are effectively excluded since as is usual in statistical mechanics the system of interest is to be thought of as weakly coupled to the external world.

<sup>9</sup> It is perhaps worth pointing out that (2.7) is the analog of the familiar metastability criterion of classical mechanics for a particle which is in the immediate vicinity of a local minimum of a potential field of force.

<sup>10</sup> A similar criterion has been employed in the problem of a persistent electric current at zero temperature in a Bose-Einstein model of a superconductor by F. Bloch and H. E. Rorschach, Phys. Rev. **128**, 1697 (1962).

that for simplicity the particles interact via the two-body potential  $V_{ij} = \lambda \delta^3(\mathbf{r}_i - \mathbf{r}_j)$ . If  $\lambda = 8\pi a$ , this choice of potential is recognized to be that describing hard spheres of diameter  $a$  in the approximation of the Fermi pseudopotential.<sup>11,12</sup> The single-particle wave functions  $\varphi_s(\mathbf{r})$  discussed in Sec. II will be of the form

$$\varphi_s(\mathbf{r}) = \varphi_{klm}(\mathbf{r}, \theta, z) = \Omega^{-1/2} e^{i(kz + l\theta)} f_{ln}(\mathbf{r}), \quad (3.1)$$

where  $l$  is an integer,  $k$  is an integral multiple of  $2\pi/L$ , and the radial function  $f_{ln}$  is real and vanishes for  $r = R$ . Thus  $\varphi_s$  satisfies the following boundary conditions

$$\varphi_s(\mathbf{r}, \theta, z + L) = \varphi_s(\mathbf{r}, \theta + 2\pi, z) = \varphi_s(\mathbf{r}, \theta, z), \quad (3.2)$$

$$\varphi_s(R, \theta, z) = 0. \quad (3.3)$$

Furthermore, the orthonormality of the  $\varphi_s$  is assured by the requirement

$$\int_0^R dr r f_{ln} f_{l'n'} = \frac{1}{2} R^2 \delta_{nn'}. \quad (3.4)$$

In the second quantized representation where the  $\varphi_s$  are basis functions the Hamiltonian of the system is

$$H = \sum_{ss'} T_{ss'} a_s^\dagger a_{s'} + \frac{1}{2} \sum_{ss'tt'} V_{stts} a_s^\dagger a_t^\dagger a_{t'} a_{s'}, \quad (3.5)$$

where

$$\begin{aligned} T_{ss'} &= T_{s's} = - \int d^3r \varphi_s^* \nabla^2 \varphi_s \\ &= - \frac{2}{R^2} \delta_{kk'} \delta_{ll'} \int_0^R dr r f_{ln} \\ &\quad \times \left[ \frac{1}{r} \frac{d}{dr} \left( \frac{d}{dr} f_{ln} \right) - \left( k^2 + \frac{l^2}{r^2} \right) f_{ln} \right], \quad (3.6) \end{aligned}$$

and

$$\begin{aligned} V_{ss'tt'} &= V(k_1 l_1 n_1, k_2 \dots, k_2' \dots, k_1' \dots) \\ &= \int d^3r_1 \int d^3r_2 \varphi_s^*(\mathbf{r}_1) \varphi_{t'}^*(\mathbf{r}_2) V_{12} \varphi_{t'}(\mathbf{r}_2) \varphi_s(\mathbf{r}_1) \\ &= (\lambda/\Omega) \delta_{k_1+k_2, k_1'+k_2'} \delta_{l_1+l_2, l_1'+l_2'} (2/R^2) \\ &\quad \times \int_0^R dr r f_{l_1 n_1} f_{l_2 n_2} f_{l_2' n_2'} f_{l_1' n_1'}. \quad (3.7) \end{aligned}$$

The selection rules on the  $z$  components of linear and angular momentum in the matrix elements (3.6) and (3.7) simply reflect the translational and rotational invariance of the system with respect to the  $z$  axis.

The first model we shall investigate as regards the existence of a persistent current is that described by the

<sup>11</sup> Except where noted to the contrary we employ units so that  $\hbar = 2m = 1$ , where  $m$  is the mass of a particle.

<sup>12</sup> For example see K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

following truncated version of (3.5)

$$\begin{aligned} H_1 &= \sum_s T_s a_s^\dagger a_s + \sum_{s,t(\neq s)} V_{stts} a_s^\dagger a_s a_t^\dagger a_t \\ &\quad + \frac{1}{2} \sum_s V_{ssss} a_s^\dagger a_s^\dagger a_s a_s, \quad (3.8) \end{aligned}$$

where  $T_s = T_{ss}$ .<sup>13</sup> The eigenvectors  $|\alpha\rangle$  and eigenvalues  $E_\alpha$  of  $H_1$  can be written down at once [see Eqs. (2.1)–(2.3)]:

$$|\alpha\rangle = |\{N_s\}\rangle = \prod_s [(N_s!)^{-1/2} (a_s^\dagger)^{N_s}] |0\rangle, \quad \sum_s N_s = N, \quad (3.9)$$

$$\begin{aligned} E_\alpha &= \sum_s T_s N_s + \sum_{s,t(\neq s)} V_{stts} N_s N_t \\ &\quad + \frac{1}{2} \sum_s V_{ssss} N_s (N_s - 1). \quad (3.10) \end{aligned}$$

Despite their simple structure the eigenvectors (3.9) can, as is well known, partially incorporate correlations between particles due to their mutual interactions by choosing the  $\varphi_s$  as solutions of a single-particle Schrödinger equation with self-consistent potential. For example, minimizing  $E_\alpha$  of (3.10) for given occupation numbers  $N_s$  with respect to the  $\varphi_s$  yields the usual ‘‘Hartree-Fock’’ equations. We will return to this question later in this section.

We now consider an eigenvector  $|\bar{\alpha}, N_c\rangle$  of  $H_1$  with eigenvalue  $E_{\bar{\alpha}}(N_c)$  whereby a single-particle function  $\varphi_c(\mathbf{r})$  of the form (3.1) with  $l \neq 0$  is occupied by  $N_c = O(N)$  particles. As discussed in Sec. IIB, this eigenvector corresponds to a persistent macroscopic current state of the system if, for all eigenvectors  $|\bar{\alpha} + \delta\alpha, N_c\rangle$  with eigenvalues  $E_{\bar{\alpha} + \delta\alpha}(N_c)$  which can be obtained from  $|\bar{\alpha}, N_c\rangle$  by reshuffling  $o(N)$  particles [see (2.5) and (2.6)], all energy differences

$$\Delta E_{\bar{\alpha}} = E_{\bar{\alpha} + \delta\alpha}(N_c) - E_{\bar{\alpha}}(N_c)$$

are positive-definite. For nonlocalized radial functions  $f_{ln}$ , the matrix elements (3.7) are  $O(1/\Omega)$ . Because of (2.6) it then follows that these energy differences are  $o(N)$ . Thus  $\Delta E_{\bar{\alpha}}$  may be calculated as

$$\Delta E_{\bar{\alpha}} = \sum_s \left( \frac{\partial E_\alpha}{\partial N_s} \right)_{\bar{\alpha}} \delta N_s, \quad (3.11)$$

where the subscript  $\bar{\alpha}$  means that the partial derivative  $\partial E/\partial N_s$  is to be evaluated for the occupation numbers appropriate to the state  $|\bar{\alpha}, N_c\rangle$ . As the total number  $N$  of particles is fixed, i.e.,  $\sum_s \delta N_s = 0$ , we have

$$\Delta E_{\bar{\alpha}} = \sum_{(s \neq c)} \left[ \left( \frac{\partial E_\alpha}{\partial N_s} \right)_{\bar{\alpha}} - \left( \frac{\partial E_\alpha}{\partial N_c} \right)_{\bar{\alpha}} \right] \delta N_s. \quad (3.12)$$

Now the numbers  $\delta N_{s(\neq c)}$  are in the nature of independent variables. It then follows that the metastability criterion can be satisfied if and only if each term of the

<sup>13</sup> Note that for the delta function two-body potential the direct and exchange interaction matrix elements  $V_{stts}$  and  $V_{stst}$  are equal.

TABLE I. Assorted roots  $\rho_{ln}(n=1, 2, \dots)$  of the Bessel functions  $J_l(x)$ .

$l \backslash n$	0	1	2	3	4	5	6	7	8
1	2.405	3.832	5.136	6.380	7.588	8.771	9.936	11.086	12.225
2	5.520	7.016	8.417	9.761	11.065	12.339	13.589	14.821	16.038
3	8.654	10.173	11.620	13.015	14.373	15.700	17.004		
4	11.792	13.324	14.796	16.223	17.616				
5	14.931	16.471	17.960						

sum for which  $\delta N_s \neq 0$  is positive-definite.<sup>14</sup> But such is clearly impossible if  $\delta N_s$  can take on both positive and negative values! The positive definiteness of  $\Delta E_{\bar{\alpha}}$  can be ensured only if all the particles occupy the state  $\varphi_c$ , i.e.,  $N_s = N\delta_{sc}$ , in which case  $\delta N_{s(\neq c)} \geq 0$ , and further if the net energy change of the system upon removing one particle from  $\varphi_c$  and placing it in any other state  $\varphi_s$  is positive-definite, i.e.,

$$\left(\frac{\partial E_{\alpha}}{\partial N_s}\right)_{\bar{\alpha}} > \left(\frac{\partial E_{\alpha}}{\partial N_c}\right)_{\bar{\alpha}} \quad \text{all } s(\neq c). \quad (3.13)$$

Thus in the framework of the model Hamiltonian (3.8) only those of its eigenvectors (3.9) which are of the form

$$|\bar{\alpha}, N\rangle = (N!)^{-1/2} (a_c^\dagger)^N |0\rangle, \quad (3.14)$$

whereby *all* particles occupy the single-particle state  $\varphi_c$ , and which ensure that the inequalities (3.13) are satisfied will, in fact, describe a metastable persistent current.

We turn now to the question of which single-particle functions (3.1) of a given complete set are such as to ensure that (3.13) is satisfied. Using (3.10) and the fact that  $N_s = N\delta_{sc}$  for eigenvectors (3.14), one has

$$\left(\frac{\partial E_{\alpha}}{\partial N_s}\right)_{\bar{\alpha}} = T_s + 2NV_{cssc}, \quad (s \neq c); \quad (3.15)$$

$$\left(\frac{\partial E_{\alpha}}{\partial N_s}\right)_{\bar{\alpha}} = T_c + NV_{cccc}, \quad (s = c).$$

The inequality (3.13) now takes the form

$$T_s - T_c + N(2V_{cssc} - V_{cccc}) > 0. \quad (3.16)$$

But now in order to proceed further we must become more explicit concerning the radial functions  $f_{ln}$  of (3.1).

### A. Free-Particle Eigenfunctions

As a first example we assume that the  $\varphi_s$  are the solutions of the Schrödinger equation for a free particle

<sup>14</sup> It is helpful to regard the set of numbers  $\{N_s\}$  as the generalized coordinates of a point in a space. The physically meaningful sector of this space is that for which all  $N_s \geq 0$ . The constraint  $\sum_s N_s = N$  can then be visualized geometrically as the (finite) portion of a hyperplane passing through the physical sector. Now, except perhaps for a pathological  $H_1$ , the energy eigenvalue  $E_{\alpha}$  of a macroscopic system when regarded as a function of  $\{N_s\}$  has no minimum interior to the physical sector. Hence (3.13) rather than  $(\partial E_{\alpha}/\partial N_s)_{\bar{\alpha}} - (\partial E_{\alpha}/\partial N_c)_{\bar{\alpha}} = 0$ , is equivalent to the stability criterion (2.7). Indeed using (3.10) one can explicitly show that  $(\partial E_{\alpha}/\partial N_s)_{\bar{\alpha}} - (\partial E_{\alpha}/\partial N_c)_{\bar{\alpha}} = 0$  cannot be satisfied for all  $s$  if  $N \neq 0$  and  $T_s \neq T_c$ .

confined to the cylinder. Making use of the boundary condition (3.3) and the normalization condition (3.4), one finds, in this case,

$$f_{ln}(r) = C_{ln} J_l(\rho_{ln} r/R), \quad (n=1, 2, \dots), \quad (3.17)$$

where  $\rho_{ln}$  denotes the  $n$ th root of the Bessel function  $J_l(x)$ , and  $C_{ln}$ , obtained by using the identity

$$\int_0^1 dx x J_l(\rho_{lm} x) J_l(\rho_{ln} x) = \frac{1}{2} [J_l'(\rho_{ln})]^2 \delta_{mn}, \quad (3.18)$$

is given by

$$C_{ln} = 1/J_l'(\rho_{ln}). \quad (3.19)$$

Substituting (3.17) for  $f_{ln}$  in (3.6), the kinetic energy is easily found to be

$$T_s = T_{kln} = k^2 + (\rho_{ln}^2/R^2). \quad (3.20)$$

In the following the quantum numbers generically written as  $c$  and  $s$  in (3.16) will denote the two sets  $(kln)$  and  $(k'l'n')$ , respectively. Note first that if the particles are noninteracting, the inequality (3.16) which becomes

$$k'^2 - k^2 + (\rho_{l'n'}^2 - \rho_{ln}^2)/R^2 > 0, \quad \text{all } (k', l', n'),$$

can be satisfied for given  $(kln)$  only if  $k=l=0, n=1$ . This follows because  $\rho_{01}$  is the smallest of all roots of the  $J_l(x)$  (see Table I). Thus for the ideal Bose-Einstein system only the single-particle state  $\varphi_{001}$  of lowest kinetic energy, a non-current-carrying state, satisfies the stability criterion (3.16). In short, a persistent current cannot occur in an ideal Bose-Einstein system. Stated somewhat differently, in order that a persistent current be possible the *interactions* between particles must be such that the net change in energy of the system upon removing a particle from the current-carrying state  $\varphi_c$  and placing it in a different state  $\varphi_s$  even of lower kinetic energy must be positive.

Substituting (3.17) for  $f_{ln}$  in (3.7), the matrix elements  $V_{cccc}$  and  $V_{cssc}$  become

$$V_{cccc} = (2\lambda/\Omega) [J_l'(\rho_{ln})]^{-4} \int_0^1 dx x J_l^4(\rho_{ln} x), \quad (3.21)$$

$$V_{cssc} = (2\lambda/\Omega) [J_{l'}(\rho_{l'n'}) J_l'(\rho_{ln})]^{-2} \times \int_0^1 dx x J_l^2(\rho_{ln} x) J_{l'}^2(\rho_{l'n'} x). \quad (3.22)$$

The integrals in (3.21) and (3.22) have been calculated with the aid of a computer for a variety of quantum numbers ( $ln$ ) and ( $l'n'$ ).<sup>15</sup> Using these results, we have collected in Table II sufficient values of  $(\lambda/\Omega)^{-1} (2V_{cssc} - V_{cccc})$  so as to indicate when the stability criterion (3.16) is satisfied. The quantum numbers  $k$  and  $k'$  have always been set equal to zero since nonzero values of  $k'^2$  and  $k^2$  misleadingly enhance or suppress the possible positive values of the left-hand side of (3.16).

The relevant parameter in the following discussion is  $\lambda\rho R^2$ , which, roughly speaking, is the ratio of the mean interaction energy between pairs of particles to the single-particle zero-point kinetic energy. The symbol  $\rho$  denotes the mean number density  $N/\Omega$ . By consulting Table II, it can be seen that the states  $\varphi_c = \varphi_{011}$  and  $\varphi_{021}$ , although of higher kinetic energy than the state  $\varphi_{001}$ , are such that the stability criterion (3.16) is satisfied so long as  $\lambda\rho R^2$  is sufficiently large. In particular, the stability criterion is satisfied if  $\lambda\rho R^2$  is larger than 6.5 and 32.3, for  $\varphi_{011}$  and  $\varphi_{021}$ , respectively. The state  $\varphi_{031}$  is a less likely possibility for although transitions to the lower kinetic-energy states  $\varphi_{001}$ ,  $\varphi_{011}$ ,  $\varphi_{021}$ ,  $\varphi_{002}$  will not occur for sufficiently large  $\lambda\rho R^2$  there is the added difficulty that  $2V_{cssc} - V_{cccc}$  is negative even for the higher kinetic-energy states  $\varphi_{003}$ ,  $\varphi_{004}$ ,  $\varphi_{005}$ ,  $\dots$ . Finally, for the state  $\varphi_{012}$  the stability criterion (3.16) cannot be satisfied since transitions to  $\varphi_{021}$  and  $\varphi_{031}$  will occur irrespective of the value of the ratio  $\lambda\rho R^2$ . We should also point out that, according to the data of Table II, transitions are possible from  $\varphi_c = \varphi_{001}$  to states  $\varphi_s = \varphi_{031}$ ,  $\varphi_{041}$ ,  $\varphi_{051}$ ,  $\dots$ , but only if  $\lambda\rho R^2 \gtrsim 70$ . For such large values of  $\lambda\rho R^2$  the use of free-particle eigenfunctions (3.17) would be unjustified; instead one should use the Hartree eigenfunctions described in Subsec. IIIB.

The data in Table III indicate under what circumstances the system is stable against transitions from

TABLE II. Matrix elements  $(\lambda/\Omega)^{-1} (2V_{cssc} - V_{cccc})$  for the states  $\varphi_s$ ,  $s = (l_s, n_s)$ , and  $\varphi_c$ ,  $c = (l_c, n_c)$ , of Eq. (3.17), and the sign of the kinetic energy differences  $T_s - T_c$ . In all cases,  $k_s = k_c = 0$ .

$\begin{array}{c} c \\ s \end{array}$	(0,1)	(1,1)	(2,1)	(3,1)	(1,2)
(0,1)		1.37, -	0.64, -	0.14, -	1.46, -
(0,2)		0.35, +	0.24, +	0.30, -	1.26, -
(0,3)		0.48, +	0.18, +	-0.03, +	
(0,4)		0.50, +	0.19, +	-0.02, +	
(0,5)		0.52, +	0.19, +	-0.01, +	0.65, +
(1,1)	0.75, +		1.38, -	1.04, -	0.21, -
(1,2)		0.72, +	0.21, +		
(1,3)		0.61, +	0.22, +		1.05, +
(2,1)	0.00, +			1.45, -	-0.25, -
(3,1)	-0.46, +				-0.36, -
(4,1)	-0.77, +				
(5,1)	-1.00, +				

<sup>15</sup> This work made use of computer facilities at Princeton University which are supported in part by National Science Foundation Grant NSF-GP579.

TABLE III. Matrix elements  $(\lambda/\Omega)^{-1} (2V_{cssc} - V_{cccc})$  for assorted states  $\varphi_c$ ,  $c = (l_c, n_c)$  and  $\varphi_s = \varphi_{001}$ , the single-particle ground state. All single-particle states are of the type (3.17).

$(l_c, n_c)$	$(\lambda/\Omega)^{-1} (2V_{cssc} - V_{cccc})$
(1,1)	1.37
(1,2)	1.46
(2,1)	0.64
(2,2)	1.25
(3,1)	0.14
(4,1)	-0.24
(5,1)	-0.54
(6,1)	-0.78

various states  $\varphi_c$  to the single state  $\varphi_s = \varphi_{001}$ . With the possible exception of the state  $\varphi_{022}$  no states other than those mentioned in the previous paragraph satisfy the stability criterion. In fact, further analysis shows that  $\varphi_{022}$  also is unacceptable. Thus we conclude that only the single-particle states  $\varphi_{011}$ ,  $\varphi_{021}$ , and  $\varphi_{031}$ , or more properly the  $N$ -body eigenvectors (3.14) constructed from these, can support a persistent current and then only if  $\lambda\rho R^2$  is sufficiently large. Note the strong dependence of our conclusions, as to which states satisfy the stability criterion (3.16), upon the size of the radius of the container. Finally, it is important to observe that there is a critical angular momentum which a persistent current can carry; in the present model it is  $3N\hbar$ , a value which cannot be exceeded no matter how large the value of  $\lambda\rho R^2$ . The reason for this small value is that free-particle wave functions are not appropriate for describing the condensate when the interactions are strong. Such wave functions decrease the size of the matrix elements  $V_{cssc}$  from the value they would have in the actual system and thus reduce the effective two-particle interaction. This leads us to consider a more appropriate set of basis functions.

## B. Hartree Eigenfunctions

Our second choice for the set of single-particle functions  $\varphi_s(\mathbf{r})$  will be guided by our earlier finding that within the framework of the model Hamiltonian  $H_1$  persistent current eigenstates correspond to vectors  $|\bar{\alpha}, N\rangle$  of (3.14) which ensure that (3.13) is satisfied. The eigenvalue of  $H_1$  corresponding to  $|\bar{\alpha}, N\rangle$  is

$$E_{\bar{\alpha}}(N) = N(T_c + \frac{1}{2}NV_{cccc}) \\ = N \left[ - \int d^3r \varphi_c^* \nabla^2 \varphi_c + \frac{1}{2}\lambda N \int d^3r |\varphi_c|^4 \right]. \quad (3.23)$$

We will choose for  $\varphi_c$  that function of the form (3.1)

$$\varphi_c(\mathbf{r}) = \Omega^{-1/2} e^{il\theta} f_l(\mathbf{r}), \quad (l \neq 0)$$

which satisfies (3.2), (3.3), and (3.4) and which minimizes  $E_{\bar{\alpha}}(N)$ .<sup>16</sup> The minimizing function satisfies the

<sup>16</sup> In this expression for  $\varphi_c$  we have chosen  $k=0$  so that the factor  $e^{ikz}$  in (3.1) is unity; a nonzero value of  $k$  increases the eigenvalue  $\epsilon$  in (3.24).

Hartree equation

$$-\nabla^2\varphi + \lambda N |\varphi|^2\varphi = \epsilon\varphi. \quad (3.24)$$

In particular, we are interested in the solution of (3.24), satisfying the previously mentioned conditions, which for given  $l$  is associated with the smallest eigenvalue.

It is rather remarkable that the vector (3.14) [or equivalently the configuration space wave function  $\prod_{n=1}^N \varphi_c(\mathbf{r}_n)$ , where  $\varphi_c$  is the required solution of (3.24)] describes a vortex with quantized circulation.<sup>17,18</sup> We will briefly review the arguments for this interpretation. One can define the velocity of a system at a point  $\mathbf{r}$  when in a state  $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_n)$  by

$$\mathbf{v}(\mathbf{r}) = \mathbf{j}(\mathbf{r})/\rho(\mathbf{r}), \quad (3.25)$$

where  $\mathbf{j}(\mathbf{r})$  and  $\rho(\mathbf{r})$  given by

$$\mathbf{j}(\mathbf{r}) = \langle \Psi | \frac{\hbar}{2mi} \sum_{i=1}^N [\nabla_i \delta^3(\mathbf{r}_i - \mathbf{r}) + \delta^3(\mathbf{r}_i - \mathbf{r}) \nabla_i] | \Psi \rangle, \quad (3.26)$$

and

$$\rho(\mathbf{r}) = \langle \Psi | \sum_{i=1}^N \delta^3(\mathbf{r}_i - \mathbf{r}) | \Psi \rangle \quad (3.27)$$

are the expectation values in the state  $|\Psi\rangle$  of the local current and particle number density operators, respectively. For the Hartree function  $\prod_i \varphi_c(\mathbf{r}_i)$ , one finds

$$\mathbf{v}(\mathbf{r}) = (\hbar l/mr)\hat{\theta}, \quad (3.28)$$

where  $\hat{\theta}$  is a unit vector in the direction of increasing azimuthal angle  $\theta$ . The vorticity  $\nabla \times \mathbf{v}$  for this fluid flow is zero except along the line  $\mathbf{r}=0$ , whereas the circulation is

$$\oint \mathbf{v} \cdot d\mathbf{r} = \hbar l/m \quad (3.29)$$

for any closed path encircling this line. These properties are characteristic of a fluid containing a single line vortex with circulation quantized in units of  $\hbar/m$ . Such flow states in liquid helium were first predicted by Onsager,<sup>19</sup> and their existence has been conclusively established experimentally in recent years.<sup>20</sup>

The objection might be raised that because (3.28) and (3.29) are independent of the form of the radial function  $f_i$  of  $\varphi_c(\mathbf{r})$  these same equations, and therefore presumably the above vortex interpretation, apply even for wave functions of the form  $\prod_i e^{i l \theta_i} J_l(\rho_{ln} r_i/R)$  which describe the noninteracting system. The answer to this

<sup>17</sup> A discussion of the vortex-type solutions of the Hartree equation (3.24) and a list of references to work by others can be found in E. P. Gross, *J. Math. Phys.* 4, 195 (1963). The series of recent articles by A. L. Fetter, *Phys. Rev.* 138, A429 (1965); 138, A709 (1965); 140, A452 (1965) should also be consulted.

<sup>18</sup> In order to conform with the usual discussion of vortices with quantized circulation we will in this paragraph employ usual units so that  $\hbar = 2\pi\hbar$  is Planck's constant and  $m$  is the mass of a particle.

<sup>19</sup> L. Onsager, *Nuovo Cimento Suppl.* 6, 2, 249 (1949).

<sup>20</sup> G. W. Rayfield and F. Reif, *Phys. Rev. Letters* 11, 305 (1963).

question derives from the essential difference between the local number density  $\rho(\mathbf{r})$  of the noninteracting system and that of the system with wave function constructed from solutions to (3.24). For the noninteracting system

$$\rho(\mathbf{r}) = \frac{N}{\Omega} \left[ \frac{J_l(\rho_{ln} r/R)}{J'_l(\rho_{ln})} \right]^2,$$

which is a function of considerable variation even for  $n=1$ . This behavior is not surprising; because the function  $e^{i l \theta} J_l(\rho_{ln} r/R)$  describes a free particle it is strongly dependent upon the form of the boundary conditions imposed at the walls of the container.<sup>21</sup> By contrast if  $\varphi$  is the required solution of (3.24) and  $l^2/R^2 \ll \lambda N/\Omega$ , as discussed in Appendix A the density is virtually uniform except in the immediate vicinity of  $r=0$  and  $R$  where it drops to zero. On this basis the vortex interpretation is justifiably limited to  $N$ -body functions based on (3.24).

In principle, a complete orthonormal set of single-particle functions can now be obtained by finding all eigenfunctions of the linear self-adjoint equation

$$-\nabla^2\varphi_s + \lambda N |\varphi_s|^2\varphi_s = \epsilon_s\varphi_s \quad (3.30)$$

subject to the boundary conditions (3.2) and (3.3). As before,  $\varphi_c$  is the required solution of (3.24). Note that  $\varphi_c$  and  $\epsilon_c = \epsilon$ , the required eigenfunction of (3.24) and the corresponding eigenvalue, satisfy (3.30). For purposes of tractability we must settle on an approximate treatment of (3.30). Based on the discussion in Appendix A, as long as  $1/\sigma^2 = \lambda N/\Omega \gg l_c^2/R^2$  it would appear reasonable when calculating  $\varphi_s (\neq c)$  to approximate  $\varphi_c$  as  $\Omega^{-1/2} e^{i l_c \theta}$  and  $\epsilon_c$  by  $\lambda N/\Omega$ . In that case the solutions of (3.30) are easily found to be

$$\varphi_s(\mathbf{r}) = \varphi_{kln}(\mathbf{r}) = \Omega^{-1/2} e^{i(kz+l\theta)} [J_l(\rho_{ln} r/R)/J'_l(\rho_{ln})], \quad (3.31)$$

$$\epsilon_{kln} = k^2 + \rho_{ln}^2/R^2 + \lambda N/\Omega, \quad (3.32)$$

with the exception that for the set of quantum numbers  $(k, l, n) = (0, l_c, 1)$  we define  $\varphi_{0l_c1}$  and  $\epsilon_{0l_c1}$  by the approximate forms of  $\varphi_c$  and  $\epsilon_c$ . That is,

$$\varphi_{0l_c1} = \varphi_c = \Omega^{-1/2} e^{i l_c \theta}, \quad (3.33)$$

and

$$\epsilon_{0l_c1} = \lambda N/\Omega. \quad (3.34)$$

Note that the eigenfunctions  $\varphi_s (\neq c)$  are identical to those considered in Subsec. IIIA. Note further that with the exception of the matrix elements  $\int d^3r \varphi_s^* \varphi_{0l_c1} \varphi_{0l_c n}$ , we have  $\int d^3r \varphi_s^* \varphi_{s'} = \delta_{ss'}$ .

In line with our earlier comments that the  $N$ -body state  $\prod_i \varphi_c(\mathbf{r}_i)$  describes a line vortex with circulation

<sup>21</sup> A similar situation occurs for a cubic container where one has standing waves or plane waves as solutions of a free-particle Schrödinger equation depending on whether rigid wall or periodic boundary conditions are prescribed.

$l_c h/m$ , the energy  $E_{\bar{\alpha}}(N)$  of this state [see Eq. (3.23)] is

$$E_{\bar{\alpha}}(N) = \frac{1}{2} \lambda N^2 / \Omega + 2\pi l_c^2 (N/\Omega) L \ln(R/l\sigma), \quad (3.35)$$

where

$$\sigma = (\lambda\rho)^{-1/2}. \quad (3.36)$$

As discussed in Appendix A,  $l\sigma$  is the distance from the axis of the cylinder beyond which the Hartree function  $\varphi_c$  is uniform. Equivalently,  $l\sigma$  can be thought of as the core radius of the line vortex. The result (3.35) is obtained by assuming that  $\varphi_c$  is given by (3.33) in the range  $l\sigma \leq r \leq R$  and zero in the range  $0 \leq r \leq l\sigma$ .<sup>22</sup> This choice of  $\varphi_c$  is an adequate facsimile of the exact solution of the Hartree equation (3.24). Note that the second term on the right-hand side of (3.35) has the same form as that of the energy of a classical line vortex.

Using the single-particle wave functions (3.31) and (3.33), the matrix elements  $V_{cscs}$  and  $V_{cccc}$  are found to be

$$V(k_c \cdots, k_s \cdots, k_s \cdots, k_c \cdots) \\ = V(k_c \cdots, k_s \cdots, k_c \cdots, k_s \cdots) = \lambda/\Omega, \quad (3.37)$$

so that the stability criterion (3.16) is easily found to take the form

$$\lambda\rho + \frac{\rho v n^2}{R^2} - 2 \frac{l_c^2}{R^2} \ln\left(\frac{R}{l_c \sigma}\right) > 0. \quad (3.38)$$

Now even if we drop the positive term  $\rho v n^2/R^2$ , this inequality which becomes  $x - \ln x > 0$ , where  $x = \lambda\rho R^2/l_c^2$ , is satisfied for all values of  $x$ . That is to say, so long as  $\lambda\rho \gg l_c^2/R^2$ , in which case (3.31) and (3.33) are good approximate solutions of (3.30), the  $N$ -body eigenvectors (3.14) constructed from (3.33) describing single line vortices with circulation  $l_c(h/m)$  correspond to persistent current-carrying states of the system. When the strong form of the inequality fails to hold, (3.31) and (3.33) no longer comprise the approximate solutions of (3.30). In fact, for successively smaller values of the ratio  $\lambda\rho R^2/l_c^2$ , the more nearly does (3.24) become the Schrödinger equation for a free particle in the cylinder and the analysis of Subsec. IIIA becomes relevant. Thus if  $\lambda\rho R^2/l_c^2$  is decreased to a certain critical value the system becomes incapable of supporting a persistent current for the single-particle angular momentum  $l_c$ .

We remark at this point that the fact that our condensate wave function  $\varphi_c$  describes a single line vortex does not imply that our results are invalid for a system throughout which there are distributed many vortices. The crucial point here is that (3.37) holds solely because  $\varphi_c$  is approximately constant almost

<sup>22</sup> Inasmuch as the matrix elements  $V_{cscs}$  and  $V_{cccc}$  (see (3.7)) remain finite when calculated using (3.31) and (3.33) there is no need to replace (3.33) by an expression which shall vanish as  $r \rightarrow 0$  as does the exact solution  $\varphi_c$  of (3.24). Furthermore, the resulting error in the matrix elements is ignorable since as discussed in Appendix A the radial part of  $\varphi_c$  is constant except within a distance  $l(\lambda\rho)^{-1/2} \ll R$  of the cylinder axis.

everywhere. In a system where  $\varphi_c$  described many vortices, this would still be true so that  $V_{cscs}$  would still be  $\approx \lambda/\Omega$ . On the other hand, for a given total system angular momentum,  $T_c$  would be lowered by the distribution of vortices throughout the volume, as is well known from the theory of superfluid hydrodynamics. We then see from the form of the stability criterion (3.16) that in this case our basic conclusion would still be valid.

Summarizing the work of Subsecs. IIIA and IIIB, we have found that the model Hamiltonian (3.8) does, in fact, possess eigenvectors which describe persistent macroscopic current-carrying states of the system. However, in Subsec. IIIA we found that no matter how large the value of  $\lambda\rho R^2$  the number of single-particle functions  $\varphi_c$  for which the stability criterion (3.16) is satisfied does not exceed a particular finite number. By contrast, for the single-particle functions of Subsec. IIIB we have found that so long as  $\lambda\rho R^2 \gg l_c^2$ ,  $\varphi_c$  given by (3.33) is such as to satisfy the stability criterion.

#### IV. QUASIPARTICLE MODEL ( $T=0^\circ\text{K}$ )

It is a simple truism that the replacement of a physical system by a model is credible only if there are strong reasons for believing that the essential features of the real system are reflected in the model. Now although the properties of the model studied in the previous section are quite satisfying and give considerable insight into the nature of a persistent current in a many-boson system, there is little basis for claiming that the model is an accurate facsimile of the actual system described by the Hamiltonian (3.5). In this section we shall formulate a model which is not only tractable but also has a basis as a reasonable approximation to the actual system.

It will be recalled that in his classic work on the nonideal boson gas Bogoliubov<sup>23</sup> was led to construct a model replacement for the actual Hamiltonian by invoking the following argument: At sufficiently low temperatures one expects that a macroscopic number  $N_0 = O(N)$  of particles of a system of interacting bosons will occupy the single-particle state of zero momentum (Bose-Einstein condensation), paralleling the behavior of the ideal boson gas. It is reasonable then in an approximate treatment to retain only those terms of the complete second-quantized Hamiltonian which involve products of two or more zero-momentum single-particle creation and destruction operators  $a_0^{(\dagger)}$ . In addition, Bogoliubov<sup>23</sup> argued that as a further consequence of the Bose-Einstein condensation it is plausible to replace the operators  $a_0$  and  $a_0^\dagger$  by the  $c$  number  $N_0^{1/2}$ . Analogously, we argue that if a macroscopic number of particles occupy a *current-carrying* single-particle state  $\varphi_c$ , then it is a reasonable procedure to retain only those terms of (3.5) which involve products of two or more

<sup>23</sup> N. N. Bogoliubov, J. Phys. (U.S.S.R.) 11, 23 (1947).



$a_c^{(\dagger)}$  operators and further to replace these operators by  $N_c^{1/2}$ . Assuming that only one single-particle state  $\varphi_c$  is macroscopically occupied, we obtain a Hamiltonian of the form<sup>24</sup>:

$$H_2 = (T_c - \mu)N_c + \frac{1}{2}N_c(N_c - 1)V_{cccc} \\ + \sum'_{qm} [f_{qm}a_{k+q, l+m}^\dagger a_{k+q, l+m} \\ + \frac{1}{2}h_{qm}(a_{k-q, l-m}^\dagger a_{k+q, l+m}^\dagger \\ + a_{k+q, l+m} a_{k-q, l-m})], \quad (4.1)$$

where

$$f_{qm} = T_{k+q, l+m} - \mu \\ + 2N_c V(k+q, l+m; kl; kl; k+q, l+m), \quad (4.2)$$

and

$$h_{qm} = h_{-q, -m} = N_c V(k-q, l-m; k+q, l+m; kl; kl). \quad (4.3)$$

In obtaining (4.1) we have eliminated terms of the form<sup>25</sup>  $N_c^{1/2} \sum_s' (T_{sc} + N_c V_{cccc})(a_s + a_s^\dagger)$ . The presence of these terms can be a source of great difficulty, for upon diagonalizing the Hamiltonian which includes them one finds, in addition to the consistent result that the single-particle state  $\varphi_c = \varphi_{kl_n}$  is macroscopically occupied, that all states  $\varphi_{kl_n'} (\neq n)$  are likewise macroscopically occupied. Such a result contradicts the starting premise that the sole "preferred" single-particle state is  $\varphi_c$ . This difficulty is avoided by choosing the single-particle functions  $\varphi_s$  as solutions of<sup>26</sup>

$$-\nabla^2 \varphi_c + \lambda N_c |\varphi_c|^2 \varphi_c = \epsilon_c \varphi_c, \\ -\nabla^2 \varphi_s + \lambda N_c |\varphi_c|^2 \varphi_s = \epsilon_s \varphi_s, \quad (s \neq c), \quad (4.4)$$

subject to the boundary conditions (3.2) and (3.3). These equations differ from those of (3.30) only in that  $N_c$  is a number which may differ from  $N$ ; the actual value of  $N_c$  will be determined later in this section. A consequence of these equations is that  $T_{sc} + N_c V_{cccc} = 0$  as claimed above.

We have further simplified the Hamiltonian by discarding all terms involving operators  $a_s^{(\dagger)}$  relating to a state  $\varphi_s$ ,  $s = (k_s, l_s, n_s)$ , for which  $n_s \neq 1$ . The justification for this procedure stems from the fact that the single-particle state with  $n_s = 1$  corresponds to the smallest eigenvalue  $\epsilon_s$  for the given quantum numbers  $k_s, l_s$  and therefore transitions to or from higher energy states  $n_s > 1$  are of less importance. Finally, in (4.1) and throughout the following, a prime on a summation sign means that  $m$  and  $q$  cannot both be zero.

<sup>24</sup> In the following it will prove convenient to add the terms  $-\mu \sum_s a_s^\dagger a_s$  to the Hamiltonian (3.5), where  $\mu$  is a Lagrangian multiplier. One should not identify  $\mu$  with the usual chemical potential of a system, a parameter characterizing the thermal equilibrium state of the system. The actual definition of  $\mu$  will be given somewhat later in this section.

<sup>25</sup> The linear terms arise because of the absence of any selection rules for the quantum number  $n$  in the matrix elements of (3.6) and (3.7).

<sup>26</sup> This procedure has been used by E. P. Gross, *Nuovo Cimento* **20**, 454 (1961).

In the following it is assumed that the single-particle functions satisfy (4.4) and thus the linear terms which would otherwise appear in (4.1) are absent. In particular, if the macroscopically occupied state is  $\varphi_c = \varphi_{kl_1}$  then, as discussed in Appendix A, if  $\lambda \rho_c R^2 \gg l^2$ , the approximate eigenfunctions of (4.4) are given by

$$\varphi_c(\mathbf{r}) = \varphi_{kl_1}(\mathbf{r}) = \Omega^{-1/2} e^{i(kz+l\theta)}, \quad (4.5)$$

$$\varphi_s (\neq c) = \varphi_{k'l'1}(\mathbf{r}) \\ = \Omega^{-1/2} e^{i(k'z+l'\theta)} [J_{l'}(\rho_{l'1} r/R) / J_{l'}(\rho_{l'1})]. \quad (4.6)$$

The diagonalization of (4.1) is readily achieved by introducing new boson destruction and creation operators  $b_{k-q, l-m}$  and  $b_{k-q, l-m}^\dagger$ , respectively, defined by

$$a_{k-q, l-m} = u_{qm} b_{k-q, l-m} + v_{qm} b_{k+q, l+m}^\dagger, \quad (4.7)$$

where the  $c$  numbers  $u_{qm}$  and  $v_{qm}$  are such that  $u_{qm} = u_{-q, -m} = u_{qm}^*$  and  $v_{qm} = v_{-q, -m} = v_{qm}^*$ . To ensure that these operators satisfy the Bose-Einstein commutation relations, we must impose the restriction that

$$u_{qm}^2 - v_{qm}^2 = 1. \quad (4.8)$$

Substitution of (4.7) into (4.1) yields an expression which is diagonal in the new representation if

$$(f_{qm} + f_{-q, -m}) u_{qm} v_{qm} + h_{qm} (u_{qm}^2 + v_{qm}^2) = 0. \quad (4.9)$$

The simultaneous equations (4.8) and (4.9) have as their solutions

$$u_{qm}^2 = \frac{1}{2} [\frac{1}{2} \epsilon_{qm}^{-1} (f_{qm} + f_{-q, -m}) + 1], \\ v_{qm}^2 = \frac{1}{2} [\frac{1}{2} \epsilon_{qm}^{-1} (f_{qm} + f_{-q, -m}) - 1], \quad (4.10)$$

where

$$\epsilon_{qm} = \epsilon_{-q, -m} = [\frac{1}{4} (f_{qm} + f_{-q, -m})^2 - h_{qm}^2]^{1/2}. \quad (4.11)$$

As a result of this transformation,  $H_2$  becomes

$$H_2 = W + \sum'_{q, m} \omega_{qm} b_{k+q, l+m}^\dagger b_{k+q, l+m}, \quad (4.12)$$

where

$$W = (T_c - \mu)N_c + \frac{1}{2}N_c(N_c - 1)V_{cccc} \\ + \frac{1}{2} \sum'_{qm} [\epsilon_{qm} - \frac{1}{2} (f_{qm} + f_{-q, -m})], \quad (4.13)$$

and

$$\omega_{qm} = \epsilon_{qm} + \frac{1}{2} (f_{qm} - f_{-q, -m}) \neq \omega_{-q, -m}. \quad (4.14)$$

The form of (4.12) shows that  $H_2$  possesses a ground-state eigenvector, i.e., the eigenvalue spectrum of  $H_2$  has a finite lower bound, if in fact

$$\omega_{qm} > 0, \quad (\text{all } q, m \neq 0). \quad (4.15)$$

This eigenvector, denoted by  $|0\rangle$ , describes a state with no  $b$  excitations:

$$b_{qm} |0\rangle = 0, \quad (\text{all } q, m \neq 0). \quad (4.16)$$

The ground-state energy of  $H_2$ , again only when (4.15)

holds, is  $W$ . Note carefully that because

$$N_c = \langle 0 | a_c^\dagger a_c | 0 \rangle = O(N)$$

the ground-state eigenvector of  $H_2$  corresponds to a macroscopic current-carrying state of the system.

The parameters  $\mu$  and  $N_c$  are determined by the auxiliary conditions, first, that the total number of particles in the system is  $N$ , and second, that  $W$  is minimized with respect to variations of  $N_c$ ,<sup>27</sup> that is,

$$N_c = N - \sum'_{qm} \langle 0 | a_{k-q, l-m}^\dagger a_{k-q, l-m} | 0 \rangle \quad (4.17)$$

and

$$(\partial W / \partial N_c)(N_c, \mu) = 0. \quad (4.18)$$

Upon using (4.13), one easily finds that (4.18) becomes

$$\mu = T_c + N_c V_{cccc}. \quad (4.19)$$

In obtaining this result we have ignored a term of the form  $N_c V_{cccc} (\rho_c \lambda^3)^{1/2} \times F(\lambda \rho_c R^2)$ , when  $F$  is a function only of the indicated variable. It is well known that the Fermi pseudopotential  $V_{ij} = \lambda \delta^3(\mathbf{r}_i - \mathbf{r}_j)$ ,  $\lambda = 8\pi a$ , describes hard spheres, of diameter  $a$ , only if  $\rho a^3 \ll 1$ .<sup>12</sup> Thus it is justified to approximate  $\mu$  by (4.19) since the restriction  $\rho a^3 \ll 1$  nevertheless allows  $\lambda \rho_c R^2$  to be very large compared to one; as discussed in Sec. IIIB, this allows us to interpret the single-particle solutions of (4.4) in terms of line vortices. Returning now to (4.17), this equation can be rewritten with the aid of (4.7) and (4.16) as

$$N_c = N - \frac{1}{2} \sum'_{qm} [\frac{1}{2} \epsilon_{qm}^{-1} (f_{qm} + f_{-q, -m}) - 1]. \quad (4.20)$$

Using (4.2), (4.3), (4.11), and (4.19) one can solve for  $N_c$  from this equation. Note carefully that the value of  $N_c$  will depend upon  $l$  but not  $k$ .

We are now in a position to discuss the possibility of  $H_2$  describing a persistent current. The normalized eigenvectors and eigenvalues of this Hamiltonian are given by

$$|\alpha\rangle = |\{\mathbf{n}_s\}\rangle = \prod_{qm} [(n_s!)^{-1/2} (b_{k-q, l-m}^\dagger)^{n_s}] |0\rangle, \quad (4.21)$$

$$E_\alpha = W + \sum'_{qm} n_{k-q, l-m} \omega_{k-q, l-m}. \quad (4.22)$$

Note that the eigenvectors (4.21) are not subject to the auxiliary condition  $\sum_s n_s = N$  as was the case for the eigenvectors (3.9) of  $H_1$ . For those eigenvectors (4.21) for which  $\sum_s n_s$  is a finite number, the expectation values  $\langle \alpha | a_c^\dagger a_c | \alpha \rangle$  differ from  $N_c = \langle 0 | a_c^\dagger a_c | 0 \rangle$  by a number  $o(N)$ .<sup>28</sup> In terms of the notation of Sec. IIB the current-carrying ground state  $|0\rangle$  of  $H_2$  corresponds to  $|\bar{\alpha}, N_c\rangle$ , whereas the eigenvectors described in the

<sup>27</sup> N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959); A. E. Glassgold, A. N. Kaufman, and K. M. Watson, *ibid.* **120**, 660 (1960).

<sup>28</sup> This can easily be verified by using (4.7) to express  $a_c^\dagger a_c$  in terms of the  $b^{(\dagger)}$  operators.

previous sentence correspond to the eigenvectors  $|\bar{\alpha} + \delta\alpha, N_c\rangle$ . We see at once, then, that for the present model the stability criterion (2.7) is equivalent to the demand (4.15) that all excitation energies  $\omega_{qm}$  of  $H_2$  be positive-definite.<sup>29</sup> As we pointed out earlier in this section, this demand must also be satisfied in order that  $H_2$  possess a ground state. That is to say, the statements that  $H_2$  possesses a ground-state eigenvector and that it describes a metastable persistent current state of the system are entirely equivalent.

Before proceeding to study under which conditions the stability criterion (4.15) is satisfied, we shall utilize our formalism to study the metastability of linear flow through a long channel. We will find that, for this case, (4.15) reduces to Landau's<sup>30</sup> well-known criterion for linear "superfluid flow."

Assume that our system is confined to the interior of a stationary long channel with, say, a square cross section. Assume further that a macroscopic number  $N_c$  of particles occupy the single-particle state  $\Omega^{-1/2} e^{i\mathbf{k}\cdot\mathbf{r}}$ , where  $\mathbf{k}$  points along the axis of the cylinder. Instead of the wave vector  $\mathbf{k}$ , it will be useful in the following to introduce the velocity  $\mathbf{v} = 2\mathbf{k}$  (in terms of usual units  $\hbar\mathbf{k} = m\mathbf{v}$ ). For this system the interaction matrix elements  $V_{stt's'}$  of (3.7) are all given by

$$V_{stt's'} = (\lambda/\Omega) \delta(\mathbf{k}_s + \mathbf{k}_t, \mathbf{k}_{s'} + \mathbf{k}_{t'}),$$

where  $\delta(i, j)$  is the Kronecker delta function. Further, upon referring to (4.2), (4.3), and (4.19), we find

$$f_q(\mathbf{v}) = q^2 + \lambda\rho_c + \mathbf{v}\cdot\mathbf{q}, \quad h_q(\mathbf{v}) = \lambda\rho_c \quad (4.23)$$

and

$$\epsilon_q(\mathbf{v}) = q(q^2 + 2\lambda\rho_c)^{1/2}, \quad (4.24)$$

so that

$$\omega_q(\mathbf{v}) = q(q^2 + 2\lambda\rho_c)^{1/2} + \mathbf{v}\cdot\mathbf{q} = \omega_q(0) + \mathbf{v}\cdot\mathbf{q}. \quad (4.25)$$

This expression gives the energy of an excitation, with momentum  $\mathbf{q}$  relative to the drifting condensate (drift velocity  $\mathbf{v}$ ), as measured by an observer at rest in the reference frame in which the container is stationary (lab frame). It is essential to note that the second equality in (4.25) holds only because  $\rho_c$  is independent of  $\mathbf{v}$  (for  $v < v_s$ ), which is easily shown to follow from (4.20).

<sup>29</sup> One might legitimately question our result that the energy difference between the state  $|\alpha\rangle = \delta_{k+q, l+m}^\dagger |0\rangle$  and  $|0\rangle$  is  $\omega_{k+q, l+m}$ , citing the need for our calculations to reflect the fact that as one considers excited states of  $H_2$  the number  $N_c$  decreases. This could be partially incorporated by replacing  $N_c$  wherever it appears, especially in  $W$ , by the operator  $a_c^\dagger a_c$ . Then one has  $\langle \alpha | H_2 | \alpha \rangle - \langle 0 | H_2 | 0 \rangle - \omega_{k+q, l+m} = \langle \alpha | W | \alpha \rangle - \langle 0 | W | 0 \rangle$ . Now because

$$\langle \alpha | a_c^\dagger a_c | \alpha \rangle - \langle 0 | a_c^\dagger a_c | 0 \rangle = O(1),$$

one might argue that  $\langle \alpha | W | \alpha \rangle - \langle 0 | W | 0 \rangle$  is an  $O(1)$  quantity and thus not ignorable. This argument is easily countered by noting that were we to follow such a procedure the Taylor expansion of  $\langle \alpha | W | \alpha \rangle - \langle 0 | W | 0 \rangle$  is  $\langle 0 | \partial W / \partial (a_c^\dagger a_c) | 0 \rangle \delta N_c + o(1)$ , where  $\delta N_c = \langle \alpha | a_c^\dagger a_c | \alpha \rangle - \langle 0 | a_c^\dagger a_c | 0 \rangle$ . But  $\langle 0 | \partial W / \partial (a_c^\dagger a_c) | 0 \rangle$  is the same as the partial derivative  $\partial W / \partial N_c$  in (4.18) and thus is zero. Hence  $\langle \alpha | W | \alpha \rangle - \langle 0 | W | 0 \rangle = o(1)$  and thus is ignorable. Because of this result we have chosen to follow the simplified, but ultimately correct, procedure described in the text.

<sup>30</sup> L. D. Landau, J. Phys. (U.S.S.R.) **5**, 71 (1941).

According to (4.15) the metastability of the current flow is ensured if the velocity  $\mathbf{v}$  is such that

$$\omega_{\mathbf{q}}(\mathbf{v}) = \omega_{\mathbf{q}}(0) + \mathbf{v} \cdot \mathbf{q} > 0, \quad (\text{all } \mathbf{q} \neq 0), \quad (4.26)$$

that is, if

$$v < v_s, \quad (4.27)$$

where

$$v_s = (2\lambda\rho_c)^{1/2} \quad (4.28)$$

is the sound velocity in this model. As mentioned above, the metastability criterion (4.26) for linear flow was first obtained by Landau.<sup>30</sup> It is important to remark that (4.26) can be derived without basing the discussion on the Hamiltonian  $H_2$  describing a *drifting* condensate: because of the Galilean invariance of the system in

question, if the spectrum of the excitations is known for  $\mathbf{v}=0$  a simple kinematical transformation yields (4.25), the spectrum for  $\mathbf{v} \neq 0$ . The Galilean invariance of the system is reflected further in the fact that  $v_s$  is independent of  $\mathbf{v}$ . For the cylindrical geometry and the persistent rotational flow, which is the primary subject of discussion in this paper, there is no symmetry principle to invoke analogous to Galilean invariance, and thus the discussion must be based on  $H_2$ .

We turn now to a study of the stability criterion (4.15) for our system confined to the cylindrical geometry. Because the single-particle functions are given by (4.5) and (4.6), the matrix elements  $V_{ccc}$  and  $V_{ccc}$  are again  $\lambda/\Omega$  [see (3.37)]. Straightforward calculations then yield as the stability criterion

$$\omega_{qm} = \left\{ \left[ q^2 + \frac{1}{2R^2} \left( \rho_{l+m,1}^2 + \rho_{l-m,1}^2 - 2l^2 \ln \left( \frac{\lambda\rho_c R^2}{l^2} \right) \right) + \lambda\rho_c \right]^2 - \lambda^2 \rho_c^2 v^2 (l-m, l+m, l, l) \right\}^{1/2} + 2kq + (1/2R^2)(\rho_{l+m,1}^2 - \rho_{l-m,1}^2) > 0, \quad (4.29)$$

where

$$v(l-m, l+m, l, l) = 2[J_{l-m}'(\rho_{l-m,1})J_{l+m}'(\rho_{l+m,1})]^{-1} \int_0^1 dx x J_{l-m}(\rho_{l-m,1}x) J_{l+m}(\rho_{l+m,1}x), \quad (4.30)$$

and  $q$  and  $m$  cannot both be zero. We will first demonstrate the existence of a critical value for  $k$ , the  $z$  momentum of the state  $\varphi_c$ . All quantities within the square root in (4.29) are independent of  $k$ .<sup>31</sup> On the other hand, if  $|k|$  is chosen sufficiently large then for given  $|q|$  and  $m$ , because of the term  $2kq$ , it follows that  $\omega_{qm}$  can be made negative in violation of the inequality. Note also that the critical value of  $k$  is dependent upon  $l$ .

We shall now determine  $l_M$  the largest value of  $l$  for which the inequality (4.29) is satisfied when  $k=q=0$ . This quantity must be such as to satisfy the requirement  $\lambda\rho_c R^2 \gg l_M^2$  so that the single-particle functions of (4.5) and (4.6) continue to be accurate approximate solutions of the Hartree equations of (4.4). We now list several properties of the matrix element (4.30). Using the Schwarz inequality and (3.18) it is easily seen that

$$v(l-m, l+m, l, l) \leq 1. \quad (4.31)$$

The equality holds only if  $m=0$ . In fact, for fixed  $l$ , as  $m$  increases from zero the matrix element decreases monotonically, at least until  $m$  becomes about the same size as  $l$ . Further, as  $l$  increases, the value of  $v(l-1, l+1, l, l)$  approaches unity from below; that is

$$\alpha(l) \equiv 1 - v(l-1, l+1, l, l) \xrightarrow{l \rightarrow \infty} 0+. \quad (4.32)$$

This result follows from the fact that if  $\rho_{l1}'$  denotes the location of the first maximum of  $J_l(x)$ , then  $\rho_{l1}'/\rho_{l1}$  approaches unity as  $l$  increases. Utilizing these properties one finds that for given  $l$  the inequality (4.29) is

most suspect when  $m=1$ . Further, we suppose that  $\lambda\rho_c R^2 \gg l_M^2 \gg 1$ . Using (4.32) and the fact that  $\rho_{l1} \approx l$  for large  $l$ , the inequality (4.29) is found to reduce to

$$\lambda\rho_c R^2/l^2 < \exp[1 + \alpha(l)\lambda\rho_c R^2/l^2]. \quad (4.33)$$

Evidently, the critical value  $l_M$  for satisfying (4.33) will depend sensitively upon the functional form of  $\alpha(l)$ . Despite this fact, in order to avoid extensive numerical work, we have calculated  $\alpha(l)$  for large  $l$  by approximating  $J_l(\rho_{l1}x)$  in the interval  $0 \leq x \leq 1$  by a function  $f(x)$  which is only nonzero for  $2(\rho_{l1}'/\rho_{l1}) - 1 \leq x \leq 1$ . In this region it is constant and so normalized that  $\int_0^1 dx x f^2(x) = 1$ . With this approximation we obtain an  $\alpha(l)$  which for large  $l$  approaches  $2/(3l)$ . Using this result, one finds that if  $\lambda\rho_c R^2 = 10^4$  and  $10^8$ , then  $l_M \approx 13$  and  $200$ , respectively. We must emphasize, however, that these values of  $l_M$  very likely differ considerably from the values that would result if the correct form of  $\alpha(l)$  were known.

It is worth remarking that, if the matrix element  $v(l-m, l+m, l, l)$  were identically zero, (4.29) would reduce to (3.38), the stability criterion for the independent-particle model. We therefore conclude that the effect of the pair excitation terms ( $a_{k-q, l-m}^\dagger a_{k+q, l+m}^\dagger + \text{H.c.}$ ) in (4.1) is to greatly reduce  $l_M$  from its value in the case of the independent-particle model.

## V. STABILITY CRITERION ( $T > 0$ )

In these remaining sections we will extend some of our previous considerations to the case of finite temperatures ( $T > 0$ ). In particular, we will generalize the stability criterion (2.7) and then study the independent-

<sup>31</sup> A careful inspection of (4.20) will show that  $\rho_c$  is independent of  $k$ .

particle model, described by the Hamiltonian of (3.8), for nonzero temperatures.

Statistical mechanics is concerned with determining the macroscopic properties of a system of interest about which only limited information is available. This is achieved by the general procedure of determining the average behavior in an ensemble of systems, each system being specified by the same limited information which specifies the original system of interest. In addition, the composition of the ensemble is made in accordance with the postulate of equal *a priori* probabilities and random *a priori* phases for the quantum-mechanical states of the system.<sup>32</sup> For example, consider a system in statistical equilibrium for which we only know its volume  $\Omega$ , particle number  $N$ , and total energy  $E$  with an accuracy  $\Delta E$ . According to the above postulate the member systems of the representative ensemble are to be chosen to have volume  $\Omega$  and particle number  $N$ . In addition, it is necessary that when averaged over the ensemble the probability amplitude of a system being in an energy eigenstate has random values for its phase and the same magnitude for all energy eigenstates of the system lying within the specified range  $E$  and  $E+\Delta E$ . For all other energy eigenstates, the corresponding average is to be zero. The underlying idea of the postulate is that any assignment other than equal *a priori* probabilities and random *a priori* phases would favor some of the energy eigenstates with eigenvalues in the range  $E$  and  $E+\Delta E$  in preference to others; this could not be justified in the absence of more information concerning the system than is actually available. To date the use of this procedure, which is based on the notion of a representative ensemble, has been restricted mainly to the study of macroscopic systems in thermodynamic equilibrium.

In order to study persistent currents in finite temperature systems, it is convenient to exploit the notion of an ensemble of systems which correspond to a system in metastable equilibrium. A system in metastable equilibrium will be understood to mean one whose macroscopic properties do not change noticeably over periods of time which are very long compared to the time needed for the establishment of equilibrium for typical thermal phenomena. Implicit in this definition is the idea that the system in metastable equilibrium can be described during very long periods of time by one or more essentially constant macroscopic variables<sup>33</sup>  $X, Y, \dots$  besides the volume  $\Omega$ , particle number  $N$ , and temperature  $T$ . The representative ensemble must therefore be composed of systems all of which are described by the same values of *all* of these macroscopic variables. Furthermore, these systems must be distrib-

uted in accordance with the postulate of equal *a priori* probabilities and random *a priori* phases.

All these requirements can be met if one chooses as representative ensemble what we shall call the *restricted canonical ensemble*. In the representation in which the Hamiltonian of the system of interest is diagonal the elements of the density matrix describing this ensemble are to be defined as

$$\rho_{mn} = (1/\mathcal{Q})e^{-\beta E_n}\delta_{mn}I_n. \quad (5.1)$$

The quantity  $I_n$  in (5.1) is nonzero and has value unity only for energy eigenstates  $n$  such that

$$\begin{aligned} |\mathfrak{X}_{nn} - X| &= o(X), \\ |\mathfrak{Y}_{nn} - Y| &= o(Y), \end{aligned} \quad (5.2)$$

where  $\mathfrak{X}, \mathfrak{Y}, \dots$  are the quantum-mechanical operators corresponding to  $X, Y, \dots$ .<sup>34</sup> The quantity  $\beta^{-1}$  is the product of Boltzmann's constant  $\mathcal{K}$  and the absolute temperature  $T$ . The quantity  $\mathcal{Q}$  in (5.1) is a normalization factor so chosen that  $\text{Tr}\rho = \sum_n \rho_{nn} = 1$ . By analogy to the usual nomenclature for the canonical ensemble,

$$\mathcal{Q} = \sum_n e^{-\beta E_n} I_n \quad (5.3)$$

will be called the partition function of the system in metastable equilibrium. Finally, the ensemble average  $\langle \mathfrak{O} \rangle$  of any quantity described by an operator  $\mathfrak{O}$  is given as

$$\langle \mathfrak{O} \rangle = \text{Tr}(\rho\mathfrak{O}), \quad (5.4)$$

where  $\text{Tr}(\dots)$  denotes the trace operation.

Equations (5.2) ensure that  $\langle \mathfrak{X} \rangle = X$ ,  $\langle \mathfrak{Y} \rangle = Y$ ,  $\dots$ , and that the mean-square fluctuations of  $\mathfrak{X}, \mathfrak{Y}, \dots$  are small; that is,

$$[\langle \mathfrak{X}^2 \rangle - X^2]/X^2 = o(1)$$

and likewise for  $\mathfrak{Y}, \dots$ . This, in turn, guarantees that all systems composing the representative ensemble are specified by the same values of the macroscopic variables  $X, Y, \dots$  as those that specify the original system of interest. Note further that because  $X, Y, \dots$  will, in general, be temperature-dependent, it follows that the set of eigenstates for which  $\rho_{nn}$  is nonzero also changes with temperature. We should also emphasize that the elements of the density matrix (5.1) do not vary with time, for with the aid of the Liouville equation,

$$i(\partial\rho_{mn}/\partial t) = (E_m - E_n)\rho_{mn} = 0. \quad (5.5)$$

The last equality in (5.5) follows because, according to (5.1),  $\rho_{mn}$  is zero for  $m \neq n$ . Thus the ensemble average

<sup>32</sup> There are metastable systems which require for a proper treatment consideration of a superposition of nearly degenerate eigenstates, which is to be contrasted with the demands of (5.2), which gives conditions on the exact eigenstates of the Hamiltonian. One example of such a metastable process is  $\alpha$  decay. However, we feel that our treatment is sufficiently general to be valid for almost all systems of interest in statistical mechanics. We wish to thank Professor J. J. Hopfield for bringing this point to our attention.

<sup>32</sup> R. C. Tolman, *The Principles of Statistical Mechanics* (Oxford University Press, London, 1938), Chap. IX.

<sup>33</sup> By a macroscopic variable we will understand any quantity which serves to characterize a macroscopic state of the system. For example, the  $z$  component of the total angular momentum of the system is a macroscopic variable.

$\langle \Theta \rangle$  corresponding to a Schrödinger operator  $\Theta$  is time-independent. In summary, the restricted canonical ensemble differs from the ordinary canonical ensemble in that the former is composed of a considerably smaller class of systems, namely, only those systems which are specified by the same constant values of the macroscopic variables  $\Omega, N, T, X, Y, \dots$  as specify the original system of interest which is known to be in metastable thermal equilibrium.

It is extremely important to note that the restricted canonical ensemble defined by (5.1) and (5.2) must be such that the calculated mean-square fluctuation of the energy of the system must be small, that is,

$$[\langle H^2 \rangle - \langle H \rangle^2] / \langle H \rangle^2 = o(1). \quad (5.6)$$

If this fails to be the case, a trustworthy treatment of the system of interest based on the methods of statistical mechanics would be impossible.<sup>35</sup>

In the above discussion the actual system of interest is known to be in metastable thermal equilibrium. If, on the other hand, we attempt to set up a restricted canonical ensemble to represent a system which we *presume* to be in metastable equilibrium, then the values  $X, Y, \dots$  are of course not known, so that in this case  $I_n$  in (5.1) is nonzero only for energy eigenstates  $n$  such that (5.6) and

$$\begin{aligned} [\mathfrak{X}_{nn} - \langle \mathfrak{X} \rangle] &= o(\langle \mathfrak{X} \rangle), \\ [\mathfrak{Y}_{nn} - \langle \mathfrak{Y} \rangle] &= o(\langle \mathfrak{Y} \rangle), \dots \end{aligned} \quad (5.7)$$

are satisfied. Equations (5.6) and (5.7) severely restrict the number of energy eigenstates  $n$  for which  $\rho_{nn}$  is nonzero. If an ensemble satisfying these equations can be found, then it ensures the existence of a metastable state, for, as pointed out earlier, (5.1) defines a stationary ensemble. If, however, these restrictive conditions cannot be satisfied, then the presumption that the system is in metastable equilibrium is false.

The above remarks which pertain to any system in metastable thermal equilibrium are easily applied to the theoretical study of a system in which a persistent current is presumed to flow. Based on the work of earlier sections such a system is to be specified not only by  $\Omega, N, T$ , but also by a macroscopic occupation of a current-carrying single-particle state  $\varphi_c$ . The actual system of interest is replaced by the restricted canonical ensemble which corresponds to it. This ensemble is characterized by  $\Omega, N, T$ , and  $\langle a_c^\dagger a_c \rangle = O(N)$ , where, as earlier,  $\langle a_c^\dagger a_c \rangle$  is the occupation number operator for the single-particle state  $\varphi_c$ . In this case, Eqs. (5.6) and (5.7) are satisfied if

$$\langle a_c^\dagger a_c \rangle = O(N), \quad (5.8)$$

$$\sum_s |(a_s^\dagger a_s)_{nn} - \langle a_s^\dagger a_s \rangle| = o(N), \quad (5.9)$$

where  $a_c^\dagger a_c$  stands for  $\mathfrak{X}$ . Note in fact that (5.9) is the generalization of (2.6) to finite-temperature systems. Thus the question of whether or not a system at a finite temperature can support a persistent current reduces to the question of whether or not (5.8) and (5.9) can be satisfied for the restricted canonical ensemble (5.1).

## VI. INDEPENDENT-PARTICLE MODEL ( $T > 0$ )

In this section we shall find those conditions which ensure the existence of a persistent current at nonzero temperatures in the model system described by the Hamiltonian (3.8). In this model an energy eigenvector, given by (3.9), is completely specified by the set of occupation numbers  $\{N_s\}$  for the single-particle states  $\varphi_s$ . The corresponding energy eigenvalues are given by (3.10). On the basis of the discussion of the previous section, we will set up a restricted canonical ensemble of the form (5.1). Specifically, the admissible energy eigenstates, i.e., those for which the density matrix elements in (5.1) are taken to be nonzero, will be such that the occupation numbers  $\{N_s\}$  do not differ greatly from a specified set of values. We further demand that these specified values of  $N_s$  be the same as the resulting ensemble averages  $\langle N_s \rangle$  of the number operators  $a_s^\dagger a_s$ . That is, the admissible energy eigenvectors, to be denoted by  $|\bar{\alpha} + \delta\alpha\rangle$ , are described by the set of occupation numbers  $\{N_s = \langle N_s \rangle + n_s\}$  for which

$$\sum_s |n_s| = o(N). \quad (6.1)$$

The eigenvector for which  $\{N_s = \langle N_s \rangle\}$  will be denoted by  $|\bar{\alpha}\rangle$ . Now if an ensemble can be found which satisfies (6.1) and, furthermore, is such that

$$\langle N_c \rangle = \langle a_c^\dagger a_c \rangle = O(N) \quad (6.2)$$

for a current-carrying single-particle state  $\varphi_c$ , then a persistent current occurs in the system.

Because of the restriction on the size of the  $n_s$  which is required by (6.1), the eigenvalue  $E_{\bar{\alpha} + \delta\alpha}$  corresponding to a state  $|\bar{\alpha} + \delta\alpha\rangle$  is well approximated by the first two terms of a Taylor expansion

$$E_{\bar{\alpha} + \delta\alpha} = E_{\bar{\alpha}} + \sum_s n_s \bar{\epsilon}_s, \quad (6.3)$$

where<sup>36</sup>

$$\begin{aligned} \bar{\epsilon}_s &\equiv \left( \frac{\partial E_{\bar{\alpha}}}{\partial N_s} \right)_{\bar{\alpha}} \\ &= \mathcal{T}_s + (\langle N_s \rangle - \frac{1}{2}) V_{ssss} + 2 \sum_{t (\neq s)} \langle N_t \rangle V_{stts}. \end{aligned} \quad (6.4)$$

It will prove to be somewhat more convenient in the following to utilize a restricted *grand* canonical ensemble. Thus if  $\mu$  denotes a Lagrange multiplier, playing

<sup>35</sup> K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963), p. 161.

<sup>36</sup> To avoid any possible confusion, throughout this section we will use the symbols  $\mathcal{T}_s$  to denote the kinetic energy matrix element of (3.6) and  $T$  to denote the absolute temperature.

the role of the chemical potential appropriate to this ensemble, the grand partition function for a system presumed to be in metastable thermal equilibrium is

$$\mathcal{Q} = \sum_{\{n_i\}} \exp[-\beta(E_{\bar{\alpha}} - \mu N + \sum_s (\bar{\epsilon}_s - \mu)n_s)], \quad (6.5)$$

where

$$N = \sum_s \langle N_s \rangle \quad (6.6)$$

is the mean total number of particles in the system.

The allowed values of  $n_s$  in (6.5) should be chosen to be compatible with (6.1), but as regards this calculation, we can actually relax this restriction to allow each  $n_s$  to take on all values from  $-\langle N_s \rangle$  to  $\infty$ . This procedure can be justified as follows: The condition (6.1) is sufficient, but not necessary, for ensuring that the mean square fluctuation of the total energy of the system is small [see (5.6)]. It will, in fact, turn out that (5.6) is satisfied, when the sum in (6.5) is calculated without use of (6.1), as long as

$$\bar{\epsilon}_s - \mu > 0, \quad (\text{all } s). \quad (6.7)$$

Thus (6.7) is essentially equivalent to (6.1) for the purpose of satisfying (5.6), although it should be borne in mind that (6.1) is essential for the purpose of yielding (6.3) for the relevant energy eigenvalues  $E_{\bar{\alpha}+\delta\alpha}$ .

Following this procedure and using (6.6) and (6.7), one finds

$$\begin{aligned} \mathcal{Q} &= \exp[-\beta(E_{\bar{\alpha}} - \sum_s \langle N_s \rangle \bar{\epsilon}_s)] \prod_s \sum_{n_s=0}^{\infty} \exp[-n_s \beta(\bar{\epsilon}_s - \mu)] \\ &= \exp[-\beta(E_{\bar{\alpha}} - \sum_s \langle N_s \rangle \bar{\epsilon}_s)] \prod_s [1 - e^{-\beta(\bar{\epsilon}_s - \mu)}]^{-1}. \end{aligned} \quad (6.8)$$

We have written out one of the intermediate steps in this calculation to show that (6.7) is necessary to insure that the geometric series in (6.8) are all convergent.<sup>37</sup> The thermodynamic potential is then given by<sup>38</sup>

$$\tilde{\Omega} = -\mathcal{K}T \ln \mathcal{Q} = E_{\bar{\alpha}} - \sum_s \langle N_s \rangle \bar{\epsilon}_s + \mathcal{K}T \sum_s \ln[1 - e^{-\beta(\bar{\epsilon}_s - \mu)}]. \quad (6.9)$$

The mean number  $\langle N_s \rangle$  of particles occupying the state  $\varphi_s$  is easily found to be

$$\begin{aligned} \langle N_s \rangle &= \mathcal{Q}^{-1} \sum_{\{n_i\}} (\langle N_s \rangle + n_s) \\ &\quad \times \exp[-\beta(E_{\bar{\alpha}} - \mu N + \sum_t n_t (\bar{\epsilon}_t - \mu))] \\ &= [e^{\beta(\bar{\epsilon}_s - \mu)} - 1]^{-1}. \end{aligned} \quad (6.10)$$

Equation (6.10) is the familiar result for the distribution

<sup>37</sup> Note that because of (6.7) the terms in the geometric series for large values of  $n_s$  are very small, thus justifying their inclusion in (6.8).

<sup>38</sup> We have denoted the thermodynamic potential by  $\tilde{\Omega}$ , although the conventional notation for this quantity is  $\Omega$ ; throughout this paper the latter symbol is used to denote the volume of the system.

function of a gas of noninteracting bosons with single-particle energies  $\bar{\epsilon}_s$ . Note that as a consequence of (6.7) all the  $\langle N_s \rangle$  are positive.

At this point we wish to call to the reader's attention the fact that this result can also be obtained from a method based on maximizing the entropy of the system. This method, which is treated in detail in Appendix B, gives added insight into the treatment of persistent currents in finite temperature systems and complements our present approach which is based on ensemble theory.

To ensure that the current-carrying state  $\varphi_c$  is the only state which is occupied to order  $N$ , the Lagrange multiplier  $\mu$  is taken to be

$$\mu = \bar{\epsilon}_c - (\mathcal{K}T / \langle N_c \rangle). \quad (6.11)$$

This, of course, does not yet assure that  $\langle N_c \rangle$  is in fact of order  $N$ ; one needs further that the calculated value of  $N - \sum_{s(\neq c)} \langle a_s^\dagger a_s \rangle$  is of order  $N$ . The procedure we shall follow will be to assume that (6.2) is satisfied so that as regards single-particle states  $\varphi_s$ ,  $s \neq c$ , one may replace  $\mu$  by its value in the volume limit. Equation (6.10) then reads

$$\langle N_s \rangle = [e^{\beta(\bar{\epsilon}_s - \bar{\epsilon}_c)} - 1]^{-1}, \quad (s \neq c), \quad (6.12)$$

so that

$$\langle N_c \rangle = N - \sum_{s(\neq c)} [e^{\beta(\bar{\epsilon}_s - \bar{\epsilon}_c)} - 1]^{-1}. \quad (6.13)$$

The starting assumption is verified if the right-hand side of (6.13) is of order  $N$ . We will return to this question later in this section.

With  $\mu$  given by (6.11) we can rewrite (6.7) as

$$\bar{\epsilon}_s - \bar{\epsilon}_c = \left( \frac{\partial E_{\bar{\alpha}}}{\partial N_s} \right)_{\bar{\alpha}} - \left( \frac{\partial E_{\bar{\alpha}}}{\partial N_c} \right)_{\bar{\alpha}} > 0 \quad (s \neq c). \quad (6.14)$$

This requirement can be restated in the following physical terms:  $\varphi_c$  may be chosen as the macroscopically occupied state only if the net energy difference upon transferring a particle from that state to any other state  $\varphi_s$  is positive-definite. Note further that (6.14) reduces at  $T=0$  to (3.13), the stability criterion in the zero-temperature treatment of this model in Sec. III. This result follows since (6.13) and (6.14) imply that  $N_s = N \delta_{sc}$  at  $T=0$ , in agreement with our earlier work, thereby ensuring that the derivatives in (6.14) are evaluated for the same values of  $\langle N_s \rangle$  as in the zero-temperature work. As such we shall refer to (6.14) as the persistent current stability criterion for all temperatures for the independent-particle model.

At this juncture we remark that upon using the formula

$$\langle H^2 \rangle - \langle H \rangle^2 = - \left[ \frac{\partial^2}{\partial \beta^2} (\beta \tilde{\Omega}) \right]_{\Omega, z}, \quad (6.15)$$

where

$$z = e^{\beta \mu}, \quad (6.16)$$

and the expression (6.9) for  $\tilde{\Omega}$ , one finds that (5.6) is

satisfied. This important result is ultimately a consequence of (6.7) [or (6.14)], the condition which ensures that (6.9) is the correct expression for  $\bar{\Omega}$ .

In order to determine when the stability criterion (6.14) is satisfied, it will be necessary to have an explicit expression for  $\bar{\epsilon}_s - \bar{\epsilon}_c$  as a function of the temperature. Towards this end we begin by choosing the  $\varphi_s$ , which appear in (6.4) via the matrix elements  $\mathcal{T}_s$  and  $V_{stts}$  [see (3.6) and (3.7)], to be the approximate solutions (4.5) and (4.6) of the Hartree equations (4.4). It will be recalled that (4.4) explicitly takes into account the fact that the state  $\varphi_c$  is occupied by  $N_c = O(N)$  particles. Furthermore, as discussed in Appendix A, (4.5) and (4.6) will be reasonably good approximate solutions as long as  $\lambda\rho_c \gg l_c^2/R^2$ .

At first sight the prospects for obtaining an explicit expression for  $\bar{\epsilon}_s$  as a function of the temperature are poor since  $\bar{\epsilon}_s$  as given by (6.4) depends on the  $\langle N_t \rangle$ , which, in turn, are functions of the  $\bar{\epsilon}_t$  according to (6.12). In addition, the matrix elements  $V_{stts}$  and  $V_{stss}$  are given by integrals of products of four Bessel functions when  $s, t \neq c$  which further complicates (6.4). However, after making one reasonable assumption it will be possible to explicitly evaluate the  $\bar{\epsilon}_s$  without difficulty in spite of these apparent complications. Using (3.7) we rewrite (6.4) as

$$\bar{\epsilon}_s = \mathcal{T}_s + 2\lambda \int d^3r |\varphi_s|^2 \sum_i \langle N_i \rangle |\varphi_i|^2, \quad (s \neq c), \quad (6.17)$$

$$\begin{aligned} \bar{\epsilon}_c = & \mathcal{T}_c + \lambda \langle N_c \rangle \int d^3r |\varphi_c|^4 \\ & + 2\lambda \int d^3r |\varphi_c|^2 \sum_{t \neq c} \langle N_t \rangle |\varphi_t|^2. \end{aligned} \quad (6.18)$$

In obtaining (6.17) and (6.18) from (6.4), we have dropped several terms which are of order  $1/\Omega$ . Now the ensemble average of the local number density  $\rho(\mathbf{r})$  is conveniently written as

$$\rho(\mathbf{r}) = \langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \rangle, \quad (6.19)$$

where  $\psi(\mathbf{r})$  is the field operator

$$\psi(\mathbf{r}) = \sum_s a_s \varphi_s(\mathbf{r}). \quad (6.20)$$

Because  $\langle a_s^\dagger a_t \rangle = \langle N_s \rangle \delta_{st}$ , we have

$$\rho(\mathbf{r}) = \sum_s \langle N_s \rangle |\varphi_s(\mathbf{r})|^2. \quad (6.21)$$

Now in Appendix A we have pointed out that  $\rho_c(\mathbf{r}) = \langle N_c \rangle |\varphi_c(\mathbf{r})|^2$  is essentially a constant through the container except in the immediate vicinity [distances of the order of  $l_c(\lambda\rho_c)^{-1/2} \ll R$ ] of  $\mathbf{r} = 0$  (vortex core) and  $\mathbf{r} = R$  (container wall). Furthermore, we can anticipate that except in these small regions the system will be characterized by an over-all uniform density because of the repulsive interactions between particles. As such we

feel justified in the following to replace  $\rho(\mathbf{r})$  and  $\rho_c(\mathbf{r})$  by the constants  $\rho = N/\Omega$  and  $\rho_c = \langle N_c \rangle/\Omega$ , respectively. Finally, upon using the normalization condition, (3.4), (6.17), and (6.18) become

$$\bar{\epsilon}_s = \mathcal{T}_s + 2\lambda\rho, \quad (6.22)$$

$$\bar{\epsilon}_c = \mathcal{T}_c + \lambda(2\rho - \rho_c). \quad (6.23)$$

We now substitute these results into the stability criterion (6.14) to obtain

$$\mathcal{T}_s - \mathcal{T}_c + \lambda\rho_c > 0. \quad (6.24)$$

Note that at  $T = 0^\circ K$ , when  $\langle N_c \rangle = N$ , this becomes identical with (3.16) since  $V_{cssc} = V_{cccc} = \lambda/\Omega$  for the  $\varphi_s$  we are employing. Thus as long as  $\lambda\rho_c R^2 \gg l_c^2$ , in which case the  $\varphi_s$  of (4.5) and (4.6) are good approximate solutions of the Hartree equations (4.4), our finite-temperature criterion (6.24) is satisfied. This is the same conclusion that we reached at the end of Sec. IIIB in the discussion of the zero-temperature version of this model. Note that as the temperature is increased  $\rho_c$  will decrease, so for given  $l_c$  it becomes increasingly more difficult to satisfy the demand  $\lambda\rho_c R^2 \gg l_c^2$ . In order to clarify this matter we will now calculate  $\rho_c$  as a function of temperature.

Using (6.22) and (6.23) we can rewrite (6.13) as

$$\rho_c = \rho - \frac{1}{\Omega} \sum_{s \neq c} \{\exp[\beta(\mathcal{T}_s - \mathcal{T}_c + \lambda\rho_c)] - 1\}^{-1}. \quad (6.25)$$

It is an impossible task to obtain a closed expression for this sum since  $\mathcal{T}_{s \neq c}$ , given by  $k^2 + (\rho l_s^2/R^2)$ ,  $s = (k, l, n)$ , is a complicated function of  $l$  and  $n$ . We agree, however, that because  $\lambda\rho_c R^2 \gg 1$  it is justified to replace  $\mathcal{T}_s$  by the corresponding quantity for a particle in a cubic geometry. For states of low kinetic energy  $\mathcal{T}_s \approx \rho l_s^2/R^2 \ll \lambda\rho_c$ , so that altering the form of  $\mathcal{T}_s$  causes an insignificant change in (6.25); on the other hand, this procedure is justified for single-particle states of high kinetic energy (short de Broglie wavelengths) because these wave functions are necessarily insensitive to the particular boundary conditions or container geometry that we utilize. The former reason also allows us to replace the sum in (6.25) by an integral, whereby we imagine that the height  $L$  and radius  $R$  of the container become infinitely large. Equation (6.25) now reads

$$\rho - \rho_c = (4\pi\beta)^{-3/2} F_{3/2}(\lambda\rho_d\beta), \quad (6.26)$$

where

$$F_{3/2}(\lambda\rho_d\beta) = \frac{1}{\Gamma(\frac{3}{2})} \int_0^\infty dx \frac{x^{1/2}}{\exp(x + \lambda\rho_d\beta) - 1}. \quad (6.27)$$

In obtaining (6.26) we have dropped the term  $\mathcal{T}_c$  in (6.25) since  $\mathcal{T}_c = (l_c^2/R^2) \ln(\lambda\rho_c R^2/l_c^2)$  is very small compared to  $\lambda\rho_c$  when  $\lambda\rho_c R^2 \gg l_c^2$ . An analytic solution of (6.26) is readily obtained if  $\lambda\rho/\mathcal{K}T_i \ll 1$ , where

$$T_i = 4\pi\mathcal{K}^{-1}(\rho/2.612)^{2/3} \quad (6.28)$$

is the transition temperature of the ideal boson gas. For parameters appropriate to liquid He<sup>4</sup> the value of  $\lambda\rho/\mathcal{K}T_t$  is actually about 2.3, so that we have resorted to numerical methods to solve (6.30) in this case<sup>39</sup> (see Fig. 1). Despite the large value of  $\lambda\rho/\mathcal{K}T_t$  for liquid He<sup>4</sup> the analytic solution which we present in the following does not differ in a qualitative way from the correct numerical solution.

For  $T=0$ , Eq. (6.26) has as its solution  $\rho_e=\rho$ . As the temperature is raised,  $\rho_e$  decreases monotonically. However, if  $T$  is raised above  $T_t$ , the function  $\rho_e(T)$  becomes double valued as shown in Fig. 1. The physically relevant portion of the curve  $\rho_e(T)$  versus  $T$  is indicated by a full line in Fig. 1. This double-valued behavior is maintained until a temperature  $T^*$  is reached; for  $T>T^*$ , Eq. (6.26) fails to possess a solution.  $T^*$  is therefore the actual transition temperature for this system. The discussion in Appendix C shows that when  $\lambda\rho\ll\mathcal{K}T_t$ , the upper and lower branches of  $\rho_e(T)$  are given by

$$\frac{\rho_e^\pm(T)}{\rho} = \frac{1}{2}\alpha^2 \left(\frac{T}{T_t}\right)^2 - \left[ \left(\frac{T}{T_t}\right)^{3/2} - 1 \right] \pm \frac{1}{2}\alpha \left(\frac{T}{T_t}\right) \left\{ \alpha^2 \left(\frac{T}{T_t}\right)^2 - 4 \left[ \left(\frac{T}{T_t}\right)^{3/2} - 1 \right] \right\}^{1/2},$$

$$(T_t \leq T \leq T^*, \quad \alpha \ll 1), \quad (6.29)$$

where

$$\alpha^2 = 1.842(\lambda\rho/\mathcal{K}T_t). \quad (6.30)$$

Further,

$$\frac{T^*}{T_t} = \frac{2(1 - \frac{1}{2}\alpha^2)^{1/2} - 1}{1 - \frac{2}{3}\alpha^2} \approx 1 + \frac{1}{6}\alpha^2, \quad (\alpha \ll 1). \quad (6.31)$$

Finally,

$$\rho_e(T^*)/\rho = \frac{1}{4}\alpha^2[1 + O(\alpha^2)] = \frac{1}{4}[\rho_e^+(T_t)/\rho][1 + O(\alpha^2)]. \quad (6.32)$$

These results will apply in the full temperature range  $T \leq T^*$  for current-carrying states  $\varphi_e$  of the form (4.5) as long as  $\lambda\rho_e(T^*)R^2 \gg l_e^2$ . This inequality serves to determine the values of  $l_e$ , and thus the functions  $\varphi_e$ , for which the stability criterion (6.24) is satisfied. Making use of (6.30) and (6.32) one finds that stable persistent currents are characterized by values of  $l_e$  for which

$$l_e^2 \ll l_M^2 = 0.461(\lambda\rho/\mathcal{K}T_t)\lambda\rho R^2, \quad (\lambda\rho/\mathcal{K}T_t \ll 1) \\ = 43.9(\rho a^3)^{1/3}\rho a R^2, \quad (\rho a^3 \ll 1). \quad (6.33)$$

We should also point out that as long as  $l_e$  is in accord with (6.33) the form of  $\rho_e(T)$  and the value of  $T^*/T_t$  are

<sup>39</sup> To evaluate this ratio for liquid He<sup>4</sup> parameters we have taken  $\lambda = 8\pi a$  where  $a = 2.2 \text{ \AA}$  is the nearest distance of approach of two atoms as determined from measurements of the radial distribution function by D. G. Henshaw [Phys. Rev. **119**, 14 (1960)]. Furthermore, the mass density of He<sup>4</sup> at  $T=0$  is  $0.145 \text{ g/cm}^3$ .

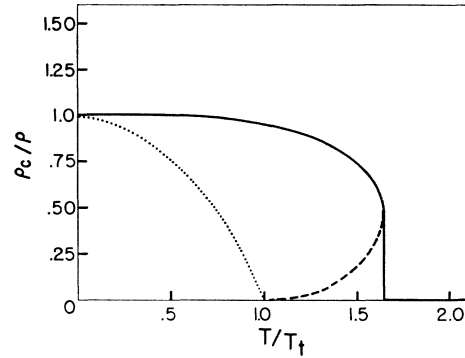


FIG. 1. The solid curve gives the fraction of particles occupying the current-carrying state  $\varphi_e$  as a function of the reduced temperature  $T/T_t$  for liquid He<sup>4</sup> parameters.  $T_t$  is the transition temperature of the corresponding ideal boson gas. The dashed curve is an unphysical solution of (6.26), and the dotted curve is the fraction of condensed particles for the ideal Bose gas. It can be seen that, in this case, (6.26) fails to have a solution when  $T/T_t > T^*/T_t \approx 1.65$ .

otherwise independent of the value of  $l_e$ . This also can be seen from (6.26) which holds even when  $\lambda\rho/\mathcal{K}T_t$  is not small compared to unity.

Briefly summarizing the results of the latter half of this section, an analysis based on a reasonable approximation procedure shows that the stability criterion (6.14) is satisfied for a large number of current-carrying single-particle functions  $\varphi_e$  of the form (4.5). In particular, if  $\lambda\rho/\mathcal{K}T_t \ll 1$  the single-particle angular momenta  $l_e$  of these states satisfy the inequality (6.37).

The following section is devoted to a thorough review of the essential results of this paper, and to a brief discussion of several questions which remain to be studied theoretically.

## VII. DISCUSSION

This work has been devoted to providing a first-principles explanation for the existence and nature of persistent macroscopic currents in He II, utilizing as a model a system of interacting bosons confined to a cylindrical container. We have argued that these currents are metastable, and we have formulated a general, model-independent criterion for their stability both at absolute zero as well as at elevated temperatures. In our formulation a fundamental requirement for the metastability of these currents is that a current-carrying single-particle state  $\varphi_e$  with angular momentum  $l_e$  is macroscopically occupied. The finite-temperature stability criterion is derived within the framework of ensemble theory, suitably generalized for metastable equilibrium situations, and the underlying method should also be useful in studying other metastable phenomena.

We have applied our general stability criterion to the study of two soluble models of interacting bosons. One of these, an independent-particle model, was studied for all temperatures, whereas the second, a quasiparticle



model, was studied only for  $T=0^\circ\text{K}$ . In a subsequent publication we will report our results for the quasiparticle model for  $T>0$ . For both models we have found that metastable circulating currents are in fact possible at  $T=0$  provided the interactions between particles are sufficiently strong, and that the angular momentum  $l_c$  of the macroscopically occupied state  $\varphi_c$  does not exceed a critical value  $l_M$ . Equivalently, the total angular momentum of a persistent current cannot exceed a particular critical value. The specific value of  $l_M$  depends sensitively upon the dimensions of the container, the nature of the single-particle basis functions employed, and the model under discussion. Of particular interest are those single-particle functions chosen as solutions of a Hartree equation, which is relevant to a description of a line vortex with quantized circulation. For the independent particle model at temperatures  $T>0$  the stability criterion can be satisfied as long as  $l_c < l_M(T)$  and  $T$  does not exceed a certain value  $T^*$ . For the single-particle functions previously described, both  $T^*$  and  $\rho_c(T)$ , the (number) density of particles occupying  $\varphi_c$ , are independent of  $l_c$  whenever  $l_c < l_M(T)$ . These results are analogous to the findings of Reppy and Depatie that the total angular momentum of a persistent current at a temperature  $T$ ,  $L_p(T)$ , is proportional to the superfluid density  $\rho_s(T)$  of stationary He II, and further that persistent currents can exist for temperatures up to the lambda point for the stationary liquid.

In this connection we are hopeful that a study of the quasiparticle model for  $T>0$  will provide a derivation of the observed relation between  $L_p$  and  $\rho_s$ . In particular, we hope to show that  $L_p(T)$  is proportional to the standard formal definition of  $\rho_s(T)$ ; we do not, however, expect to be able to derive an expression for  $\rho_s(T)$  in agreement with experiment.

One could improve upon the treatment given here by studying a more refined model, and, in addition, by considering interparticle potentials other than the Fermi pseudopotential which we have employed here for computational simplicity. Nevertheless, we believe that the present work, and in particular our general discussion built around the stability criterion does provide a satisfactory explanation for the existence of persistent currents in He II.

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#### APPENDIX A

In this Appendix we will qualitatively discuss the solutions of the Hartree equation [Eq. (3.24) in the text]

$$-\nabla^2\varphi + \lambda N|\varphi|^2\varphi = \epsilon\varphi \quad (\text{A1})$$

of the form

$$\varphi(\mathbf{r}) = \Omega^{-1/2} e^{i(kz+l\theta)} f_l(r), \quad (l \neq 0), \quad (\text{A2})$$

subject to the conditions of (3.3) and (3.4). The radial function  $f_l(r)$  satisfies the differential equation

$$f_l'' + f_l'/r + [\epsilon' - (l^2/r^2) - \lambda\rho f_l^2]f_l = 0, \quad (\text{A3})$$

where  $\epsilon' = \epsilon - k^2$ . In the following it will be useful to define the characteristic length

$$\sigma = (\lambda\rho)^{-1/2}. \quad (\text{A4})$$

Because of the normalization condition (3.4) we can typically expect  $f_l$  to be of order unity. Thus for values of  $r$  small compared to  $l\sigma$  the centrifugal potential  $l^2/r^2$  dominates the term  $\lambda\rho f_l^2$  so that in this regime  $f_l$  is approximately proportional to the Bessel function  $J_l(\epsilon^{1/2}r)$ . Now if  $l\sigma \ll R$ , for values of  $r$  large compared to  $l\sigma$  we can ignore  $l^2/r^2$  compared to  $\lambda\rho f_l^2$  so that (A3) has as an approximate solution a constant

$$f_l \approx \sigma \epsilon^{1/2} (l\sigma \ll r < R). \quad (\text{A5})$$

Finally, because of the boundary condition (3.3)  $f_l$  drops to zero at  $r=R$  within a distance of the order of  $\epsilon^{-1/2}$ . If it is assumed for the moment that the latter distance is very small compared to  $R$  we can determine  $\epsilon$  using the normalization condition (3.4) in conjunction with (A5):

$$\int_0^R dr r f_l^2 \approx \frac{1}{2} \sigma^2 \epsilon' R^2 = \frac{1}{2} R^2$$

so that

$$\epsilon = k^2 + (1/\sigma^2). \quad (\text{A6})$$

Note that the assumption  $\epsilon'^{-1/2} \ll R$  is satisfied since we have in mind those cases where  $l\sigma \ll R$ . In summary, if  $l\sigma \ll R$  then (A3) possesses a solution which in the range  $l\sigma \leq r \leq R - \sigma$  is essentially constant with value unity. For this solution the eigenvalue  $\epsilon$  is given by (A6). In addition, the number density  $\rho(\mathbf{r})$  of the system [see (3.27)] is in this same range  $l\sigma \leq r \leq R$  constant with value  $\rho = N/\Omega$ . In the opposite limit that  $\lambda\rho \ll l^2/R^2$  the nonlinear term in (A3) can be ignored and the solutions of (A3) revert to those of a free particle confined to the cylinder.

#### APPENDIX B

In Sec. V we formulated a criterion which when satisfied ensures the existence of a persistent current in a system at finite temperatures. This formulation is based on the procedure of replacing the actual system of interest by a representative ensemble of systems.

This method was subsequently applied in Sec. VI to the study of the independent particle model which is described by the Hamiltonian  $H_1$  of (3.8). In this Appendix we shall adopt a different approach to the question of the existence of a persistent current in this particular model. Our method will be based on finding that macroscopic condition of the system which is most probable, or, equivalently, is characterized by a maximal "entropy."

Consider an eigenvector  $|\bar{\alpha}\rangle$  of (3.8) which is described by a specified set of occupation numbers, of the type  $\{\bar{N}_s(\neq c) = O(1), \bar{N}_c = O(N)\}$ , for the various single-particle states  $\varphi_s$  of (3.1). The macroscopically occupied state  $\varphi_c$  is a particular current-carrying state, that is, a state for which  $I_c \neq 0$ . Consider also those eigenvectors of  $H_1$ , to be denoted by  $|\bar{\alpha} + \delta\alpha\rangle$ , which are described by occupation numbers  $\{N_s\}$  differing from  $\{\bar{N}_s\}$  by an amount which is  $o(N)$ ; that is,

$$\sum_s |N_s - \bar{N}_s| = o(N), \quad (\text{B1})$$

where the sum over  $s$  includes the term for which  $s = c$ . The energy eigenvalue  $E_{\bar{\alpha} + \delta\alpha}$  corresponding to  $|\bar{\alpha} + \delta\alpha\rangle$  is given by (3.10), but, because of the restriction of the size of the  $N_s$  which is required by (B1) it may be approximated as

$$E_{\bar{\alpha} + \delta\alpha} = E_{\bar{\alpha}} + \sum_s |N_s - \bar{N}_s| \bar{\epsilon}_s, \quad (\text{B2})$$

where

$$\begin{aligned} \bar{\epsilon}_s &= (\partial E_{\alpha} / \partial N_s)_{\bar{\alpha}} \\ &= \mathcal{T}_s + (\bar{N}_s - \frac{1}{2}) V_{ssss} + 2 \sum_{t(\neq s)} \bar{N}_t V_{stts}. \end{aligned} \quad (\text{B3})$$

For nonlocalized wave functions  $\varphi_s$  the interaction matrix elements in (B3) are  $O(1/\Omega)$  and thus the energy eigenvalues (B2) differ from each other by a quantity  $o(N)$ .

We now divide the single-particle energy spectrum of (B3) into groups of levels or "cells." The  $i$ th cell will contain a large number  $g_i$  of energy levels all of which are nearly equal to an average energy, to be denoted by  $\bar{\epsilon}_i$ . Further, let  $N_i$  denote the sum of the occupation numbers  $N_s$ , for levels situated within the  $i$ th cell. The number of distinct  $N$ -body boson energy eigenvectors  $|\bar{\alpha} + \delta\alpha\rangle$  corresponding to a set of cell occupation numbers  $\{N_i\}$  is given by<sup>40</sup>

$$W(\{N_i\}) = \prod_i \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!}. \quad (\text{B4})$$

This is a familiar result in the case of the ideal boson gas, but it applies equally well in the present discussion as a consequence of the fact that the energy eigenvectors  $|\bar{\alpha} + \delta\alpha\rangle$  are specified by single-particle occupation numbers; the validity of this formula is not

<sup>40</sup> See, for example, p. 369 of the reference cited in Footnote 32.

dependent on the specific form of the single-particle energy spectrum.

The most probable values of the cell occupation numbers, to be denoted by  $\hat{N}_i$ , are found by maximizing  $W(\{N_i\})$  subject to the constraints, first, that the allowed energy eigenvalues of the system, given by (B2), are equal to a previously specified system energy  $E$ , and, second, that the total number of particles in the system is fixed and has the value  $N$ .<sup>41</sup> At the end of the calculation we shall allow the number of levels in a given cell to be one, thereby obtaining  $\hat{N}_s$ , the most probable occupation number of a given single-particle state  $\varphi_s$ . Finally, this entire procedure is consistent only if the  $\hat{N}_s$  agree with the initially specified values  $\bar{N}_s$ . Satisfying this consistency requirement ensures that the predicted (most probable) properties of the system are actually realizable among the set of eigenvectors  $|\bar{\alpha} + \delta\alpha\rangle$  which are restricted according to (B1).<sup>42</sup> The present approach of maximizing  $W$  is well known in the theory of equilibrium statistical mechanics. We must emphasize, however, that this is only a formal similarity since in the present discussion the set of eigenvectors  $|\bar{\alpha} + \delta\alpha\rangle$ , restricted according to (B1), does not correspond to a true equilibrium state of the system. However, if the consistency requirement just stated is satisfied, and in particular  $\hat{N}_c = \bar{N}_c = O(N)$ , then a persistent current exists in this model system.

To find the set  $\{\hat{N}_i\}$  of the most probable cell occupation numbers we follow the usual procedure of maximizing

$$\ln W - \alpha \sum_i N_i - \beta \sum_i N_i \bar{\epsilon}_i,$$

where  $\alpha$  and  $\beta$  are Lagrange multipliers; according to this procedure we are maximizing  $W$  subject to the constraints stated in the previous paragraph. For the actual calculation we employ the Stirling asymptotic formula  $\log N! \approx N \log(N) - N$ . In this way, one easily finds

$$\hat{N}_i = g_i [e^{\alpha + \beta \bar{\epsilon}_i} - 1]^{-1}. \quad (\text{B5})$$

The Lagrange multiplier  $\beta$  is identified in the usual way with  $1/\mathcal{K}T$ , since the familiar results of thermodynamics

<sup>41</sup> The entropy of the system is given by  $S = \mathcal{K} \sum_{\{N_i\}} \ln W(\{N_i\})$ , where the sum extends over all cell occupation numbers which are compatible with (B1). Now if the fluctuations of the  $N_i$  are small one can approximate  $S$  by  $\mathcal{K} \ln W(\{\hat{N}_i\})$ . Thus the  $\hat{N}_i$  can be regarded as those cell occupation numbers which, subject to the stated constraints, maximize the entropy. Finally, as discussed in Sec. VI, the fluctuations of the  $N_i$  are in fact small.

<sup>42</sup> There is a dual purpose in our having selected a restricted set of eigenvectors  $|\bar{\alpha} + \delta\alpha\rangle$ , conforming to (B1), for this discussion. To compute  $W(\{N_i\})$  presupposes a procedure for dividing the single-particle energies into cells. This in turn assumes that for a single-particle state  $\varphi_s$  there is associated but one energy  $\epsilon_s$ . Now, in contrast to the ideal gas, the  $\epsilon_s$  are functions of all the occupation numbers  $\{N_i\}$ . Only by specifying a particular set of occupation numbers, and we have chosen  $\{\hat{N}_i\}$ , is one able to have a unique energy,  $\epsilon_s$ , for a given state  $\varphi_s$ . Secondly, calculus provides us with a procedure for finding a local, rather than a global, maximum of  $W$ . Thus, only those values  $N_i$  which are nearly equal to those,  $\hat{N}_i$ , which maximize  $W$  are of any interest.

must apply during the very long time span when the system is in metastable equilibrium. Finally,  $\alpha$  is identified with  $-\beta\mu$ , where  $\mu$  is the chemical potential of the system, which satisfies the equation

$$N = \sum_i g_i [e^{\beta(\bar{\epsilon}_i - \mu)} - 1]^{-1}. \quad (\text{B6})$$

The most probable occupation number  $\hat{N}_s$  for the state  $\varphi_s$ , which must equal  $\bar{N}_s$ , can be written, using (B5),

$$\bar{N}_s = [e^{\beta(\bar{\epsilon}_s - \mu)} - 1]^{-1}, \quad (\text{B7})$$

simply because  $\hat{N}_s$  is proportional to  $g_s$ , the number of single-particle energy levels in the  $i$ th cell. Finally, in order to ensure that the  $\bar{N}_s$  of (B7) are positive we must impose the requirement

$$\bar{\epsilon}_s > \mu, \quad (\text{all } s). \quad (\text{B8})$$

In fact, we shall choose

$$\mu = \bar{\epsilon}_c - (\mathcal{K}T/\bar{N}_c) \quad (\text{B9})$$

so as to ensure that only the current-carrying state  $\varphi_c$  is macroscopically occupied. Since  $\bar{N}_c$  is of order  $N$ , as regards single-particle states  $\varphi_s$ ,  $s \neq c$ , one can rewrite (B7) as

$$\bar{N}_s = [e^{\beta(\bar{\epsilon}_s - \bar{\epsilon}_c)} - 1]^{-1}, \quad (\text{B10})$$

and (B8) as

$$\bar{\epsilon}_s > \bar{\epsilon}_c, \quad (s \neq c). \quad (\text{B11})$$

We conclude then that a persistent current occurs in the independent-particle system if (B3), (B10), and

$$\bar{N}_c = N - \sum_{s \neq c} [e^{\beta(\bar{\epsilon}_s - \bar{\epsilon}_c)} - 1]^{-1} \quad (\text{B12})$$

possess consistent solutions satisfying the inequality (B11). These equations are seen to be formally identical to (6.4), (6.12), and (6.13) which were derived in Sec. VI. The only difference is that the latter equations depend upon the  $\langle N_s \rangle$ , which are the average single-particle occupation numbers for the systems composing the restricted grand canonical ensemble. We now see that these two treatments, determination of the ensemble averages  $\langle N_s \rangle$ , on the one hand, and determination of the most probable occupation numbers  $\hat{N}_s$ , on the other, yield identical results for the single-particle

energies and occupation numbers, as well as for the metastability criterion for a persistent current.

### APPENDIX C

In this Appendix we shall obtain an approximate solution of

$$\rho - \rho_c = (4\pi\beta)^{-3/2} F_{3/2}(\lambda\rho_c\beta), \quad (\text{C1})$$

which is valid when  $\lambda\rho/\mathcal{K}T_i \ll 1$  [see (6.26) and (6.28)]. For small values of  $x$  the function  $F_{3/2}(x)$  possesses the following expansion<sup>43</sup>:

$$F_{3/2}(x) = -2\sqrt{\pi}x^{1/2} + \sum_{n=0}^{\infty} \frac{\zeta(\frac{3}{2}-n)}{n!} (-x)^n. \quad (\text{C2})$$

For  $T \geq T_i$  the quantity  $\lambda\rho_c\beta$  is surely smaller than  $\lambda\rho/\mathcal{K}T_i$  since  $\rho_c$  cannot exceed  $\rho$ . Thus for sufficiently small values of  $\lambda\rho/\mathcal{K}T_i$  one can legitimately drop all but the first two terms of the expansion (C2) of  $F_{3/2}(\lambda\rho_c\beta)$ . With  $y = \rho_c(T)/\rho$ ,  $x = T/T_i$ , and  $\alpha^2$  given by (6.30),  $y$  is found to satisfy the quadratic equation

$$y^2 + y[2(x^{3/2}-1) - \alpha^2 x^2] + (x^{3/2}-1)^2 = 0, \quad (x \geq 1). \quad (\text{C3})$$

The solutions of (C3) are given by

$$y^{\pm} = \frac{1}{2}\alpha^2 x^2 - (x^{3/2}-1) \pm \frac{1}{2}\alpha x [\alpha^2 x^2 - 4(x^{3/2}-1)]^{1/2}, \quad (x \geq 1), \quad (\text{C4})$$

and they are displayed in Fig. 1. Finally, the value  $x^* = T^*/T_i$  at which (C4) no longer possesses a solution is such that

$$\alpha^2 (x^*)^2 - 4[(x^*)^{3/2} - 1] = 0. \quad (\text{C5})$$

Although (C5) is a quartic equation for  $x^*$ , the root of interest for small values of  $\alpha$  is easily obtained. Noting that if  $\alpha=0$ , the relevant root of (C5) is  $x^*=1$ , it follows that  $x^* \approx 1$  for small values of  $\alpha^2$ . Thus we can write  $(x^*)^{3/2} = [1 + (x^*-1)]^{3/2} \approx 1 + \frac{3}{2}(x^*-1) + \frac{3}{8}(x^*-1)^2$ . Equation (C5) then simplifies to a quadratic equation for  $x^*$  with solution

$$\frac{T^*}{T_i} = \frac{2(1 - \frac{1}{2}\alpha^2)^{1/2} - 1}{1 - \frac{2}{3}\alpha^2} \approx 1 + \frac{1}{6}\alpha^2. \quad (\text{C6})$$

<sup>43</sup> F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II, Appendix.