Coherent States in the Theory of Superfluidity*

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It is shown that the coherent-state representation of a many-boson wave function may be identified with the order-parameter function conventionally used to describe a superfluid. The statistical mechanics of the many-boson system is reformulated in terms of the coherent states, and a theory of the Ginzburg-Landau form is recovered in an obvious approximation. The formalism is particularly useful for describing metastable states of finite superflow and the fluctuations which may cause spontaneous decay of such states.

I. INTRODUCTION: THE PHENOMENOLOGICAL MODEL

A SLIGHTLY generalized interpretation of the Ginzburg-Landau phenomenological model of superfluidity leads to several novel conclusions regarding the nature of superfluid flow. These conclusions have been published in two recent papers,[1,2] and are summarized in this introductory section. The remainder of this paper is devoted to a systematic derivation of the Ginzburg-Landau model in the form in which we wish to use it for many-boson systems. The derivation makes use of the coherent-state representation of boson fields, a formalism which turns out to be very appropriate for the discussion of superfluidity.

In the Ginzburg-Landau model,[3,4] the states of the system are described by a complex-valued order parameter $\psi(\mathbf{r})$, which is a function of position $\mathbf{r}$. The function $\psi(\mathbf{r})$ ordinarily is interpreted as a wave function for the superfluid component of the system. In particular,

$$n_s(\mathbf{r}) = |\psi(\mathbf{r})|^2 \tag{1.1}$$

is the superfluid number density, and the corresponding current density is

$$\mathbf{j}_s(\mathbf{r}) = (1/2i)(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{1.2}$$

(We shall work always in units $\hbar = 1$.) ψ is supposed to have the time dependence $\exp(i\mu t)$ [or $\exp(2i\mu t)$ for a superconductor], where μ is the chemical potential. More generally, if we choose two separate points in the superfluid, we may write

$$\Delta\mu = (\partial/\partial t)\Delta(\arg\psi), \tag{1.3}$$

where $\Delta\mu$ is the difference in chemical potential between the two points and $\Delta(\arg\psi)$ the corresponding difference in phase of ψ. Equation (1.3), in combination with (1.2), describes the acceleration of the supercurrent by a potential gradient, and thus characterizes the intrinsically superfluid properties of the system.[5,6]

Our specific phenomenological picture is based on the assumption that the space of all functions $\psi(\mathbf{r})$ satisfying suitable boundary conditions is appropriate for the representation of an isothermal canonical ensemble. That is, statistical fluctuations of the system, caused by interactions with a constant-temperature bath, are to be visualized as a continuous random motion of the system point $\psi(\mathbf{r})$ in the function space, the neighborhood of each point being visited by the system with a frequency proportional to the Boltzmann factor $\exp(-F\{\psi\}/k_BT)$. Here $F\{\psi\}$ will be taken to be of the form of the usual Ginzburg-Landau free-energy functional:

$$F\{\psi\} = \int d\mathbf{r}[|\nabla\psi|^2 - A|\psi|^2 + \tfrac{1}{2}B|\psi|^4 + \cdots], \tag{1.4}$$

where A and B are temperature-dependent constants. In particular, A passes through zero at some T_0, being positive for $T < T_0$.

The fact that A and B are temperature-dependent implies that $F\{\psi\}$ is already some sort of coarse-grained free energy, i.e., that a partial partition sum has been performed in order to obtain $F\{\psi\}$. It is just this point that will be amplified in the following analysis. Here, however, it is important to emphasize that, although the state ψ_0 which minimizes $F\{\psi\}$ is the most probable state of the system, $F\{\psi_0\}$ is not the correct free energy. Rather, the true free energy is

$$-k_BT \ln\left\{\int \delta\psi(\mathbf{r}) \exp(-F\{\psi\}/k_BT)\right\}, \tag{1.5}$$

where the symbol $\int \delta\psi(\mathbf{r})\cdots$ denotes an integration over the space of functions $\psi(\mathbf{r})$. It is only when this integral may be approximated by the largest value of the integrand that the usual Ginzburg-Landau (mean field) theory is valid.

The above formulation is particularly well suited to

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[1] J. S. Langer and M. E. Fisher, Phys. Rev. Letters **19**, 560 (1967), hereafter referred to as I.
[2] J. S. Langer and V. Ambegaokar, Phys. Rev. **165**, 498 (1967), hereafter referred to as II.
[3] V. L. Ginzburg and L. D. Landau, Zh. Eksperim. i Teor. Fiz. **20**, 1064 (1950). For a more recent review of the Ginzburg-Landau theory as applied to metallic superconductors, see P. G. de Gennes, *Superconductivity of Metals and Alloys* (W. A. Benjamin, Inc., New York, 1966), Chaps. 6 and 7.
[4] The use of a Ginzburg-Landau equation for the description of superfluid helium was proposed by E. P. Gross [Nuovo Cimento **20**, 454 (1961)] and by V. L. Ginsburg and L. P. Pitaevskii, Zh. Eksperim. i Teor. Fiz. **34**, 1240 (1958) [English transl.: Soviet Phys.—JETP **7**, 858 (1958)]. See also L. P. Pitaevskii, Zh. Eksperim. i Teor. Fiz. **40**, 646 (1961) [English transl.: Soviet Phys.—JETP **13**, 451 (1961)].
[5] B. D. Josephson, Advan. Phys. **14**, 419 (1965).
[6] P. W. Anderson, Rev. Mod. Phys. **38**, 298 (1966).

the discussion of metastable states. If only continuous deformations of ψ are permitted—the perturbations are small in some sense—then any local minimum of $F\{\psi\}$ locates a stable or metastable state. The stability condition is therefore

$$\delta F/\delta\psi(\mathbf{r})=0, \tag{1.6}$$

to which we add the requirement that the matrix

$$\delta^2 F/\delta\psi(\mathbf{r})\delta\psi(\mathbf{r}') \tag{1.7}$$

must be positive definite. Equation (1.6) is just the Ginzburg-Landau equation for general F.

The following properties of metastable states have been discussed in Refs. 1 and 2.

A. Constant-Current States

We choose F in the form (1.4) and impose periodic boundary conditions. Then the solutions of Eq. (1.6) are

$$\psi_{\mathbf{k}}(\mathbf{r})=f_k e^{i\mathbf{k}\cdot\mathbf{r}}, \quad f_k^2=(A-k^2)/B, \tag{1.8}$$

and carry current

$$\mathbf{j}_{\mathbf{k}}=\mathbf{k}f_k^2=\mathbf{k}(A-k^2)/B. \tag{1.9}$$

For $k^2<\frac{1}{3}A$ (the conventional Ginzburg-Landau critical wave vector[7]), each of the states (1.8) locates an isolated local minimum of F. For $\frac{1}{3}\leq k^2<A$, however, the matrix (1.7) is no longer positive definite.[8] In fact, these states are unstable against deformations of the form

$$\psi_{\mathbf{k}}\rightarrow\psi_{\mathbf{k}}+\delta_{\mathbf{q}}e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}, \tag{1.10}$$

where $\mathbf{q}$ is small and preferably parallel to $\mathbf{k}$ and $\delta_{\mathbf{q}}$ is an infinitesimal amplitude whose phase depends on $\mathbf{q}$.

B. Current-Reducing Fluctuations

An important feature of any fluctuation which carries the system from one constant-current state to another is that the wave function $\psi(\mathbf{r})$ must pass through zero somewhere during the transition.[9] For example, consider a ring of circumference L in which the superflow is characterized by the state $\psi_{\mathbf{k}}$. The states ψ in the neighborhood of ψ_k all will have the property that $\arg\psi$ increases by exactly kL around the ring. But if the fluctuation away from $\psi_{\mathbf{k}}$ is large enough that ψ vanishes somewhere, then the total change in $\arg\psi$ around the ring is indefinite for that particular wave function, and the system point may pass continuously from the region of states with total phase change kL to those with, say, $k'L$.

This point is particularly significant in view of the fact that it is the phase fluctuations which preclude off-diagonal long-range order in one- or two-dimensional superfluids.[10,11] Clearly, if the amplitude of ψ never vanishes, no fluctuations in the way the phase varies from point to point can possibly modify the total change of phase around a ring. In fact, if the amplitude of ψ remains constant, then the dc component of the current also must remain constant. It follows that we might expect a system to behave like a superfluid whenever there exists an energy barrier to inhibit fluctuations in the amplitude of ψ, whether or not there occurs a true phase transition with long-range order.

C. The Free-Energy Barrier

It is obvious topologically that, in order for the system point to pass from one local minimum of $F\{\psi\}$ to another, it must overcome a free-energy barrier. The lowest barrier, and thus the least improbable fluctuation which will effect the required transition, occurs at a saddle point between the two minima. Thus the current-reducing fluctuation, say $\bar{\psi}(\mathbf{r})$, satisfies the Ginzburg-Landau equation (1.6); but the matrix (1.7) must have a single negative eigenvalue at $\bar{\psi}$ determining the direction in ψ space along which the fluctuation is most likely to progress.

The properties of the saddle-point fluctuation $\bar{\psi}$ have been studied recently in several different connections. In general, $\bar{\psi}$ describes a state which is almost everywhere the same as the metastable state ($\psi_{\mathbf{k}}$ in our case), but which contains a single localized fluctuation. The simplest example of such a fluctuation is the well-known critical droplet which nucleates the condensation of a supersaturated vapor.[12,13] In the case of liquid helium, we have argued in I that $\bar{\psi}$ must describe a vortex ring of a critical size determined by the velocity of the superfluid.[14] Because ψ vanishes at the vortex core, an expanding, singly quantized, vortex ring will eventually subtract 2π from the total phase change across the system. Paper II was devoted to the study of an effectively one-dimensional superconductor, in which case the Ginzburg-Landau equation is exactly soluble and the relevant amplitude fluctuations can be examined in detail.

The point to be emphasized is that a state of nonzero superflow is truly metastable as opposed to stable in the sense that there always exists a nonzero probability for transitions to states of lower current and lower free energy. This transition probability in all cases depends on the frequency of nucleation of certain localized amplitude fluctuations, and is therefore independent of the size of the system. Rather than trying to compute this transition probability directly,[15] in I and II we

[7] J. Bardeen, Rev. Mod. Phys. **34**, 667 (1962).
[8] See II, Appendix C.
[9] The following argument owes much to the work of W. A. Little, Phys. Rev. **156**, 396 (1967).
[10] T. M. Rice, Phys. Rev. **140**, A1889 (1965).
[11] P. Hohenberg, Phys. Rev. **158**, 383 (1967).
[12] J. Frenkel, *Kinetic Theory of Liquids* (Dover Publications, Inc., New York, 1955), Chap. 7.
[13] J. S. Langer, Ann. Phys. (N. Y.) **41**, 108 (1967).
[14] See also S. V. Iordanskii, Zh. Eksperim. i Teor. Fiz. **48**, 708 (1965) [English transl.: Soviet Phys.—JETP **21**, 467 (1965)].
[15] A brief discussion of the difficulties encountered in trying to make a direct calculation of the transition probability for creation of a vortex ring has been given by W. F. Vinen, in *Proceedings of the International School of Physics, "Enrico Fermi," Course XXI*, edited by G. Careri (Academic Press Inc., New York, 1963), p. 336. Our point of view differs from Vinen's in that we imagine the critical ring to be created in a very large number of small steps rather than in a single quantum jump.

have simply invoked an ergodic hypothesis and have said that the frequency of transitions has the form

$$\tau_0^{-1}\exp(-\Delta F/k_BT), \tag{1.11}$$

where ΔF is the height of the free-energy barrier and τ_0 is some sort of characteristic time for microscopic processes. (Actual calculations of, say, critical currents or resistivities turn out to be very insensitive to the choice of τ_0.) The results of these calculations are relaxation rates for states of finite superflow which are always extremely rapidly varying functions of temperature and current, being unobservably small throughout most of the conventional superfluid region. For example, in II we estimated that the width of the observable resistive transition in a tin wire about $1\,\mu^2$ in cross section would be of the order of 10^{-4}°K. In principle, however, the wire would have a finite resistivity below this transition; but one would have to make measurements over cosmologically long times in order to observe it.

II. COHERENT STATES

The preceding discussion has been based on a phenomenological model which is slightly more general than the conventional Ginzburg-Landau theory and therefore requires additional justification. In particular, we must question whether it is possible to formulate a completely general characterization of a many-body system, including both normal and superfluid phases, in terms of an order-parameter function $\psi(\mathbf{r})$. In the following we shall attempt to show that a very simple such characterization can be constructed for many-boson systems. Hopefully, an equally simple formulation can be found for superconducting many-fermion systems.[16]

The order parameter ψ for a many-boson system is conventionally defined to be the thermodynamic expectation value of the boson field operator, the superfluid phase transition usually being associated with the loss of symmetry which allows this expectation value to be nonzero. In the preceding development, however, ψ somehow characterized the pure quantum states of the system, and was not itself a thermodynamic quantity. Our assertion is that the order parameter ψ, as we have used it above, may conveniently be chosen to be the coherent-state representation of the pure quantum states.

Consider the boson field operator, $\Psi_{\rm op}(\mathbf{r})$, which satisfies the commutation relation[17]

$$[\Psi_{\rm op}(\mathbf{r}),\Psi_{\rm op}^{\dagger}(\mathbf{r}')]=\delta(\mathbf{r}-\mathbf{r}'). \tag{2.1}$$

We shall often work in the Fourier representation:

$$\Psi_{\rm op}(\mathbf{r})=\frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2.2}$$

where

$$[a_{\mathbf{k}},a_{\mathbf{k}'}^{\dagger}]=\delta_{\mathbf{k},\mathbf{k}'},\quad [a_{\mathbf{k}},a_{\mathbf{k}'}]=[a_{\mathbf{k}}^{\dagger},a_{\mathbf{k}'}^{\dagger}]=0, \tag{2.3}$$

and V is the quantization volume. The right eigenstates of the annihilation operator $a_{\mathbf{k}}$,

$$a_{\mathbf{k}}|\alpha_{\mathbf{k}}\rangle=\alpha_{\mathbf{k}}|\alpha_{\mathbf{k}}\rangle, \tag{2.4}$$

are the so-called "coherent states"[18–21]:

$$|\alpha_{\mathbf{k}}\rangle=\exp(-\tfrac{1}{2}|\alpha_{\mathbf{k}}|^2)\sum_{n\mathbf{k}=0}^{\infty}\frac{\alpha_{\mathbf{k}}{}^n}{\sqrt{n_{\mathbf{k}}!}}|n_{\mathbf{k}}\rangle, \tag{2.5}$$

where the $|n_{\mathbf{k}}\rangle$ are the number states for the $\mathbf{k}$th mode of the Bose field, and $\alpha_{\mathbf{k}}$ can be any complex number. Then the order parameter $\psi(\mathbf{r})$ turns out to be

$$\psi(\mathbf{r})=\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}\alpha_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{2.6}$$

The states given by Eq. (2.5) are normalized but not orthogonal. In fact,

$$\langle\alpha_{\mathbf{k}}|\beta_{\mathbf{k}}\rangle=\exp(\alpha_{\mathbf{k}}{}^*\beta_{\mathbf{k}}-\tfrac{1}{2}|\alpha_{\mathbf{k}}|^2-\tfrac{1}{2}|\beta_{\mathbf{k}}|^2). \tag{2.7}$$

They do, however, form a complete set:

$$\frac{1}{\pi}\int d^2\alpha_{\mathbf{k}}|\alpha_{\mathbf{k}}\rangle\langle\alpha_{\mathbf{k}}|=1_{\rm op}, \tag{2.8}$$

where the integration is performed over the two-dimensional complex α plane. Thus the set of all states of the form

$$\begin{aligned}&\prod_{\mathbf{k}}|\alpha_{\mathbf{k}}\rangle\equiv|\{\alpha\}\rangle\equiv|\{\psi\}\rangle,\\ &\Psi_{\rm op}(\mathbf{r})|\{\psi\}\rangle=\psi(\mathbf{r})|\{\psi\}\rangle\end{aligned} \tag{2.9}$$

is a complete set for the many-boson system. We shall use the notations introduced in (2.9) interchangeably throughout the rest of the paper.

The coherent states are most useful for dealing with many-body systems which behave in some sense classically, that is, systems in which the boson modes are highly occupied. When this is true, the function $\psi(\mathbf{r})$ becomes a classical Schrödinger field which describes the complete many-boson system in just the

[16] In an earlier paper [J. S. Langer, Phys. Rev. **134**, A553 (1964)], the problem of superconductivity has been formulated in terms of a functional integral which resembles that derived in Sec. III of the present paper. The main difference is that, for the superconductor, ψ depends on an extra timelike variable.

[17] We shall use the subscript "op" to denote second-quantized operators.

[18] R. J. Glauber, Phys. Rev. **131**, 2766 (1963).

[19] P. Carruthers and M. M. Nieto, Am. J. Phys. **33**, 537 (1965).

[20] P. Carruthers and K. S. Dy, Phys. Rev. **147**, 214 (1966). The problem of the anharmonic crystal discussed in this reference is closely related mathematically to the interacting-Boson problem discussed in the present paper.

[21] The relevance of the coherent states to the theory of superfluidity has previously been pointed out by F. W. Cummings and J. R. Johnston, Phys. Rev. **151**, 105 (1966).

same way that the Maxwell field describes the classical limit of quantum electrodynamics. Indeed, the most fruitful application of the coherent states has been in the systematic quantum-mechanical description of intense radiation fields for which classical electrodynamics provides a valid, although incomplete, description.[18] Our point is that, for many-particle Bose systems as opposed to many-photon systems, the validity of the classical description implies superfluidity.

It will be useful to discuss briefly the properties of the coherent states in the classical limit. The discussion is slightly complicated by the fact that the $|\alpha_{\mathbf{k}}\rangle$ are eigenstates of the annihilation operator $a_{\mathbf{k}}$, which is not Hermitian. It is a bit simpler to pursue the classical limit by introducing a coordinate q and its conjugate momentum p (we drop the subscript $\mathbf{k}$ for the moment):

$$q_{\rm op}=\frac{1}{\sqrt{2}}(a^\dagger+a), \quad p_{\rm op}=\frac{i}{\sqrt{2}}(a^\dagger-a). \tag{2.10}$$

Let the eigenstates of $q_{\rm op}$ be denoted $|q'\rangle$. Then it is easy to show that[18]

$$\langle q'|\alpha\rangle=\pi^{-1/4}\exp\{-\tfrac{1}{2}(q'-q)^2+ip(q'-q)+\tfrac{1}{2}p^2\}, \tag{2.11}$$

where

$$\alpha\equiv\frac{1}{\sqrt{2}}(q+ip). \tag{2.12}$$

Thus the coherent state is a Gaussian wave packet centered at the coordinate q. Similarly, in the momentum representation, it is a wave packet centered at p. This wave packet, in either representation, becomes extremely narrow in the classical limit. To see this, note that

$$\langle n\rangle=\langle\alpha|a^\dagger a|\alpha\rangle=|\alpha|^2\gg 1 \text{ (classical)}. \tag{2.13}$$

That is, $\hbar|\alpha|^2$ is a quantity which remains finite as $\hbar\to 0$, so that (2.11) becomes a δ function. It follows that the coherent states provide an acceptable (but by no means unique) representation for the quantum-mechanical analysis of classical or semiclassical systems. The representation is particularly convenient from an analytic point of view because of the direct relationship between α and the annihilation operator, and also because of the simplicity of the canonical transformation (2.12).

Now consider boson modes $\mathbf{k}$ with occupations $|\alpha_{\mathbf{k}}|^2$ large enough that a classical approximation has some validity. The Hamiltonian equations of motion are

$$dp_{\mathbf{k}}/dt=-\partial H/\partial q_{\mathbf{k}}, \quad dq_{\mathbf{k}}/dt=\partial H/\partial p_{\mathbf{k}}. \tag{2.14}$$

Starting with (2.14) we may make a sequence of canonical transformations to derive the equations of motion for the complex field $\psi(\mathbf{r})$ which describes the classical limit of the many-boson system. From (2.12) and its complex conjugate, we have

$$d\alpha_{\mathbf{k}}/dt=-i\partial H/\partial\alpha_{\mathbf{k}}^*, \quad d\alpha_{\mathbf{k}}^*/dt=i\partial H/\partial\alpha_{\mathbf{k}}. \tag{2.15}$$

Equivalently,[22]

$$\begin{aligned} d\psi(\mathbf{r})/dt&=-i\delta H/\delta\psi^*(\mathbf{r}),\\ d\psi^*(\mathbf{r})/dt&=i\delta H/\delta\psi(\mathbf{r}). \end{aligned} \tag{2.16}$$

Finally, it is conventional to use the notation

$$\psi(\mathbf{r})=f(\mathbf{r})\exp[i\phi(\mathbf{r})], \tag{2.17}$$

where f and ϕ are real functions of $\mathbf{r}$. In a pure coherent state, or in the classical limit, f^2 is just the local number density $n(\mathbf{r})$:

$$n(\mathbf{r})=\langle\Psi_{\rm op}^\dagger(\mathbf{r})\Psi_{\rm op}(\mathbf{r})\rangle=|\psi(\mathbf{r})|^2=f^2(\mathbf{r}). \tag{2.18}$$

If we transform to the conjugate variables n and ϕ (action and angle variables), we obtain

$$dn(\mathbf{r})/dt=\delta H/\delta\phi(\mathbf{r}), \quad d\phi(\mathbf{r})/dt=-\delta H/\delta n(\mathbf{r}). \tag{2.19}$$

These are exactly the superfluid equations of motion discussed by Anderson.[23] It must be emphasized, however, that Eqs. (2.14), (2.15), (2.16), or (2.19) represent, at best, a semiclassical approximation to the equations of motion for the quantum-mechanical many-body system.

III. FREE-ENERGY FUNCTIONAL

We turn now to the statistical mechanics of the many-boson system as described by the coherent states. Our entire analysis hinges on the fact that the states (2.9) form a complete set, so that we can evaluate the grand-canonical partition function as follows:

$$\begin{aligned} Z&=\mathrm{Tr}\exp\left(-\frac{H_{\rm op}-\mu N_{\rm op}}{k_BT}\right)\\ &=\prod_{\mathbf{k}}\left(\int\frac{d^2\alpha_{\mathbf{k}}}{\pi}\right)\langle\{\alpha\}|\exp\left(-\frac{H_{\rm op}-\mu N_{\rm op}}{k_BT}\right)|\{\alpha\}\rangle\\ &\equiv\int\delta\psi(\mathbf{r})\exp(-F\{\psi\}/k_BT). \end{aligned} \tag{3.1}$$

In the final form of (3.1) we have defined again the functional-integral notation first introduced in (1.5), and also have made the important identification

$$F\{\psi\}=-k_BT\ln\left[\langle\{\psi\}|\exp\left(-\frac{H_{\rm op}-\mu N_{\rm op}}{k_BT}\right)|\{\psi\}\rangle\right]. \tag{3.2}$$

In this section we shall consider the evaluation of the free-energy functional $F\{\psi\}$.

Consider first the case of noninteracting bosons. We

[22] In this form, the equations of motion reduce to the nonlinear differential equation studied by E. P. Gross, Ann. Phys. (N. Y.) 4, 57 (1958).

[23] P. W. Anderson, Ref. 6, p. 300. The same equations are mentioned in a coherent-state formalism by P. Carruthers and M. M. Nieto (unpublished).

have (in units $\hbar=m=1$)

$$H_{\rm op}^{(0)}=\sum_{\mathbf{k}}\tfrac{1}{2}k^2a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \tag{3.3}$$

so that

$$\langle\{\alpha\}|\exp\left(-\frac{H_{\rm op}^{(0)}-\mu N_{\rm op}}{k_BT}\right)|\{\alpha\}\rangle$$

$$=\prod_{\mathbf{k}}\langle\alpha_{\mathbf{k}}|\exp\left(-\frac{\tilde{\epsilon}_{\mathbf{k}}}{k_BT}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right)|\alpha_{\mathbf{k}}\rangle, \tag{3.4}$$

where

$$\tilde{\epsilon}_{\mathbf{k}}\equiv\tfrac{1}{2}k^2-\mu. \tag{3.5}$$

Inserting the representation (2.5) for the coherent states, we obtain

$$\langle\alpha_{\mathbf{k}}|\exp\left(-\frac{\tilde{\epsilon}_{\mathbf{k}}}{k_BT}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\right)|\alpha_{\mathbf{k}}\rangle$$

$$=\exp[(e^{-\tilde{\epsilon}_{\mathbf{k}}/k_BT}-1)|\alpha_{\mathbf{k}}|^2]. \tag{3.6}$$

Finally,

$$F^{(0)}\{\psi\}=-k_BT\sum_{\mathbf{k}}(e^{-\tilde{\epsilon}_{\mathbf{k}}/k_BT}-1)|\alpha_{\mathbf{k}}|^2$$

$$=-k_BT\int d\mathbf{r}\,\psi^*(\mathbf{r})\times\left[\exp\left(\frac{-\frac{1}{2}\nabla^2+\mu}{k_BT}\right)-1\right]\psi(\mathbf{r}). \tag{3.7}$$

Equation (3.7) assumes a more familiar form if we restrict our attention to slowly varying functions ψ and remember that, near the Bose condensation, μ is small and negative. Then we may keep only the first term in an expansion of the exponent:

$$F^{(0)}\{\psi\}\cong\int d\mathbf{r}[\tfrac{1}{2}|\nabla\psi|^2+|\mu||\psi|^2]. \tag{3.8}$$

The functional $F^{(0)}\{\psi\}$ given by (3.7) is a quadratic form in ψ. This means, first, that the partition function Z is a product of Gaussian integrals which may be evaluated easily and which give exactly the correct result for noninteracting bosons. More important, however, is the fact that (3.7) predicts no metastable states; that is, there are no isolated minima of $F^{(0)}\{\psi\}$ except the one at $\psi=0$ and, therefore, no superfluidity according to our criteria. The mathematical mechanism of the Bose condensation, as obtained via the coherent-state formulation, is very reminiscent of the spherical model of a ferromagnet[24]; and it is interesting to note that the spherical model is also unrealistic in its description of the ferromagnetic phase transition because it predicts no metastable states.[25]

[24] T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).
[25] J. S. Langer, Phys. Rev. **137**, A1531 (1965).

What is needed in order to make (3.7) or (3.8) describe a system which can support metastable superflow is a higher-order term in the integrand of $F\{\psi\}$ of the form, say, $|\psi|^4$. Such a term, with the correct sign, will be generated by a repulsive two-body interaction in the original Hamiltonian. If we add a term like (2.25) to H, however, we no longer can evaluate $F\{\psi\}$ exactly. What we shall do in the following is evaluate $F\{\psi\}$ as a power series in ψ, the term of order $|\psi|^4$ being the lowest-order term involving the two-body interaction.

The technique required for evaluating $F\{\psi\}$ as a power series in ψ is the same as that used in most field-theoretic or many-body perturbation expansions. We shall use the notation

$$H_{\rm op}-\mu N_{\rm op}=K_{\rm op}+H_{\rm op}',$$

$$K_{\rm op}=\sum_{\mathbf{k}}\tilde{\epsilon}_{\mathbf{k}}a_{\mathbf{k}}^\dagger a_{\mathbf{k}},$$

$$H_{\rm op}'=\frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\tilde{v}(\mathbf{q})a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'}a_{\mathbf{k}}, \tag{3.9}$$

where $v(\mathbf{q})$ is the Fourier transform of the two-body interaction potential. The relevant expansion is

$$\exp\left(-\frac{H_{\rm op}-\mu N_{\rm op}}{k_BT}\right)=\exp\left(-\frac{K_{\rm op}}{k_BT}\right)\times\sum_{n=0}^{\infty}(-1)^n\int_0^{(k_BT)^{-1}}d\lambda_1\int_0^{\lambda_1}d\lambda_2\cdots\int_0^{\lambda_{n-1}}d\lambda_n\times H_{\rm op}'(\lambda_1)\cdots H_{\rm op}'(\lambda_n), \tag{3.10}$$

$H_{\rm op}'(\lambda)$ being the interaction representation of $H_{\rm op}'$:

$$H_{\rm op}'(\lambda)\equiv e^{\lambda K_{\rm op}}H_{\rm op}'e^{-\lambda K_{\rm op}}. \tag{3.11}$$

Our procedure is to evaluate, term by term, the diagonal matrix element of (3.10) for the state $|\{\alpha\}\rangle$ and then to exponentiate the resulting series to obtain a free energy F which is proportional to a single factor of the volume V. This exponentiation amounts to a linked-cluster expansion.

In evaluating the matrix element of a term in (3.10), we first make use of the fact that the interaction representation of the annihilation or creation operators always may be written in the form

$$a_{\mathbf{k}}(\lambda)=e^{-\lambda\tilde{\epsilon}_{\mathbf{k}}}a_{\mathbf{k}},\quad a_{\mathbf{k}}^\dagger(\lambda)=e^{\lambda\tilde{\epsilon}_{\mathbf{k}}}a_{\mathbf{k}}. \tag{3.12}$$

All the λ-dependent quantities now appear simply as numerical factors, and may be brought outside of the matrix element.

The next step is to bring the annihilation operators $a_{\mathbf{k}}$ to the right and the creation operators $a_{\mathbf{k}}^\dagger$ to the left. This is done by using the Bose commutation relations (2.3). The result is a product of matrix

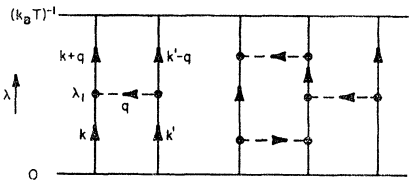

FIG. 1. A typical diagram occurring in the expansion of the partition function. The diagram contains five particle lines and four interaction lines. There are two disconnected parts, only the left-hand one of which is shown with complete momentum and λ labeling.

elements of the form

$$\langle\alpha_{\mathbf{k}}|\exp\left(-\frac{\tilde{\epsilon}_{\mathbf{k}}}{k_BT}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right)(a_{\mathbf{k}}^{\dagger})^s(a_{\mathbf{k}})^t|\alpha_{\mathbf{k}}\rangle, \quad (3.13)$$

one such factor for each mode $\mathbf{k}$. This expression may be evaluated as follows. Use the completeness relation (2.8) and the number-state representation (2.5) to write (3.13) in the form

$$\int\frac{d^2\beta_{\mathbf{k}}}{\pi}|\langle\alpha_{\mathbf{k}}|\beta_{\mathbf{k}}\rangle|^2(\beta_{\mathbf{k}}^*)^s(\alpha_{\mathbf{k}})^t \times\exp[(e^{-\tilde{\epsilon}_{\mathbf{k}}/k_BT}-1)\alpha_{\mathbf{k}}^*\beta_{\mathbf{k}}]. \quad (3.14)$$

The integration over $\beta_{\mathbf{k}}$ can be performed using the second of the following integration formulas, valid for any function $f(\alpha)$ which has a power series in α [see Ref. 20, Eqs. (2.6)]:

$$\int\frac{d^2\beta}{\pi}e^{\alpha^*\beta-|\beta|^2}\beta^n f(\beta^*)=\left(\frac{\partial}{\partial\alpha^*}\right)^n f(\alpha^*),$$
$$\int\frac{d^2\beta}{\pi}e^{\alpha\beta^*-|\beta|^2}(\beta^*)^n f(\beta)=\left(\frac{\partial}{\partial\alpha}\right)^n f(\alpha). \quad (3.15)$$

The final form of (3.13) is then

$$\exp[(e^{-\tilde{\epsilon}_{\mathbf{k}}/k_BT}-1)|\alpha_{\mathbf{k}}|^2] \times\exp(-s\tilde{\epsilon}_{\mathbf{k}}/k_BT)(\alpha_{\mathbf{k}}^*)^s(\alpha_{\mathbf{k}})^t. \quad (3.16)$$

The left-hand factor in (3.16) is just the quantity we computed in Eq. (3.6); therefore the quantity $\exp(-F^{(0)}\{\psi\}/k_BT)$ must factor out of each term in the perturbation expansion.

The remaining contributions are conveniently denoted by diagrams of the kind shown in Fig. 1. The variable λ increases upward from 0 to $(k_BT)^{-1}$. Vertical solid lines denote particles; horizontal dotted lines denote interactions. Both particle lines and interaction lines are labeled by momenta, and momentum is conserved at each interaction.

The rules for evaluation of these diagrams are the following:

(1) For each particle line of momentum $\mathbf{k}$ starting at $\lambda=0$, write a factor $\alpha_{\mathbf{k}}$. For each line ending at $\lambda=(k_BT)^{-1}$, write a factor $\alpha_{\mathbf{k}}^*$.

(2) For each particle line of momentum $\mathbf{k}$ starting at λ' and ending at λ, write a factor

$$\exp[-(\lambda-\lambda')\tilde{\epsilon}_{\mathbf{k}}].$$

The points λ and λ' may be either interaction vertices or the end points 0 and $(k_BT)^{-1}$.

(3) For an interaction line carrying momentum $\mathbf{q}$, write a factor

$$(1/V)\tilde{v}(\mathbf{q}).$$

(4) Sum over all momenta subject to momentum conservation at each vertex. Integrate over the λ's, observing the limits of integration indicated in (3.10).

(5) Multiply by the standard symmetry factors to avoid overcounting diagrams when performing summations over momentum variables.

The above procedure yields

$$\langle\{\alpha\}|\exp\left(-\frac{H_{o\rho}-\mu N_{op}}{k_BT}\right)|\{\alpha\}\rangle =\exp(-F^{(0)}\{\alpha\}/k_BT)\sum_{\Gamma}W_{\Gamma}\{\alpha\}, \quad (3.17)$$

where $W_{\Gamma}\{\alpha\}$ denotes the numerical contribution of the diagram Γ as determined by the preceding rules. The conventional linked-cluster analysis then tells us that

$$F\{\alpha\}-F^{(0)}\{\alpha\}=k_BT\sum_{\Gamma^{(c)}}W_{\Gamma^{(c)}}\{\alpha\}, \quad (3.18)$$

where now only connected diagrams, $\Gamma^{(c)}$, are included in the sum. By "connected," we mean that every particle line is connected to the rest of the diagram by at least one interaction line.

According to rule (1) above, a diagram with l particle lines is formally of order $|\alpha|^{2l}$; that is, it contains l factors $\alpha_{\mathbf{k}}$, $\alpha_{\mathbf{k}'}$, etc., and l factors $\alpha_{\mathbf{p}}^*$, $\alpha_{\mathbf{p}'}^*$, etc. To obtain the entire contribution to $F\{\alpha\}$ of order $|\alpha|^4$, we must sum all the two-body diagrams like those shown in Fig. 2. The three-body diagrams will make contributions of order $|\alpha|^6$, and so forth.

For completeness, we quote the numerical contribution to F of the first diagram shown in Fig. 2:

$$\frac{k_BT}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\tilde{v}(\mathbf{q})\left(\frac{e^{-E/k_BT}-e^{-E'/k_BT}}{E'-E}\right) \times\alpha_{\mathbf{k}+\mathbf{q}}^*\alpha_{\mathbf{k}'-\mathbf{q}}^*\alpha_{\mathbf{k}'}\alpha_{\mathbf{k}}, \quad (3.19)$$

where $E=\tilde{\epsilon}_{\mathbf{k}}+\tilde{\epsilon}_{\mathbf{k}'}$, $E'=\tilde{\epsilon}_{\mathbf{k}+\mathbf{q}}+\tilde{\epsilon}_{\mathbf{k}'-\mathbf{q}}$. If the two-body interaction contains a hard core or is otherwise too strong to permit the use of (3.19), then the entire series of ladder diagrams must be summed. At this point our formalism is very similar to that developed by Lee and Yang,[26] and the reader is referred to their papers for the details of such calculations.

[26] T. D. Lee and C. N. Yang, Phys. Rev. 113, 1165 (1959).

In conclusion, we note that we have constructed a free-energy functional $F\{\psi\}$ of basically the Ginzburg-Landau form, Eq. (1.4), the only real difference being that the derivatives of ψ enter in a rather more complicated manner when ψ varies rapidly with position. The simple form of the quartic term in (1.4) will be correct for ψ's which vary slowly over distances of the order of the two-body scattering length. Finally, the crucial temperature dependence of A, the coefficient of $|\psi|^2$, is essentially the same as the temperature dependence of the chemical potential μ, which must be chosen to fix the number of particles. For noninteracting particles, we know that μ is negative at high temperatures and goes to zero at the Bose-Einstein condensation point. When we add the effect of repulsive interactions, i.e., the term $B|\psi|^4$ with positive B, then μ may be expected to become positive below some critical temperature, as required by the phenomenological model.

IV. THERMODYNAMIC AVERAGES AND THE TWO-FLUID MODEL

The functional

$$\rho(\{\alpha^*\},\{\alpha\})=\frac{1}{Z}\langle\{\alpha\}|\exp\left(-\frac{H_{\rm op}-\mu N_{\rm op}}{k_BT}\right)|\{\alpha\}\rangle$$
$$=(1/Z)\exp(-F\{\psi\}/k_BT) \quad (4.1)$$

is the diagonal element of the density matrix in the coherent-state representation. We should like to interpret (4.1) as simply the probability that the system will be found in state ψ, but it must be recognized that the density matrix is not quite diagonal in this representation. For example, consider the expectation value of the number density, which is given for a pure state ψ by Eq. (2.18). We have [see Ref. 20, Eq. (2.16)]

$$n_{\mathbf{k}}=\mathrm{Tr}(a_{\mathbf{k}}{}^{\dagger}a_{\mathbf{k}}\rho_{\rm op})$$
$$=\prod_{\mathbf{k}'}\left(\int\frac{d^2\alpha_{\mathbf{k}'}}{\pi}\right)\alpha_{\mathbf{k}}{}^*\left(\alpha_{\mathbf{k}}+\frac{\partial}{\partial\alpha_{\mathbf{k}}{}^*}\right)\rho(\{\alpha^*\},\{\alpha\}), \quad (4.2)$$

which is derived by means of the integration formulas (3.15). An integration by parts turns out to be legal, so that

$$n_{\mathbf{k}}=\prod_{\mathbf{k}'}\left(\int\frac{d^2\alpha_{\mathbf{k}'}}{\pi}\right)(|\alpha_{\mathbf{k}}|^2-1)\rho(\{\alpha^*\},\{\alpha\})$$
$$=\langle|\alpha_{\mathbf{k}}|^2\rangle_\psi-1, \quad (4.3)$$

where the angular brackets denote an average over ψ or α space with (4.1) as the statistical weight.

It is important to note that the expected identity between $n_{\mathbf{k}}$ and $\langle|\alpha_{\mathbf{k}}|^2\rangle_\psi$ is a good approximation only in the classical limit, $n_k\gg1$. The identity is exactly correct only when the mode is occupied macroscopically, i.e., n_k is of order N.

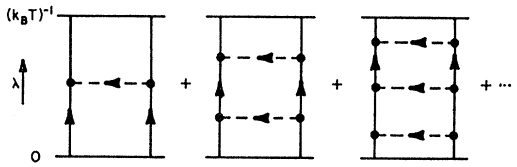

FIG. 2. The sequence of two-body ladder diagrams which must be summed to obtain the entire contribution to F of order $|\alpha|^4$.

The total density can be written in the form

$$n=\frac{1}{V}\sum_{\mathbf{k}}n_{\mathbf{k}}=\frac{1}{V}\int d\mathbf{r}\,\langle|\psi(\mathbf{r})|^2\rangle_\psi-\frac{1}{V}\sum_{\mathbf{k}}1. \quad (4.4)$$

Here it is obvious that we must expect a short-wavelength (large $\mathbf{k}$) divergence in $\langle|\psi(\mathbf{r})|^2\rangle_\psi$. In fact, this divergence is the same one which appears in similar field-theoretic calculations, and it is reassuring to see how it is subtracted out in Eq. (4.4). This divergence disappears in the formula for the current density:

$$\mathbf{j}=\frac{1}{V}\sum_{\mathbf{k}}\mathbf{k}n_{\mathbf{k}}=\frac{1}{V}\int d\mathbf{r}\left\langle\frac{1}{2i}(\psi^*\nabla\psi-\psi\nabla\psi^*)\right\rangle_\psi. \quad (4.5)$$

The Ginzburg-Landau theory, and the two-fluid model, emerge only when it is possible to evaluate the above formulas by what amounts to a mean-field calculation, augmented by a random-phase approximation. Suppose that $\rho\{\psi\}$, Eq. (4.1), is sharply peaked at some ψ, say ψ_s. In fact, let us assume that ψ_s is overwhelmingly the most probable state in its part of the function space, so that it must describe a stable or metastable state of the system. Then we can associate with ψ_s a superfluid density n_s and a supercurrent $\mathbf{j}_s$:

$$n_s=|\psi_s|^2, \quad \mathbf{j}_s=\frac{1}{2i}(\psi_s{}^*\nabla\psi_s-\psi_s\nabla\psi_s{}^*). \quad (4.6)$$

In order for the quantities defined in (4.6) to be meaningful, ψ_s must be of order unity (not, say, order $N^{-1/2}$) throughout the system. That is, ψ_s must have the properties of the classical field discussed in Sec. II, and, in particular, must obey the superfluid equations of motion, Eqs. (2.19). Thus, the most probable ψ appears to describe a superfluid component of the system.

It should be recognized, however, that the most probable ψ is not the same thing as the average ψ, nor are n_s and $\mathbf{j}_s$ the same as the average or expected values of n and $\mathbf{j}$ as defined in Eqs. (4.4) and (4.5). In order to evaluate the correct density or current, one must take proper account of the width of the peak in $\rho\{\psi\}$ near ψ_s. That is, one must include the fluctuations. There is no known way of doing this rigorously (except in one dimension), but the following procedure probably gives qualitatively correct results at temperatures far

enough away from the critical point that the fluctuations are small.

In principle, we want to expand $F\{\psi\}$ out to terms quadratic in $\psi-\psi_s$ and then perform the resulting Gaussian integrals.[27] This procedure is slightly complicated by the fact that $F\{\psi\}$ is independent of the phase of ψ, so that the phase fluctuations always will be appreciable and must be handled separately. Suppose that ψ_s is one of the uniform current-carrying states given by Eq. (1.8):

$$\psi_s = f_k e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{4.7}$$

Then we follow essentially Rice's procedure[10] and write

$$\psi(\mathbf{r}) = (f_k + \nu(\mathbf{r}))\exp[i\mathbf{k}\cdot\mathbf{r} + i\phi(\mathbf{r})], \tag{4.8}$$

where ν and ϕ are real functions of $\mathbf{r}$. It then makes sense to expand $F\{\psi\}$ out to terms quadratic in ν and ϕ. For the $F\{\psi\}$ given in Eq. (1.4),

$$F\{\psi\} \cong F\{\psi_s\} + \int d\mathbf{r}\,[(\nabla\nu)^2 + f_k^2(\nabla\phi)^2 + 4f_k\nu\mathbf{k}\cdot\nabla\phi + \kappa^2\nu^2], \tag{4.9}$$

where

$$\kappa^2 = 2Bf_k^2 = 2(A - k^2). \tag{4.10}$$

If we use the more general $F\{\psi\}$ computed in Sec. III, especially with the quadratic term $F^{(0)}\{\psi\}$ given by (3.7) which is necessary in order to allow for rapidly varying ψ's, then the relevant quadratic form becomes more complicated but remains qualitatively similar to (4.9). We arrive at expressions of the form

$$n = n_s + \langle\nu^2\rangle - \frac{1}{V}\sum_{\mathbf{k}'} 1 \tag{4.11}$$

and

$$\mathbf{j} = \mathbf{j}_s + 2f_k\langle\nu\nabla\phi\rangle + \mathbf{k}\langle\nu^2\rangle, \tag{4.12}$$

where the angular brackets here represent averages with respect to the above Gaussian approximation for the weight factor $\rho\{\psi\}$. In Eqs. (4.11) and (4.12), the fluctuations contribute additively to n and $\mathbf{j}$, and appear to describe a normal component of the fluid.

Special calculations of this kind have been published by Rice,[10] who has emphasized the fact that the phase fluctuations preclude off-diagonal long-range order in one or two dimensions. The reader may check from Rice's results that the formulas for n and $\mathbf{j}$ remain well defined in all cases except where the fluctuations become anomalously large near an apparent critical point. The fact that the method breaks down in some temperature range, especially in one or two dimensions, says nothing at all about whether a phase transition occurs, nor does it necessarily invalidate the qualitative results in regions where the fluctuations are small enough that the method seems self-consistent. In fact, the known features of the soluble one-dimensional model of the kind discussed here, using the simplest Ginzburg-Landau form for $F\{\psi\}$, are also the most striking features of the above approximation. That is, there is no long-range order, but the amplitude of ψ has a nonzero most probable value and, for low enough temperatures, is very unlikely to vanish. Thus the one-dimensional model may, in some sense, be a superfluid.

Both this one-dimensional model and further analysis concerning the behavior of the normal component as described by fluctuations will, hopefully, be the subjects of later communications.

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[27] The mathematical significance of performing these integrations in the neighborhood of a ψ_s which is not the absolute minimum of $F\{\psi\}$ is discussed in Ref. 13.