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Two Kinds of Bosons and Bose Condensates*

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This paper deals with ordinary material systems whose elementary constituents are fermions. It is pointed out that in such systems there can occur two kinds of bosons with quite different physical and mathematical characteristics. Type I bosons are bound complexes of an even number of fermions (such as ^{4}He); and type II bosons are elementary excitations which are bound complexes of fermions and their holes (such as excitons). When the first type condenses, a superfluid state results with so-called off-diagonal, long-range order; while when the second type condenses, there is no superfluidity, but a change in spatial order. Thus both kinds of long-range order are related to Bose condensation.

CONTENTS

1. INTRODUCTION

Bose condensation is one of the most striking phenomena exhibited by macroscopic systems. The condensation of a macroscopic fraction of the particles of an ideal Bose–Einstein gas into the lowest-energy single-particle state at sufficiently low temperatures was first predicted theoretically by Einstein in 1924. By considering ^{4}He atoms as bosons, London (1938) showed that the condensed Bose gas provided a model for the explanation of the remarkable superfluid properties of helium (II). The work of London and the pioneering paper of Bogoliubov (1947) on a microscopic model of a weakly interacting Bose gas, in which again a single momentum state is macroscopically occupied at low temperature, have laid the basis for much of our present theoretical knowledge about liquid helium.† Penrose and Onsager (Penrose, 1951; Penrose and Onsager, 1956) generalized the concept of Bose condensation to apply also to strongly interacting Bose systems. They characterized the Bose condensed state by the following form of the one-particle density matrix:

$$\rho(\mathbf{r},\mathbf{r}')=\chi^*(\mathbf{r})\chi(\mathbf{r}')+g(\mathbf{r},\mathbf{r}'), \qquad (1.1)$$

where $g(\mathbf{r},\mathbf{r}')\to 0$ as $|\mathbf{r}-\mathbf{r}'|\to\infty$ and

$$\int |\chi(\mathbf{r})|^2\, d\mathbf{r}$$

is a macroscopic number. This Bose condensation gives rise to superfluidity in helium II.

In real material systems the basic constituent particles are fermions, but often there exist complexes of even numbers of fermions and/or fermion holes which obey Bose–Einstein statistics at least in an approximate sense. The present paper is concerned with such composite bosons and related Bose-condensed states.*

Helium 4 is the most familiar example of a system of composite bosons and, below the condensation temperature, is a superfluid. Superconductors cannot quite so easily be regarded from this point of view since, above the condensation temperature, there exist no well-defined composite bosons. Nevertheless, as has been shown by Yang (1962), below the superconducting transition temperature, the two-particle density matrix has a form analagous to Eq. (1.1), so that the superconducting state can also be naturally considered as a Bose-condensed state. (Schafroth, 1954; Schafroth, 1955; Bardeen, Cooper, and Schrieffer, 1957).† Qualita-

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† For more recent work on helium II the reader is referred to articles in the book *Quantum Fluids*, D. F. Brewer, Ed. (1966) and to I. M. Khalatnikov (1965), *Theory of Superfluidity.*

* All particles will be considered in the nonrelativistic limit.

† For more discussion of metallic superconductivity the reader is referred to the standard texts; for example: J. R. Schrieffer (1964), *Theory of Superconductivity*; J. M. Blatt (1964), *Theory of Superconductivity*; G. Rickayzen (1965), *Theory of Superconductivity.*

tively one may regard the Cooper pair as the underlying boson.

Both ^{4}He atoms and Cooper pairs consist of an even number of fermions. Recently there has also been much interest in condensates of bosons which are complexes of equal numbers of fermions and fermion holes. In particular there have been studies of condensates of real excitons* and of the so-called excitonic phase.† The latter is predicted to occur when a normal semiconductor or semimetal becomes unstable against the formation of a coherent condensate of bound electron-hole pairs. By analogy with helium II and superconductors, some authors‡ have been led to believe that these Bose condensates will also exhibit superfluid behavior. However, explicit calculations showing that the excitonic phase does not exhibit a Meissner effect (Jerome, Rice, and Kohn, 1967), is not electrically superconducting (Zittartz, 1968a), and does not possess superthermal conductivity (Zittartz, 1968b) have strongly implied that this view is incorrect.

In the present paper we hope to clarify this situation by highlighting the existence of two entirely different types of composite bosons and Bose condensates, and exhibiting and relating their fundamental physical and mathematical characteristics.

A boson of type I is a bound complex which consists essentially of an even number of fermions, or an even number of fermion holes. A ^{4}He atom is an example of this type. Such a boson, when in motion, carries real mechanical momentum. When a system of such bosons condenses, the resulting state is superfluid. In this state there is what London called an order in momentum space, or, in the terminology of Yang (1962), off-diagonal long-range order (ODLRO).

On the other hand, a boson of type II is an elementary excitation of a many-body system which is essentially a bound complex of equal numbers of fermions and their holes. An exciton is an example of this type. Bosons of type II, when in motion, may or may not carry mechanical momentum. When they condense, the resultant state is not superfluid. In the terminology of Yang (1962) there is no ODLRO but there is a change of long-range order in coordinate space, i.e., of the diagonal long-range order (DLRO). The appearance of a superlattice is an example of such a change of order.

In the following portions of this paper we shall demonstrate these properties for two representative examples. We shall also exhibit and contrast the general mathematical features of the states characterizing these two types of bosons and show how the stated physical properties follow from these mathematical features.

2. BOSONS OF TYPE I

A type I boson is a complex of an even number of fermions (or fermion holes).*

While the ^{4}He atom is the most familiar boson of this type, we shall, for reasons of simpler exposition, discuss here the example of a hypothetical bound pair of spin-$\frac{1}{2}$ fermions. The singlet, S-state eigenfunction of such a pair, which corresponds to a total momentum $\mathbf{k}$, is of the form

$$\Phi_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2) = (1/\Omega^{1/2}) \exp\{i\mathbf{k}\cdot[\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)]\}\varphi(\mathbf{r}_1-\mathbf{r}_2)\chi_0, \tag{2.1}$$

where Ω is the normalization volume, φ is the normalized internal wave function, and χ_0 is the singlet spin function. The characteristic features of this pair appear most clearly in momentum space. Hence we Fourier analyze the internal wave function φ, using periodic boundary conditions on the surface of a cube:

$$\varphi(\mathbf{r}_1-\mathbf{r}_2) = (1/\Omega^{1/2})\sum_{\mathbf{q}} f(\mathbf{q}) \exp[i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)], \tag{2.2}$$

where

$$(1/\Omega)\sum |f(\mathbf{q})|^2 = 1. \tag{2.3}$$

The total momentum space wave function of the pair is then

$$F_{\mathbf{k}}(\mathbf{p}_1, \mathbf{p}_2) \equiv \Omega^{-1}\int \Phi_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2) \times \exp[-i(\mathbf{p}_1\cdot\mathbf{r}_1+\mathbf{p}_2\cdot\mathbf{r}_2)]\, d\mathbf{r}_1 d\mathbf{r}_2$$
$$= f(\tfrac{1}{2}(\mathbf{p}_1-\mathbf{p}_2))\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{k})\chi_0. \tag{2.4}$$

In the notation of second quantization, the state vector of this boson has the form

$$\Psi_{\mathbf{k}} = (1/\Omega^{1/2})\sum_{\mathbf{q}} f(\mathbf{q}) c^*_{\mathbf{k}/2-\mathbf{q},\downarrow} c^*_{\mathbf{k}/2+\mathbf{q},\uparrow}\Psi_{\text{vac}}, \tag{2.5}$$

where $c_{\mathbf{p}}^*$ is a plane-wave creation operator and Ψ_{vac} is the vacuum state.

We wish to draw particular attention to the occurrence of the δ-function factor $\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{k})$ in Eq. (2.4), which involves the *sum* of an even number of momentum variables. This δ-function factor expresses conservation of total momentum. (In type II bosons, momentum conservation takes an essentially different form.)

We may also note incidentally that the 1-boson state carries real mechanical momentum.†

We wish now to pass from this special model to a general mathematical characterization of type I bosons.

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* J. M. Blatt, K. W. Boer, and W. Brandt (1962), J. Casella (1963), S. A. Moskalenko (1962), V. M. Agranovich and B. S. Toshich (1967), L. V. Keldysh and A. N. Kozlov (1967), L. V. Keldysh and A. N. Kozlov (1968), V. A. Gergel', R. F. Kazarinov, and R. A. Suris (1968).

† For recent reviews (including bibliographies) see W. Kohn (1968), "Metals and Insulators," in *Many-Body Physics*, C. DeWitt and R. Balian, Eds.; B. I. Halperin and T. M. Rice (1968a, 1968b).

‡ Moskalenko (1962), Arganovich and Toshich (1967), Keldysh and Kozlov (1967, 1968), Gergel', Kazarinov, and Suris (1968), Kozlov and Maksimov (1966).

* When such a complex is in a material medium, with which it interacts, it will of course be "dressed" by virtual excitations.

† By this we mean that during the motion of a wave packet there is a displacement of the center of mass. Mechanical momentum is in general different from crystal momentum which is a translational quantum number.

For this purpose we introduce the density matrices (or Green's functions) which have a well-defined meaning even for complicated many-body systems, such as a boson moving in a material medium. For a 2-fermion boson the two-particle density matrix is appropriate.* This is defined, (Yang, 1962) in the plane-wave representation, as

$$(\mathbf{p}_1', \mathbf{p}_2' \mid \rho^{(2)} \mid \mathbf{p}_1, \mathbf{p}_2) \equiv \langle c_{\mathbf{p}_2}{}^* c_{\mathbf{p}_1}{}^* c_{\mathbf{p}_1'} c_{\mathbf{p}_2'} \rangle, \quad (2.6)$$

where $\langle\ \rangle$ denotes, for a pure state, the expectation value and, for a thermal ensemble, the thermal average. Appropriate spin indices, which would encumber the notation, have been suppressed. In the state $\Psi_{\mathbf{k}}$, Eq. (2.5), in which one di-fermion is present, we find

$$(\mathbf{p}_1', \mathbf{p}_2' \mid \rho^{(2)} \mid \mathbf{p}_1, \mathbf{p}_2) = \delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{k})\delta(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{k}) \times (1/\Omega) f^*(\tfrac{1}{2}(\mathbf{p}_1-\mathbf{p}_2)) f(\tfrac{1}{2}(\mathbf{p}_1'-\mathbf{p}_2')). \quad (2.7)$$

We now present our general mathematical characterization, valid for a general many-body system. We say that a state contains one boson of type I if the following conditions are satisfied.

The two-particle density matrix has a structure of the following form:

$$(\mathbf{p}_1', \mathbf{p}_2' \mid \rho^{(2)} \mid \mathbf{p}_1, \mathbf{p}_2) = \alpha\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{k})\delta(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{k}) \times g(\mathbf{p}_1-\mathbf{p}_2, \mathbf{p}_1'-\mathbf{p}_2') + h(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_1', \mathbf{p}_2'); \quad (2.8)$$

α is a constant of order unity, independent of the size of the system; each δ-function contains the *sum* of two momentum variables; g is a smooth function of its arguments with unit trace

$$\sum_{\mathbf{q}} g(\mathbf{q}, \mathbf{q}) = 1; \quad (2.9)$$

h is free of the δ-function product occurring in the first term.† At the same time, the four-particle density matrix does not contain terms involving products of four δ-functions of the type appearing in Eq. (2.8).‡

Extension to bosons consisting of a larger number of fermions or of fermions of different species is straightforward.

We have already noted that our model di-fermion carries real mechanical momentum. In Appendix I we show that this is a mathematical consequence of the *sums* of momenta, such as $\mathbf{p}_1+\mathbf{p}_2$ occurring in the δ-function of (2.8). Thus all type I bosons carry mechanical momentum.

In Sec. 4 we shall see that the δ-function structure of $\rho^{(2)}$, shown in (2.8), is the mathematical basis of the fact that when type I bosons condense, the resulting system is superfluid.

* Alternatively, one may use the anomalous, particle nonconserving density matrix $(0 \mid c_{p_1} c_{p_2} \mid 1)$, where $(0 \mid$ and $\mid 1)$ denote, respectively, states with 0 and 1 boson present.

† If a periodic crystal potential is present, there will also occur δ functions of the form $\delta(\mathbf{p}_1+\mathbf{p}_2+\mathbf{K}_\nu-\mathbf{k})$, where $\mathbf{K}_\nu$ is a reciprocal lattice vector.

‡ This rules out the presence of more than one boson.

3. BOSONS OF TYPE II

A type II boson is an elementary excitation of a many-body system which is a bound complex of equal numbers of fermions and their holes. The term "collective excitation" is commonly used for such bosons. Examples are excitons, spin waves, zeroth sound in ^{3}He, phonons in solids, phonons and rotons in ^{4}He, etc.

As an example, we shall treat in some detail a simple model of an exciton in an insulator. For our present purposes we consider the nuclei as nondynamical and merely as giving rise to a periodic potential. We shall consider only spin-conserving excitations of the spin-up electrons and hence can omit the spin-down electrons from further consideration. We denote the (self-consistent) Bloch functions and energy eigenvalues in the usual way by $\varphi_{n,\mathbf{p}}$ and $\epsilon_{n,\mathbf{p}}$, and the corresponding (spin-up) creation and annihilation operators by $b_{n,\mathbf{p}}{}^*$ and $b_{n,\mathbf{p}}$.

We take as the insulating ground state the state in which the band $n=0$ is fully occupied while all other bands are completely empty. This state we write as

$$\Psi_0 = \prod_{\mathbf{p}} b_{0,\mathbf{p}}{}^* \Psi_{\text{vac}}, \quad (3.1)$$

where $\mathbf{p}$ runs over the fundamental Brillouin zone.

An exciton of wave vector $\mathbf{k}$ must be regarded as a coherent linear combination of electron–hole pairs whose net crystal momentum is $\mathbf{k}$. Thus we write the 1-exciton state as

$$\Psi_{\mathbf{k}}' = (1/\Omega^{1/2}) \sum_{\mathbf{q}} f'(\mathbf{q}) b^*_{1,\mathbf{k}/2+\mathbf{q}} b_{0,-\mathbf{k}/2+\mathbf{q}} \Psi_0. \quad (3.2)$$

The function f' is the internal wave function of the bound electron–hole pair. Clearly $f'(\mathbf{q}+\mathbf{K}_\mu) = f'(\mathbf{q})$, where $\mathbf{K}_\mu$ is any reciprocal lattice vector.

The formal analogy of $\Psi_{\mathbf{k}}'$ with the state vector $\Psi_{\mathbf{k}}$ of the di-fermion [Eq. (2.5)] is evident. However, we shall see that the physical differences are profound. Here we note that while all type I bosons carry mechanical momentum, an exciton in an insulator does not. However, other type II bosons, e.g., plasmons, do carry momentum. (See Appendix I.)

To pass from this special example to a general mathematical characterization of type II bosons, we study again the two-particle density matrix.* The change of this matrix, due to the presence of an exciton, clearly contains terms of the form

$$\Delta(\mathbf{p}_1', \mathbf{p}_2' \mid \rho^{(2)} \mid \mathbf{p}_1, \mathbf{p}_2) = \alpha'\delta(\mathbf{p}_2'-\mathbf{p}_1-\mathbf{k}) \times \delta(\mathbf{p}_2-\mathbf{p}_1'-\mathbf{k}) g'(\tfrac{1}{2}(\mathbf{p}_1+\mathbf{p}_2'), \tfrac{1}{2}(\mathbf{p}_2+\mathbf{p}_1')) + \cdots; \quad (3.3)$$

α' is again a constant of order unity, independent of the size of the system, and g' has unit trace

$$\sum_{\mathbf{q}} g'(\mathbf{q}, \mathbf{q}) = 1; \quad (3.4)$$

* Alternatively, one may use the off-diagonal density matrix $(0 \mid c_{p_1}{}^* c_{p_2} \mid 1)$, where $(0 \mid$ and $\mid 1)$ denote, respectively, states with 0 and 1 boson of type II present.

there are other terms, not explicitly written down, which are of similar structure and allow for the antisymmetry of $\rho^{(2)}$ and for the presence of Umklapp terms. One δ function comes from the destruction of the exciton [see Eq. (2.6)] and the other one from its re-creation.

We now present our general mathematical characterization, valid for a general many-body system. We say that a state contains one type II boson if the following conditions are met:

The two-particle density matrix contains terms of the form

$$\alpha'\delta(\mathbf{p}_2'-\mathbf{p}_1-\mathbf{k})\delta(\mathbf{p}_2-\mathbf{p}_1'-\mathbf{k})g'(\tfrac{1}{2}(\mathbf{p}_1+\mathbf{p}_2'),\tfrac{1}{2}(\mathbf{p}_2+\mathbf{p}_1')) \tag{3.5}$$

and their antisymmetrized and Umklapp partners. Each of the δ-functions contains a *difference* of two momentum variables, such as $\mathbf{p}_2'-\mathbf{p}_1$. The function g' has a trace of unity [see Eq. (3.4)]. At the same time, the four-particle density matrix does not contain products of four δ-functions of the form occurring in (3.5).*

Extension to bosons consisting of a larger number of fermions and holes, or of fermions and holes of different species, is straightforward.

Concerning mechanical momentum we quote here the conclusion derived in Appendix I: Some type II bosons carry mechanical momentum, others do not.

4. CONDENSED STATES OF TYPE I

A system of noninteracting elementary bosons condenses below a critical temperature. In the condensed state, a finite fraction of all particles occupy the state $\mathbf{k}=0$.

Now let us consider the di-fermions of Sec. 2. Let us assume that they interact with each other in a manner similar to ^{4}He atoms. Then, if we have a sufficiently dilute system, the interactions between these type I bosons will be unimportant and, at low temperatures, they will condense very much like elementary bosons. For example, at $T=0°$, the ground state will be approximately given by

$$\Psi_0=(B_0^*)^N\Psi_{\text{vac}}, \tag{4.1}$$

where B_0^* is the creation operator of one di-fermion in the state $\mathbf{k}=0$ [cf. Eq. (2.5)]

$$B_0^*\equiv(1/\Omega^{1/2})\sum_{\mathbf{q}}f(q)c_{-\mathbf{q},\downarrow}^*c_{\mathbf{q},\uparrow}^*. \tag{4.2}$$

With N bosons now occupying the state $\mathbf{k}=0$, it is clear, by reference to Eq. (2.8), and may be checked by direct calculation, that $\rho^{(2)}$ contains a term of the form

$$(\mathbf{p}_1',\mathbf{p}_2'\mid\rho^{(2)}\mid\mathbf{p}_1,\mathbf{p}_2)=\gamma N\delta(\mathbf{p}_1+\mathbf{p}_2-0)\times\delta(\mathbf{p}_1'+\mathbf{p}_2'-0)G(\mathbf{p}_1-\mathbf{p}_2,\mathbf{p}_1'-\mathbf{p}_2')+\cdots, \tag{4.3}$$

with γ of order unity and G a smooth function of its arguments with unit trace. The factor N is of course characteristic of the Bose condensation.

From this model we arrive at the following general characterization: We call a state a condensed state of type I, wave vector $\mathbf{k}$, and degree 2, if the two-particle density matrix contains a term of the form

$$(\mathbf{p}_1',\mathbf{p}_2'\mid\rho^{(2)}\mid\mathbf{p}_1,\mathbf{p}_2)=\gamma N\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{k})\times\delta(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{k})G(\mathbf{p}_1-\mathbf{p}_2,\mathbf{p}_1'-\mathbf{p}_2'), \tag{4.4}$$

where γ and G have the same properties as above.*

We now present some discussion:

(a) The degree of the condensed state is the order of the lowest density matrix in which a delta-function structure of the type (4.4) appears (for He atoms the degree would be 6).

(b) The characterization (4.4) implies off-diagonal long-range order (ODLRO) in the sense of Yang (1962). This is immediately verified by Fourier transformation;

$$\begin{aligned}(\mathbf{r}_1',\mathbf{r}_2'\mid\rho^{(2)}\mid\mathbf{r}_1,\mathbf{r}_2)&=(1/\Omega^2)\sum\exp[i(\mathbf{p}_1'\cdot\mathbf{r}_1'+i\mathbf{p}_2'\cdot\mathbf{r}_2'-\mathbf{p}_1\cdot\mathbf{r}_1-\mathbf{p}_2\cdot\mathbf{r}_2)]\\&\quad\times(\mathbf{p}_1',\mathbf{p}_2'\mid\rho^{(2)}\mid\mathbf{p}_1,\mathbf{p}_2)\\&=\exp\{i\mathbf{k}\cdot[\tfrac{1}{2}(\mathbf{r}_1'+\mathbf{r}_2')-\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)]\}\\&\quad\times F(\mathbf{r}_1'-\mathbf{r}_2',\mathbf{r}_1-\mathbf{r}_2),\end{aligned} \tag{4.5}$$

where

$$F(\mathbf{r}_1'-\mathbf{r}_2',\mathbf{r}_1-\mathbf{r}_2)\equiv(\gamma N/\Omega^2)\sum G(\mathbf{q},\mathbf{q}')\times\exp\{i[\mathbf{q}'\cdot\tfrac{1}{2}(\mathbf{r}_1'-\mathbf{r}_2')-\mathbf{q}\cdot\tfrac{1}{2}(\mathbf{r}_1-\mathbf{r}_2)]\} \tag{4.6}$$

and

$$\int F(\mathbf{r}_1-\mathbf{r}_2,\mathbf{r}_1-\mathbf{r}_2)\,d\mathbf{r}_1d\mathbf{r}_2=\gamma N. \tag{4.7}$$

In particular we see that $\rho^{(2)}$ remains finite in the limit where $\mathbf{r}_1\approx\mathbf{r}_2$, $\mathbf{r}_1'\approx\mathbf{r}_2'$, but $\mathbf{r}_1-\mathbf{r}_1'\to\infty$. As Yang (1962) has stated, and as we show in detail in Sec. 6, the structure (4.4) of the density matrix implies superfluidity.

(c) A condensed state of type I, as here defined, occurs—if it does at all—below some critical temperature T_c. Above T_c we may encounter two kinds of situations. In some systems, such as ^{4}He, it is appropriate to regard the system as a collection of type I bosons, although, because of interactions, this description is only approximate. The transition through T_c can then be regarded as a modification of a free Bose–Einstein condensation. On the other hand, for example, in a B.C.S. superconductor, there are no real bosons present above T_c, although below T_c one may regard the system as similar to a condensed state of Cooper pairs. The transition through T_c then of course cannot be viewed as a condensation of bosons.

* This condition rules out the presence of more than one boson. We do not count here δ-functions of the type $\delta(\mathbf{p}_2'-\mathbf{p}_1+\mathbf{K}_\mu)$ which are characteristic of the ground state.

* For some purposes, the equivalent form

$$\tfrac{1}{2}\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_1'-\mathbf{p}_2')\delta(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_1'+\mathbf{p}_2'-2\mathbf{k})$$

of the δ-function factors is useful (see Sec. 6).

5. CONDENSED STATES OF TYPE II

As a prototype of a condensed state of type II, let us consider the following situation. At zero temperature we shine light on an insulator creating a substantial number N of excitons. Suppose that their recombination time is much longer than the time to reach thermal equilibrium among themselves. Then because of their Bose statistics and, assuming that interactions between them play a minor role, these excitons will Bose condense. Suppose that the exciton of lowest energy has crystal momentum $\mathbf{k}(\neq 0)$* and let us call the operator creating one exciton with crystal momentum $\mathbf{k}$, $B_{\mathbf{k}}'^*$, where by Eq. (3.2)

$$B_{\mathbf{k}}'^* \approx (1/\Omega^{1/2}) \sum_{\mathbf{q}} f'(\mathbf{q}) b^*_{1,\mathbf{k}/2+\mathbf{q}} b_{0,-\mathbf{k}/2+\mathbf{q}}. \quad (5.1)$$

Then the totally condensed state of these excitons will be given approximately by

$$\Psi_N' \approx (B_{\mathbf{k}}'^*)^N \Psi_0, \quad (5.2)$$

where Ψ_0 is the insulating ground state. With N excitons now occupying the state $\mathbf{k}$, it is clear by reference to Eq. (3.4) and may be checked by direct calculation that $\rho^{(2)}$ contains a term of the form

$$(\mathbf{p}_1', \mathbf{p}_2' \mid \rho^{(2)} \mid \mathbf{p}_1, \mathbf{p}_2) = \gamma' N \delta(\mathbf{p}_2' - \mathbf{p}_1 - \mathbf{k}) \times \delta(\mathbf{p}_2 - \mathbf{p}_1' - \mathbf{k}) G'(\tfrac{1}{2}(\mathbf{p}_1 + \mathbf{p}_2'), \tfrac{1}{2}(\mathbf{p}_2 + \mathbf{p}_1')) + \cdots \quad (5.3)$$

plus its antisymmetrized and Umklapp partners as well as other terms which do not have such a δ-function structure.† The constant γ is of order unity and G' is a smooth function of its arguments.

From this model we arrive at the following general characterization: We call a state a condensed state of type II, wave vector $\mathbf{k}$, and degree 2 if the two-particle density matrix contains terms of the structure (5.3).

We now present some discussion:

(a) The degree of the condensed state is the order of the lowest density matrix in which a δ-function structure of the type (5.3) occurs. Thus the condensed state of bound *pairs* of excitons is of degree 4 and gives rise in $\rho^{(4)}$ to a product of δ functions of the form $\delta(\mathbf{p}_3' + \mathbf{p}_4' - \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{k}) \delta(\mathbf{p}_3 + \mathbf{p}_4 - \mathbf{p}_1' - \mathbf{p}_2' - \mathbf{k})$.

(b) The characterization (5.3) implies long-range order in the ordinary sense, i.e., in coordinate space, or diagonal long-range order (as opposed to Yang's "off diagonal"). This may be verified by Fourier transformation of (5.3). In analogy with (4.5) this gives

$$(\mathbf{r}_1', \mathbf{r}_2' \mid \rho^{(2)} \mid \mathbf{r}_1, \mathbf{r}_2) = \exp\{i\mathbf{k} \cdot [\tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2') - \tfrac{1}{2}(\mathbf{r}_2 + \mathbf{r}_1')]\} \times F'(\mathbf{r}_1' - \mathbf{r}_2, \mathbf{r}_1 - \mathbf{r}_2') + \cdots, \quad (5.4)$$

where

$$F'(\mathbf{r}_1' - \mathbf{r}_2, \mathbf{r}_1 - \mathbf{r}_2') = (\gamma' N/\Omega^2) \sum G'(\mathbf{q}, \mathbf{q}') \times \exp\{i[\mathbf{q}' \cdot (\mathbf{r}_1' - \mathbf{r}_2) - q \cdot (\mathbf{r}_1 - \mathbf{r}_2')]\} \quad (5.5)$$

and

$$\int F'(\mathbf{r}_1 - \mathbf{r}_2, \mathbf{r}_1 - \mathbf{r}_2)\, d\mathbf{r}_1 d\mathbf{r}_2 = \gamma' N. \quad (5.6)$$

In particular we see that the density–density correlation function shows a characteristic long-range order governed by the wave vector $\mathbf{k}$:

$$\langle n(\mathbf{r}_2) n(\mathbf{r}_1) \rangle = -(\mathbf{r}_2, \mathbf{r}_1 \mid \rho^{(2)} \mid \mathbf{r}_1, \mathbf{r}_2) = -\exp[i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)] F(0, 0) + \cdots \quad (\mathbf{r}_1 \neq \mathbf{r}_2). \quad (5.7)$$

(c) Although there is long-range order in the density–density correlation function (5.7), the one-particle density itself,

$$n(\mathbf{r}) = (N-1)^{-1} \int (\mathbf{r}, \bar{\mathbf{r}} \mid \rho^{(2)} \mid \mathbf{r}, \bar{\mathbf{r}})\, d\bar{\mathbf{r}} = \int F'(\mathbf{r} - \bar{\mathbf{r}}, \mathbf{r} - \bar{\mathbf{r}})\, d\mathbf{r} + \cdots = (\gamma N/\Omega) \sum G'(\mathbf{q}, \mathbf{q}) + \cdots = (\gamma N/\Omega) + \cdots, \quad (5.8)$$

shows no long-range oscillation of wave vector $\mathbf{k}$.

This last conclusion can also be reached directly by noting that the condensed state in question is an eigenstate of the crystal translation operators T_l, which move all coordinates through the lattice vectors $\mathbf{R}_l$,

$$T_l \Psi_N' = [\exp(i\mathbf{k} \cdot \mathbf{R}_l)]^N \Psi_N'; \quad (5.9)$$

from this we conclude at once that

$$n(\mathbf{r} + \mathbf{R}_l) = n(\mathbf{r}), \quad (5.10)$$

so that $n(\mathbf{r})$ has only Fourier components with wave vectors $\mathbf{K}_\nu$.

This state of affairs is analogous to a crystal lattice in a state Ψ of uniform translational motion, described by a total wave vector $\mathbf{K}$. Here we have for an arbitrary translation operator $T(\mathbf{R})$

$$T(\mathbf{R}) \Psi = \exp(i\mathbf{K} \cdot \mathbf{R}) \Psi,$$

so that

$$n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r}) = n_0. \quad (5.11)$$

Thus the mean density is entirely uniform. However the density–density correlation function [cf. Eq. (5.7)] exhibits of course the internal crystal structure and contains Fourier components of the form $\exp[i\mathbf{K}_\nu \cdot (\mathbf{r}_1 - \mathbf{r}_2)]$.

(d) There is another kind of condensed state of type II, in which the one-particle density itself *does* show a long-range oscillation proportional to $\exp(i\mathbf{k} \cdot \mathbf{r})$. A good example is the so-called excitonic state* of a two-band solid, with a valence band $n=0$, having its

* We also assume that $\mathbf{k}$ is incommensurate with the reciprocal lattice vectors $\mathbf{K}_\nu$ and we disregard here the existence of other equivalent excitons, such as that with crystal momentum $-\mathbf{k}$.

† For some purposes the equivalent form

$$\tfrac{1}{2}\delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2') \delta((\mathbf{p}_2' - \mathbf{p}_1') + (\mathbf{p}_2 - \mathbf{p}_1) - 2\mathbf{k})$$

of the δ-function factors is useful (see Sec. 6).

* See, for example, W. Kohn (1968), Halperin and Rice (1968a), and Jerome, Rice, and Kohn (1967).

maximum at the origin of $\mathbf{k}$ space, and a conduction band $n=1$, with minimum at $\mathbf{k}$. In Hartree–Fock approximation the state is written as

$$\Psi'=\prod_{\mathbf{p}}(u_{\mathbf{p}}{}^{*}b_{0,\mathbf{p}}{}^{*}-v_{\mathbf{p}}{}^{*}b_{1;\mathbf{k}+\mathbf{p}}{}^{*})\Psi_{\mathrm{vac}}, \tag{5.12}$$

where $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ are coefficients which can be determined by minimizing the energy. To assure normalization we set

$$|u_{\mathbf{p}}|^2+|v_{\mathbf{p}}|^2=1. \tag{5.13}$$

It is elementary to evaluate explicitly the one- and two-particle density matrices with the following results:

The one-particle density matrix $\rho^{(1)}$ contains δ functions of the following structure:

$$\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{K}_\mu), \tag{5.14a}$$

$$\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{K}_\mu\pm\mathbf{k}); \tag{5.14b}$$

and the two-particle density matrix $\rho^{(2)}$

$$\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{K}_\mu)\delta(\mathbf{p}_2-\mathbf{p}_2'-\mathbf{K}_\nu) \tag{5.15a}$$

$$\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{K}_\mu-\mathbf{k})\delta(\mathbf{p}_2-\mathbf{p}_2'-\mathbf{K}_\nu-\mathbf{k}) \tag{5.15b}$$

$$\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{K}_\mu)\delta(\mathbf{p}_2-\mathbf{p}_2'-\mathbf{K}_\nu\pm\mathbf{k}) \tag{5.15c}$$

$$\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{K}_\mu\mp\mathbf{k})\delta(\mathbf{p}_2-\mathbf{p}_2'-\mathbf{K}_\nu\pm\mathbf{k}) \tag{5.15d}$$

and their antisymmetrized partners.

The one-particle density matrix, characterized by (5.14), gives rise to a density of the form

$$n(\mathbf{r})=\sum_\nu A_\nu\exp(i\mathbf{K}_\nu\cdot\mathbf{r})+\sum_\nu A_\nu'\exp[i(\mathbf{K}_\nu+\mathbf{k})\cdot\mathbf{r}]+\text{c.c.} \tag{5.16}$$

showing an additional long-range order characterized by the wave vector $\mathbf{k}$. This additional order comes from (5.14b) or, after contraction, from (5.15c).

We shall now try to explain the relationship between the state Ψ_N' of N condensed excitons, Eq. (5.2), and the excitonic state Ψ', Eq. (5.12). It is evident by inspection that the excitonic state is *not* an eigenstate of the crystal translation operators since $\varphi_{0,\mathbf{p}}$ and $\varphi_{1,\mathbf{k}+\mathbf{p}}$ correspond to different eigenvalues of this operator. However Ψ' may be written as a superposition of such states

$$\Psi'=\sum C_N\Psi_N, \tag{5.17}$$

where

$$T_l\Psi_N=[\exp(i\mathbf{k}\cdot\mathbf{R}_l)]^N\Psi_N \tag{5.18}$$

and

$$\sum_N|C_N|^2=1. \tag{5.19}$$

Thus

$$\Psi_0=\prod_{\mathbf{p}}b_{0,\mathbf{p}}{}^{*}\Psi_{\mathrm{vac}}, \tag{5.20}$$

$$\Psi_1=(1/\Omega^{1/2})\sum f(\mathbf{q})\,b_{1,\mathbf{k}+\mathbf{q}}{}^{*}b_{0,\mathbf{q}}\Psi_0, \tag{5.21}$$

$$f(\mathbf{q})=(\text{const})[v^{*}(\mathbf{q})/u^{*}(\mathbf{q})],$$
etc.

Clearly Ψ_0 is the insulating ground state; Ψ_1 has the structure of a state with one exciton of wave vector $\mathbf{k}$ [cf. Eq. (3.2)]*; similarly Ψ_N may be qualitatively thought of as a state containing N excitons. The coefficients C_N have a sharp maximum at some value $N=N_0$, of width $\Delta N\sim N_0{}^{1/2}$.

We may remark that, because of crystal momentum conservation,

$$(\Psi_N, H\Psi_{N'})=E_N\delta_{NN'}, \tag{5.22}$$

so that a particular linear combination of the Ψ_N must be established by some small perturbation which does not have the periodicity of the lattice (e.g., a local strain).†

Now, by (5.17), we may write

$$(\Psi', \rho^{(i)}\Psi')=\sum C_N{}^{*}C_{N'}(\Psi_N, \rho^{(i)}\Psi_{N'}), \qquad i=1, 2. \tag{5.23}$$

Only terms with $N'-N=0, \pm1$ contribute in the case of $\rho^{(1)}$; Eq. (5.14a) comes from $N'-N=0$ and (5.14b) from $N'-N=\pm1$. Only terms with $N'-N=0, \pm1, \pm2$ contribute in the case of $\rho^{(2)}$. Equations (5.15a) and (5.15b) come from $N'-N=0$, Eq. (5.15c) from $N'-N=\pm1$, and Eq. (5.15d) from $N'-N=\pm2$.

Thus we see that, for example, the coefficient of (5.14b) depends on the relative phase of C_N and C_{N+1}, and in view of (5.22), this phase is determined by some external nonperiodic perturbation.† Only such a perturbation can "pin" the additional density fluctuations of wave numbers $\pm\mathbf{k}+\mathbf{K}_\nu$ in a definite phase relationship to the periodic background density associated with (5.14a).

(e) We observe that, according to our definition, the electrons of an ordinary crystal (like Na or NaCl) are in a condensed state of type II, wave vectors $\mathbf{K}_\mu$, and degree 2 because of the presence in $\rho^{(2)}$ of δ-function products of the type (5.15a). If an ordinary insulator undergoes an excitonic transition, it remains a condensed state of type II and degree 2, but its characteristic wave vectors are augmented by the set $\mathbf{k}+\mathbf{K}_\mu$.

(f) A type II condensed state may or may not arise as a result of a process of condensation of type II bosons. An example where the condensate of wave vector $\mathbf{k}$ arises from such a process was given at the beginning of this section. On the other hand, for a system with an excitonic phase there are (at least according to the present theories) no free excitons above the transition temperature.‡

(g) The point of view of this section appears to have some relevance for several classes of phase transitions. Many distortive transitions can be viewed as due to the

* When the normal insulator has just become unstable against the excitonic transition, $f(q)$ is *exactly* the exciton wave function (see W. Kohn, 1968).

† This conclusion holds only if k is noncommensurate with the $\mathbf{K}_\nu$; on the other hand, e.g., for $\mathbf{k}=\mathbf{K}_\nu/2$, higher-order terms introduce couplings between Ψ_N and $\Psi_{N\pm1}$.

‡ See, for example, W. Kohn (1968), Halperin and Rice (1968a) and Jerome, Rice, and Kohn (1967).

formation of type II condensates consisting of soft phonons; magnetic phases can be viewed as condensates of magnons or paramagnons; and certain liquid-to-solid transitions (e.g., noble gases) may usefully be thought of as type II Bose-like condensations of soft phonons in the liquid.

(h) Some systems are simultaneously Bose condensates of type I and II (e.g., a crystalline superconducting metal); they combine the physical and mathematical characteristics of both types.

6. NECESSARY AND SUFFICIENT CONDITION FOR SUPERFLUIDITY

In this section we shall show that a system is superfluid if and only if it exhibits off-diagonal long-range order (ODLRO). This result has already been indicated by Yang (1962) but without formal proof.

We consider the system to be contained within two closely spaced concentric circular cylinders which may be rotated together with small angular velocity ω (see Fig. 1). We use the following characterization of normal and superfluid systems. A normal system rotates rigidly with the cylinders and its free energy differs from the free energy of the system at rest only by the classical inertial kinetic energy. In a superfluid there are (periodic) deviations from this behavior.*

The Hamiltonian in the rotating system is (Blatt, Butler, and Schafroth, 1955)

$$H=H_0-\omega L, \tag{6.1}$$

where H_0 is the Hamiltonian in the stationary system and L is the angular-momentum operator. For simplicity we discuss here systems in which there is only one kind of dynamical particle, e.g., electrons. When there is also an external lattice, this is regarded as rigidly attached to the walls of the cylinder. We consider the limiting situation in which the average radius R of the cylinders becomes large, while their separation d and the velocity of rotation ωR remain finite. Then H can be written as

$$H=H_K+\tfrac{1}{2}M(\omega R)^2, \tag{6.2}$$

where M is the total mass of the particles and

$$H_K=\sum_{\mathbf{k}}(1/2m)(\mathbf{k}-\mathbf{K})^2c^*(\mathbf{k})c(\mathbf{k}) + \sum_{\mathbf{kl}}(\mathbf{k}\mid V\mid \mathbf{l})c^*(\mathbf{k})c(\mathbf{l}) + \tfrac{1}{2}\sum_{\mathbf{klmn}}(\mathbf{kl}\mid U\mid \mathbf{mn})c^*(\mathbf{k})c^*(\mathbf{l})c(\mathbf{m})c(\mathbf{n}); \tag{6.3}$$

here

$$K\equiv m(\omega R); \qquad \mathbf{K}\equiv(K,0,0), \tag{6.4}$$

and the x, y, and z directions have the meaning shown in Fig. 1; V is the external lattice potential (if present) and U is the interparticle interaction.

A system is then normal if the free energy F_K, calculated in the usual way from H_K, is independent of K; and it is superfluid if F_K depends on K. We may remark that for a singly connected bounded system K could be removed from H_K by a simple gauge transformation, and F_K is then formally independent of K. In the present geometry such a gauge transformation in general violates the periodic boundary conditions which follow from the equivalence of the points x and $x+2\pi R$. Only for $K=n/R$ (n an integer) can K be formally removed from H_K by a gauge transformation involving the phase factor e^{iKx}.

We shall prove the assertion, stated at the beginning of this section, by a consideration of the hierarchy of thermal Green's function equations. The first of these, which is representative for our purposes, has the form

$$[i(\partial/\partial t)-(1/2m)(\mathbf{k}-\mathbf{K})^2+\mu]G_{1,K}(\mathbf{k}t;\mathbf{k}'t') + \sum_{\mathbf{l}}(\mathbf{k}\mid V\mid \mathbf{l})G_{1,K}(\mathbf{l}t;\mathbf{k}'t')=\delta(\mathbf{k}-\mathbf{k}') + i\sum_{\mathbf{l,m,n}}(\mathbf{kl}\mid U\mid \mathbf{mn})G_{2,K}(\mathbf{m}t,\mathbf{n}t^-;\mathbf{l}t^+,\mathbf{k}'t'), \tag{6.5}$$

where μ is the chemical potential, $t^-=t-0$, $t^+=t+0$, and $G_{1,K}$, $G_{2,K}$ are the K-dependent one- and two-particle Green's functions.*

We now translate all momentum variables, $\mathbf{k}-\mathbf{K}\to\mathbf{k}$, etc., and, recalling that V and U depend only on momentum transfers, obtain

$$[i(\partial/\partial t)-(1/2m)\mathbf{k}^2+\mu]G_{1,K}(\mathbf{k}+\mathbf{K}t;\mathbf{k}'+\mathbf{K}t') + \sum_{\mathbf{l}}(\mathbf{k}\mid V\mid \mathbf{l})G_{1,K}(\mathbf{l}+\mathbf{K}t;\mathbf{k}'+\mathbf{K}t') = \delta(\mathbf{k}-\mathbf{k}')+i\sum_{\mathbf{l,m,n}}(\mathbf{kl}\mid U\mid \mathbf{mn}) \times G_{2,K}(\mathbf{m}+\mathbf{K}t,\mathbf{n}+\mathbf{K}t^-;\mathbf{l}+\mathbf{K}t^+,\mathbf{k}'+\mathbf{K}t'). \tag{6.6}$$

From the structure of this equation, and the similar higher-order equations of the hierarchy, we see that if the Green's functions,

$$G_{\nu,0}(\mathbf{k}_1t_1,\mathbf{k}_2t_2,\cdots;\mathbf{k}_1't_1',\mathbf{k}_2't_2',\cdots), \tag{6.7}$$

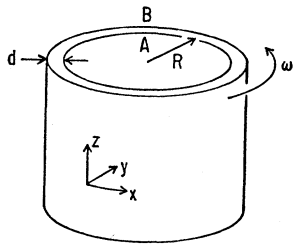

FIG. 1. Geometry used in Sec. 6. A and B are concentric cylinders between which the system under consideration is contained. $R\gg d\gg a_0$ (interatomic distance). The system rotates with an angular velocity ω. The coordinate system is such that the x direction is everywhere circumferential.

* This characterization, which refers to the most literal aspect of a superfluid—namely incomplete dragging by slowly rotating walls—appears first to have been used by Blatt and Butler (1955). It is directly applicable to neutral superfluids. For charged superfluids, equivalent criteria are the Meissner effect (Schafroth, 1955b) or flux quantization (Byers and Yang, 1961; Brenig, 1961; and Yang, 1962). Strictly speaking we leave open the possibility that a system which is *not* superfluid in our sense might have some other superfluid property, e.g., superthermal conductivity. No example of this kind is known. Furthermore, having recognized that a Bose condensate of type II is simply a system with long-range spatial order, such a possibility would now appear about as unlikely as the possibility of superfluid properties in solid NaCl.

* See, e.g., L. P. Kadanoff and G. Baym (1962).

TABLE I. Single bosons of types I and II.

	Type I	Type II
Example	^{4}He atoms	Exciton
Nature	Complexes of even number of real fermions	Particle–hole bound complexes
Form of Green's functions and density matrices	Singular as functions of momentum sum variables	Singular as functions of momentum difference variables
Momentum properties	Carry mechanical momentum	May or may not carry mechanical momentum

for $K=0$ are known, then *formally*, for $K\neq 0$, we have

$$G_{\nu,K}(\mathbf{k}_1t_1, \mathbf{k}_2t_2, \cdots; \mathbf{k}_1't_1', \mathbf{k}_2't_2', \cdots)$$
$$=G_{\nu,0}(\mathbf{k}_1-\mathbf{K}t_1, \mathbf{k}_2-\mathbf{K}t_2, \cdots; \mathbf{k}_1'-\mathbf{K}t_1', \mathbf{k}_2'-\mathbf{K}t_2', \cdots). \quad (6.8)$$

However $G_{\nu,0}(\mathbf{q}_1t_1, \cdots)$ is defined only for the discrete values

$$q_{ix}=n_i(1/R), \qquad n_i=0, \pm 1, \cdots, \quad (6.9)$$

so that for arbitrary values of K, the right-hand side is, in general, undefined.

To proceed further we introduce as new variables the sum variables $\mathbf{Q}_\nu$ and the difference variables $\mathbf{q}_\nu$, $\mathbf{q}_i$, and $\mathbf{q}_i'$:

$$\mathbf{Q}_\nu\equiv(\mathbf{k}_1+\mathbf{k}_2+\cdots\mathbf{k}_\nu)+(\mathbf{k}_1'+\mathbf{k}_2'+\cdots\mathbf{k}_\nu'),$$
$$\mathbf{q}_\nu\equiv(\mathbf{k}_1+\mathbf{k}_2+\cdots\mathbf{k}_\nu)-(\mathbf{k}_1'+\mathbf{k}_2'+\cdots\mathbf{k}_\nu'),$$
$$\mathbf{q}_i\equiv\mathbf{k}_{i+1}-\mathbf{k}_i;$$
$$\mathbf{q}_i'\equiv\mathbf{k}_{i+1}'-\mathbf{k}_i' \qquad (i=1, \cdots\nu-1). \quad (6.10)$$

Then, suppressing the time arguments, Eq. (6.8) can be written as

$$G_{\nu,K}(\mathbf{Q}_\nu; \mathbf{q}_\nu; \mathbf{q}_1, \mathbf{q}_2, \cdots; \mathbf{q}_1', \mathbf{q}_2', \cdots)$$
$$=G_{\nu,0}(\mathbf{Q}_\nu-2\nu\mathbf{K}; \mathbf{q}_\nu; \mathbf{q}_1, \mathbf{q}_2, \cdots; \mathbf{q}_1', \mathbf{q}_2', \cdots). \quad (6.11)$$

We now have two possible cases:

(A) Every $G_{\nu,0}$ is a smooth* function of the discrete sum variable $\mathbf{Q}_\nu$. This is the situation for systems without ODLRO. For in such systems, singular behavior in momentum space occurs only in the difference variables $\mathbf{q}_\nu$, $\mathbf{q}_i$, and $\mathbf{q}_i'$. Thus a factor $\delta(\mathbf{q}_\nu)$ is common to all systems with translational invariance, and factors like $\delta(q_i'+q_i-2k)$ occur in condensed states of type II [see Eq. (5.3) and asterisk footnote on p. 5]. In this case, the right-hand side is to be interpreted in the sense of an interpolation between the discrete values of $\mathbf{Q}_\nu$. The $G_{\nu,K}$, so defined, satisfy the equations of the hierarchy, such as (6.5). This follows at once, since—in view of the smooth dependence of the $G_{\nu,K}$ on the sum variables—summation over these variables may be replaced by integrations and, by a shift of variables, the equations can then be reduced to those for $K=0$. Similarly the free energy F_K, which is expressible as an integral involving $G_{1,K}$ and $G_{2,K}$, can by a shift of variables be shown to be identical to F_0. Hence such a system is normal.

(B) Some Green's functions $G_{\nu,0}$ have a δ-function dependence on the sum variables Q_ν. For example, in the B.C.S. theory we have $\delta(Q_2)$ occurring in $G_{2,0}$. In view of Sec. 4 [see especially Eq. (4.4) and footnote on p. 4] this is the case only for a condensed state of type I, or equivalently, for a state with ODLRO. In this case, for a general value of K, we, of course, cannot use interpolation over the discrete sum variables to obtain $G_{\nu,K}$ from $G_{\nu,0}$ from Eq. (6.11).* Thus $G_{\nu,K}$ is not expressible in terms of $G_{\nu,0}$ by a simple shift of variables.† Since all Green's functions are interconnected by the equations of motion, it follows that in particular $G_{1,K}$ and $G_{2,K}$ (even if themselves free of the critical δ functions) cannot be expressed by a shift of variables in terms of $G_{1,0}$ and $G_{2,0}$. Thus, for a general K, the free energy F_K cannot be reduced to F_0 and hence such a system is superfluid.

7. CONCLUDING REMARKS

In the preceding sections we have pointed out the existence of two quite different types of bosons. We have observed that when the first type condenses, the resulting system shows a macroscopic "off-diagonal" order which leads to superfluid properties; while when the second type condenses, there results a long-range macroscopic order of the usual type as is familiar from crystalline solids. In this way we have related both known kinds of long-range order to Bose condensation.

This point of view gives some insight into many kinds of phase transitions, such as superfluid, superconducting, distortive, excitonic, magnetic, and liquid–solid transitions.

Some systems may be viewed as simultaneously containing condensates of several type II bosons. Thus a

* For the present purpose, "smooth" means absence of Kronecker δ-functions.

* For special discrete values of K, $G_{\nu,K}$ *can* be expressed in terms of $G_{\nu,0}$. This gives rise to the well-known periodic behavior of F_K as a function of K (Byers and Yang, 1961; Brenig, 1961).

† In fact, for example for small K, the arguments of the critical δ functions remain unshifted.

TABLE II. Condensed states of types I and II.

	Type I	Type II
Example	He II	Excitonic Phase
Type of additional order	Off-diagonal long-range order	Diagonal long-range order
Superfluidity	Yes	No
Form of Green's functions and density matrices	Macroscopic singularities as functions of momentum sum variables	Macroscopic singularities as functions of momentum difference variables

crystal may be regarded as a simultaneous condensate of three bosons, with wave vectors corresponding to three principal reciprocal lattice vectors, $\mathbf{K}_1$, $\mathbf{K}_2$, and $\mathbf{K}_3$. Other systems, such as a crystalline superconductor may be viewed as a condensate of type I bosons (Cooper pairs), in a condensate of type II bosons (the normal host crystal).

Thus we have a broad framework for describing all manifestations of macroscopic order in terms of condensates of appropriate bosons.

For convenience, we summarize the main points of this paper in Tables I and II.

We wish to make two other closing remarks.

Our discussion has been limited to systems with translational invariance. This was done since one is accustomed to associate definite wave vectors with isolated bosons. However, Yang's (1962) work on off-diagonal long range order indicates an approach for dealing with systems lacking such invariance.

Secondly, the reader may be puzzled by our discussion of distortive transitions in terms of Bose condensations since, e.g., a distortive lattice transition might very well be discussed in terms of purely classical (i.e., nonquantum) lattice dynamics. In fact there is no paradox in this. We show in Appendix II that a classical lattice distortion can be regarded as a Bose condensation of phonons.

APPENDIX I. MOMENTUM PROPERTIES OF THE TWO KINDS OF BOSONS

We show first that a type I boson, characterized by Eq. (2.8) (or its generalization), carries mechanical momentum. The essential feature of (2.8), for the present purpose, is the appearance of momentum sums such as $\mathbf{p}_1+\mathbf{p}_2$ in the arguments of the δ functions.

For simplicity we discuss a many-fermion system, consisting of a single species, in which a single 2-fermion boson is present [see Eq. (2.8)]. An insulator, with an additional two fermions in a bound state, might be an example. We consider the system enclosed in a cube of volume $\Omega=L^3$, on which periodic boundary conditions are imposed.

It is convenient to introduce, as a formal device, a constant vector potential in the x direction

$$\mathbf{A}=-(c/e)\mathbf{K}, \qquad \mathbf{K}=(K,0,0), \qquad \text{(AI.1)}$$

and to define the following K-dependent Hamiltonian (Kohn, 1964),

$$H(K)=\sum(1/2m)(\mathbf{p}+\mathbf{K})^2 c_{\mathbf{p}}{}^* c_{\mathbf{p}}+V+U; \qquad \text{(AI.2)}$$

here V and U represent, respectively, interaction with an external potential and mutual interaction. Let the set $E_\alpha(K)$ be the complete spectrum of $H(K)$ for all crystal momenta $\mathbf{k}$, each $E_\alpha(K)$ being an analytic function of K. Then, from (AI.2) we obtain directly for the x component of the total momentum

$$(\alpha \mid P_x \mid \alpha)=m\left(\alpha \left| \left[\frac{dH}{dK}\right]_{K=0} \right| \alpha\right)=m\left.\frac{dE_\alpha(K)}{dK}\right|_{K=0}. \qquad \text{(AI.3)}$$

Thus we see that the system carries momentum in the state α if and only if $E_\alpha(K)$ has a K dependence (barring accidental vanishing of the derivative).

For certain discrete values of K,

$$K_n=(2\pi/L)n, \qquad n=0,\pm1,\cdots, \qquad \text{(AI.4)}$$

K may be removed from $H(K)$ by the unitary gauge transformation

$$\Phi\rightarrow\Phi\exp[-iK_n(x_1+x_2+\cdots x_N), \qquad E\rightarrow E \qquad \text{(AI.5)}$$

on the wave function.*

Hence the spectra of $H(0)$ and $H(K_n)$ must be identical:

$$\{E_\alpha(0)\}=\{E_\alpha(K_n)\}. \qquad \text{(AI.6)}$$

This of course does *not* imply that, for a *given* α, $E_\alpha(K_n)=E_\alpha(0)$. Instead one could have $E_\beta(K_m)=E_\alpha(0)$ [see Fig. 2, where, e.g., $E_2(K_1)=E_1(0)$].

Now let $\rho_\alpha{}^{(2)}(0)$ and $E_\alpha(0)$ be, respectively, the two-particle density matrix and eigenvalue of $H(K)$ corresponding to the 1-boson state of wave vector $\mathbf{k}$, and $K=0$; also let $\rho_\alpha{}^{(2)}(K)$ and $E_\alpha(K)$ be the analytic continuations of these quantities. Let $\rho_\beta{}^{(2)}(K_1)$ and $E_\beta(K_1)$ [$=E_\alpha(0)$] be the density matrix and eigenvalue

* For other values of K, the transformation (AI.5) violates the periodic boundary conditions.

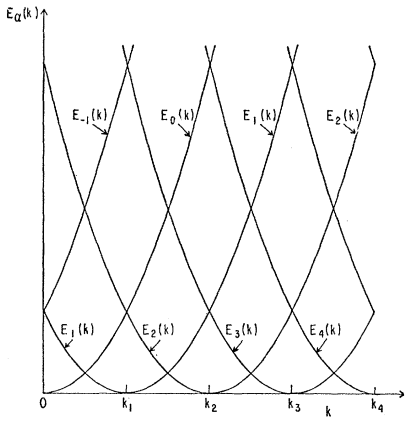

FIG. 2. Dependence of the one-boson energy spectrum on the gauge parameter K (schematic).

of $H(K)$ for $K=K_1$ and the same physical 1-boson state. Then, by (AI.5),

$$(\mathbf{p}_1', \mathbf{p}_2' \mid \rho_\beta^{(2)}(K_1) \mid \mathbf{p}_1, \mathbf{p}_2)$$
$$= (\mathbf{p}_1'+\mathbf{K}_1, \mathbf{p}_2'+\mathbf{K}_1 \mid \rho_\alpha^{(2)}(0) \mid \mathbf{p}_1+\mathbf{K}_1, \mathbf{p}_2+\mathbf{K}_1). \quad \text{(AI.7)}$$

Now $(\mathbf{p}_1', \mathbf{p}_2' \mid \rho_\alpha^{(2)}(0) \mid \mathbf{p}_1, \mathbf{p}_2)$ contains a factor $\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{k})$ and hence, by (AI.7),

$$(\mathbf{p}_1', \mathbf{p}_2' \mid \rho_\beta^{(2)}(K_1) \mid \mathbf{p}_1, \mathbf{p}_2)$$

contains a factor $\delta(\mathbf{p}_1+\mathbf{p}_2+2\mathbf{K}_1-\mathbf{k})$. As the arguments of the two δ-functions are discrete and different, we see that $\rho_\beta^{(2)}(K_1)$ is *not* the analytic continuation of $\rho_\alpha^{(2)}(0)$. Thus $\beta\neq\alpha$. Since, however, by definition, $E_\beta(K_1)=E_\alpha(0)$, it follows that (barring accidental degeneracies)

$$E_\alpha(K_1)\neq E_\alpha(0). \quad \text{(AI.8)}$$

Thus $E_1(K)$ is K dependent and hence,

$$(1 \mid P_x \mid 1)\neq 0, \quad \text{(AI.9)}$$

except for special circumstances such as $\mathbf{k}=0$.

We now turn to type II bosons. The discussion through Eq. (AI.7) applies equally to them. However the two-particle density matrix $\rho_\alpha^{(2)}(0)$ now contains δ-functions whose arguments are *differences* of momenta such as $\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{k})$, and hence, by (AI.7), $\rho_\beta^{(2)}(K_1)$ contains the *same* δ function $\delta((\mathbf{p}_1'+\mathbf{K}_1)-(\mathbf{p}_1+\mathbf{K}_1)-\mathbf{k})=\delta(\mathbf{p}_1'-\mathbf{p}_1-\mathbf{k})$. Therefore we can no longer conclude that $\beta\neq\alpha$ or that $E_\alpha(K_1)\neq E_\alpha(0)$, and thus we cannot use the previous argument to show that the momentum is nonvanishing.

Do type II bosons then carry momentum or not? An exciton in an insulator does not. This follows at once from the fact that the motion of a bound pair of fermion and fermion hole in an insulator does not shift the center of mass of the system.* On the other hand, zeroth sound in ^{3}He has a real momentum given by $\mathbf{P}=\mathbf{k}$, which follows at once from the translational invariance of the Hamiltonian. Thus we see that type II bosons may or may not carry mechanical momentum.

* The absence of momentum may also be derived more formally from the "disconnectedness property" of the many-body wave function discussed in Kohn (1964).

APPENDIX II. LATTICE DISTORTION AS BOSE CONDENSATION OF PHONONS

Consider a monatomic crystal in an original configuration C at $T=0°$. Let the mass M be very large, so that quantum zero-point fluctuations are small, and write the wave function as

$$\Phi(\mathbf{u}(1), \mathbf{u}(2), \cdots, \mathbf{u}(N)), \quad \text{(AII.1)}$$

where $\mathbf{u}(l)$ is the displacement of the lth nucleus from its equilibrium position $\mathbf{R}(l)$.

Next consider a slightly distorted configuration C' in which the nuclei vibrate about new lattice positions:

$$\mathbf{R}'(l)=\mathbf{R}(l)+\mathbf{v}(l). \quad \text{(AII.2)}$$

Let the new wave function be

$$\Phi'(\mathbf{u}(1), \mathbf{u}(2), \cdots)=\Phi(\mathbf{u}(1)-\mathbf{v}(1), \mathbf{u}(2)-\mathbf{v}(2), \cdots), \quad \text{(AII.3)}$$

where, while we allow for the changes of the equilibrium positions, we ignore as unessential other changes in the wave function. This is reasonable when both the excursions $\mathbf{u}(l)$ and displacements $\mathbf{v}(l)$ are small compared to the lattice spacing. The new wave function can evidently be written in the form

$$\Phi'(\mathbf{u}(1), \mathbf{u}(2), \cdots)$$
$$= \exp\{-\sum_{i,l} v_i(l)[\partial/\partial u_i(l)]\}\Phi(\mathbf{u}(1), \mathbf{u}(2), \cdots), \quad \text{(AII.4)}$$

since, by Taylor's theorem, the operator $\exp[a(\partial/\partial x)]$ is just a displacement operator.

The sum occurring in the exponent can be written in terms of phonon operators. As an illustration we consider the formation of a simple superlattice in which the atomic displacements are alternately $\mathbf{v}(l)=\pm\mathbf{v}$. We may write this as

$$\mathbf{v}(l)=\mathbf{v}\exp[i\mathbf{k}_0\cdot\mathbf{R}(l)], \quad \text{(AII.5)}$$

where

$$\mathbf{k}_0=\mathbf{K}_1/2 \quad \text{(AII.6)}$$

and $\mathbf{K}_1$ is an appropriate reciprocal lattice vector.

We recall the normal mode expansion for a Bravais lattice,

$$u_i(l)=\sum_s[\hbar/2MN\omega(s)]^{1/2}e_i(s)$$
$$\times\{a(s)\exp[i\mathbf{k}\cdot\mathbf{R}(l)]+a^*(s)\exp[-i\mathbf{k}\cdot\mathbf{R}(l)]\} \quad \text{(AII.7)}$$

where s stands for both k and the polarization index j, $\mathbf{e}(s)$ is a polarization vector, and $a(s)$ and $a^*(s)$ are phonon destruction and creation operators satisfying

the commutation rules

$$[a(s), a^*(s')]=\delta_{ss'}. \tag{AII.8}$$

From (AII.7) we derive

$$\partial/\partial u_i(l) = (i/h)\, p_i(l) = i(M/\hbar)\dot{u}_i(l)$$
$$=\sum_s (M\omega(s)/2\hbar N)^{1/2} e_i(s)$$
$$\times\{a(s)\,\exp[i\mathbf{k}\cdot\mathbf{R}(l)]-a^*(s)\,\exp[-i\mathbf{k}\cdot\mathbf{R}(l)]\}. \tag{AII.9}$$

Combining now (AII.5) and (AII.9) gives the desired result

$$\sum_{i,l} v_i(l)[\partial/\partial u_i(l)]=\sum_j [MN\omega(\mathbf{k}_0, j)/2\hbar]^{1/2}[\mathbf{e}(\mathbf{k}_0, j)\cdot\mathbf{v}]$$
$$\times[a(\mathbf{k}_0, j)-a^*(\mathbf{k}_0, j)]. \tag{AII.10}$$

Let us further assume for simplicity that $\mathbf{v}$ is parallel to one of the polarization vectors, say $\mathbf{e}(\mathbf{k}_0, 1)$. Then (AII.10) simplifies to

$$\sum_{i,l} v_i(l)[\partial/\partial u_i(l)]=\alpha(a-a^*), \tag{AII.11}$$

where

$$\alpha\equiv (MN\omega/2\hbar)^{1/2} \tag{AII.12}$$

and

$$a\equiv a(\mathbf{k}_0, 1), \qquad \omega\equiv\omega(\mathbf{k}_0, 1); \tag{AII.13}$$

and Eq. (AII.4) now becomes

$$\Phi'=\exp[-\alpha(a-a^*)]\Phi. \tag{AII.14}$$

Of course the exponential acts only on the wave function of the oscillator $(\mathbf{k}_0, 1)$. In second-quantized language, the state of this oscillator is changed from the original zero-phonon ground state $|0\rangle$ to a new state $|\alpha\rangle$ given by

$$|\alpha\rangle=\exp[-\alpha(a-a^*)]\,|0\rangle. \tag{AII.15}$$

This is just a coherent state in the sense used by Glauber (1963) for photon oscillators. Using the fact that $[a, a^*]=1$, we have the identity

$$\exp[-\alpha(a-a^*)]=\exp(-\tfrac{1}{2}\alpha^2)\cdot\exp(\alpha a^*)\exp(-\alpha a) \tag{AII.16}$$

which gives

$$|\alpha\rangle=\exp(-\tfrac{1}{2}\alpha^2)\exp(\alpha a^*)\,|0\rangle$$
$$=\exp(-\tfrac{1}{2}\alpha^2)\sum_n[\alpha^n/(n!)^{1/2}]\,|n\rangle. \tag{AII.17}$$

Thus the new state is a coherent linear combination of n-phonon states. The maximum amplitude occurs for $\alpha/n^{1/2}=1$, or for

$$n=(M\omega v^2/2\hbar)N. \tag{AII.18}$$

We may verify that the excitation energy of these phonons,

$$E=n\hbar\omega=N(M\omega^2/2)v^2, \tag{AII.19}$$

is just the classical potential energy of distortion. Since the new state has present a macroscopic number of phonons in a single mode, it is a Bose-condensed state.

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