Concept of Off-Diagonal Long-Range Order and the Quantum Phases of Liquid He and of Superconductors

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I. INTRODUCTION

We consider a many-particle system with fixed number of particles, with a density matrix ρ. We define the reduced density matrices $\rho_1, \rho_2, \cdots$ by

$$\mathrm{Sp}\ \rho = 1\ , \tag{1}$$

$$\langle j|\rho_1|i\rangle = \mathrm{Sp}\ a_j \rho a_i^\dagger$$
$$\langle kl|\rho_2|ij\rangle = \mathrm{Sp}\ a_k a_l \rho a_j^\dagger a_i^\dagger \tag{2}$$
$$\text{etc.},$$

where $i, j, \cdots$ represent single particle states and a_i, a_j the annihilation operators for these states. In all our discussions, unless explicitly stated otherwise, we consider a collection of identical particles, either fermions or bosons.

1. This paper is concerned with the concept that in a many-body system of bosons or fermions, it is possible to have an off-diagonal long-range order (ODLRO) of the reduced density matrices in the coordinate space representation. The onset of such an order leads to a new thermodynamic phase of the system. It is reasonable to assume that superfluid He II and the superconductors are phases characterized by the existence of such an order.

2. The general characteristics of the gaseous, the liquid, and the solid phases are well known and are describable in classical mechanical terms. In particular, the solid phase is characterized by the existence of a long-range correlation. However, the long-range correlation in the solid is exhibited in quantum mechanics in the diagonal element of ρ_2 in coordinate space and is quite *different* from the off-diagonal-long-range-order that we shall discuss in this paper. Since off-diagonal elements have no classical analog, the off-diagonal long-range order discussed in this paper is a quantum phenomenon not describable in classical mechanical terms.

3. The long-range correlation in a solid is the basis of essentially all approximate calculations of the properties of a solid. If ODLRO is the characteristic of the phases He II and superconductors, it seems that a reasonable calculation of their properties can only be made with ODLRO explicitly built into the physical picture.

4. We shall show that the existence of ODLRO in ρ_n implies its existence in reduced density matrices ρ_m with $m > n$. [In fact for $m \geqq 2n$, the ODLRO occurs in a more intensified form.] The *smallest* n for which ODLRO occurs gives the collection of n particles that, in a sense, forms a basic group [hereafter called the basic group] exhibiting the long-range correlation. Of course, the system of particles that we consider may be a collection of particles of different kinds, such as nuclei and electrons. We shall give reasons to believe that the basic group must be composed of bosons and an *even* number of fermions. The phenomena of ODLRO is therefore fundamentally related to that of Bose-Einstein condensation. Or, more precisely, Bose-Einstein condensation is the simplest form of an ODLRO.

5. For a system of bosons the possible existence of ODLRO in ρ_1 was discussed in a paper by Penrose[1] and later in a paper by Penrose and Onsager.[2]

For the fermions, the ideas discussed in this paper are clearly related to the ideas of "long-range order of the average momentum," "macroscopic quantum state," etc., of London.[3] They are also clearly related to the ideas based on quasi-boson condensation in the papers of Schafroth, Butler, and Blatt.[4] Furthermore, since the wave functions assumed by Bardeen, Cooper, and Schrieffer[5] and by Bogoliubov[6] (as an *ansatz*) do have the ODLRO, the contents of

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[1] O. Penrose, Phil. Mag. **42**, 1373 (1951).
[2] O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).
[3] F. London, *Superfluids* (John Wiley & Sons, Inc., Vol. 1, 1950, Vol. 2, 1954).
[4] M. R. Schafroth, Phys. Rev. **96**, 1442 (1954); M. R. Schafroth, S. T. Butler, and J. M. Blatt, Helv. Phys. Acta **30**, 93 (1957).
[5] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[6] N. N. Bogoliubov, Nuovo cimento **7**, 794 (1958).

the present paper are clearly also related to their work. However, it seems to us that in none of the previous works has the question of the detailed mathematical characterization of the superconducting state been raised. [Within the context of this question, the pairing idea of Bardeen, Cooper, and Schrieffer seems to be the closest in its implications to the ideas discussed in this paper.] Nor has there been an explicit understanding of exactly in what sense are the characterization of superfluidity and that of superconductivity similar, a similarity that London had emphasized.

6. It will be shown in Sec. IV that the existence of ODLRO gives rise to the phenomena of quantized magnetic flux. Furthermore, for cases where the basic group is two electrons, the unit of magnetic flux is $hc/2e$, as it was experimentally found.[7]

7. There is no discussion in this paper of the properties of the Hamiltonian that is needed to ensure the existence of ODLRO at low temperatures.

In the solid phase the existence of long-range correlation makes it necessary to introduce additional macroscopic variables, (namely, the strain) to describe the thermodynamics of the system. It is important to recognize that similarly the onset of ODLRO necessitates the introduction of additional macroscopic variables. What these variables are, however, is not discussed in this paper, except for a speculation about the fraction of superfluid in Sec. 10 and one about the penetration depth in Sec. 40.

II. PROPERTIES OF ρ_n

8. The reduced density matrices of Sec. 1 have the following properties:

$$\rho_n = \text{positive definite or semidefinite}, \tag{3}$$

$$\begin{aligned} \mathrm{Sp}\,\rho_1 &= N\,, \\ \mathrm{Sp}\,\rho_2 &= N(N-1)\,, \\ \mathrm{Sp}\,\rho_3 &= N(N-1)(N-2)\,, \quad \text{etc.}\,, \end{aligned} \tag{4}$$

where N = total number of particles.

It is obvious that if we perform a unitary transformation on the operators a_i, the reduced density matrices ρ_n undergo a similar transformation. In fact, the transformation from, e.g., the coordinate to the momentum space representation of the ρ's follows the same law as the usual operators.

The following formulas are easy to prove:

$$\begin{aligned} \textstyle\sum_i \langle ij|\rho_2|ik\rangle &= (N-1)\langle j|\rho_1|k\rangle\,, \\ \textstyle\sum_i \langle ijk|\rho_3|ilm\rangle &= (N-2)\langle jk|\rho_2|lm\rangle\,, \quad \text{etc.} \end{aligned} \tag{5}$$

[7] B. S. Deaver and W. M. Fairbank, Phys. Rev. Letters **7**, 43 (1961); R. Doll and M. Näbauer, *ibid.* **7**, 51 (1961).

In defining the reduced density matrix ρ_2 in (2), we allow the indices i and j to run freely over all states. Clearly, there is a symmetry or antisymmetry when we switch i and j. There is, of course, a natural way to reject the superfluous elements of ρ_2, $\rho_3\cdots$ due to these symmetries by considering ρ_2, $\rho_3,\cdots$ to operate only on states of the correct symmetry. A whole mathematical formalism can be neatly worked out for this process. We shall, however, not go into it, as it does not really add to the clarity of the physics of the problem.

9. We define λ_n as the largest eigenvalue of ρ_n. From (3) and (4) it is obvious that all eigenvalues of ρ_n are $\geqq 0$, and,

$$\begin{aligned} \lambda_1 &\leqq N\,, \\ \lambda_2 &\leqq N(N-1)\,, \\ \lambda_3 &\leqq N(N-1)(N-2)\,, \\ &\text{etc.} \end{aligned} \tag{6}$$

10. *Theorem 1.* $\lambda_2 \geqq \lambda_1^2 - \lambda_1$ for a system of bosons.

Proof. Let f_i be the normalized eigenvector for $\langle i'|\rho_1|i\rangle$ with eigenvalue λ_1.

$$\text{Define} \quad F = \textstyle\sum f_i^* a_i\,.$$

$$\text{Then} \quad \mathrm{Sp}\,F^\dagger F\rho = \lambda_1\,.$$

Use $f_i f_j$ as a trial wave function for $\langle i'j'|\rho_2|ij\rangle$. Clearly,

$$\lambda_2 \geqq \text{trial expectation value of } \rho_2 = \mathrm{Sp}\,F^\dagger F^\dagger F F\rho\,. \tag{7}$$

But $$F^\dagger F = FF^\dagger - 1\,.$$

Thus $$\lambda_2 \geqq \mathrm{Sp}\,F^\dagger F F^\dagger F\rho - \lambda_1\,.$$

$$\text{Using } 0 \leqq \mathrm{Sp}\,(F^\dagger F - \lambda_1)^2\rho = \mathrm{Sp}\,F^\dagger F F^\dagger F\rho - \lambda_1^2 \tag{8}$$

we obtain $$\lambda_2 \geqq \lambda_1^2 - \lambda_1\,, \quad \text{Q.E.D.}$$

Theorem 2. $\lambda_3 \geqq \lambda_1^3 - 2\lambda_1^2 - \lambda_2$ for a system of bosons.

Proof. Use the same notation as the proof of Theorem 1.

$$\begin{aligned} \lambda_3 &\geqq \mathrm{Sp}\,F^\dagger F^\dagger F^\dagger F F F\rho \\ &= \mathrm{Sp}\,F^\dagger F^\dagger (FF^\dagger - 1) F F\rho \\ &\geqq \mathrm{Sp}\,F^\dagger F^\dagger F F^\dagger F F\rho - \lambda_2\,. \end{aligned}$$

$$\begin{aligned} \text{But,}\quad 0 &\leqq \mathrm{Sp}\,F^\dagger (F^\dagger F - \lambda_1)^2 F\rho = \mathrm{Sp}\,F^\dagger F^\dagger F F^\dagger F F\rho \\ &\quad - 2\lambda_1\,\mathrm{Sp}\,F^\dagger F^\dagger F F\rho + \lambda_1^3 = \mathrm{Sp}\,F^\dagger F^\dagger F F^\dagger F F\rho \\ &\quad - 2\lambda_1\,\mathrm{Sp}\,F^\dagger F F^\dagger F\rho + 2\lambda_1\,\mathrm{Sp}\,F^\dagger F\rho + \lambda_1^3 \end{aligned}$$

By (8), therefore,

$$\text{Sp } F^\dagger F^\dagger FF^\dagger FF\rho \geq 2\lambda_1 \text{ Sp } F^\dagger FF^\dagger F\rho - 2\lambda_1^2 - \lambda_1^3$$
$$\geqq 2\lambda_1^3 - 2\lambda_1^2 - \lambda_1^3 = \lambda_1^3 - 2\lambda_1^2 .$$

Thus $\lambda_3 \geqq \lambda_1^3 - 2\lambda_1^2 - \lambda_2$, Q.E.D.

Theorem 3. $\lambda_4 \geqq \lambda_2^2 - 4\lambda_3 - 2\lambda_2$ for a system of bosons.

Proof. Let f_{12} be the normalized eigenvector of $\langle 1'2'|\rho_2|12\rangle$ with eigenvalue λ_2. Define

$$F = \sum_{1,2} f_{12}^* a_1 a_2 .$$

The proof follows essentially the same lines as that of Theorem 1. In place of (8) one uses

$$0 \leqq \text{Sp } (F^\dagger F - \lambda_2)^2\rho = \text{Sp } (F^\dagger F)^2\rho - \lambda_2^2 .$$

In place of (7) one uses

$$\lambda_4 \geqq \text{Sp } F^\dagger F^\dagger FF\rho ,$$

obtained by taking a product trial wave function for ρ_4. By carrying out the detailed computation of

$$F^\dagger[F^\dagger F - FF^\dagger]F$$

one easily obtains

$$\lambda_4 \geqq \lambda_2^2 - 4\lambda_3 - 2\lambda_2 , \quad \text{Q.E.D.}$$

Theorem 4. $\lambda_4 \geqq \lambda_2^2 - 2\lambda_2$ for a system of fermions. This theorem can be proved in the same way as Theorem 3.

Notice that for fermions if we follow the reasoning that led to Theorem 1, we do not obtain any useful results.

Theorem 1 has been stated before[8] without proof. It is clear that theorems establishing lower bounds for $\lambda_5, \lambda_6, \cdots$ can be obtained in a similar fashion. These theorems presumably will show that if ρ_n has[9] an eigenvalue of the order of N, $\rho_{n+1}, \rho_{n+2}, \cdots$ have also large eigenvalues. Furthermore for the boson case, if λ_1 is of the order of N, $(\lambda_2)^{1/2}$ $(\lambda_3)^{1/3}\cdots$ form a monotonically increasing series $\leqq N$. Thus they approach a limit and it is tempting[8] to identify this limit with the size of the superfluid component of the system, if ρ is the density matrix for thermal equilibrium.

11. *Theorem 5.* For fermions, $\lambda_1 \leqq 1$.

Proof. This follows from the fact that the expectation value of $a_i^\dagger a_i$ where a_i is the annihilation operator for any states is $\leqq 1$. Q.E.D.

Theorem 6.

$$\lambda_2 \leqq N(M - N + 2)/M \tag{9}$$

for a system of N fermions in M states. We assume both M and N to be even.

This theorem is proved in Appendix A. The proof will also show that the upper limit for λ_2 given by (9) can be reached, and can be reached in essentially only one way.

Notice that for any value of M, for fermions,

$$\lambda_2 \leqq N .$$

Theorems 5 and 6 suggest the following generalization:

Conjecture. There exists numerical constants β_3, $\beta_4, \cdots$ so that

$$\lambda_n \leqq (N)^{n/2}\beta_n \quad \text{for} \quad n = \text{even} ,$$
$$\lambda_n \leqq (N)^{(n-1)/2}\beta_n \quad \text{for} \quad n = \text{odd} ,$$

for a system of identical fermions.

These theorems demonstrate that large eigenvalues in the reduced density matrices for fermions essentially originate from pairs of fermions forming Bose-Einstein degeneracy.

12. *Theorem 7.* For a system of N_b bosons and N_f fermions, consider

$$\langle b'f'|\rho_2|bf\rangle , \tag{10}$$

where b and f label boson and fermion states, respectively. Its largest eigenvalue is $\leqq 1 + \lambda_1$ where λ_1 is the largest eigenvalue of $\langle b'|\rho_1|b\rangle$.

Proof. Consider the normalized eigenfunction f_{bf} for (10) with the largest eigenvalue λ. By a unitary transformation on the states of the fermion and one on the states of the boson, f_{bf} can be reduced to a paired form:

$$F \equiv \sum_{b,f} f_{bf} a_b \alpha_f = \xi_1 a_1 \alpha_1 + \xi_2 a_2 \alpha_2 + \cdots , \tag{11}$$

where α are the annihilation operators for the fermion states and a those of the boson states. In (11) all ξ's are $\geqq 0$. Now

$$F^\dagger F + FF^\dagger = \xi_1^2(a_1^\dagger a_1 + \alpha_1\alpha_1^\dagger) + \xi_2^2(a_2^\dagger a_2 + \alpha_2\alpha_2^\dagger) + \cdots .$$

But $\lambda = \text{Sp } F^\dagger F\rho \leqq \text{Sp } (F^\dagger F + FF^\dagger)\rho$.

Furthermore, $\text{Sp } \alpha_i\alpha_i^\dagger\rho \leqq 1$,

$$\sum \xi_1^2 = 1 ,$$
$$\text{Sp } (a_i^\dagger a_i)\rho \leqq \lambda_1 .$$

Thus $\lambda \leqq \lambda_1 + 1$, Q.E.D.

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[8] C. N. Yang, Physica **26**, S49 (1960).

[9] We use the term "of the order of N" to apply loosely to a quantity $\geqq \alpha N$ where α is a fixed number independent of N.

This theorem suggests the following generalization:

Conjecture. In a mixture of particles, consider

$$\langle a'b',c'\cdots|\rho_n|a,b,c,\cdots\rangle \tag{12}$$

where a, b, c are states of bosons or fermions. If the collection of particles in $a, b, c,\cdots>$ contains an odd number of fermions, then the largest eigenvalue of (12) is $\leqq$ a function, independent of N, of the largest eigenvalues of the reduced density matrices

$$\langle a''',b''',\cdots|\rho_m|a'',b'',c'',\cdots\rangle\,,$$

where a'', b'', $c'',\cdots$ is a subgroup of particles in (12).

It follows from this conjectured theorem that if all lower order ρ's have no eigenvalues as large as of the order of N, then (12) also does not have such a large eigenvalue, if a, b, $c,\cdots\rangle$ contains an odd number of fermions. In the next chapter we shall demonstrate the equivalence of the existence for ρ_n of large eigenvalues and that of an off-diagonal long-range order. The above conjecture forms, then, the basis of the discussion in Sec. 4 about the basic group.

III. OFF-DIAGONAL LONG-RANGE ORDER (ODLRO)

13. We shall now discuss the equivalence of the existence for ρ_n of eigenvalues of the order of N and that of an off-diagonal long-range order. To illustrate the concept consider a system of N free fermions or bosons in a periodic box of volume Ω in thermal equilibrium. ρ commutes with the total momentum. Therefore in the momentum representation ρ_1 is diagonal:

$$\langle\mathbf{p}'|\rho_1|\mathbf{p}\rangle = \delta_{\mathbf{pp}'}n_{\mathbf{p}}\,,$$

where the diagonal element $n_{\mathbf{p}}$ is the average occupation number of the single particle state $\mathbf{p}$.

$$n = \frac{\mu e^{-p^2/T}}{1 \pm \mu e^{-p^2/T}}\,. \tag{13}$$

In coordinate representation

$$\langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle = (1/\Omega)\sum n_{\mathbf{p}}\exp i\mathbf{p}(\mathbf{x}' - \mathbf{x}) = g(\mathbf{x}' - \mathbf{x})\,. \tag{14}$$

For fermions, or for free bosons at high temperatures, all n are finite and

$$\langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle \to 0 \quad \text{as} \quad |\mathbf{x} - \mathbf{x}'| \to \infty\,. \tag{15}$$

But for free bosons below the Bose-Einstein transition temperature, $n_0 = N\alpha$, where α is a finite fraction. Therefore,

$$\langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle \to N\alpha/\Omega \quad \text{as} \quad |\mathbf{x} - \mathbf{x}'| \to \infty\,. \tag{16}$$

The existence of a Bose-Einstein condensation is thus characterized by the nonvanishing behavior of $\langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle$ as $|\mathbf{x} - \mathbf{x}'| \to \infty$.

14. If the condensation is in a state with $\mathbf{p} \neq 0$, it is clear that

$$\langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle \to (N\alpha/\Omega)\exp i\mathbf{p}(\mathbf{x}' - \mathbf{x})\,,$$
$$\text{as} \quad |\mathbf{x}' - \mathbf{x}| \to \infty\,. \tag{17}$$

It seems that the general criterion for Bose-Einstein condensation is

$$\int_\Omega \langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle d\mathbf{x}\langle\mathbf{x}|\rho_1|\mathbf{x}'\rangle = \text{order of } \Omega\,. \tag{18}$$

15. We now consider the case of N particles with any boundary condition and any density matrix ρ. By taking the trial wave function $\psi = 1/(\Omega)^{1/2}$ it is obvious that (16) implies the existence of a large eigenvalue of the order of $N\alpha$ for ρ_1. Conversely, if ρ_1 has a large eigenvalue $N\alpha$ with an eigenfunction $\phi(\mathbf{x})$, we can make a spectral resolution of ρ_1:

$$\langle x'|\rho_1|x\rangle = N\alpha\phi(\mathbf{x}')\phi^*(\mathbf{x}) + \rho_1' \tag{19}$$

where ρ_1' is a positive operator. It is reasonable to assume $\phi(\mathbf{x})$ to contain the normalization factor $1/(\Omega)^{1/2}$. Equation (19) shows that

$$\langle\mathbf{x}'|\rho_1|x\rangle \nrightarrow 0 \quad \text{as} \quad |\mathbf{x} - \mathbf{x}'| \to \infty\,. \tag{20}$$

16. We shall take (20) or (18) as the definition of the existence of an off-diagonal long-range order (ODLRO) in ρ_1. Its existence is equivalent to that of the existence of a large eigenvalue for ρ_1 of the order of N.

Proposition 1. The phase He II of liquid He is characterized by the existence of ODLRO in ρ_1 for the equilibrium density matrix of the interacting He atoms. This ODLRO is defined either by (20), or equivalently, by the condition that ρ_1 has an eigenvalue of the order of N.

17. For a system of bosons, if ODLRO exists in ρ_1, $\langle\mathbf{x}'|\rho_1|\mathbf{x}\rangle$ remains, in general, nonvanishing for all values of $\mathbf{x}$ and $\mathbf{x}'$. What is the characteristic of $\langle\mathbf{x}_1'\mathbf{x}_2'|\rho_2|\mathbf{x}_1\mathbf{x}_2\rangle$ in such a case? It is clear that a large contribution to ρ_2 comes from

$$\langle\mathbf{x}_1'|\rho_1|\mathbf{x}_1\rangle\langle\mathbf{x}_2'|\rho_1|\mathbf{x}_2\rangle$$

and therefore, in general, ρ_2 remains nonvanishing for all values of $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_1'$, and $\mathbf{x}_2'$.

The above statement is well illustrated by the example of the free Bose gas in equilibrium. In that

case, it is simplest to treat the equilibrium grand canonical ensemble. It is clear that

$$\langle \mathbf{p}_1'\mathbf{p}_2'|\rho_2|\mathbf{p}_1\mathbf{p}_2\rangle = \delta_{\mathbf{p}_1\mathbf{p}_1'}\delta_{\mathbf{p}_2\mathbf{p}_2'}n_{\mathbf{p}_1}n_{\mathbf{p}_2} + \delta_{p_1p_2}'\delta_{p_2p_1}'n_{\mathbf{p}_1}n_{\mathbf{p}_2} + \delta_{p_1p_1}'\delta_{p_2p_2}'\delta_{p_1p_2}m_{p_1}\,, \tag{21}$$

where $m_{\mathbf{p}}$ is the average of $M^2 - M - 2n_{\mathbf{p}}^2$ for the state $\mathbf{p}$, M being the occupation number of the state. A simple calculation shows that $m_p = 0$ for the equilibrium distribution. Thus

$$\langle \mathbf{x}_1'\mathbf{x}_2'|\rho_2|\mathbf{x}_1\mathbf{x}_2\rangle = g(\mathbf{x}_1' - \mathbf{x}_1)g(\mathbf{x}_2' - \mathbf{x}_2) + g(\mathbf{x}_1' - \mathbf{x}_2)g(\mathbf{x}_2' - \mathbf{x}_1)\,. \tag{22}$$

Therefore, for a free Bose gas, for the grand canonical ensemble,

$$\text{with ODLRO in } \rho_1, \qquad \rho_2 \not\approx 0 \text{ for all } x_1, x_1', x_2, x_2'\,; \tag{23}$$

without ODLRO in ρ_1, $\rho_2 \approx 0$ except in the neighborhood of

$$\text{(a) } \mathbf{x}_1 = \mathbf{x}_1',\ \mathbf{x}_2 = \mathbf{x}_2'\,; \qquad \text{and (b) } \mathbf{x}_1 = \mathbf{x}_2',\ \mathbf{x}_2 = \mathbf{x}_1'\,. \tag{24}$$

18. The two cases (23) and (24) are also characterized by the fact that the largest eigenvalue of ρ_2 is of the order of N^2 and is finite, respectively. What happens if it is of the order of N? This case cannot obtain for a *free* Bose gas in equilibrium, but may obtain for other systems. Following the argument in Sec. 15 for the ODLRO in ρ_1 we make a spectral separation of ρ_2, separating the largest eigenvalue

$$\langle \mathbf{x}_1'\mathbf{x}_2'|\rho_2|\mathbf{x}_1\mathbf{x}_2/ = N\alpha\varphi(\mathbf{x}_1'\mathbf{x}_2')\phi^*(\mathbf{x}_1\mathbf{x}_2) + \rho_2'\,, \tag{25}$$

where ρ_2' is positive. The eigenfunction $\phi(\mathbf{x}_1,\mathbf{x}_2)$, one can expect, is zero for large separations $|\mathbf{x}_1 - \mathbf{x}_2|$ and is $\sim 1/(\Omega)^{1/2}$ for microscopic separations for $\mathbf{x}_1$ and $\mathbf{x}_2$. Thus, we have a type of behavior intermediate between (23) and (24):

With ODLRO in ρ_2, but not in ρ_1:

$\rho_2 \approx 0$ except in the neighborhood of

$$\text{(a) } \mathbf{x}_1 = \mathbf{x}_1'\,,\quad \mathbf{x}_2 = \mathbf{x}_2'\,; \qquad \text{(b) } \mathbf{x}_1 = \mathbf{x}_2'\,,\quad \mathbf{x}_2 = \mathbf{x}_1'\,;$$

$$\text{and (c) } \mathbf{x}_1 = \mathbf{x}_2\,,\ \mathbf{x}_1' = \mathbf{x}_2' \text{ (but} |\mathbf{x}_1 - \mathbf{x}_2'| \text{may be } \infty)\,. \tag{26}$$

It is clear that if (26) obtains, ρ_2 has an eigenvalue of the order of N.

19. For a system of fermions, Theorem 5 shows that ODLRO cannot obtain for ρ_1. Theorem 6 shows, however, that ρ_2 may have eigenvalues of the order of N. Thus, for fermions ODLRO may occur in ρ_2 in the sense of (26).

Two examples are illuminating in this connection. For a system of free fermions in equilibrium, all eigenvalues of ρ_2 are finite (i.e., not of the order of N). Thus, neither in ρ_1 nor ρ_2 is there ODLRO. For a system in which the pair occupation hypothesis of Bardeen, Cooper, and Schrieffer[5] (BCS) is legitimate, it is easy to show that ρ_2 has an eigenvalue of the order of N. In fact in the proof of Theorem 6, in order to find a system with a maximum eigenvalue for ρ_2, one is forced to have pair occupation of single particle states exactly in the manner of the BCS ansatz.

20. *Proposition* 2. The superconducting state is characterized by the existence of ODLRO in

$$\langle e_1'e_2'|\rho_2|e_1e_2\rangle\,, \tag{27}$$

where e_1, e_2, e_1', e_2' represent electron states, for the ensemble in thermal equilibrium. This ODLRO is defined either by (26), or equivalently, by the condition that (27) has an eigenvalue of the order of N, the number of electrons in the system.

21. Actually the two propositions above are more restrictive than they need be. Take the case of He. To describe liquid He as a collection of He atoms is only an approximation. A much better description is a collection of electrons and He nuclei. A general characterization of a new phase exhibiting ODLRO should apply both to liquid He as a collection of He atoms and to liquid He as a collection of electrons and He nuclei. It is evident that in the latter description ODLRO first occurs in

$$\langle \mathrm{He}',e_1',e_2'|\rho_3|\mathrm{He},e_1,e_2\rangle$$

because any reduced density matrix of lower order would mostly describe only the internal structure of the He atom.

It thus seems that in a macroscopic system, ODLRO can set in at ρ_n. The theorems of II indicate that the reduced density matrix, to be called ρ_m, of lowest order which has ODLRO must operate on a basic group that consists of an even number of fermions and any number of bosons. For liquid He II the basic group is the He atom; for superconductors, the basic group is a set of two electrons. For ρ_m the largest eigenvalue is of the order of N. It has an ODLRO in the sense that in coordinate representation, when the unprimed coordinates are microscopically close to a point $\mathbf{x}$, and the primed coordinates are microscopically close to another point $\mathbf{x}'$, with $\mathbf{x}$ and $\mathbf{x}'$ *macroscopically* apart, ρ_m remains nonvanishing. For fixed unprimed coordinates microscopically close together, the region of the primed coordinates where ρ_m remains nonvanishing is thus a

"tube" with one 3-space dimension extending macroscopically. The volume of the region is

$$\Omega \times (\text{microscopic dimension})^{m-1} .$$

For higher order reduced density matrices with particle groups containing one or more basic groups, the corresponding region would have one or more 3-space dimensions extending macroscopically.

Physically the concepts of ODLRO and of the basic group are therefore directly related to the *dimensionality* of the macroscopic regions in space where the matrix elements of ρ_1, $\rho_2, \cdots$ are not vanishingly small.

22. It is easy to believe that the onset of ODLRO in an equilibrium system would lead to a phase transition. Consider, for example, a system of Bose (or Fermi) particles in thermal equilibrium. The thermodynamical function of the system can be obtained[10] as the maximum of a functional of ρ_1. This variational principle also determines ρ_1. The functional is expressed as a series of terms each of which involves integrations over products of matrix elements of ρ_1. It has been shown[11] that if an eigenvalue of ρ_1 attains the order of N, the series contains progressively larger terms and a rearrangement is necessary. Such a rearrangement is, of course, what is required by every phase transition.

The formalism of reference 10 has been generalized by De Dominicis[12] to the case where ρ_2 is also explicitly used in the argument of the functional. It is not difficult to find the successive terms in his formalism that become progressively larger when ρ_2 has a large eigenvalue of the order of N. Thus there is to be expected also a phase transition when ODLRO first sets in in ρ_2.

23. The existence of ODLRO in ρ_1 [or ρ_2] implies the possible separation (19) [or (25)]. If there is only one large eigenvalue of the order of N, then ρ_1' [or ρ_2'] vanishes as $\mathbf{x}$ becomes far separated from $\mathbf{x}'$ [or as $\mathbf{x}_1$, $\mathbf{x}_2$ become far separated from $\mathbf{x}_1'$, $\mathbf{x}_2'$]. Thus, at large spatial separations ρ_1 [or ρ_2] assumes a product form. ρ_1 thus behaves, in some respects, like a single (double) particle system in a *pure state*. It is worth noticing that the hypothesis of a product form for ρ_2 underlies many[13] discussions on superconductivity.

24. For nonequilibrium systems the existence of ODLRO requires a reformulation of transport properties. However, it is doubtful that much real progress can be made without a first understanding of the microscopic basis of the additional macroscopic equilibrium variables required by ODLRO. [Cf. Sec. 7.]

25. It is obvious that the basic group may form a bound state, as in liquid He II; or it may not form a bound state, as in superconductors.

It is also evident from these examples that ODLRO may occur in a liquid, and it may also occur in a solid. But in a solid the basic group cannot contain particles that are localized, such as the nuclei.

26. In an insulator, the electrons, because of energy considerations, have no usable empty states. Effectively, in the notation of Theorem 6, $M = N$. Thus, by that theorem, ρ_2 cannot have an eigenvalue of the order of N and consequently it cannot have an ODLRO. Thus, an insulator cannot satisfy the characterization of a superconductor as given in Sec. 20.

IV. MAGNETIC FLUX QUANTIZATION

27. To discuss the question of magnetic flux quantization we recall that[14] for a superconducting ring P with a magnetic field in the hole O, but no magnetic field in P, the vector potential can be transformed away by a gauge transformation (See Fig. 1). The Schrödinger equation for the electrons

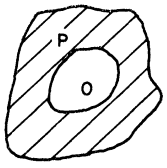

FIG. 1. Superconducting ring.

in P is then the same as that for the case where there is no magnetic field in O, but the boundary condition is that the wave function changes by a phase factor $\exp [i(e/c\hbar)\Phi]$ every time an electron is brought around the ring. The symbol Φ stands for the total magnetic flux through O. The Schrödinger equation together with the boundary condition determine the energy levels, and consequently the free energy $N^{-1} \ln Q$ of the system. The arguments of reference 14 show that if

$$L^2 N^{-1} \ln Q \tag{28}$$

varies as Φ is changed, then the system would have magnetic flux quantization (because body currents would be generated if Φ is not quantized). The quantity L is the circumference of the ring.

[10] T. D. Lee and C. N. Yang, Phys. Rev. **117**, 22 (1960).
[11] T. D. Lee and C. N. Yang, Phys. Rev. **117**, 897 (1960).
[12] C. De Dominicis (to be published).
[13] See e.g., L. P. Gor'kov, J. Exptl. Theoret. Phys. U.S.S.R. **34**, 735 (1958) [translation: Soviet Phys.—JETP **7**, 505 (1958)].
[14] N. Byers and C. N. Yang, Phys. Rev. Letters **7**, 46 (1961.)

28. It is convenient for the present discussion to change slightly the geometry of the mathematical problem formulated above. Instead of a ring-shaped body P we consider a periodic box, i.e., a box of dimension $L \times L' \times L''$ with strict periodicity condition in the y and z directions:

$$\psi(y + L') = \psi(y) , \quad \psi(z + L'') = \psi(z) , \quad (29)$$

and periodicity with a phase factor in the x direction:

$$\psi(x + L) = \exp [i(e/c\hbar)\Phi]\psi(x) , \quad (30)$$

where Φ is a parameter. If the quantity (28) shows a variation with Φ, it is reasonable to assume that the same obtains for the ring geometry, and the physical system would show a quantization of flux, of a unit that is equal to the period in Φ of (28).

29. The periodicity conditions (29) and (30) assume a particularly simple form in the momentum representation: The lattice in momentum space is displaced from the origin by $e\Phi/cL$ in the x direction. The quantization of flux therefore depends on whether the free energy of the system changes with this displacement.

For a free Fermi gas it is not difficult to demonstrate that the free energy is independent of this displacement, as stated in reference 14. Thus, a free Fermi gas shows no magnetic flux quantization.

For a free Bose gas the same obtains for temperatures above the Bose-Einstein transition temperature. But below the Bose-Einstein transition temperature, the momentum state closest to the origin (in momentum space) is degenerate to a degree proportional to N and (28) varies with Φ quadratically for small Φ. Thus, a free Bose gas below the transition temperature should exhibit the phenomena of quantized flux. The period in Φ is clearly ch/e, which is therefore the unit of quantization.

30. While for a free particle system it is convenient to examine in momentum space the large occupation numbers, hence the large eigenvalues of ρ_1, for an interacting system of particles, it is convenient to examine the problem in coordinate space. Also, we shall use an equilibrium density matrix R with a different normalization from that of ρ as given in (1).

$$R \equiv \exp (-H/kT) . \quad (31)$$

Defining the normalization constant as Q, one has

$$R = Q\rho , \quad (32)$$

where $$Q = \mathrm{Sp}\, R = \text{partition function} . \quad (33)$$

The contracted density matrices R_n are defined as

$$R_n = Q\rho_n . \quad [Q = \text{a number, not a matrix.}] \quad (34)$$

Through (4) and (34) we easily obtain

$$\begin{aligned} Q &= N^{-1}\, \mathrm{Sp}\, R_1 , \\ Q &= [N(N-1)]^{-1}\, \mathrm{Sp}\, R_2 , \\ &\text{etc.} \end{aligned} \quad (35)$$

Let us consider the matrix elements of R_1:

$$\langle \mathbf{x}'|R_1|\mathbf{x}\rangle .$$

The periodicity conditions (29) and (30) imply

$$\begin{aligned} \langle x' + L|R_1|x\rangle &= \langle x'|R_1|x - L\rangle \\ &= \exp [i(e/c\hbar)\Phi]\langle x'|R_1|x\rangle , \end{aligned} \quad (36)$$

$$\langle y' + L|R_1|y\rangle = \langle y'|R_1|y - L\rangle = \langle y'|R_1|y\rangle , \text{etc.} \quad (37)$$

31. We shall symbolically represent a 3-space $\mathbf{x}$ by one dimension. In what region of $\mathbf{x}$ and $\mathbf{x}'$ is R_1 nonvanishingly small, relative to its value near $\mathbf{x} = \mathbf{x}'$? The free Bose gas example of Secs. 13 and 14 shows the following:

(A) Without ODLRO, the region consists of narrow parallel strips running along

$$\begin{aligned} x &= x' , \\ x &= x' \pm L , \\ x &= x' \pm 2L , \\ &\text{etc.} \end{aligned} \quad (38)$$

(Cf. Fig. 2.) The values of R_1 between the strips

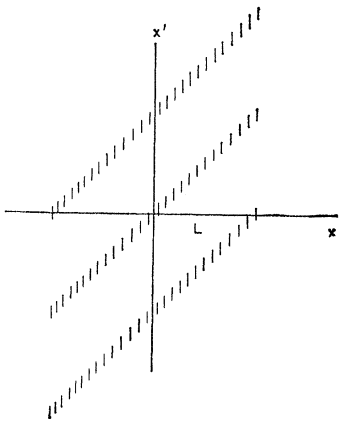

FIG. 2. Region of relatively nonvanishing values of R_1, in absence of ODLRO.

are vanishingly small. The values of R_1 in two neighboring strips, by (36), are different only by a phase factor $\exp [i(e/c\hbar)\Phi]$. The width of the strips is microscopic, but the distance between the strips is macroscopic.

(B) With ODLRO, the strips merge into each other, and R_1 is nonvanishing everywhere. The phase

change by a factor exp $[i(e/c\hbar)\Phi]$ at distances L, however, remains.

The behavior of R_1 along a cut in the $\mathbf{x}\,\mathbf{x}'$ plane at $\mathbf{x}+\mathbf{x}'=0$ is *schematically* illustrated in Fig. 3.

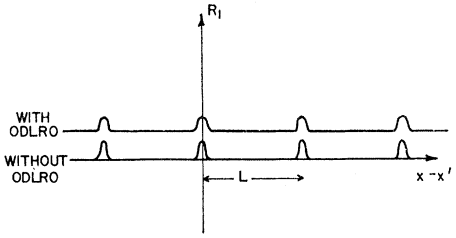

FIG. 3. Schematic plot of R_1 against $\mathbf{x}-\mathbf{x}'$. Notice that with $\Phi \neq 0$, R_1 is, in general, complex.

Notice that the merging of the strips occurs not as a consequence of the broadening of the strips, but as that of the sudden lifting of the value of R_1 between the strips.

32. The above discussion of the region of (relatively) nonvanishing values for R_1 for the cases with and without ODLRO is obviously valid for interacting particles as well.

33. When the parameter Φ is changed, it is clear from Fig. 3 that with ODLRO, the whole dependence of R_1 on $\mathbf{x}-\mathbf{x}'$ must change. Consequently, by (35) the partition function Q changes with Φ and quantization of flux follows.

If on the other hand ODLRO is not present in ρ_1, the different strips are separated from each other and the phase change at distances L can be effected by a simple multiplicative factor, as in the free Bose gas discussed in Sec. 31. Thus quantization of flux need not be present.

The difference in the behavior of R under changes in Φ for the cases with and without ODLRO is quite similar to the Bloch eigenvalue problem[15] in a periodic potential. Bloch showed that wave functions should be sought that changes by a phase factor $e^{i\Phi}$ for each lattice displacement. How does the wave function depend on Φ? If the wave function remains finite between lattice points, the energy value and the wave function would be dependent on Φ. If, however, the wave function becomes very small in a region between lattice points, caused by, e.g., a potential barrier, then the energy and the wave function would not be very much dependent on Φ. For an infinite potential barrier in between the atoms, the wave function vanishes in the barrier, and the energy levels would be independent of Φ while the wave function only picks up phase factors $e^{i\Phi}$ from one atom to the next.

The physical meaning of the effect of the presence of ODLRO on the phase condition (36) is that ODLRO preserves the memory of phases over macroscopic distances. Also in this sense, one can interpret for the Bloch problem, the effect of the small nonvanishing interatomic value of the wave function on the Φ dependence of the energy: The nonvanishing interatomic value of the wave function preserves the memory of phases from one atom to the next.

34. In the absence of an ODLRO in ρ_1 it becomes necessary to examine ρ_2. The region of relatively nonvanishing values of R_2 can be obtained from (24) if ODLRO is absent in ρ_2, and from (26) if ODLRO is present in ρ_2. To simplify matters we suppress as before y and z dimensions and consider the element

$$\langle x_1'x_2'|R_2|x_1x_2\rangle$$

as a function of

$$\begin{aligned} \xi &= x_1 - x_2\,, \\ \eta &= x_1' - x_2'\,, \\ \text{and}\quad \zeta &= x_1 + x_2 - x_1' - x_2'\,. \end{aligned} \tag{39}$$

Invariance under uniform displacement ensures that, for equilibrium, R_2 is independent of the fourth coordinate

$$x_1 + x_2 + x_1' + x_2'\,.$$

The periodicity conditions (29) and (30) imply

$$\begin{aligned} \langle x_1'+L,x_2'|R_2|x_1,x_2\rangle &= \langle x_1',x_2'+L|R_2|x_1,x_2\rangle \\ &= \langle x_1',x_2'|R_2|x_1-L,x_2\rangle = \langle x_1',x_2'|R_2|x_1,x_2-L\rangle \\ &= \exp\,[i(e/c\hbar)\Phi]\langle x_1',x_2'|R_1|x_1,x_2\rangle\,. \end{aligned} \tag{40}$$

Repeated application of these conditions shows that in the (ξ,η,ζ) space a face-centered cubic lattice of displacements can be formed.

Displacements by ($n_1,n_2,n_3 = \pm$ integers, $n_1+n_2+n_3$ = even)

$$(\xi,\eta,\zeta) \rightarrow (\xi+n_1L,\eta+n_2L,\zeta+n_3L)$$

changes the value of R by a factor exp $[-in_3(e/c\hbar)\Phi]$. (41)

35. If ODLRO is not present in ρ_2, the region D of (relatively) nonvanishing values of R_2 is given by (24) in case $L=\infty$. It consists of the two lines

$$\xi=\eta\,,\quad \zeta=0 \quad\text{and}\quad \xi=-\eta\,,\quad \zeta=0\,,$$
and their microscopic neighborhoods. (42)

For finite L all displacements of (42) by the lattice

[15] F. Bloch, Z. Physik **52**, 555 (1928).

(41) should also be included in the region D. Thus, D consists of

$$\xi - \eta = m_1 L\,, \quad \zeta = m_3 L\,;$$
$$\text{and} \quad \xi + \eta = m_1 L\,, \quad \zeta = m_3 L\,;$$
$$\text{and their microscopic neighborhoods,}$$

$$(\text{where } m_1,\ m_3 = \pm \text{ integers}, m_1 + m_3 = \text{even})\,. \quad (43)$$

Geometrically, D consists of parallel plane square nets. Those in the even planes $\zeta = m_3 L$, m_3 = even, are plotted in Fig. 4 in horizontal shading and those in the odd planes $\zeta = m_3 L$, m_3 = odd, are plotted in vertical shading.

36. The values of R not on the nets are (relatively) vanishing. The dependence condition on Φ is contained in (41). Now (41) says (i) that nets in different planes should have a relative phase factor $\exp[i(\Delta m_3)(e/c\hbar)\Phi]$, and (ii) that the value of R on each net is periodic *with no phase factor* under the displacements $(\xi,\eta,\zeta) \rightarrow (\xi + n_1 L, \eta + n_2 L, \zeta)$ $n_1 + n_2$ = even.

Since different nets are not connected to each other, (41) can be satisfied by a mere phase change from net to net, and (35) demonstrates that the free energy need not vary with Φ. Thus, there need not be a quantization of flux.

37. In case ODLRO is present in ρ_2 but not in ρ_1, the discussions of the last two sections have to be modified. The region D is now to be generated from (26). It consists of the nets (43) plus the rods

$$\xi = l_1 L\,, \quad \eta = l_2 L\,, \quad l_1, l_2 = \pm \text{ integers} \qquad (44)$$
$$\text{and their microscopic neighborhoods}\,.$$

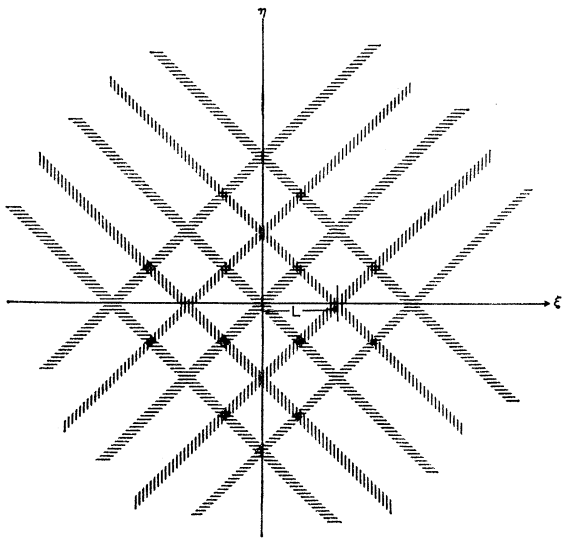

FIG. 4. Projection in $\zeta = 0$ plane of region of relatively nonvanishing values of R_2, in absence of ODLRO.

Now the rods (44) are perpendicular to the planes of the nets and connect all the nets in the even planes together, and also connect all the nets in the odd planes together. But nets in different even (odd) planes have phase-factor differences which are powers of

$$\exp 2i(e/c\hbar)\Phi\,. \qquad (45)$$

Thus, R_2 changes when Φ varies, and we have the phenomena of flux quantization. The unit of quantization is, from (45),

$$ch/2e\,.$$

38. The discussions above can be generalized to the case where the basic group (Secs. 4 and 21) is of any size. If the sum of charges of the particles in the basic group is

$$\sum e \neq 0\,,$$

quantization of flux should take place with a unit of quantization $ch/(\sum e)$.

39. It is clear that the discussions above are in many respects similar to the discussions of reference 14 which was in terms of the BCS pairs. It is also similar to the discussions of Onsager in terms of a boson picture[16] and of Bardeen[17] in terms of the Ginsburg-Landau equation of a doubly charged single-particle system. Furthermore, the discussions of the present paper are based on a series of propositions and guesses. However, we believe these propositions and guesses, in fact, give the common general physical basis of the phenomena of a type of quantum phase in a many-body system.

40. We conclude this paper with a speculation. For superconductors, an important experimental quantity is the penetration depth, defined, for example, in London's book. Is it related to the function (28)? We have some arguments to indicate that it is. In fact,

$$\text{penetration depth} = \left[-4\pi L^2 \frac{\partial^2}{\Omega \partial \Theta^2}\,(kT \ln Q)\right]^{-1/2}$$
$$\text{at } \Phi = 0\,, \qquad (46)$$

where Ω is the volume of the box.

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[16] L. Onsager, Phys. Rev. Letters **7**, 50 (1961).
[17] J. Bardeen, Phys. Rev. Letters **7**, 162 (1961).

sohn, T. D. Lee, J. G. Valatin, and B. Zumino. He is much indebted to B. S. Deaver and W. M. Fairbank for informing him of their beautiful experiment and for many discussions. This paper was largely written while the author was a visitor at CERN. The financial support of CERN and of the Guggenheim Foundation is gratefully acknowledged.

APPENDIX A

To prove Theorem 6, the following lemma is useful:

Lemma. Let X be an antisymmetrical matrix

$$X = -\tilde{X} .$$

There exists a unitary matrix U so that $UX\tilde{U}$ is zero everywhere except for 2×2 diagonal blocks of the form

$$\begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix},$$

where all a's are real and positive.

Proof. Let ψ be a normalized eigenvector of $X^\dagger X$: ($\dagger$ = Hermitian conjugate)

$$X^\dagger X\psi = a^2\psi , \quad a > 0 \tag{A1}$$

Then
$$X^* X\psi = -a^2\psi . \tag{A2}$$

Define
$$\phi = -a^{-1}X^*\psi^* . \tag{A3}$$

By (A1)
$$X\phi = a\psi^* . \tag{A4}$$

By (A3)
$$X\psi = -a\phi^* . \tag{A5}$$

From (A4) and (A5),

$$\tilde{\psi}\phi^* = 0 ,$$

and
$$\tilde{\phi}\phi^* = \tilde{\psi}\psi^* = 1 .$$

Thus ψ and ϕ are orthogonal unit vectors. Taking them as the first two columns of $\tilde{U}$, one easily proves the lemma by induction.

Proof of Theorem 6. (a) To prove the theorem it is necessary and sufficient to prove it for the case that ρ is the density matrix of an N particle pure state Ψ.

(b) Consider any normalized antisymmetrical trial function f_{ij} for ρ_2: Let

$$F = \textstyle\sum_{ij} f_{ij}^* a_i a_j . \tag{A6}$$

Then the expectation value of ρ_2 is

$$\mathrm{Sp}\, F\rho F^\dagger = \Psi^\dagger F^\dagger F\Psi . \tag{A7}$$

Under a unitary transformation U on a_i, the matrix f_{ij} is transformed like the matrix X of the lemma. Thus, we can take f_{ij} to be of the diagonal 2×2 block form of the lemma. In other words, we can take without loss of generality,

$$F = \alpha_1(a_1a_2 - a_2a_1) + \alpha_2(a_3a_4 - a_4a_3) + \cdots , \tag{A8}$$

where
$$\alpha_i \geqq 0 \quad \text{and} \quad 2\textstyle\sum \alpha_i^2 = 1 , \tag{A9}$$

and Theorem 6 is equivalent to the assertion that

$$\Psi^\dagger F^\dagger F\Psi \leq N(M - N + 2)/M . \tag{A10}$$

(c) Consider that Ψ and F which are of the form of (A8), and maximize $\Psi^\dagger F^\dagger F\Psi$. Not all α are 0. Without loss of generality we can assume

$$\alpha_1 > 0$$

We write

$$G = F - 2\alpha_1 a_1 a_2, K = \sum_{3,4,\ldots} a_i^\dagger a_i \tag{A11}$$

so that G and K only operate on states 3, 4, 5, $\cdots$. We write Ψ in the form of

$$\Psi = \begin{Vmatrix} \phi_{00} \\ \phi_{01} \\ \phi_{10} \\ \phi_{11} \end{Vmatrix} \tag{A12}$$

where the subscripts of ϕ represent the occupation numbers of states 1 and 2. In this notation

$$F = \begin{Vmatrix} G & & & 2\alpha_1 \\ & G & & \\ & & G & \\ & & & G \end{Vmatrix} . \tag{A13}$$

The condition on Ψ is

$$K\Psi = \begin{Vmatrix} N & & & \\ & N\text{-}1 & & \\ & & N\text{-}1 & \\ & & & N\text{-}2 \end{Vmatrix} \Psi . \tag{A14}$$

Thus both the operator $F^\dagger F$ and the condition on Ψ do not mix the subspace spanned by ϕ_{00} and ϕ_{11} with that spanned by ϕ_{01} and ϕ_{10}. Hence for maximum $\Psi^\dagger F^\dagger F\Psi$, either $\phi_{00} = \phi_{11} = 0$ or $\phi_{10} = \phi_{01} = 0$. But in the former case we can always increase $\Psi^\dagger F^\dagger F\Psi$ by proportionally increasing α_2, $\alpha_3, \cdots$, and simultaneously decreasing α_1 to keep (A9) satisfied [so that G is proportionally increased]. Hence we can put

$$\phi_{10} = \phi_{01} = 0 \tag{A15}$$

which means that the states 1 and 2 are either both empty or both occupied. [Cf. Sec. 19.]

(d) Equations (A13), (A15), and Schwartz's inequality lead to

$$\begin{aligned} \Psi^\dagger F^\dagger F\Psi &= \phi_{00}^\dagger G^\dagger G\phi_{00} + 2\alpha_1[\phi_{00}^\dagger G^\dagger \phi_{11} + \text{c.c.}] \\ &\quad + 4\alpha_1^2\phi_{11}^\dagger\phi_{11} + \phi_{11}^\dagger G^\dagger G\phi_{11} \\ &\leqq \phi_{00}^\dagger G^\dagger G\phi_{00} + 4\alpha_1^2\phi_{11}^\dagger\phi_{11} + \phi_{11}^\dagger G^\dagger G\phi_{11} \\ &\quad + 4\alpha_1[(\phi_{11}^\dagger\phi_{11})(\phi_{00}^\dagger G^\dagger G\phi_{00})]^{1/2} . \end{aligned} \tag{A16}$$

(e) Let $B(M,N)$ be the maximum for $\Psi^\dagger F^\dagger F\Psi$. (A16) implies

$$\Psi^\dagger F^\dagger F\Psi \leqq X^2\beta^2 B(M-2,N) + 4\alpha_1^2(1-X^2) + \beta^2(1-X^2)B(M-2,N-2) + 4\alpha_1(1-X^2)^{1/2}X\beta[B(M-2,N)]^{1/2}, \quad \text{(A17)}$$

where

$$\beta = (1-2\alpha_1^2)^{1/2} \geqq 0, \quad X = (\phi_{00}^\dagger\phi_{00})^{1/2} \geqq 0.$$

(f) We can now prove by induction that for even M and N

$$B(M,N) = N(M-N+2)/M \quad \text{(A18)}$$

as follows: Substitute (A18) into the right-hand side of (A17) and maximize the resultant expression with respect to α_1 and X. After some straightforward algebra, one finds the only maximum of the right-hand side of (A17) at

$$X^2 = (M-N)/M, \quad \alpha_1^2 = 1/M,$$

where it assumes the value of $B(M,N)$ in (A18). The induction is then easily completed. Q.E.D.

It is clear from the above that the only maximum of $\Psi^\dagger F^\dagger F\Psi$ with F having the form (A8) is obtained when

$$\alpha_1 = \alpha_2 = \cdots = M^{-1/2}. \quad \text{(A19)}$$

Furthermore, each pair of states (1,2), (3,4),$\cdots$ is never occupied singly. For such a problem it is easy to see that we can define $M/2$ sets of Pauli spin matrices so that

$$F = M^{-1/2}\sum_{M/2}(\sigma_i^x + i\sigma_i^y).$$

Thus, $$F^\dagger F = M^{-1}[(\sum \boldsymbol{\sigma})^2 - (\sum \sigma^z)^2 - 2\sum \sigma^z]. \quad \text{(A20)}$$

The condition that the total number of particles is N is

$$\sum \tfrac{1}{2}(1-\sigma^z) = N/2. \quad \text{(A21)}$$

Equations (A20) and (A21) show that there is only one largest eigenvalue for $F^\dagger F$ consistent with (A21).

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Effective Interactions and Coupling Schemes in Nuclei*

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I. INTRODUCTION

SHELL-model calculations of nuclear-energy levels can be carried out only by using *effective interactions* between the nucleons. The interaction between *free* nucleons is highly singular and leads to strong short-range correlations between them. Shell-model wave functions contain no such correlations and therefore do not furnish an exact description of nuclear states. Still, under certain conditions, these functions can be used for energy calculations. To do this, it is necessary to introduce the effect of the short-range correlations into the interaction Hamiltonian. Under favorable conditions this modification results in the replacement of the free-nucleon interaction by a reaction matrix or effective interaction.

The derivation of the effective interaction in finite nuclei has not yet been carried out. It is, therefore, impossible to know in advance whether the shell model can be used for the calculation of nuclear energies. The only way to find the answer to this question is by trying to carry out such calculations. In the past, many such attempts have been made. The main difficulty has been the lack of information about the effective interaction to be used. In the last few years an approach which avoids this difficulty has been used. The effective nuclear interaction was determined in several cases from the experimental energies. The consistency of the shell-model description of these cases was checked as follows. If the effective interaction between nucleons is, indeed, a two-body interaction, its matrix elements in n-

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