EXPECTATION VALUES OF OPERATORS IN THE QUASI CHEMICAL EQUILIBRIUM THEORY.

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Abstract

Expectation values of one-particle and two-particle operators are evaluated in the quasi-chemical equilibrium (pair correlation) approximation to statistical mechanics. Certain reductions, corresponding to the "quenching" of interactions by the Pauli exclusion principle, are carried out quite generally. More specific reductions, which lead to immediately useful expressions, are possible on the assumption of extreme Bose-Einstein condensation of the correlated pairs.

1. Introduction

Some time ago, an approximation to statistical mechanics was suggested based on the retention of dynamical pair correlations, retention of statistical correlations of all orders, but omission of dynamical triplet and higher correlations [9, 10]. This represents a natural extension of the independent particle model, in which all dynamical correlations are ignored, and only statistical correlations are retained. It was shown that this so-called "quasi-chemical equilibrium approximation" leads in a natural way to a chemical equilibrium between single particles and correlated pairs; furthermore, that under certain conditions the chemical equilibrium can shift suddenly towards a large number of correlated pairs, all of which are in one eigenstate of the pair correlation matrix. This phenomenon is closely analogous to a Bose-Einstein condensation of the quasi-molecules. If the particles in question are electrons in a metal, it is reasonable to expect that the transition is one to a superconducting state, since it is well-known [6, 7, 11] that the condensed ideal Bose-Einstein gas exhibits a Meissner effect.

The formalism of reference 1 has since been extended and simplified [2], and a proof of Bose-Einstein condensation has been given, valid even under conditions in which the "pairs" completely overlap and in which there need not be any energy gap [8]. The relation of the quasi-chemical equilibrium

465

approach, to the theory of superconductivity developed by Bogoliubov [5], Valatin [12] and others [1] has been established [3].

In order to carry out self-consistent calculations with the quasi-chemical equilibrium formalism, it is necessary to have simple expressions for expectations values of one-particle and two-particle operators. Reference [8] does not cover this case, since it is concerned with the evaluation of the trace of the statistical matrix itself (i.e., with the evaluation of the normalization integral). We now consider averages of type

(1.1)
$$\langle J \rangle = \frac{\text{Trace } J\mathscr{U})}{\text{Trace } (\mathscr{U})}$$

and

(1.2)
$$\langle K \rangle = \frac{\text{Trace } (K\mathscr{U})}{\text{Trace } (\mathscr{U})}$$

where J is a one-particle operator:

(1.3)
$$J = \sum_{k,k'} J_{kk'} a_k^+ a_{k'}$$

and K is a two-particle operator

(1.4)
$$K = \sum_{lml'm'} K_{lm,l'm'} a_l^+ a_m^+ a_{m'} a_{l'}$$

Here the indices k, l, etc. include both momentum and spin, the operators a and a^+ are the usual destruction and creation operators, satisfying Fermi-Dirac anti-commutation rules.

(1.5) $\quad a_k a_m^+ + a_m^+ a_k = \delta_{km} \quad a_k a_m + a_m a_k = a_k^+ a_m^+ + a_m^+ a_k^+ = 0$

Finally, $\mathscr{U}$ is the statistical matrix in the quasi-chemical equilibrium approximation, as defined in reference [2], equation (2.12).

The reduction of the rather complicated expressions (1.1), (1.2) is carried out in two stages. The first stage, contained in section 2, consists of separating the expressions into contributions from single particles, contributions from correlated pairs, and contributions representing interactions between single particles and particles within pairs. This part of the reduction is completely general, and shows the "quenching" of interaction strengths due to the Pauli exclusion principle in a natural fashion. No assumption of Bose-Einstein condensation is made in section 2.

The expressions derived in section 2, though generally valid, are still too complicated for immediate use. Further reductions are possible under the assumption that the pair correlations are completely Bose-Einstein condensed, i.e., only one eigenstate of the pair correlation matrix contributes significantly. Note that we need *not* assume that single particles are absent; on the contrary, the single particles can form a Fermi sea, with the pairs made

up only out of particles above this Fermi sea, without affecting the validity of the formulae derived here. To this extent, then, we have gone beyond the theories of references [5], [12] and [1]. There is a more important generalization, however, included within our formalism. This refers to the nature of the pair wave function. In references [5, 12, 1], the nature of the pair wave function was severely restricted by the requirement: [1]

(1.6) $\varphi(\mathbf{k}_1 s_1, \mathbf{k}_2 s_2) = 0$ unless $\mathbf{k}_2 = -\mathbf{k}_1$ and $s_2 = -s_1$

We shall refer to this special case as "simple" pairs. With such restrictions on the pair wave function, gauge invariance of the formalism is destroyed, since a gauge transformation applied to a wave function of type (1.6) leads to a transformed wave function not of this type. *It is thus impossible to establish a Meissner effect in these theories, without going beyond the original formalism.* [2]

The expressions derived in sections 3, 4 and 5 of the present paper are valid for an arbitrary pair wave function $\varphi(\mathbf{k}_1 s_1, \mathbf{k}_2 s_2)$, not merely for "simple" pairs. In section 3 we establish a general algebra and show that the expectation values (1.1) and (1.2) can be written in terms of traces of certain operators, in well-defined and limited combinations. In sections 4 and 5, we use the special case of "simple" pairs to get explicit expressions for the general case.

The application of these formulae to a gauge-invariant calculation of the Meissner effect in the quasi-chemical equilibrium theory is contained in a separate paper [4].

The work here applies to straightforward interactions between electrons, of type (1.4). Interactions transmitted via phonons are not included. Extension of the formalism to include phonons explicitly is now under way, and will be reported in a later publication.

2. Separation of Single-Particle and Pair Contributions

Throughout this section we use the notation of reference [2] and we shall denote formulas of this reference by $(I; \cdots)$. Let us consider the numerator of (1.1). Using equation $(I; 2.12)$ and the fact that cyclic permutations leave traces unaltered, we get

(2.1) $\mathrm{Tr}\,(J\mathscr{U}) = \mathrm{Tr}(J\omega \exp(Q^+)\mathscr{V} \exp(Q)\omega)$
$$= \mathrm{Tr}\,(\mathscr{V} \exp(Q)\omega J \omega \exp(Q^+))$$

Next, we use the same argument which led from $(I; 3.2)$ to $(I; 3.4)$ to write (2.1) in the form

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[1] Here we have broken up the formal index k of (1.3)—(1.5) into a momentum $\mathbf{k}$ and a spin coordinate s.

[2] More recent theories of the Meissner effect will be discussed in reference [4].

(2.2) $\text{Tr } (J\mathscr{U}) = \text{Tr } (\mathscr{V}\omega \exp (P) J \exp (P^+)\omega)$

It is desirable to rearrange the expression in such a way that, in the factor multiplying the operator $\mathscr{V}$, all creation operators are to the right, all destruction operators to the left. We therefore use the commutation rule (1.5) and the explicit expression (1.3) for J to rewrite (2.2) in the form:

(2.3) $\text{Tr } (J\mathscr{U}) = \text{Tr } \{\mathscr{V}\omega \exp (P)[\sum_{kk'} J_{kk'}(\delta_{kk'} - a_{k'}a_k^+)] \exp (P^+)\omega\}$

We can now employ the "quenching identity" of reference [2]; let $F(a \cdots)$ be an operator containing only destruction operators; let $G(a^+ \cdots)$ be an operator containing only creation operators. Then

(2.4) $\text{Tr } (\mathscr{V} FG) = \text{Tr } (\mathscr{V})\langle 0|\tilde{F}\tilde{G}|0\rangle$

where $\tilde{F}$ and $\tilde{G}$ are obtained from F and G, respectively, by the replacements

$$a_k \to \tilde{a}_k = (1 + u_k)^{-\frac{1}{2}} a_k$$
(2.5)
$$a_k^+ \to \tilde{a}_k^+ = (1 + u_k)^{-\frac{1}{2}} a_k^+$$

As we shall see in a moment, the average number of particles in single-particle state k is given by

(2.6) $$\bar{n}_k = \frac{u_k}{1 + u_k}$$

Hence the factor $(1 + u_k)^{-\frac{1}{2}}$ in equations (2.5) can also be written as $(1 - \bar{n}_k)^{\frac{1}{2}}$. This is the "quenching" of interaction strengths associated with the Pauli exclusion principle. If a state k is already fully occupied, i.e., $\bar{n}_k = 1$, the quenching factor becomes zero, and this state can not appear in the product $\tilde{F}\tilde{G}$ in (2.4). The quenching identity (2.4) is proved in section 3 of reference [2].

We now apply (2.4) to (2.3), and use the commutation relations (1.5) once more. Furthermore, we note that the trace of the statistical matrix itself is given by formula (I; 3.10) as

(2.7) $\text{Tr } (\mathscr{U}) = \text{Tr } (\mathscr{V})\langle 0|\exp (\tilde{P}) \exp (\tilde{P}^+)|0\rangle$

We then get for the ratio (1.1):

(2.8) $$\langle J \rangle = \sum_k \bar{n}_k J_{kk} + \frac{\langle 0|\exp (\tilde{P})\tilde{J} \exp (\tilde{P}^+)|0\rangle}{\langle 0|\exp (\tilde{P}) \exp (\tilde{P}^+)|0\rangle}$$

where

(2.9) $$\tilde{J} = \sum_{kk'} \frac{J_{kk'}}{(1 + u_k)^{\frac{1}{2}}(1 + u_{k'})^{\frac{1}{2}}} a_k^+ a_{k'} = \sum_{kk'} \tilde{J}_{kk'} a_k^+ a_{k'}$$

The interpretation of (2.8) is clear: the first term is the contribution of the

single particles, the second term is the contribution of the correlated pairs. In this latter term, all the operators are "quenched" by the exclusion principle. If we set $J_{kk'} = \delta_{kk'}$, the operator J is just the operator for the number of particles in the system; the first term of (2.8) is then a sum over the $\bar{n}_k$, thereby justifying our earlier interpretation of $\bar{n}_k$, (2.6), as the number of single particles in state k.

Exactly the same reductions can be carried out on two-particle operators to obtain an expression for $\langle K \rangle$, equation (1.2) and (1.4). We shall only quote the result here. We define the operator $\tilde{K}^{(1)}$ by

$$(2.10a) \qquad \tilde{K}^{(1)} = \sum_{kk'} \tilde{K}^{(1)}_{kk'} a_k^+ a_{k'}$$

$$(2.10b) \qquad \tilde{K}^{(1)}_{kk'} = \sum_m \bar{n}_m \frac{K_{mk,mk'} + K_{km,k'm} - K_{km,mk'} - K_{mk,k'm}}{(1 + u_k)^{\frac{1}{2}}(1 + u_{k'})^{\frac{1}{2}}}$$

This operator is, qualitatively speaking, the scattering of a particle within a correlated pair, from state k to state k', due to interaction with the single particles in the various states m. Furthermore, we introduce the quenched interaction operator for particles within pairs

$$(2.11a) \qquad \tilde{K} = \sum_{k,m,k',m'} \tilde{K}_{km,k'm'} a_k^+ a_m^+ a_{m'} a_{k'}$$

$$(2.11b) \qquad \tilde{K}_{km,k'm'} = \frac{K_{km,k'm'}}{[(1 + u_k)(1 + u_m)(1 + u_{k'})(1 + u_{m'})]^{\frac{1}{2}}}$$

In terms of these, the expectation value $\langle K \rangle$, equation (1.2), reduces to:

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\begin{aligned}
(2.12) \qquad \langle K \rangle = {}& \sum_{k,m} (K_{km,km} - K_{km,mk}) \bar{n}_k \bar{n}_m \\
& + \frac{\langle 0| \exp(\tilde{P}) \tilde{K}^{(1)} \exp(\tilde{P}^+)|0\rangle}{\langle 0| \exp(\tilde{P}) \exp(\tilde{P}^+)|0\rangle} \\
& + \frac{\langle 0| \exp(\tilde{P}) \tilde{K} \exp(\tilde{P}^+)|0\rangle}{\langle 0| \exp(\tilde{P}) \exp(\tilde{P}^+)|0\rangle}
\end{aligned}
$$

The first line of (2.12) is the conventional Hartree-Fock expectation value over the single-particle distribution; the second line represents the interaction between single particles and particles within correlated pairs; and the last line is the interaction between particles, both of which are members of correlated pairs.

Although expressions (2.8) and (2.12) are simpler than the original formulae, they are by no means directly amenable to calculation. The following two sections are devoted to further reductions of these expressions for an

important special case, namely that of Bose-condensed pair correlations.[3]

3. A Commutator Algebra for Bose-condensed Pairs

Let us consider the evaluation of the second term in (2.8) for the special case of Bose-condensed pair correlations. The operator $\tilde{P}$ is given in general by equations (I; 3.24) and (I; 3.25). The extreme Bose-Einstein condensation means that we retain only one term in the sum (I; 3.25) so that $\tilde{P}$ becomes, explicitly:

(3.1) $$\tilde{P} = v^{1/2} bA$$

with [4]

(3.2) $$b = 2^{-1/2} \sum_{k,k'} \varphi^*(k, k') a_k a_{k'}$$

v is a constant, related to the chemical potential, $\varphi(k, k')$ is the wave function of the correlated electron pair, and A is a formal, labelling operator with Bose-Einstein commutation rules:

(3.3) $$[A, A^+]_- = 1$$

The pair wave function $\varphi(k, k')$ is normalized in the usual way:

(3.4) $$\sum_{k,k'} |\varphi(k, k')|^2 = 1$$

We now insert these expressions into the numerator of the second term in (2.8); using the commutation rule (3.3), we obtain:

(3.5) $$\langle 0|\exp(\tilde{P})\tilde{J}\exp(\tilde{P}^+)|0\rangle = \sum_{N=0}^{\infty} \frac{v^N}{N!} \langle 0|b^N \tilde{J}(b^+)^N|0\rangle$$

Next, we use the explicit expression (2.9) for $\tilde{J}$ together with the commutation rule (1.5) to write:

(3.6) $$\langle 0|b^N \tilde{J}(b^+)^N|0\rangle = \langle 0|b^N [\sum_{k,k'} \tilde{J}_{kk'}(\delta_{kk'} - a_{k'} a_k^+)](b^+)^N|0\rangle$$

We observe that b commutes with all the a_k, and b^+ with all the a_k^+. Thus the

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[3] In references [2] and [8] a method of Dyson, developed for spin-waves, was shown to be extremely useful in reducing the complexity of the expression for the trace of the statistical operator itself. Unfortunately, we have so far been unable to use the Dyson formalism for expectation values. The trouble arises from the fact that closure is used (see reference [8], end of section 2); infinite sums, representing closure expansions, then appear in exponentials, and serious convergence difficulties arise. We have tried, without success so far, to modify the Dyson formalism so as to overcome this difficulty. The alternative formalism given in the next three sections solves the problem for the special case of extreme Bose-Einstein condensation, but more work is needed for the general case.

[4] In reference [2], the complex conjugate sign on φ was omitted by mistake. This makes no difference normally, but would cause trouble in calculations involving magnetic fields, where the pair wave function φ cannot be made completely real.

operator $a_{k'}$ in (3.6) can be transferred all the way to the left, the operator a_k^+ all the way to the right, to give the result

(3.7) $\langle 0|b^N \tilde{J}(b^+)^N|0\rangle = \text{tr}\,(\tilde{J})\langle 0|b^N(b^+)^N|0\rangle - \sum_{k,k'} \tilde{J}_{kk'}\langle 1_{k'}|b^N(b^+)^N|1_k\rangle$

where the symbol "tr" stands for a trace over the k-space:

(3.8) $\text{tr}\,(\tilde{J}) = \sum_k \tilde{J}_{kk}$

and $|1_k\rangle$ denotes a state with only one electron present, in state k, i.e.

(3.9) $|1_k\rangle = a_k^+|0\rangle$

We observe that b gives zero when operating on the vacuum state from the left

(3.10) $b|0\rangle = 0$

and also when operating on a one-particle state

(3.11) $b|1_k\rangle = 0$

Hence we would like, if possible, to permute the b^N and the $(b^+)^N$ in (3.7), so as to bring the factors b to the extreme right. Unfortunately, the operators b do *not* obey Bose-Einstein commutation rules. Rather we have the commutation relation (I; 3.26) which can be rewritten (for $\alpha = \beta$) in the form

(3.12a) $[b, b^+] = \sum_{k,k'} \langle k|q|k'\rangle (a_k^+ a_{k'} - a_{k'} a_k^+) \equiv Q_1$

where

(3.12b) $\langle k|q|k'\rangle = \sum_{k''} \varphi(k, k'')\varphi^*(k'', k')$

Thus the very first commutation operation introduces a new type of operator. Fortunately, however, the subsequent commutation operations lead back to operators of the same *types* already encountered; for example, the commutator $[b, Q_1]$ is an operator of the same *type* as b itself, only with a different wave function instead of $\varphi(k, k')$. We shall state the results first, and prove them thereafter.

We define a sequence of wave functions $\varphi_n(k, k')$ recursively by

(3.13a) $\varphi_0(k, k') = \varphi(k, k')$

(3.13b) $\varphi_n(k, k') = \sum_{k''} \langle k|q|k''\rangle \varphi_{n-1}(k'', k')$

For example,

(3.14) $\varphi_1(k, k') = \sum_{k'',k'''} \varphi(k, k'')\varphi^*(k'', k''')\varphi(k''', k')$

φ_2 is a similar structure with 2 factors φ^* and 3 factors φ. In general, φ_n has n factors φ^* interlaced within $n + 1$ factors φ, and is an antisymmetric function of its arguments if φ is itself anti-symmetric:

(3.15) $$\varphi_n(k', k) = -\varphi_n(k, k')$$

Next we define operators b_n in analogy to (3.2):

(3.16) $$b_n = 2^{-\frac{1}{2}} \sum_{k,k'} \varphi_n^*(k, k') a_k a_{k'}$$

and a sequence of operators Q_n by

(3.17) $$Q_n = \sum_{k,k'} \langle k|q^n|k'\rangle (a_k^+ a_{k'} - a_{k'} a_k^+)$$

We note that Q_1, (3.12) is the first member of this set.

We now assert that the set of operators b_n, b_n^+, and Q_n forms the basis of a *commutator ring*, that is, an algebraic structure allowing the operations of addition, subtraction, multiplication by scalars, and commutation, without having to go beyond the ring. The basic commutation relations are:

(3.18a) $$[b_n, b_m^+] = Q_{n+m+1}$$

(3.18b) $$[b_n, Q_m] = 4b_{n+m}$$

(3.18c) $$[Q_m, b_n^+] = 4b_{n+m}^+$$

(3.18d) $$[Q_n, Q_m] = 0$$

Commutator rings are well known, in particular in connection with the theory of Lie groups; the infinitesimal operations of the group form a commutator ring, the Lie ring of the group. Unlike conventional Lie rings, however, the present commutator ring has an infinite number of basis elements.[5]

We now prove these commutation relations. Straightforward use of (1.5) and (3.16), together with the antisymmetry of the functions φ_n, gives:

(3.19) $$[b_n, b_m^+] = \sum_{kk'k''} \varphi_m(k, k'') \varphi_n^*(k'', k')(a_k^+ a_{k'} - a_{k'} a_k^+)$$

By using the expanded forms for the functions φ_n, of which (3.14) is the simplest example, we see that the following identity holds:

(3.20) $$\sum_{k''} \varphi_m(k, k'') \varphi_n^*(k'', k') = \langle k|q^{n+m+1}|k'\rangle$$

In fact, both sides of (3.20) are structures with equally many $(n + m + 1)$ factors φ and φ^* interlaced, the only free indices being k and k'. Combination of (3.19) and (3.20) proves (3.18a).

[5] The Dyson formalism used in reference [8] is obtained by expanding the set of functions $\varphi_n(k, k')$ in terms of a complete orthonormal set φ_α, such that φ_0 is one of the φ_α.

Next, we use (1.5) to get

(3.21) $[b_n, Q_m] = 2\sqrt{2} \sum_{kk'k''} \varphi_n^*(k, k'') \langle k''|q^m|k' \rangle a_k a_{k'}$

By using the expanded forms, of φ_m^* as well as of q^m, we easily establish the identity

(3.22) $\sum_{k''} \varphi_n^*(k, k'') \langle k''|q^m|k' \rangle = \varphi_{n+m}^*(k, k')$

Both sides of (3.22) are structures with $n + m$ factors φ interlaced between $n + m + 1$ factors φ^*, the only free indices being k and k'. Combination of (3.21) and (3.22) establishes (3.18b).

Since (3.18c) is simply the Hermitean conjugate equation to (3.18b), no separate proof is necessary. Finally

(3.23) $[Q_n, Q_m] = 4 \sum_{kk'k''} \langle k|q^n|k'' \rangle \langle k''|q^m|k' \rangle a_k^+ a_{k'}$

$- 4 \sum_{kk'k''} \langle k|q^m|k'' \rangle \langle k''|q^n|k' \rangle a_k^+ a_{k'}$.

The sums over k'' lead to matrix elements of the product $q^n q^m = q^m q^n = q^{n+m}$, therefore (3.23) cancels term by term, and vanishes identically.

The commutation rules (3.18), which we have now established, allow us to transform products $b^N (b^+)^N = (b_0)^N (b_0^+)^N$ into equivalent expressions in which all the factors b_n^+ are to the left, all the factors b_m to the right, and all factors Q_n in the middle. For example:

(3.24) $bb^+ = b_0^+ b_0 + Q_1$

and

(3.25) $b^2(b^+)^2 = (b_0^+)^2(b_0)^2 + 4b_0^+ Q_1 b_0 + 8b_1^+ b_0 + 8b_0^+ b_1 + 2Q_1^2 + 4Q_2$

According to (3.7), we are interested in the vacuum expectation value of structures of this form, and in matrix elements of this form between one-particle states. The relations (3.10) and (3.11) hold not only for the operator $b = b_0$, but for *all* the operators b_n. Hence, the only terms which contribute to (3.7) are those made up out of factors Q_n exclusively; for example, only the last two terms of equation (3.25) make any contribution to (3.7).

Next, note that the operators Q_n conserve the number of particles. In particular, applying Q_n to the vacuum state gives:

(3.26) $Q_n|0\rangle = -\text{tr}\,(q^n)|0\rangle$

Thus, the vacuum expectation value of (3.25) is:

(3.27) $\langle 0|b^2(b^+)^2|0\rangle = 2[\text{tr}\,(q)]^2 - 4\,\text{tr}\,(q^2)$

where the symbol "tr" is defined by (3.8). More generally, *the vacuum ex-*

pectation value $\langle 0|b^N(b^+)^N|0\rangle$ *is a multinomial in the quantities* tr (q^n). This is the first main result of our commutator algebra.

Let us now consider the second term of (3.7). Direct application of the definition (3.17) gives the result:

(3.28) $$Q_n|1_k\rangle = 2\sum_{k'}\langle k'|q^n|k\rangle|1_{k'}\rangle - \text{tr }(q^n)|1_k\rangle$$

This equation can be applied successively, for example

(3.29) $$(Q_1)^2|1_k\rangle = [\text{tr }(q)]^2|1_k\rangle - 4\text{ tr }(q)\sum_{k'}\langle k'|q|k\rangle|1_{k'}\rangle + 4\sum_{k'}\langle k'|q^2|k\rangle|1_{k'}\rangle$$

Using this equation in conjunction with (3.25), we obtain the result:

(3.30) $$\begin{aligned}\langle 1_{k'}|b^2(b^+)^2|1_k\rangle &= \langle 1_{k'}|2Q_1^2 + 4Q_2|1_k\rangle \\ &= \{2[\text{tr }(q)]^2 - 4\text{ tr }(q^2)\}\delta_{kk'} - 8\text{ tr }(q)\langle k'|q|k\rangle \\ &\quad + 16\langle k'|q^2|k\rangle\end{aligned}$$

We are interested, according to (3.7), in the sum of this over k and k', weighted with a factor $J_{kk'}$. Thus we obtain:

(3.31) $$\begin{aligned}\sum_{k,k'}J_{kk'}\langle 1_{k'}|b^2(b^+)^2|1_k\rangle &= \{2[\text{tr }(q)]^2 - 4\text{ tr }(q^2)\}\text{ tr }(J) \\ &\quad - 8\text{ tr }(q)\text{ tr }(Jq) + 16\text{ tr }(Jq^2)\end{aligned}$$

The only thing of concern to us here is the *structure* of this expression. It is a multinomial in the quantities tr (q^n) and tr (Jq^n), with the factors tr (Jq^n) appearing only linearly. It is easily seen that this result holds for arbitrary N in (3.7). Since tr $(J) \equiv$ tr (Jq^0) is a special case of tr (Jq^n), the first term of (3.7) has the same structure. We have therefore established the following *theorem*:

(3.32) $$\langle 0|b^N J(b^+)^N|0\rangle = \sum_{n=0}^{N} M_n \text{ tr }(Jq^n)$$

where M_n is a multinomial in the quantities tr (q^m).

An explicit evaluation of the multinomials M_n is possible by means of our algebra. For example, combination of (3.7), (3.27) and (3.31) gives, for $N = 2$,

(3.33) $$\langle 0|b^2 J(b^+)^2|0\rangle = 8\text{ tr }(q)\text{ tr }(Jq) - 16\text{ tr }(Jq^2)$$

i.e., in the notation of (3.38), $M_0 = 0$, $M_1 = 8$ tr (q), $M_2 = -16$. However, this method of evaluation is extremely awkward; for example, the term proportional to tr (J) always cancels out, but in this way of doing the evaluation this cancellation is by no means obvious. We shall therefore use an indirect method, described in the next section.

4. Expectation Values of One-Particle Operators

Let us consider the special case of "simple" pairs, defined by the condition (1.6) on the wave function $\varphi(\mathbf{k}_1 s_1, \mathbf{k}_2 s_2)$. We introduce the notation $\varphi(\mathbf{k})$ for the non-zero values of this wave function, i.e.,

(4.1) $$\varphi(\mathbf{k}\uparrow, -\mathbf{k}\downarrow) = -\varphi(-\mathbf{k}\downarrow, \mathbf{k}\uparrow) \equiv \varphi(\mathbf{k})$$

Straightforward substitution into the definition (3.12b) shows that q is now a diagonal operator, with matrix elements:

(4.2) $$\langle \mathbf{k}s|q|\mathbf{k}'s'\rangle = -\delta_{\mathbf{k}\mathbf{k}'}\,\delta_{ss'}\,|\varphi(\mathbf{k})|^2$$

The traces which we were led to in section 3 then assume the forms:

(4.3) $$\text{tr}\,(q^n) = (-1)^n\,2\sum_{\mathbf{k}}|\varphi(\mathbf{k})|^{2n}$$

(the factor 2 arises because of the sum over spin indices), and

(4.4) $$\text{tr}\,(\tilde{J}q^n) = (-1)^n\sum_{\mathbf{k}}(\tilde{J}_{\mathbf{k}\uparrow,\,\mathbf{k}\uparrow} + \tilde{J}_{-\mathbf{k}\downarrow,\,-\mathbf{k}\downarrow})\,|\varphi(\mathbf{k})|^{2n}$$

Thus, if we can evaluate the expectation value of $\tilde{J}$, equation (2.8), for the special case of "simple" pairs, we can write the result entirely in terms of the traces (4.3) and (4.4), and, expressed in *that* form, the result must be generally valid, according to the work of section 3. Thus, consideration of the special case of "simple" pairs allows us to bypass the detailed discussion of the multinomials M_n in equation (3.32).

To illustrate the method, we start with the vacuum expectation value which appears in the trace of the density matrix, equation (2.7). Using (3.1)—(3.3) and an expansion of both exponentials, we obtain

(4.5) $$\langle 0|\exp(\tilde{P})\exp(\tilde{P}^+)|0\rangle = \sum_{N=0}^{\infty}\frac{v^N}{N!}\langle 0|b^N(b^+)^N|0\rangle$$

Substitution of (1.6) and (4.1) into the definition (3.2) of b yields, for "simple" pairs:

(4.6) $$b = 2^{\frac{1}{2}}\sum_{\mathbf{k}}\varphi^*(\mathbf{k})\beta_k$$

where

(4.7) $$\beta_k = a_{\mathbf{k}\uparrow}\,a_{-\mathbf{k}\downarrow}$$

The operators β_k commute with each other:

(4.8) $$[\beta_k, \beta_{k'}] = 0$$

and the square of each β_k vanishes identically:

(4.9) $$(\beta_k)^2 = 0$$

Substitution of (4.6) for b leads to

$$\langle 0|b^N(b^+)^N|0\rangle = 2^N \sum_{\mathbf{k}_1\cdots\mathbf{k}_N\mathbf{l}_1\cdots\mathbf{l}_N} \varphi^*(\mathbf{k}_1)\varphi^*(\mathbf{k}_2)\cdots\varphi^*(\mathbf{k}_N)\varphi(\mathbf{l}_1)\cdots\varphi(\mathbf{l}_N)$$

(4.10)

$$\langle 0|\beta_{\mathbf{k}_1}\beta_{\mathbf{k}_2}\cdots\beta_{\mathbf{k}_N}\beta^+_{\mathbf{l}_1}\beta^+_{\mathbf{l}_2}\cdots\beta^+_{\mathbf{l}_N}|0\rangle$$

We now make use of the properties (4.8) and (4.9). According to (4.9), no two $\mathbf{k}_i$ can be equal, and the same is true of the set $\mathbf{l}_i$. Furthermore, according to (4.8), the order in which the $\mathbf{k}_i$ and $\mathbf{l}_i$ appear is quite irrelevant. Finally, the vacuum expectation value vanishes unless the configuration $\{\mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_N\}$ [6] agrees identically with the configuration $\{\mathbf{l}_1, \mathbf{l}_2, \cdots, \mathbf{l}_N\}$. If this condition is satisfied, the vacuum expectation value on the right side of (4.10) gives unity. Therefore we obtain:

(4.11) $$\langle 0|b^N(b^+)^N|0\rangle = 2^N(N!)^2 \sum_{\{\mathbf{k}_1\cdots\mathbf{k}_N\}} |\varphi(\mathbf{k}_1)|^2 |\varphi(\mathbf{k}_2)|^2 \cdots |\varphi(\mathbf{k}_N)|^2$$

The sum is over different configurations, and the factor $(N!)^2$ is the number of terms in (4.10) arising from any one configuration.

When we substitute (4.11) into (4.5), we get an expression containing a factor $N!$ for each term of the sum over N. We use the identity

(4.12) $$N! = \int_0^\infty dt\, e^{-t} t^N$$

together with the general identity

(4.13) $$\sum_{N=0}^\infty \sum_{\{\mathbf{k}_1\cdots\mathbf{k}_N\}} X(\mathbf{k}_1)X(\mathbf{k}_2)\cdots X(\mathbf{k}_N) = \prod_{\mathbf{k}} [1 + X(\mathbf{k})]$$

to obtain

(4.14) $$\langle 0|\exp(\tilde{P})\exp(\tilde{P}^+)|0\rangle = \int_0^\infty dt\, e^{-t} \prod_{\mathbf{k}} (1 + 2vt|\varphi(\mathbf{k})|^2)$$

Let us consider the logarithm of the infinite product in (4.14). It is

(4.15) $$\sum_{\mathbf{k}} \ln[1 + 2vt|\varphi(k)|^2] = \tfrac{1}{2}\operatorname{tr}\ln(1 - 2vtq)$$

where we have used (4.2). We can therefore rewrite (4.14) as

(4.16) $$\langle 0|\exp(\tilde{P})\exp(\tilde{P}^+)|0\rangle = \int_0^\infty dt \exp[-t + \tfrac{1}{2}\operatorname{tr}\ln(1 - 2vtq)]$$

Since the only operator which appears is q, and thus (4.16) involves only the traces of q^n, this is precisely of the form which we have shown, in section 3, to be universally valid. *Thus, although (4.16) has been derived in this section for the special case of "simple" pairs only, (4.16) is actually a general formula*

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[6] We shall use curly brackets to indicate a configuration, i.e., the set $\mathbf{k}_1, \cdots, \mathbf{k}_N$ irrespective of the order in which the $\mathbf{k}$'s appear, with the restriction that no two $\mathbf{k}$'s can be equal.

applicable to arbitrary pair wave functions $\varphi(\mathbf{k}s, \mathbf{k}'s')$. As a check, we observe that (4.16) is identical with equation (3.10) of reference [8], which latter equation was derived by means of the Dyson formalism. As a second check, we may expand the quantity $\exp\left[\frac{1}{2} \operatorname{tr} \ln (1 - 2vtq)\right]$ in a power series in v, and integrate (4.16) term by term. The term proportional to v^2 then agrees with equations (3.27) and (4.5).

The explicit form (4.16) also shows that it would have been very difficult indeed to analyze the multinomials M_n in (3.32) in detail. The algebraic formulation of section 3 is well suited to elucidating the general structure of the expressions which occur, but is not at all well suited to explicit evaluation.

Next, we consider expectation values of one-particle operators for the special case of "simple" pairs. Using (4.6), we obtain

(4.17)
$$\langle 0|b^N \tilde{J}(b^+)^N|0\rangle = 2^N \sum_{\mathbf{k}_1\cdots\mathbf{k}_N} \sum_{\mathbf{l}_1\cdots\mathbf{l}_N} \sum_{m,s,m',s'} \tilde{J}_{ms,m's'}$$
$$\varphi^*(\mathbf{k}_1)\varphi^*(\mathbf{k}_2)\cdots\varphi^*(\mathbf{k}_N)\varphi(\mathbf{l}_1)\cdots\varphi(\mathbf{l}_N)$$
$$\langle 0|\beta_{k_1}\beta_{k_2}\cdots\beta_{k_N} a_{ms} a_{m's'} \beta^+_{l_1}\cdots\beta^+_{l_N}|0\rangle$$

Let us analyze the vacuum expectation value on the right hand side of this equation. First of all, the operator $a_{m's'}$ gives zero on the vacuum state. Hence N must be at least unity. Secondly, the state $\mathbf{m}'s'$ must occur in one of the operators β^+; i.e., if s' is an up-spin, $\mathbf{m}'$ must be one of the $\mathbf{l}_i$, if s' is a down spin, $-\mathbf{m}'$ must be one of the $\mathbf{l}_i$. One of the "pairs" created by the operators β^+ is thus broken by $a_{m's'}$. Let us suppose that $\mathbf{m}, s$ is not identically equal to $\mathbf{m}', s'$. Then this mutilated pair is not restored, and the application of pair destruction operators β_k cannot lead back to the vacuum state. Thus, the vacuum expectation value vanishes unless $\mathbf{m} = \mathbf{m}'$, $s = s'$. If this condition *is* satisfied, the subsequent analysis is the same which led from (4.10) to (4.11), and we therefore obtain, for $N \geqq 1$,

(4.18)
$$\langle 0|b^N J(b^+)^N|0\rangle = 2^N (N!)^2 \sum_m (\tilde{J}_{m\uparrow,m\uparrow} + \tilde{J}_{-m\downarrow,-m\downarrow})|\varphi(m)|^2$$
$$\sum_{\{\mathbf{k}_1\cdots\mathbf{k}_{N-1}\}}' |\varphi(\mathbf{k}_1)|^2 |\varphi(\mathbf{k}_2)|^2 \cdots |\varphi(\mathbf{k}_{N-1})|^2$$

where the prime on the sum over configurations means that none of the $\mathbf{k}_i$ can equal $\mathbf{m}$.

We substitute (4.18) into (3.5) and use (4.12) and (4.13) to obtain

(4.19)
$$\langle 0|\exp(\tilde{P})J\exp(\tilde{P}^+)|0\rangle$$
$$= \int_0^\infty dt\, e^{-t} \sum_m (\tilde{J}_{m\uparrow,m\uparrow} + \tilde{J}_{-m\downarrow,-m\downarrow})\, 2vt|\varphi(m)|^2 \prod_{k\neq m} [1 + 2vt|\varphi(\mathbf{k})|^2]$$

We can eliminate the awkward restriction on the indices k within the infinite product in (4.19), by multiplying and dividing by the factor $1 + 2vt|\varphi(\mathbf{m})|^2$. This gives, together with (4.15), the identity

$$\langle 0|\exp{(\check{P})}\check{J}\exp{(\check{P}^+)}|0\rangle = \int_0^\infty dt \exp{\left[-t + \tfrac{1}{2}\operatorname{tr}\ln{(1 - 2vtq)}\right]}$$

(4.20)

$$\sum_{\mathbf{m}}(\check{J}_{\mathbf{m}\uparrow,\,\mathbf{m}\uparrow} + \check{J}_{-\mathbf{m}\downarrow,\,-\mathbf{m}\downarrow})\frac{2vt|\varphi(\mathbf{m})|^2}{1 + 2vt|\varphi(\mathbf{m})|^2}$$

Let us introduce the k-space operator $\langle k|h|k'\rangle = \langle \mathbf{k}s|h|\mathbf{k}'s'\rangle$ by

(4.21)
$$h = \frac{-2vtq}{1 - 2vtq} = -\sum_{n=1}^\infty (2vt)^n q^n$$

For "simple" pairs, this operator is diagonal since q is diagonal, and is given by

(4.22a)
$$\langle \mathbf{k}s\,|h|\mathbf{k}'s'\rangle = \delta_{\mathbf{k},\,\mathbf{k}'}\delta_{s,\,s'}h_k$$

(4.22b)
$$h_k = \frac{2vt|\varphi(\mathbf{k})|^2}{1 + 2vt|\varphi(\mathbf{k})|^2}$$

Equation (4.4) then shows that the sum over $\mathbf{m}$ in (4.20) is simply the trace of the operator $\check{J}h$. We therefore get

(4.23) $\langle 0|\exp{(\check{P})}\,\check{J}\exp{(\check{P}^+)}|0\rangle = \int_0^\infty dt \exp{\left[-t + \tfrac{1}{2}\operatorname{tr}\ln{(1 - 2vtq)}\right]}\operatorname{tr}{(\check{J}h)}$

(4.23) is the desired result, which is generally valid according to the arguments of section 3.

Equations (4.23) and (4.16) are exact, and their substitution into (2.8) gives an exact and explicit expression for the expectation value $\langle J\rangle$ of any single-particle operator.

This expression involves the *ratio* of the integrals (4.23) and (4.16). If v exceeds unity, as it does in the Bose-Einstein condensation region, both integrals can be evaluated approximately by means of the saddle point method. The case of (4.16) has been discussed in great detail in reference [8], section 3. The value of t for the saddle point is proportional to the volume of the box.[7] The factor $\operatorname{tr}(\check{J}h)$ in (4.23) is a function of t, since t enters into the definition of the operator h, (4.21). However, $\operatorname{tr}(\check{J}h)$ is a slowly varying function of t compared to the exponential factor, and therefore does not alter the position of the saddle point to a first approximation. With this approximation, we see that the ratio of (4.23) to (4.16) can be replaced by $\operatorname{tr}(\check{J}h)$, where h is to be evaluated with $t = t_{\max}$. In this approximation, therefore, (2.8) assumes the extremely simple form:

(4.24)
$$\langle J\rangle = \sum_k \bar{n}_k \check{J}_{kk} + \operatorname{tr}{(\check{J}h)}$$

[7] In fact, one can show quite generally that $t_{\max} = N_s$, where N_s is the number of Bose-condensed pairs.

Unlike (4.23) and earlier formulae, (4.24) is only approximately true, and in particular fails if the number of pairs is comparable to 1. However, when (4.24) is valid, it is much simpler to use than (4.23) and gives equivalent results. The only thing needed is the value of t to use in h, equation (4.21). This can be obtained by putting J equal to the number operator $\mathcal{N}$, i.e., $J_{kk'} = \delta_{kk'}$. This leads to the condition

$$(4.25) \qquad N = \sum_k \bar{n}_k + \sum_k (1 - \bar{n}_k) h_{kk}$$

If the one-particle occupation numbers $\bar{n}_k$ are known, (4.25) involves only one adjustable parameter on the right hand side, namely the t which appears in the operator h. Thus (4.25) becomes an implicit definition of t.

We emphasize once more that (4.24) and (4.25) are not restricted to "simple" pairs, but are valid for arbitrary pair wave functions $\varphi(k, k') = \varphi(\mathbf{k}s, \mathbf{k}'s')$.

5. Expectation Values of Pair Operators

We now apply the same methods to the expectation value of pair operators, as given by equation (2.12). The first two lines of equation (2.12) represent no difficulty, since $\tilde{K}^{(1)}$, equation (2.10), has the structure of a single-particle operator. Thus our main concern is the evaluation of the last term in (2.12). We shall do this in two steps: (1) By use of the commutator algebra of section 3, we shall determine the general structure of the contributing terms, and (2) by special methods applicable to "simple" pairs, and subsequent identification of the structures which appear, we shall arrive at our explicit result.

We first use (3.1)—(3.3) to write:

$$(5.1) \qquad \langle 0 | \exp(\tilde{P}) \, \tilde{K} \, \exp(\tilde{P}^+) | 0 \rangle = \sum_{N=0}^{\infty} \frac{v^N}{N!} \langle 0 | b^N \tilde{K} (b^+)^N | 0 \rangle$$

Next, we use the commutation relations (1.5) in the explicit form (2.11a) of $\tilde{K}$ in order to bring the operators a_k to the left, the operators a_k^+ to the right. In that position, the a_k can be commuted through the factor b^N, and the a_k^+ through the factor $(b^+)^N$. This leads to the equation

$$\langle 0 | b^N \tilde{K} (b^+)^N | 0 \rangle = \sum_{k, l} (K_{kl, kl} - K_{kl, lk}) \langle 0 | b^N (b^+)^N | 0 \rangle$$

$$(5.2) \qquad\qquad - 2 \sum_{k, k', l} (K_{kl, k'l} - K_{kl, lk'}) \langle 1_{k'} | b^N (b^+)^N | 1_k \rangle$$

$$+ \sum_{k, l, k', l'} K_{kl, k'l'} \langle 1_{k'} 1_{l'} | b^N (b^+)^N | 1_k 1_l \rangle$$

The first two lines of (5.2) contain matrix elements of $b^N(b^+)^N$ which we have encountered already, in section 3. For our present purpose, it is convenient to introduce the following operators in the two-particle space:

(5.3) $\langle kl|p_{nm}|k'l'\rangle = \langle k|q^n|k'\rangle\langle l|q^m|l'\rangle - \langle k|q^n|l'\rangle\langle l|q^m|k'\rangle$

We note that p_{00} is the unit operator, properly antisymmetrized: we also introduce the notation tr_2 for a trace over the two-particle space:

(5.4) $\mathrm{tr}_2(\tilde{K}) = \sum_{k,\,l} \tilde{K}_{kl,\,kl}$

Then we get the identity

(5.5) $\mathrm{tr}_2(\tilde{K}p_{nm}) = \sum_{k,\,l,\,k',\,l'} (K_{kl,\,k'l'} - K_{kl,\,l'k'})\,\langle k|q^n|k'\rangle\,\langle l|q^m|l'\rangle$

Using the result of section 3, the first line of (5.2) has the structure

$$\mathrm{tr}_2(\tilde{K}p_{00})M_0$$

where M_0 is a multinomial in the quantities $\mathrm{tr}(q^n)$. Similarly, the second line of (5.2) has the structure

$$\sum_n \mathrm{tr}_2(\tilde{K}p_{n0})M'_n$$

where again each M'_n is a multinomial in the quantities $\mathrm{tr}(q^m)$.

   It remains to explore the structure of the third line of (5.2). We use the commutation relations of section 3 to rewrite $b^N(b^+)^N$ in an equivalent form in which all operators b_n^+ are to the left, all operators b_n to the right, and operators Q_n in the middle; equations (3.24) and (3.25) provide examples. For one-particle matrix elements of $b^N(b^+)^N$, the only surviving terms were the ones made up out of factors Q_n entirely. Now, however, we need two-particle matrix elements, and a new type of term enters; namely terms with one factor b_n^+ to the left, one factor b_m to the right, and any number of factors Q in the middle. For example, in equation (3.25) only the very first term gives zero matrix elements between two-particle states; all the other terms contribute.

   We use the general relations

(5.6) $b_n|1_k 1_l\rangle = 2^{\frac{1}{2}}\varphi_n^*(k,l)|0\rangle$

and

(5.7) $Q_n|1_k 1_l\rangle = \mathrm{tr}(q^n)|1_k 1_l\rangle - 2\sum_{k'}\langle k|q^n|k'\rangle|1_{k'}1_l\rangle - \sum_{l'}\langle l|q^n|l'\rangle|1_k 1_{l'}\rangle$

which follow directly from the definitions and the commutation relations (1.5). Using (5.6) we get the identity

(5.8) $\langle 1_{k'}1_{l'}|b_n^+ Q_r \cdots Q_s b_m|1_k 1_l\rangle = 2\varphi_n(k',l')\varphi_m^*(k,l)\langle 0|Q_r \cdots Q_s|0\rangle$

where $Q_r \cdots Q_s$ denotes any sequence of factors Q. Substitution into the last line of (5.2) shows that terms of this type lead to structures of the form

$$(\varphi_m, \tilde{K}\varphi_n)M''_{mn}$$

where M''_{mn} is a multinomial in the quantities tr (q^r), and the matrix element is defined by

(5.9) $$(\varphi_m, \tilde{K}\varphi_n) = \sum_{k,l,k',l'} \varphi_m^*(k, l)\tilde{K}_{kl,k'l'}\varphi_n(k', l')$$

On the other hand, it is easily seen from (5.7) that terms made up out of factors Q exclusively, lead to traces $\mathrm{tr}_2(\tilde{K}p_{nm})$ multiplied by multinomials in tr (q^r).

Combining all the results so far, we get

(5.10) $$\langle 0|b^N\tilde{K}(b^+)^N|0\rangle = \sum_{n,m} [\mathrm{tr}_2 (\tilde{K}p_{nm})M^{(1)}_{nm} + (\varphi_n, \tilde{K}\varphi_m)M^{(2)}_{nm}]$$

where the $M^{(i)}_{nm}$ are multinomials in the quantities tr (q^r). As an example of a formula of this type, we quote a result easily obtained from the explicit expressions (3.25), (5.2), (5.6), and (5.7):

(5.11)
$$\langle 0|b^2\tilde{K}(b^+)^2|0\rangle = 16(\varphi_1, \tilde{K}\varphi_0) + 16(\varphi_0, \tilde{K}\varphi_1)$$
$$- 8 \, \mathrm{tr} \, (q)\,(\varphi_0, \tilde{K}\varphi_0) + 16 \, \mathrm{tr}_2 \, (\tilde{K}p_{11})$$

At this point we leave the commutator algebra, and consider the *special case of "simple" pairs*. Using equations (4.6)—(4.7) we obtain:

$$\langle 0|b^N\tilde{K}(b^+)^N|0\rangle = 2^N \sum_{k_1\cdots k_N} \sum_{k'_1\cdots k'_N} \sum_{lml'm'} \tilde{K}_{lm, l'm'}$$

(5.12)
$$\varphi^*(k_1)\varphi^*(k_2)\cdots \varphi^*(k_N)\varphi(k'_1)\cdots \varphi(k'_N)$$
$$\langle 0|\beta_{k_1}\beta_{k_2}\cdots\beta_{k_N}a_l^+a_m^+a_{m'}a_{l'}\beta^+_{k'_1}\cdots\beta^+_{k'_N}|0\rangle$$

We now analyze the vacuum expectation values which appear on the right side of (5.12). There are two quite separate cases, depending upon whether l' and m' are "associated" or not. We call l' and m' "associated" if

(5.13) $$\mathbf{l}' = -\mathbf{m}' \text{ and } s'_l = -s'_m \qquad \text{(Def. of association)}$$

s being the spin index in each case. Since the operators β_k^+ and β_k create or destroy a pair of associated states at a time, it follows immediately that, if l' and m' are associated states, then l and m must also be associated states; and vice versa. We now follow through these two cases separately:

1) *l and m are associated, and so are l' and m'*:

The factor $a_l^+a_m^+$ now equals $\pm\beta^+_{\pm m}$, the signs depending on whether m has up-spin (plus signs) or down-spin (minus signs). Similarly, $a_{m'}a_{l'} = \pm \beta_{\pm m}$.

By permutation of commuting operators, we can make $\mathbf{k}_N = \pm\mathbf{m}$ and $\mathbf{k}'_N = \pm\mathbf{m}'$. Terms of this type then give the following contribution to (5.12):

$$\text{Type 1 contribution to (5.12)} = 2^N(N!)^2 \sum_{\mathbf{m},\mathbf{m}'} \varphi^*(\mathbf{m})L(\mathbf{m},\mathbf{m}')\varphi(\mathbf{m}')$$

(5.14)

$$\sum_{\{\mathbf{k}_1\cdots\mathbf{k}_{N-1}\}}'' |\varphi(\mathbf{k}_1)|^2 |\varphi(\mathbf{k}_2)|^2 \cdots |\varphi(\mathbf{k}_{N-1})|^2$$

where the double prime on the sum means that none of the $\mathbf{k}_i$ may equal either $\mathbf{m}$ or $\mathbf{m}'$, and where $L(\mathbf{m},\mathbf{m}')$ is defined by

(5.15)
$$L(\mathbf{m},\mathbf{m}') = \tilde{K}_{\mathbf{m}\uparrow,-\mathbf{m}\downarrow;\,\mathbf{m}'\uparrow,-\mathbf{m}'\downarrow} - \tilde{K}_{-\mathbf{m}\downarrow,\mathbf{m}\uparrow;\,\mathbf{m}'\uparrow,-\mathbf{m}'\downarrow}$$
$$- \tilde{K}_{\mathbf{m}\uparrow,-\mathbf{m}\downarrow;\,-\mathbf{m}'\downarrow,\mathbf{m}'\uparrow} + \tilde{K}_{-\mathbf{m}\downarrow,\mathbf{m}\uparrow;\,-\mathbf{m}'\downarrow,\mathbf{m}'\uparrow}$$

We now substitute (5.14) into (5.1), and use the identities (4.12), (4.13), and (4.15) to get

(5.16)   Type 1 contribution to (5.1) $= \int_0^\infty dt \exp\left[-t + \tfrac{1}{2}\operatorname{tr}\ln(1 - 2vtq)\right]T$

where

(5.17) $$T = \sum_{\mathbf{m},\mathbf{m}'} \frac{(2vt)^{\frac{1}{2}}\varphi^*(\mathbf{m})}{1 + 2vt|\varphi(\mathbf{m})|^2} L(\mathbf{m},\mathbf{m}') \frac{(2vt)^{\frac{1}{2}}\varphi(\mathbf{m}')}{1 + 2vt|\varphi(\mathbf{m}')|^2}$$

We must rewrite (5.17) as an expression of the right form to fit (5.10). For the special case of "simple" pairs, the operator q is given by (4.2). Hence we have, remembering the definitions (3.13):

(5.18) $$\frac{(2vt)^{\frac{1}{2}}}{1 + 2vt|\varphi(\mathbf{m})|^2}\,\varphi(\mathbf{m}) = \sum_{n=0}^\infty (2vt)^{n+\frac{1}{2}}q^n\varphi = \sum_{n=0}^\infty (2vt)^{n+\frac{1}{2}}\varphi_n(\mathbf{m}\uparrow,-\mathbf{m}\downarrow)$$

This is of the right form for the general case. We therefore introduce the definition

(5.19) $$\psi(k,k') = \sum_{n=0}^\infty (2vt)^{n+\frac{1}{2}}\varphi_n(k,k') = \sum_{k''}\left\langle k\left|\frac{\sqrt{2vt}}{1-2vtq}\right|k''\right\rangle \varphi(k'',k')$$

Direct substitution into (5.17) then yields the identity:

(5.20) $$T = (\psi,\tilde{K}\psi) = \sum_{n,n'=0}^\infty (2vt)^{n+n'+1}(\varphi_n,\tilde{K}\varphi_{n'})$$

The combination of (5.16) and (5.20) is exactly of the right form to agree with the second term on the right hand side of (5.10). This concludes the analysis of the type 1 contribution.

2) *l and m are not associated, and neither are l' and m', in* (5.12).

In this case, the operator $a_{m'}a_{l'}$ breaks up two separate associated pairs, and the vacuum expectation value on the right of (5.12) vanishes unless

$a_l^+ a_m^+$ restores these same two pairs. Thus the only non-vanishing contributions come from (i) $l = l'$, $m = m'$, and (ii) $l = m'$, $m = l'$. Once this is recognized, the usual arguments lead to the result:

(5.21)

$$\text{Type 2 contribution to } (5.12) = 2^N (N!)^2 \sum_{l,m} |\varphi(\mathbf{l})|^2 |\varphi(\mathbf{m})|^2$$

$$(\tilde{K}_{lm,\,lm} - \tilde{K}_{lm,\,ml}) \sum_{\{\mathbf{k}_1 \cdots \mathbf{k}_{N-2}\}}'' |\varphi(\mathbf{k}_1)|^2 \cdots |\varphi(\mathbf{k}_{N-2})|^2$$

We substitute this contribution into (5.1), use the identities (4.12), (4.13), and (4.15), and the relation (4.22b) to get

(5.22)

$$\text{Type 2 contribution to } (5.1) =$$

$$= \int dt \, \exp\left[-t + \tfrac{1}{2} \operatorname{tr} \ln (1 - 2vtq)\right] T'$$

where

(5.23)
$$T' = \sum_{l,m} h_l h_m (\tilde{K}_{lm,\,lm} - \tilde{K}_{lm,\,ml})$$

Consideration of the general form (5.3) now suggests the definition

(5.24a) $$\langle kl|p|k'l'\rangle = \langle k|h|k'\rangle \langle l|h|l'\rangle - \langle k|h|l'\rangle \langle l|h|k'\rangle$$

so that

(5.24b)
$$p = \sum_{n,\,n'=1}^{\infty} (2vt)^{n+n'} p_{nn'}$$

With this definition, the quantity T', (5.23), can be rewritten in the form

(5.25)
$$T' = \operatorname{tr}_2 (\tilde{K}p)$$

The combination of (5.22) and (5.25) is exactly of the right form to agree with the first term on the right hand side of (5.10). This concludes the analysis of the quantity (5.1). The final and exact result is:

(5.26)
$$\langle 0|\exp(\tilde{P}) \tilde{K} \exp(\tilde{P}^+)|0\rangle$$
$$= \int_0^{\infty} dt \, \exp\left[-t + \tfrac{1}{2} \operatorname{tr} \ln (1 - 2vtq)\right] \left(\operatorname{tr}_2 (\tilde{K}p) + (\psi, \tilde{K}\psi)\right)$$

Just as before, this integral can be approximated by the saddle point method in the Bose-Einstein condensation region. Under those conditions, combination of (2.12), (4.16), (4.23), and (5.26) gives

(5.27) $$\langle K \rangle = \sum_{k,l} (K_{kl,\,kl} - K_{kl,\,lk}) \bar{n}_k \bar{n}_l + \operatorname{tr} (\tilde{K}^{(1)} h) + \operatorname{tr}_2 (\tilde{K}p) + (\psi, \tilde{K}\psi)$$

This, unlike (5.26), is only an approximation, but the error is of order (volume)$^{-1}$ in the Bose-condensation region.

Equations (4.24) and (5.27) are the main results of this paper. They can be used, among other things, for a completely gauge-invariant derivation of the

Meissner-Ochsenfeld effect, in the quasi-chemical equilibrium theory of superconductivity [4].

The function $\psi(k, k')$, (5.19), and the operator h, (4.21), are easily seen to be related by the identity

$$(5.28) \qquad \sum_{k''} \psi(k, k'')\psi^*(k'', k') = -\langle k|h(1-h)|k'\rangle$$

For the special case of "simple" pairs, the only non-vanishing values of ψ are

$$(5.29) \qquad \psi(\mathbf{k}\uparrow, -\mathbf{k}\downarrow) = -\psi(-\mathbf{k}\downarrow, \mathbf{k}\uparrow) \equiv \psi(\mathbf{k})$$

The general identity (5.28) then leads to

$$(5.30) \qquad \psi(k) = \pm\sqrt{h_k(1-h_k)}$$

Quite apart from the sign ambiguity, the relation (5.30) can*not* be generalized to arbitrary pair wave functions. h is a simpler structure than ψ in the general case, and there is no hope of expressing ψ in terms of h.

(5.28) does appear to allow expression of h in terms of an operator made up from ψ. However, (5.28) leads to a quadratic equation for h, and the natural sign ambiguity in the root of a quadratic equation makes real trouble here, since both signs must actually be used.

We conclude that, in the general case, one can neither express ψ in terms of h, nor h in terms of ψ, without encountering serious sign ambiguities and other troubles. The basic quantity in the quasi-chemical equilibrium theory is the pair correlation matrix with its eigenfunctions; in the extreme Bose-Einstein condensation limit, the basic quantity is the eigenfunction $\varphi(k, k')$ of the condensed pairs. Only in terms of $\varphi(k, k')$ can we obtain generally valid, unambiguous expressions. The accidental relation (5.30), valid only for "simple" pairs, has misled some into attributing basic significance to the quantities h_k and to the simple pairing condition (1.6), a basic significance which they do not possess.

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