EXPECTATION VALUES OF OPERATORS IN THE QUASI-CHEMICAL EQUILIBRIUM THEORY
PART II

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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. Earlier work was restricted to the case of extreme Bose-Einstein condensation of the correlated pairs; the new formulas are not so restricted, but are correspondingly more complicated to evaluate practically. However, a simple result can be obtained for the expectation value of the number of particles.

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 [1, 2]. Further work on this formalism, with particular application to the theory of superconductivity, has been given in a number of papers since [3—9].

The exploitation of any approximation in statistical mechanics requires a method for evaluating the rather complex expressions which arise, in particular for expectation values of operators which enter into the Hamiltonian of the system. Thus, one-particle and two-particle operators are of primary interest. In reference [6], we were able to derive closed and explicit expressions for such expectation values, but only by means of a drastic simplification of the problem. The simplification was the assumption of an extreme Bose-Einstein condensation of the correlated pairs, i.e., only one wave function for the correlated pairs was permitted. Surprisingly enough, this suffices to get a workable theory of superconductivity — there is actually Bose-Einstein condensation, as shown in reference [4], and thus this apparently extreme assumption is nonetheless physically reasonable.

However, in the *proof* of the existence of Bose-Einstein condensation, i.e., in reference [4], no such assumption is possible, since it would amount to assuming what we wish to prove. This proof has been criticized recently by A. Katz [10], on the grounds that the formula for the number of pairs in a given quantum state of the pairs, is not really justified within the paper. Rather, this formula was taken from general statistical mechanics, whereas the quasi-chemical equilibrium approximation is only an approximation to statistical mechanics, not an exact equivalence. Thus, it is possible that the formula used in reference [4] for the average number $\bar{N}_\alpha$ of pairs in pair state α, is actually inconsistent with the basic Ansatz of the quasi-chemical equilibrium approximation. If this were true, it would vitiate the proof of condensation, i.e., the proof of the statement that $\bar{N}_1$ is of order volume, $\bar{N}_2$ of much lower order, where 1 and 2 are the ground state and first excited state of the pairs, respectively. Since the number operator is a typical one-particle operator, we require expectation values of such operators.

Quite apart from this difficulty, it would of course be highly desirable to have general expressions for expectation values in the quasi-chemical equilibrium theory, in order to be able to attack the problem of self-consistency without making the initial assumption of full Bose-Einstein condensation. The discussion of the presence or absence of an energy gap depends on such formulas. *

In the present paper, we use the Dyson formalism [11] to get fully general expressions for expectation values. One-particle operators are discussed in section 2, two-particle operators in section 3. Section 4 shows how the general formulas reduce to the special expressions of reference [6], and also derives a general result for the number operator, which justifies the formula used in reference [4].

2. Expectation Values of Single-Particle Operators

The typical single-particle operator has the second-quantized form:

$$J = \sum_{k,k'} J_{kk'} a_k^+ a_{k'} \tag{2.1}$$

and we are interested in the statistical average

$$J = \frac{\text{Trace } (J\mathscr{U})}{\text{Trace } (\mathscr{U})} \tag{2.2}$$

* The usual discussions are rather incomplete; an energy gap is proved for excitations in which at least one pair is broken up, but there is difficulty with excitations in which one or more pairs are moved out of the pair ground state, into a pair excited state, without actual breakup of pairs. Such excitations are treated as "collective excitations", whereas they are really not "collective" at all.

where $\mathscr{U}$ is the statistical matrix in the quasi-chemical equilibrium approximation, as defined in (Q, 2.12).

A considerable reduction of this complicated expression was carried out already in reference [6], leading eventually to equation (E, 2.8), which we repeat here for ready reference:

$$J = \sum \bar{n}_k J_{kk} + \frac{\langle 0| \exp(P)\tilde{J} \exp(P^+)|0\rangle}{\langle 0| \exp(P) \exp(P^+)|0\rangle} \tag{2.3}$$

where the symbols mean the following: $\bar{n}_k$ is the average number of unpaired particles in single-particle state k. The operator $\tilde{J}$ is the "quenched" form of J, equation (2.1), the "quenching" being due to the Pauli exclusion principle; the matrix elements $J_{kk'}$ in (2.1) are replaced by

$$\tilde{J}_{kk'} = (1 - \bar{n}_k)^{\frac{1}{2}} J_{kk'} (1 - \bar{n}_{k'})^{\frac{1}{2}} \tag{2.4}$$

The operator P in (2.3) is formed as follows: Let $\varphi_\alpha(k, k')$ be the wave function of pair state number α; let v_α be the associated eigenvalue of the "quenched pair correlation matrix"; the operator which destroys a pair of type α is *

$$b_\alpha = 2^{-\frac{1}{2}} \sum_{k, k'} \varphi^*_\alpha(k, k') a_k a_{k'} \tag{2.5}$$

Let A_α be a set of formal "counting" operators, obeying Bose-Einstein commutation rules:

$$[A_\alpha, A^+_\beta]_- = \delta_{\alpha\beta}$$

Then P in (2.3) is defined by:

$$P = \sum_\alpha v^{\frac{1}{2}}_\alpha b_\alpha A_\alpha \tag{2.7}$$

The problem before us is to find a method of reducing the (quite unmanageable) second term of (2.3), the contribution of the paired particles, to a form which can be evaluated, at least in special cases. Paper E did this for one special case, namely the one of complete Bose-Einstein condensation of the pairs; mathematically, this means that all the v_α vanish, except a single one of them, so that the infinite sum (2.7) reduces to one term.

In this paper, we carry out a significant reduction in the general case, where (2.7) is an infinite sum. To do this, we use the Dyson method [11] as described in Q. The "physical boson" operators b_α satisfy awkward commutation rules, namely **

* This equation differs from (Q, 3.24) by the complex conjugate sign on the wave function of the pair. This correction was already made in E, and will be carried through in the present paper also.

** The commutation rule (2.8) differs from (Q, 3.26) by complex conjugates of pair wave functions. Definition (2.9) is identical with (C, 2.9), and reduces to (E, 3.12b) for a single quantum state of the pair.

$$[b_\alpha, b_\beta^+] = \delta_{\alpha\beta} + \sum_{k,k'} \langle k|q_\alpha^\beta|k'\rangle a_{k'}^+ a_k \tag{2.8}$$

where

$$\langle k|q_\beta^\alpha|k'\rangle = \sum_{k''} \varphi_\alpha(k, k'')\varphi_\beta^*(k'', k') \tag{2.9}$$

In the Dyson method, the "physical boson" operators b_α are replaced by "ideal boson" operators B_α, the latter satisfying the ordinary commutation rules

$$[B_\alpha, B_\beta^+]_- = \delta_{\alpha\beta} \tag{2.10}$$

The precise nature of the correspondence is defined in section 4 of Q, equations (Q, 4.9) and (Q, 4.10). A useful method for finding the ideal operator corresponding to some physical operator is given in equations (Q, 4.13)–(Q, 4.15), and this method will now be employed to find the Dyson image of the operator $\tilde{J}$. Since $\tilde{J}$, acting on the vacuum state $|0\rangle$, gives zero, the coefficients defined in (Q, 4.14a) vanish. Next, we require the commutator of $\tilde{J}$ and b_α^+. Straightforward calculation yields:

$$[\tilde{J}, b_\alpha^+] = -2^{-\frac{1}{2}} \sum_{k,l,m} \tilde{J}_{kl}[\varphi_\alpha(l, m) - \varphi_\alpha(m, l)]a_k^+ a_m^+ \tag{2.11}$$

We now apply closure to the defining equation (2.5), or rather to its complex conjugate

$$b_\alpha^+ = 2^{-\frac{1}{2}} \sum_{k,k'} [\varphi_\alpha(k, k') - \varphi_\alpha(k', k)]a_{k'}^+ a_k^+ \tag{2.12}$$

The explicit antisymmetrization of the wave function φ_α in (2.12) is not necessary for the validity of the formula itself, since antisymmetry is assured anyway by the fact that the creation operators anti-commute. However, in order to apply closure, we must sum over a *complete* set of wave functions φ_α, including the symmetrical functions. The explicit anti-symmetrization in (2.12) ensures that the symmetric functions do not contribute after the closure operation has been performed.

We multiply (2.12) on both sides by $\varphi_\alpha^*(m, m') - \varphi_\alpha^*(m', m)$ and sum over all α. We employ the closure relation

$$\sum_\alpha \varphi_\alpha^*(m, m')\varphi_\alpha(k, k') = \delta_{mk}\delta_{m'k'} \tag{2.13}$$

to obtain the identity

$$a_k^+ a_{k'}^+ = 2^{-\frac{1}{2}} \sum_\alpha [\varphi_\alpha^*(k, k') - \varphi_\alpha^*(k', k)]b_\alpha^+ \tag{2.14}$$

We now substitute this identity into (2.12), replacing the dummy index α by β. Using the definition of q_β^α, equation (2.9), and noting that the wave

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functions in (2.9) are meant to be antisymmetric, we obtain our final identity:

$$[\mathcal{J}, b_\alpha^+]_- = -2\sum_{k,k'}\sum_{\beta} \mathcal{J}_{kk'}\langle k'|q_\beta^\alpha|k\rangle b_\beta^+ \tag{2.15}$$
$$= -2\sum_{\beta} \mathrm{tr}_1(\mathcal{J}q_\beta^\alpha) b_\beta^+$$

where the symbol tr_1 denotes a trace over a one-particle operator in k-space. The sums over β in (2.15) are restricted to values of β for which the pair wave function φ_β is antisymmetric.

Equation (2.15) defines the coefficients in (Q, 4.14b); since all higher commutators with the operators b_α^+ vanish obviously, all higher coefficients vanish. Substitution of these results into (Q, 4.15) yields the following Dyson image for the operator $\mathcal{J}$;

$$\mathcal{J} \to -2\sum_{\alpha,\beta} \mathrm{tr}_1(\mathcal{J}q_\beta^\alpha) B_\beta^+ B_\alpha \tag{2.16}$$

The Dyson images of the other operators in the second term of (2.3) have been obtained already in earlier work, namely equations (Q, 4.19), (C: 2.1, 2.2, 2.3, 2.24). We repeat the final formulas here for easier reference. The operators R and M are defined by

$$R = \sum_{\alpha} v_\alpha^{\frac{1}{2}} A_\alpha B_\alpha \tag{2.17}$$

$$M = 2\sum_{\alpha,\beta} q_\alpha^\beta (v_\alpha)^{\frac{1}{2}} A_\alpha B_\beta \tag{2.18}$$

It should be noted that M, unlike R, is also a (one-particle) operator in the k-space, not merely an operator in the space of the formal occupation numbers $A_\alpha^+ A_\alpha$ and $B_\beta^+ B_\beta$.

The relevant Dyson images are then:

$$\exp(P) \to \exp(S) \exp[\tfrac{1}{2}\,\mathrm{tr}_1 \ln(1-M)] \tag{2.19}$$

where S is defined in (C, 2.3), but will not be needed in what follows since $(0|\exp(S) = (0|$. The other Dyson image is:

$$\exp(P^+) \to \exp(R^+) \tag{2.20}$$

Substituting these Dyson images, and making use of the fact that vacuum expectation values are preserved under the Dyson transformation, we obtain the identity:

$$\langle 0|\exp(P) J \exp(P^+)|0\rangle \tag{2.21}$$
$$= -2(0|\exp[\tfrac{1}{2}\,\mathrm{tr}_1 \ln(1-M)] \sum_{\alpha,\beta} \mathrm{tr}_1(Jq_\beta^\alpha) B_\beta^+ B_\alpha \exp(R^+)|0)$$

This formula, though correct, is highly awkward and, unless handled with

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considerable care, likely to give misleading results. The difficulty was mentioned in C, at the end of section 2. If there are closure reductions still possible in (2.21), then all these closure reductions should be carried out *first*. The easiest way to ensure that no further closure reductions are possible, is to see to it that all operators to the left of $\exp(R^+)$ in (2.21) commute with each other. This is not true in (2.21) as written, because B_β^+ does not commute with M, (2.16). However, there is the identity

$$(0|B_\beta^+ = 0 \tag{2.22}$$

which in turn implies

$$(0|\exp[\tfrac{1}{2}\,\mathrm{tr}_1\ln(1-M)]B_\beta^+ = (0|[\exp[\tfrac{1}{2}\,\mathrm{tr}_1\ln(1-M)], B_\beta^+]_- \tag{2.23}$$

The commutator on the right of (2.23) is easily evaluated by the general rule (derivable from (2.10))

$$[f(B_1, B_2, \cdots), B_\alpha^+] = \frac{\partial f}{\partial B_\alpha} \tag{2.24}$$

where the right side of (2.24) contains a formal derivative. Carrying out this process on the right side of (2.21) yields the new identity

$$\begin{aligned}&\langle 0|\exp(P)\mathcal{J}\exp(P^+)|0\rangle\\ &\quad = +2\sum_{\alpha,\beta,\gamma}\mathrm{tr}_1(\mathcal{J}q_\beta^\alpha)(0|\exp[\tfrac{1}{2}\,\mathrm{tr}_1\ln(1-M)]\,\mathrm{tr}_1[(1-M)^{-1}q_\alpha^\beta]\\ &\qquad\qquad (v_\gamma)^{\frac{1}{2}}A_\gamma B_\alpha\exp(R^+)|0)\end{aligned} \tag{2.25}$$

At this stage, we notice the possibility of a closure reduction on the index β. Carrying out this reduction, with due regard for antisymmetry, leads to replacing the two traces involving q-operators by the single trace $\mathrm{tr}(\mathcal{J}h)$ where h is given by the following complicated formula (for later convenience, the initial factor 2 in (2.25) is included in this definition):

$$\begin{aligned}\langle k|h|k'\rangle = \tfrac{1}{2}\sum_{\alpha,\gamma}[\varphi_\alpha(k,m)-\varphi_\alpha(m,k)][\varphi_\gamma^*(k',m')-\varphi_\gamma^*(m',k')]\\ \langle m'|(1-M)^{-1}|m\rangle(v_\gamma)^{\frac{1}{2}}A_\gamma B_\alpha\end{aligned} \tag{2.26}$$

Although this definition appears very awkward, we show, in small print below, that it is identical with the much simpler definition:

$$\langle k|h|k'\rangle = \left\langle k\left|\frac{-M}{1-M}\right|k'\right\rangle \tag{2.27}$$

To prove the identity of (2.25) and (2.26), we expand the operator $(1-M)^{-1}$ in a power series, and compare term for term. As an example, consider the second term of the two series. (2.27) gives, for this second term:

$$\langle k|-M^2|k'\rangle = -4\langle k|q_\alpha^\beta|k''\rangle\langle k''|q_\gamma^\delta|k'\rangle(v_\alpha v_\gamma)^{\frac{1}{2}}A_\alpha B_\beta A_\gamma B_\delta \tag{2.28}$$

where summation over all repeated indices is understood. The second term in the expansion of (2.26) is (assuming now that φ_α, φ_γ are properly antisymmetric)

$$\begin{aligned} 2\varphi_\alpha(k, m)\varphi_\gamma^*(k', m')2\langle m'|q_\gamma^\beta|m\rangle (v_\gamma v_\delta)^{\frac{1}{2}} A_\delta B_\beta A_\gamma B_\alpha \\ = -4\varphi_\alpha(k, m)\varphi_\gamma^*(m', k')\varphi_\beta(m', m'')\varphi_\delta^*(m'', m)(v_\gamma v_\delta)^{\frac{1}{2}} A_\delta B_\beta A_\gamma B_\alpha \end{aligned} \tag{2.29}$$

where we have used the definitions of M, (2.18), of q, (2.9), and the antisymmetry of φ_γ. Using the antisymmetry of the other wave functions, this can be rewritten as

$$\begin{aligned} -4\varphi_\alpha(k, m)\varphi_\delta^*(m, m'')\varphi_\beta(m'', m')\varphi_\gamma^*(m', k')(v_\gamma v_\delta)^{\frac{1}{2}} A_\delta B_\alpha A_\gamma B_\beta \\ = -4\langle k|q_\gamma^\alpha|m''\rangle\langle m''|q_\gamma^\beta|k'\rangle (v_\gamma v_\delta)^{\frac{1}{2}} A_\delta B_\alpha A_\gamma B_\beta \end{aligned} \tag{2.30}$$

Except for renaming of dummy indices, the last line of (2.30) agrees precisely with (2.28). Direct inspection shows that this reduction is possible, in an analogous fashion, for every term of the power series, thereby proving the identity between (2.26) and (2.27).

Combining the formulas obtained so far, we obtain the result

$$\langle 0|\exp(P)\tilde{J}\exp(P^+)|0\rangle = (0|\exp[\tfrac{1}{2}\,\mathrm{tr}_1 \ln(1-M)]\mathrm{tr}_1(\tilde{J}h)\exp(P^+)|0) \tag{2.31}$$

There is an obvious formal resemblance between (2.31) and (E, 4.23), its counterpart in the case of a single quantum state of the pair. The detailed reduction of (2.31) to (E, 4.23) will be carried out in section 4 of this paper.

By substitution into (2.3), the final result for the statistical expectation value of any single-particle operator J becomes:

$$J = \sum_k \bar{n}_k J_{kk} + \frac{(0|\exp[\frac{1}{2}\,\mathrm{tr}_1 \ln(1-M)]\,\mathrm{tr}_1(\tilde{J}h)\exp(R^+)|0)}{(0|\exp[\frac{1}{2}\,\mathrm{tr}_1 \ln(1-M)]\exp(R^+)|0)} \tag{2.32}$$

This final result looks still fairly complicated. However, it is much simpler than the original expression (2.3), since all the operators in (2.32) obey simple Bose-Einstein commutation rules. We shall reduce (2.32) to the special case (of only one pair state) derived in E, and we shall obtain, from (2.32), a particularly simple result for the expectation value of the number operator. Both these things will be done in section 4.

Just as in earlier work, it is sometimes convenient to shift factors $(v_\alpha)^{\frac{1}{2}}$ from $\exp(R^+)$ to the other factors in (2.32). This can be done by the following simple replacements:

$$M \to M' = 2\sum_{\alpha,\beta} q_\alpha^\beta (v_\alpha v_\beta)^{\frac{1}{2}} A_\alpha B_\beta \tag{2.33a}$$

$$h \to h' = \frac{-M'}{1-M'} \tag{2.33b}$$

$$R^+ \to (R')^+ = \sum_\alpha A_\alpha^+ B_\alpha^+ \tag{2.33c}$$

Formula (2.32) remains valid when M, h, R are replaced by M', h', R' respectively.

3. Expectation values of two-particle operators

We now consider a typical two particle operator

$$K = \sum K_{lm,\, l'm'} a_l^+ a_m^+ a_{m'} a_{l'} . \tag{3.1}$$

There is already a considerable reduction for its expectation value, which was carried out in E and has led to equation (E, 2.12), which we reproduce here for easier reference

$$\begin{aligned} \langle K \rangle = \sum_{l,m} (K_{lm,\,lm} - K_{lm,\,ml}) \bar{n}_l \bar{n}_m + \frac{\langle 0|\exp(P)\tilde{K}^{(1)}\exp(P^+)|0\rangle}{\langle 0|\exp(P)\exp(P^+)|0\rangle} \\ + \frac{\langle 0|\exp(P)\tilde{K}\exp(P^+)|0\rangle}{\langle 0|\exp(P)\exp(P^+)|0\rangle} . \end{aligned} \tag{3.2}$$

The first term in this equation is an ordinary Hartree-Fock expectation value due to the unpaired particles. The second term arises from the interaction between unpaired particles and particles within pairs. The quantity $\tilde{K}^{(1)}$ is defined by

$$\tilde{K}^{(1)} = \sum_{k,k'} \tilde{K}^{(1)}_{kk'} a_k^+ a_{k'} \tag{3.3a}$$

$$\tilde{K}^{(1)}_{kk'} = (1 - \bar{n}_k)^{\frac{1}{2}} (1 - \bar{n}_{k'})^{\frac{1}{2}} \sum_l \bar{n}_l (K_{kl,\,k'l} + K_{lk,\,lk'} - K_{kl,\,lk'} - K_{lk,\,k'l}). \tag{3.3b}$$

The last term in (3.2) is the contribution of particles within pairs. The operator $\tilde{K}$ has the same form as (3.1) except that the matrix elements are now quenched. That is

$$\tilde{K}_{lm,\,l'm'} = [(1 - \bar{n}_l)(1 - \bar{n}_m)(1 - \bar{n}_{l'})(1 - \bar{n}_{m'})]^{\frac{1}{2}} K_{lm,\,l'm'} . \tag{3.4}$$

Since $\tilde{K}^{(1)}$ is a one particle operator, it needs no further discussion and we shall concentrate entirely on the last term of (3.2). As a first step we require the Dyson image of the operator $a_l^+ a_m^+ a_{m'} a_{l'}$. The Dyson transformation is linear. Thus we may consider the factors $a_l^+ a_m^+$ and $a_{m'} a_{l'}$ separately and combine them at the end. We use (2.14) together with the fact that the Dyson image of b_α^+ is B_β^+. This gives

$$a_l^+ a_m^+ \to 2^{-\frac{1}{2}} \sum_\alpha [\varphi_\alpha^*(l, m) - \varphi_\alpha^*(m, l)] B_\alpha^+ \tag{3.5}$$

The Dyson transformation, although linear, does not preserve Hermitean conjugates, thus b_β does not map into B_β, but rather into (see equation (Q, 4.18))

$$b_\beta \to B_\beta - \tfrac{1}{2} \sum_{\beta'\gamma\delta} C_{\gamma\delta}^{\beta\beta'} B_{\beta'}^+ B_\gamma B_\delta \tag{3.6}$$

where*

* This equation differs from (Q, 4.3) by correction for complex conjugates of wave functions.

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(3.6a) $$C^{\alpha\beta}_{\gamma\delta} = 4 \sum_{k_1k_2k_3k_4} \varphi^*_\alpha(k_1k_2)\varphi^*_\beta(k_3k_4)\varphi_\gamma(k_2k_3)\varphi_\delta(k_4k_1)$$

Taking the Hermitean conjugates of (2.14) and using (3.6) we get the following Dyson image

(3.7) $$a_{m'}a_{l'} \to 2^{-\frac{1}{2}} \sum_\beta [\varphi_\beta(m', l') - \varphi_\beta(l', m')][B_\beta - \tfrac{1}{2} \sum_{\beta'\gamma\delta} C^{\beta\beta'}_{\gamma\delta} B^+_{\beta'} B_\gamma B_\delta]$$

In accordance with our general procedure, we make use of closure contractions wherever possible and as soon as possible. There is clearly a closure contraction on the index β in the last term of (3.7). We define the quantity

(3.8) $$\varphi_{\gamma\beta\delta}(m', l') = \sum_{k_1k_2} \varphi_\gamma(m'k_1)\varphi^*_\beta(k_1k_2)\varphi_\delta(k_2l')$$

and use closure on (3.7) to get

(3.9) $$a_{m'}a_{l'} \to 2^{-\frac{1}{2}} \sum_\beta [\varphi_\beta(m', l') - \varphi_\beta(l', m')]B_\beta - 2^{-\frac{1}{2}} \sum_{\beta\gamma\delta} [\varphi_{\gamma\beta\delta}(m', l') - \varphi_{\gamma\beta\delta}(l', m')] \times B^+_\beta B_\gamma B_\delta$$

So far everything has been written in correct antisymmetric form. Howevery, since the formulas would become unreasonably long if we continued this, we shall henceforth deliberately do it unsymmetrically; for example, we shall replace $\varphi_\beta(m', l') - \varphi_\beta(l', m')$ by $2\varphi_\beta(m', l')$, and so on. At the very end of the derivation we shall recover the correct antisymmetric form by antisymmetrizing in (l, m) and (m', l').

We substitute (2.19), (2.20), (3.5) and (3.9) into the last term of (3.2). In the resulting vacuum expectation value, we eliminate the operator B^+_α, as before, by commutation through the left side. It is now possible to contract with the wave function $\varphi^*_\alpha(l, m)$ according to

(3.10) $$\sum_\alpha \varphi^*_\alpha(l, m)\langle k|q^\alpha_{\alpha'}|k'\rangle = \delta_{lk}\varphi^*_{\alpha'}(m, k')$$

This gives rise to the identity

(3.11) $$\sum_{\alpha,\alpha'} \varphi^*_\alpha(l, m) \operatorname{tr}_1 [(1-M)^{-1}q^\alpha_{\alpha'}] = \sum_{\alpha'} \varphi^*_{\alpha'}(m, k') \left\langle k' \left| \frac{1}{1-M} \right| l \right\rangle.$$

Combining the result so far we obtain

(3.12) $$\begin{aligned}(0|\exp(P)a^+_l a^+_m a_{m'}a_{l'} \exp(P^+)|0) &= 2(0|\exp[\tfrac{1}{2}\operatorname{tr}_1 \ln(1-M)] \\ &\times \left[\sum_{\alpha,k} \varphi^*_\alpha(m, k) \left\langle k \left| \frac{1}{1-M} \right| l \right\rangle v^{\frac{1}{2}}_\alpha A_\alpha\right] \\ &\times [\sum_\beta \varphi_\beta(m', l')B_\beta + 2\sum_{\beta\gamma\delta} \varphi_{\gamma\beta\delta}(m', l')B^+_\beta B_\gamma B_\delta] \\ &\times \exp(R^+)|0) = I_1 + I_2.\end{aligned}$$

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This expression is still subject to antisymmetrization later on.

We now proceed to eliminate the factor B_β^+ by commuting it through everything to the left of it. We use (2.24) and the identity

$$\frac{\partial}{\partial B_\beta}\left(\frac{1}{1-M}\right) = \frac{1}{1-M}\frac{\partial M}{\partial B_\beta}\frac{1}{1-M} \tag{3.13}$$

to get

$$\frac{\partial}{\partial B_\beta}\left\{\exp\left[\tfrac{1}{2}\,\mathrm{tr}_1 \ln(1-M)\right]\left\langle k'\left|\frac{1}{1-M}\right|l\right\rangle\right\}$$

$$= \exp\left[\tfrac{1}{2}\,\mathrm{tr}_1 \ln(1-M)\right]\left\{-\tfrac{1}{2}\,\mathrm{tr}\left(\frac{1}{1-M}\frac{\partial M}{\partial B_\beta}\right)\left\langle k'\left|\frac{1}{1-M}\right|l\right\rangle\right. \tag{3.14}$$

$$\left. + \left\langle k'\left|\frac{1}{1-M}\right|k''\right\rangle\left\langle k''\left|\frac{\partial M}{\partial B_\beta}\right|k'''\right\rangle\left\langle k'''\left|\frac{1}{1-M}\right|l\right\rangle\right\}$$

We observe that

$$\frac{\partial M}{\partial B_\beta} = 2\sum_\sigma q_\sigma^\beta (v_\sigma)^{\frac{1}{2}} A_\sigma \tag{3.15}$$

At this stage it is possible to make a contraction on the index β according to

$$\sum_{\beta\gamma\delta}\left\langle k_1\left|\frac{\partial M}{\partial B_\beta}\right|k_2\right\rangle\varphi_{\gamma\beta\delta}(m'l')B_\gamma B_\delta = -2\sum_{\sigma\gamma\delta}\langle l'|q_\sigma^\delta|k_2\rangle\varphi_\gamma(m',k_1)(v_\sigma)^{\frac{1}{2}}A_\sigma B_\gamma B_\delta$$

$$= -\langle l'|M|k_2\rangle\sum_\gamma \varphi_\gamma(m',k_1)B_\gamma \tag{3.16}$$

Using this result we get the following expression for the term I_2, the second sum in (3.12) *

$$I_2 = -4(0|\exp\left[\tfrac{1}{2}\,\mathrm{tr}_1\ln(1-M)\right]\varphi_\alpha^*(m,k)\,(v_k)^{\frac{1}{2}}A_\alpha\cdot\varphi_\gamma(m',k_1)B_\gamma\cdot\langle l'|M|k_2\rangle$$

$$\cdot\left[\left\langle k\left|\frac{1}{1-M}\right|k_1\right\rangle\left\langle k_2\left|\frac{1}{1-M}\right|l\right\rangle - \tfrac{1}{2}\left\langle k_2\left|\frac{1}{1-M}\right|k_1\right\rangle\left\langle k\left|\frac{1}{1-M}\right|l\right\rangle\right]$$

$$\cdot\exp(R^+)|0) = I_{2,1} + I_{2,2}. \tag{3.17}$$

We have again broken this into two separate parts. Remembering the definition of h, equation (2.27), the first part becomes

$$I_{2,1} = 2(0|\exp\left[\tfrac{1}{2}\,\mathrm{tr}_1\ln(1-M)\right]\langle l'|h|l\rangle\langle m'|h|m\rangle\exp(R^+)|0) \tag{3.18}$$

At this stage we antisymmetrize. We define the two particle operator p by

$$\langle l'm'|p|lm\rangle = \langle l'|h|l\rangle\langle m'|h|m\rangle - \langle m'|h|l\rangle\langle l'|h|m\rangle \tag{3.19}$$

* We use the summation convention that all repeated indices are to be summed over, in order to decrease the length of these formulas somewhat.

to get as a properly antisymmetrized form of $I_{2,1}$

$$(3.20)\qquad I_{2,1} = (0|\exp[\tfrac{1}{2}\mathrm{tr}_1 \ln(1-M)]\langle l'm'|p|lm\rangle \exp(R^+)|0)$$

The term $I_{2,2}$ is given by

$$(3.21)\qquad \begin{aligned} I_{2,2} = {} & 2(0|\exp[\tfrac{1}{2}\mathrm{tr}_1 \ln(1-M)]\left\langle l'\left|\frac{M}{1-M}\right|k_1\right\rangle \varphi_\gamma(k_1, m') \\ & \cdot \varphi_\alpha^*(m,k)\left\langle k\left|\frac{1}{1-M}\right|l\right\rangle (v_\alpha)^{\frac{1}{2}} A_\alpha B_\gamma \exp(R^+)|0) \end{aligned}$$

It turns out to be useful to employ the identity

$$(3.22)\qquad \left\langle l'\left|\frac{M}{1-M}\right|k_1\right\rangle = -\delta_{l'k_1} + \left\langle l'\left|\frac{1}{1-M}\right|k_1\right\rangle$$

We now combine this term with I_1 in (3.21). By judicious juggling of dummy indices, we find that the $\delta_{l'k_1}$ in (3.22) gives rise to a term which exactly cancels I_1, if the wave function φ_γ is antisymmetric. It turns out to be convenient to define an operator wave function (operator in the AB space, wave function in the kl space) by

(3.23)

$$\psi_\alpha(l', m') = 2^{-\frac{1}{2}} \sum_{k'} \left[\left\langle l'\left|\frac{1}{1-M}\right|k'\right\rangle \varphi_\alpha(k', m') - \left\langle m'\left|\frac{1}{1-M}\right|k'\right\rangle \varphi_\alpha(k', l')\right]$$

In (3.23) we have already carried out the required antisymmetrization. Carrying out that same antisymmetrization on the result so far, we find that the correctly antisymmetrized form becomes

$$(3.24)\qquad \begin{aligned} I_1 + I_{2,2} = {} & (0|\exp[\tfrac{1}{2}\mathrm{tr}_1 \ln(1-M)]\cdot \psi_\gamma(l', m')\psi_\alpha^*(l, m) \\ & \cdot (v_\alpha)\tfrac{1}{2} A_\alpha B_\gamma \exp(R^+)|0). \end{aligned}$$

At this state all that remains is to multiply by $\tilde{K}_{lm,l'm'}$ and sum over l, m, l' and m'. We define the trace of a two particle operator in the usual way (see E, 5.4) and we also define

$$(3.25)\qquad (\psi_\alpha, \tilde{K}\psi_\beta) = \sum_{l,m,l',m'} \psi_\alpha^*(l, m)\tilde{K}_{lm,l'm'}\psi_\beta(l', m').$$

This gives us our final result

$$(3.26)\qquad \begin{aligned} \langle 0|\exp(P)\tilde{K}\exp(P^+)|0\rangle = {} & (0|\exp[\tfrac{1}{2}\mathrm{tr}_1 \ln(1-M)] \\ & \cdot \{\mathrm{tr}_2(\tilde{K}p) + \sum_{\alpha,\beta}(\psi_\alpha, \tilde{K}\psi_\beta)(v_\alpha)^{\frac{1}{2}} A_\alpha B_\beta\} \cdot \exp(R^+)|0). \end{aligned}$$

There is of course a very strong formal resemblance between (3.26) and equation (E, 5.26). All other terms in equation (3.2) are already under control.

We close this section by remarking that we can again throw all factors $v^{\frac{1}{2}}$ to the left-hand side. In addition to the replacements (2.33), all we require is the additional replacement, in (3.26)

$$(3.27) \qquad (v_\alpha)^{\frac{1}{2}} A_\alpha A_\beta \to (v_\alpha v_\beta)^{\frac{1}{2}} A_\alpha B_\beta$$

Equation (3.26) then remains a valid equation.

4. Discussion

We start by showing how these formulas reduce to the results of paper E. Thus we now assume that only one eigenvalue of the quenched pair correlation matrix differs from zero

$$(4.1) \qquad v_1 \neq 0, \quad v_2 = v_3 = \cdots = 0.$$

By using the replacements (2.33), it is now obvious that only $\alpha = \beta = 1$ makes any contribution whatever. We therefore drop the subscripts $\alpha, \beta, \cdots$. Furthermore, we note that B occurs only combined with A, in the product AB. Thus B has as its only function the supplying of a factor $n!$ for a term of order n. We thus use the same reduction as in C, section 3, which led to equation (C, 3.10). In effect, the operator AB wherever it occurs is replaced by a c-number t. Thus, in particular, we get the correspondence

$$(4.2) \qquad M' = 2q\, vAB \to 2vtq$$

$$(4.3) \qquad h' = \frac{-M}{1-M} \to \frac{-2vtq}{1-2vtq}.$$

This gives an exact correspondence with the results of paper E. Compare, for example, (4.3) and (E, 4.21). The correspondence is equally exact for the two particle operators, that is (3.26) reduces directly to (E, 5.26).

It turns out that there exists a useful identity for the expectation value of the number operator in the case where all particles are paired, but the pairs are not necessarily Bose condensed. The number operator is

$$(4.4) \qquad N = \sum_k a_k^+ a_k$$

This is a special case of (2.1), with $J_{kk'} = \delta_{kk'}$. If there are no unpaired particles (as we shall assume henceforth), then there is no quenching and $\bar{J} = J$.

Let us now consider the expression for the partition function taken from (C, 2.25)

$$(4.5) \qquad \exp(-\beta\Omega_M) = (0|\exp[\tfrac{1}{2}\operatorname{tr}_1 \ln(1-M')]\exp[(R')^+]|0)$$

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We operate on both sides of this equation with $v_\alpha(\partial/\partial v_\alpha)$, sum over α and multiply by 2

$$
\begin{aligned}
(4.6) \qquad & 2\sum_\alpha v_\alpha \frac{\partial}{\partial v_\alpha}(-\beta\Omega_M) \\
&= \exp(+\beta\Omega_M)(0|\exp[\tfrac{1}{2}\operatorname{tr}_1\ln(1-M')]\operatorname{tr}_1\left(\frac{-1}{1-M'}\sum_\alpha v_\alpha\frac{\partial M'}{\partial v_\alpha}\right) \\
&\times \exp(R^+)|0)
\end{aligned}
$$

Since M', equation (2.33a) is homogeneous of first degree in the quantity v_α, Euler's theorem gives

$$(4.7) \qquad \sum_\alpha v_\alpha \frac{\partial M'}{\partial v_\alpha} = M'$$

Thus the one particle trace in equation (4.6) is simply the trace of the operator h', equation (2.33b), which is just what is needed for the expectation value of the number operator. We therefore obtain

$$(4.8) \qquad N = 2\sum_\alpha v_\alpha \frac{\partial}{\partial v_\alpha}(-\beta\Omega_M) = \sum_\alpha N_\alpha.$$

If we interpret the individual terms of this sum as the number of particles bound in pairs of type α, then these are exactly the expressions we used in paper C to establish the existence of a Bose condensation. Furthermore, it is easy to show that for other operators also, besides the number operator, the second pair state contributes an amount of relative order $1/N$, compared to the lowest pair state, in the condensation region.

Although the identification of $\langle N_\alpha\rangle$ as the number of particles in pairs of type α is quite natural, this analogy must not be pushed too far. In particular, if J is an arbitrary one-particle operator, it is well to observe that

$$(4.9) \qquad \langle J\rangle \neq \sum_\alpha \langle N_\alpha\rangle(\varphi_\alpha, J\varphi_\alpha)$$

However, such an identity is by no means required to establish the existence of a Bose condensation.

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References

[1] Schafroth, M. R., Phys. Rev., 96, 1442 (1954) L.
[2] Schafroth, M. R., Butler, S. T. and Blatt, J. M., Helv. Phys. Acta, 30, 93 (1957).
[3] Blatt, J. M. and Matsubara, T., Prog. Theor. Phys., 20, 533 (1958), called Q henceforth.
[4] Matsubara, T. and Blatt, J. M., Prog. Theor. Phys., 23, 451 (1960), called C henceforth.
[5] Blatt, J. M., Prog. Theor. Phys., 23, 447 (1960).

[6] Blatt, J. M., J. Aust. Math. Soc., 1, 465 (1960), called E henceforth.
[7] Blatt, J. M., Prog. Theor. Phys., 24, 851 (1960).
[8] Blatt, J. M., Phys. Rev. Letters, 7, 82 (1961).
[9] Blatt, J. M. Prog. Theor. Phys., 26, 761 (1961).
Of these, references [3], [4] and [6] are directly related to the present work, and formulas from these references will be used frequently. We shall refer to these papers by the letters Q (for quasi-chemical equilibrium theory), C (for Bosé-Einstein Condensation), and E (for Expectation values) henceforth; equation (C, 2.24) means equation (2.24) of paper C, i.e., of reference (4).
[10] Katz, A., private communication.
[11] Dyson, F. J., Phys. Rev., 102, 1217 (1956).

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