A PERTURBATION APPROACH TO BOSE-CONDENSED PAIRS

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(received 17 April 1962)

Abstract

A perturbation method is developed, and is used to obtain approximate expressions for the expectation values of one-particle and two particle operators in the quasi-chemical equilibrium (pair correlation) approximation to statistical mechanics, for the case of non-extreme Bose-Einstein condensation of the correlated pairs. To lowest order, the approximate results reproduce the results obtained previously for the case of extreme Bose-Einstein condensation.

1. Introduction

It has been shown [1, 2], that under certain conditions the quasi-chemical equilibrium approximation exhibits a transition phenomenon closely analagous to a Bose-Einstein condensation of the quasi-molecules. Furthermore, 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 [3] that the condensed ideal Bose-Einstein gas exhibits a Meissner effect.

In order to carry out self consistent calculations with the quasi-chemical equilibrium formalism, it is necessary to have simple expressions for the expectation values of one-particle and two-particle operators. This was done in [4] for the special case of extreme Bose-Einstein condensation, i.e. only one pair state is occupied. Surprisingly enough, this suffices to get a workable theory of superconductivity — there is actually Bose-Einstein condensation [5], and thus this apparently extreme assumption is nonetheless physically reasonable. However, to carry out more detailed calculations on the theory of superconductivity (in particular, calculations for finite temperatures), we require expectation values for the case of non-extreme Bose-Einstein condensation, i.e. there is an infinite number of pair states, of which only one is highly occupied.

In [6], general expressions for the expectation values of one-particle and two-particle operators were obtained, and in sections 3 and 4 of this paper, we evaluate approximate expressions for these formulae using the perturbation method developed in section 2.

Throughout this paper, we shall:

(a) Ignore spins,

(b) restrict the pair wavefunctions $\varphi_\alpha(k_1, k_2)$ to be real, "simple pair" wavefunctions (C.1.2):

$$\varphi_\alpha(k_1, k_2) = \delta(k_1 + k_2 - K_\alpha) w_\alpha[\tfrac{1}{2}(k_1 - k_2)] \tag{1.1}$$

and (c) assume that $w_\alpha(k_1, k_2) = w_{-\alpha}(k_1, k_2)$ and $v_\alpha = v_{-\alpha}$, where v_α are the eigenvalues of the "pair correlation matrix".

Assumptions (a) and (c) are reasonable but the restriction to simple pairs requires justification; a discussion on this restriction is given in section 5.

2. The trace of the statistical matrix

The statistical matrix $\mathscr{U}$ [7], in the quasi-chemical equilibrium theory has trace (Q3.10):

$$\mathrm{Tr}(\mathscr{U}) = \mathrm{Tr}(\mathscr{V})\langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle \tag{2.1}$$

The value of $\mathrm{Tr}(\mathscr{V})$ is well known, so we confine our attention to (C.2.5):

$$e^{-\beta\Omega_M} = \langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle = \langle 0|\exp\{\tfrac{1}{2}\mathrm{Tr}\ln(1-M)\}\exp\{R^+\}|0\rangle \tag{2.2}$$

where:

$$M = 2\sum_{\alpha,\beta} q_\alpha^\beta \sqrt{v_\alpha v_\beta}\, A_\alpha B_\beta \tag{2.3a}$$

and

$$R^+ = \sum_\alpha A_\alpha^+ B_\alpha^+ \tag{2.3b}$$

The A_α and the B_α are operators operating in disjoint Hilbert spaces, and both sets of operators obey Bose-commutation rules:

$$[A_\alpha, A_\beta^+] = [B_\alpha, B_\beta^+] = \delta_{\alpha\beta}, \text{ all others zero} \tag{2.4}$$

and the q_α^β are defined by (C.2.9):

$$\langle k|q_\alpha^\beta|k'\rangle = \sum_{k''} \varphi_\beta(k, k'')\varphi_\alpha^*(k'', k'). \tag{2.5a}$$

Under restriction (b), to simple pairs, this reduces to the form:

$$\langle k|q_\alpha^\beta|k'\rangle = -\delta(k + K_\alpha - [k' + K_\beta]) w_\beta(k - \tfrac{1}{2}K_\beta) w_\alpha(k - K_\beta + \tfrac{1}{2}K_\alpha). \tag{2.5b}$$

Equation (2.2) has been evaluated for some simple cases in paper C, namely, the case of extreme Bose-Einstein condensation, and the case of two quantum states only. In this section we evaluate $e^{-\beta\Omega_M}$ approximately by neglecting all but a few terms in the expansion of $\mathrm{Tr}\ln(1-M)$. The final result is expressed as an integral.

First, we take "state number 0" to be the ground state, (i.e. v_0 is the largest eigenvalue of the pair correlation matrix, corresponding to the condensed state) and separate out from M:

(2.6a) $$M_0 = 2q_0^0 v_0 A_0 B_0$$

(2.6b) $$M_1 = 2\sum_{\alpha\neq 0}\sqrt{v_0 v_\alpha}(q_0^\alpha A_0 B_\alpha + q_\alpha^0 A_\alpha B_0)$$

(2.6c) $$M_2 = 2\sum_{\alpha,\beta\neq 0} q_\alpha^\beta \sqrt{v_\alpha v_\beta} A_\alpha B_\beta$$

so that

(2.6d) $$M = M_0 + M'$$

where

(2.6e) $$M' = M_1 + M_2.$$

We now expand $\ln(1-(M_0+M'))$ (formally) in a power series (M_0 and M' do not commute) thus:

(2.7)
$$\begin{aligned}\ln(1-(M_0+M')) = &-(M_0+M') - \tfrac{1}{2}(M_0^2 + M_0M' + M'M_0 + M'^2)\\ &-\tfrac{1}{3}(M_0^3 + M_0^2M' + M_0M'M_0 + M'M_0^2 + M_0M'^2\\ &\qquad + M'M_0M' + M'^2M_0 + M'^3)\\ &-\cdots.\end{aligned}$$

Taking the trace of (2.7) and using $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ we obtain:

(2.8)
$$\begin{aligned}\mathrm{Tr}\ln(1-(M_0+M'))\\ &= \mathrm{Tr}\left(-M_0 - \frac{M_0^2}{2} - \frac{M_0^3}{3} - \cdots\right) - \mathrm{Tr}([1+M_0+M_0^2+\cdots]M')\\ &\quad -\tfrac{1}{2}\mathrm{Tr}([1+M_0+M_0^2+\cdots]M'[1+M_0+M_0^2+\cdots]M') - \cdots\\ &= \mathrm{Tr}\ln(1-M_0) - \mathrm{Tr}\left(\frac{1}{1-M_0}M'\right) - \tfrac{1}{2}\mathrm{Tr}\left(\frac{1}{1-M_0}M\frac{1}{1-M_0}M'\right)\\ &\quad -\cdots.\end{aligned}$$

We now neglect terms in (2.8) of degree higher than the first in v_α (e.g. $v_\alpha v_\beta \alpha, \beta \neq 0$ is of order 1, $\sqrt{v_0 v_\alpha}$ $\alpha \neq 0$ is of order $\frac{1}{2}$ etc.) and substitute into (2.2):

(2.9)
$$\begin{aligned}\langle 0|e^{P}e^{P^+}|0\rangle \cong \langle 0|\exp&\left\{\tfrac{1}{2}\mathrm{Tr}\ln(1-M_0) - \tfrac{1}{2}\mathrm{Tr}\left(\frac{1}{1-M_0}M_1\right)\right.\\ &\left.-\tfrac{1}{2}\mathrm{Tr}\left(\frac{1}{1-M_0}M_2\right) - \tfrac{1}{4}\mathrm{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\right)\right\}\exp\{\sum_\alpha A_\alpha^+ B_\alpha^+\}|0\rangle\end{aligned}$$

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By (2.5) $\langle k|q_0^0|k'\rangle = -\delta_{kk'}w_0^2(k)$, so M_0 is diagonal, therefore:

$$\text{Tr}\left(\frac{1}{1-M_0}M_1\right) = \sum_k \frac{1}{1-\langle k|M_0|k\rangle}\langle k|M_1|k\rangle \tag{2.10}$$

where [1])

$$\begin{aligned}\langle k|M_1|k\rangle &= 2{\sum_\alpha}' \sqrt{v_0 v_\alpha}(\langle k|q_0^\alpha|k\rangle A_0 B_\alpha + \langle k|q_\alpha^0|k\rangle A_\alpha B_0)\\ &= 0 \text{ by (2.5b).}\end{aligned} \tag{2.11}$$

Also,

$$\text{Tr}\left(\frac{1}{1-M_0}M_2\right) = \sum_k \frac{1}{1-\langle k|M_0|k\rangle}\langle k|M_2|k\rangle \tag{2.12}$$

where

$$\begin{aligned}\langle k|M_2|k\rangle &= 2\sum_{\alpha,\beta\neq 0}\langle k|q_\alpha^\beta|k\rangle\sqrt{v_\alpha v_\beta}A_\alpha B_\beta\\ &= -2\sum_{\alpha,\beta\neq 0}\delta(K_\alpha - K_\beta)w_\beta(k-\tfrac{1}{2}K_\beta)w_\alpha(k-\tfrac{1}{2}K_\alpha)\sqrt{v_\alpha v_\beta}A_\alpha B_\beta\\ &= -2{\sum_\alpha}' w_\alpha^2(k-\tfrac{1}{2}K_\alpha)v_\alpha A_\alpha B_\alpha\end{aligned} \tag{2.13}$$

since by assumption (a) $K_\alpha = K_\beta$ implies $\alpha=\beta$. So,

$$-\tfrac{1}{2}\text{Tr}\left(\frac{1}{1-M_0}M_2\right) = {\sum_\alpha}'\sum_k \frac{w_\alpha^2(k-\frac{1}{2}K_\alpha)v_\alpha A_\alpha B_\alpha}{1+2v_0A_0B_0w_0^2(k)} \tag{2.14}$$

next,

$$\begin{aligned}-\tfrac{1}{4}\text{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\right) = -\tfrac{1}{4}\sum_{k,k'}\frac{1}{1-\langle k|M_0|k\rangle}\langle k|M_1|k'\rangle\\ \cdot\frac{1}{1-\langle k'|M_0|k'\rangle}\langle k'|M_1|k\rangle.\end{aligned} \tag{2.15}$$

The A_α and B_α all commute so:

$$\begin{aligned}&-\tfrac{1}{4}\text{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\right)\\ &\qquad = -\tfrac{1}{4}\sum_{k,k'}\frac{\langle k|M_1|k'\rangle\langle k'|M_1|k\rangle}{(1-\langle k|M_0|k\rangle)(1-\langle k'|M_0|k'\rangle)}\end{aligned} \tag{2.16}$$

$$\begin{aligned}\langle k|M_1|k'\rangle\langle k'|M_1|k\rangle &= 4v_0\sum_{\alpha,\beta\neq 0}\sqrt{v_\alpha v_\beta}(\langle k|q_0^\alpha|k'\rangle A_0B_\alpha + \langle k|q_\alpha^0|k'\rangle A_\alpha B_0)\\ &\qquad\cdot(\langle k'|q_0^\beta|k\rangle A_0 B_\beta + \langle k'|q_\beta^0|k\rangle A_\beta B_0)\\ &= \text{I}+\text{II}+\text{III}+\text{IV}\end{aligned} \tag{2.17}$$

[1] The primed sum means summation over all α except $\alpha = 0$.

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I, II, III, and IV are defined by:

$$(2.18a)\quad \begin{aligned} \mathrm{I} &= 4v_0 \sum_\alpha{}' \sqrt{v_\alpha v_{-\alpha}} \langle k|q_0^\alpha|k-K_\alpha\rangle\langle k-K_\alpha|q_0^{-\alpha}|k\rangle A_0^2 B_\alpha B_{-\alpha}\delta_{k',k-K_\alpha} \\ &= 4v_0 \sum_\alpha{}' v_\alpha w_0(k) w_0(k-K_\alpha) w_\alpha^2(k-\tfrac{1}{2}K_\alpha) A_0^2 B_\alpha B_{-\alpha}\delta_{k',k-K_\alpha} \end{aligned}$$

$$(2.18b)\quad \begin{aligned} \mathrm{II} &= 4v_0 \sum_\alpha{}' \sqrt{v_\alpha v_{-\alpha}} \langle k|q_\alpha^0|k+K_\alpha\rangle\langle k+K_\alpha|q_{-\alpha}^0|k\rangle B_0^2 A_\alpha A_{-\alpha}\delta_{k',k+K_\alpha} \\ &= 4v_0 \sum_\alpha{}' v_\alpha w_0(k) w_0(k+K_\alpha) w_\alpha^2(k+\tfrac{1}{2}K_\alpha) B_0^2 A_\alpha A_{-\alpha}\delta_{k',k+K_\alpha} \end{aligned}$$

$$(2.18c)\quad \begin{aligned} \mathrm{III} &= 4v_0 \sum_\alpha{}' v_\alpha \langle k|q_0^\alpha|k-K_\alpha\rangle\langle k-K_\alpha|q_\alpha^0|k\rangle A_0 B_0 A_\alpha B_\alpha\delta_{k',k-K_\alpha} \\ &= 4v_0 \sum_\alpha{}' v_\alpha w_0^2(k-K_\alpha) w_\alpha^2(k-\tfrac{1}{2}K_\alpha) A_0 B_0 A_\alpha B_\alpha\delta_{k',k-K_\alpha} \end{aligned}$$

$$(2.18d)\quad \begin{aligned} \mathrm{IV} &= 4v_0 \sum_\alpha{}' v_\alpha \langle k|q_\alpha^0|k+K_\alpha\rangle\langle k+K_\alpha|q_0^\alpha|k\rangle A_0 B_0 A_\alpha B_\alpha\delta_{k',k+K_\alpha} \\ &= 4v_0 \sum_\alpha{}' v_\alpha w_0^2(k) w_\alpha^2(k+\tfrac{1}{2}K_\alpha) A_0 B_0 A_\alpha B_\alpha\delta_{k',k+K_\alpha} \end{aligned}$$

where we have used: (1) equation (2.5b); (2) assumption (c); and (3) $K_\alpha = -K_\beta$ implies $\alpha = -\beta$ and $K_\alpha = K_\beta$ implies $\alpha = \beta$ (since we are ignoring spins).

By substituting (2.17) into (2.16) and shifting the k-origins of the terms corresponding to I and III to $k+K_\alpha$, the contributions from I and II, and from III and IV combine and we obtain:

$$(2.19)\quad \begin{aligned} &-\tfrac{1}{4}\mathrm{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\right) \\ &= -\sum_\alpha{}'\sum_k \frac{w_0^2(k)w_\alpha^2(k+\frac{1}{2}K_\alpha)2v_0A_0B_0v_\alpha A_\alpha B_\alpha}{(1+2v_0A_0B_0w_0^2(k))(1+2v_0A_0B_0w_0^2(k+K_\alpha))} \\ &\quad -\sum_\alpha{}'\sum_k \frac{w_0(k)w_0(k+K_\alpha)w_\alpha^2(k+\frac{1}{2}K_\alpha)v_0v_\alpha}{(1+2v_0A_0B_0w_0^2(k))(1+2v_0A_0B_0w_0^2(k+K_\alpha))} \\ &\quad\cdot\{A_0^2B_\alpha B_{-\alpha}+B_0^2A_\alpha A_{-\alpha}\}. \end{aligned}$$

Before continuing we establish a useful notation; h_k, ψ_k, π_α, σ_α, τ_α and $\hat{\tau}_\alpha$ being defined by:

$$(2.20a)\quad h_k = \frac{2v_0A_0B_0w_0^2(k)}{1+2v_0A_0B_0w_0^2(k)}$$

$$(2.20b)\quad \psi_k = \frac{\sqrt{2v_0A_0B_0}\,w_0(k)}{1+2v_0A_0B_0w_0^2(k)}$$

$$(2.20c)\quad \pi_\alpha = \sum_k (1-h_k)w_\alpha^2(k-\tfrac{1}{2}K_\alpha)$$

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(2.20d) $$\sigma_\alpha = \sum_k h_k(1-h_{k+K_\alpha})w_\alpha^2(k+\tfrac{1}{2}K_\alpha)$$

(2.20e) $$\tau_\alpha = \sum_k \psi_k\psi_{k+K_\alpha}w_\alpha^2(k+\tfrac{1}{2}K_\alpha)$$

and

(2.20f) $$\hat{t}_\alpha = \frac{\tau_\alpha}{A_0B_0}.$$

Combining (2.20), (2.19), (2.14), (2.11) and (2.9) we have:

(2.21) $$\begin{aligned}\langle 0|e^{\tilde{P}}e^{\tilde{P}+}|0\rangle \cong \langle 0|\exp[\tfrac{1}{2}\operatorname{Tr}\ln(1-M_0)+{\sum_\alpha}'(\pi_\alpha-\sigma_\alpha)v_\alpha A_\alpha B_\alpha \\ -\tfrac{1}{2}{\sum_\alpha}'\hat{t}_\alpha v_\alpha(A_0^2B_\alpha B_{-\alpha}+B_0^2A_\alpha A_{-\alpha})]\exp[\sum_\alpha A_\alpha^+B_\alpha^+]|0\rangle.\end{aligned}$$

If $w_\alpha = w_{-\alpha}$ and $v_\alpha = v_{-\alpha}$ (which we are assuming), then:

(2.22) $$\begin{aligned}{\sum_\alpha}'(\pi_\alpha-\sigma_\alpha)v_\alpha A_\alpha B_\alpha-\tfrac{1}{2}{\sum_\alpha}'\hat{t}_\alpha v_\alpha(A_0^2B_\alpha B_{-\alpha}+B_0^2A_\alpha A_{-\alpha})+\sum_\alpha A_\alpha^+B_\alpha^+ \\ =\sum_{\alpha>0}(\pi_\alpha-\sigma_\alpha)(v_\alpha A_\alpha B_\alpha+v_{-\alpha}A_{-\alpha}B_{-\alpha}) \\ -\sum_{\alpha>0}\hat{t}_\alpha v_\alpha(A_0^2B_\alpha B_{-\alpha}+B_0^2A_\alpha A_{-\alpha}) \\ +A_0^+B_0^++\sum_{\alpha>0}(A_\alpha^+B_\alpha^++A_{-\alpha}^+B_{-\alpha}^+).\end{aligned}$$

The A_α and B_α satisfy the commutation relations (2.4), so we consider the $(\alpha, -\alpha)$ terms in (2.22) separately and expand:

$$\exp\{-\hat{t}_\alpha v_\alpha A_0^2B_\alpha B_{-\alpha}\}\exp\{-\hat{t}_\alpha v_\alpha B_0^2A_\alpha A_{-\alpha}\}.$$

Noting that the first term of (2.22) involves A_α, $A_{-\alpha}$, B_α and $B_{-\alpha}$ only in the products $A_\alpha B_\alpha$ and $A_{-\alpha}B_{-\alpha}$, only equal powers in the expansions of the above exponentials can give non-zero contribution to (2.21); thus:

(2.23) $$\begin{aligned}\langle 0|e^{\tilde{P}}e^{\tilde{P}+}|0\rangle \cong \prod_{\alpha>0}\langle 0|\exp\{\tfrac{1}{2}\sum_k\ln(1+2v_0A_0B_0w_0^2(k))\} \\ \cdot\exp\{(\pi_\alpha-\sigma_\alpha)(v_\alpha A_\alpha B_\alpha+v_{-\alpha}A_{-\alpha}B_{-\alpha})\} \\ \cdot f(\tau_\alpha^2v_\alpha A_\alpha B_\alpha v_{-\alpha}A_{-\alpha}B_{-\alpha})\exp\{A_\alpha^+B_\alpha^++A_{-\alpha}^+B_{-\alpha}^+\} \\ \cdot\exp[A_0^+B_0^+]|0\rangle\end{aligned}$$

where $f(x)$ is defined by:

(2.24) $$f(x)=\sum_{n=0}^\infty\frac{x^n}{(n!)^2}.$$

Using:

(2.25) $$\langle 0|f(A_\alpha B_\alpha)e^{A_\alpha{}^+B_\alpha{}^+}|0\rangle=\int_0^\infty dt\,e^{-t}f(t)$$

where the A_α and B_α are as in (2.4) [(2.25) will be called the "t-trick"

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henceforth: see § 3 of paper C]; we can now replace each of the $(\alpha, -\alpha)$ terms in (2.23) by an integral, thus:

$$\int_0^\infty dt_\alpha \int_0^\infty dt_{-\alpha} e^{-t_\alpha - t_{-\alpha} + (\pi_\alpha - \sigma_\alpha)(v_\alpha t_\alpha + v_{-\alpha} t_{-\alpha})} f(\tau_\alpha^2 v_\alpha t_\alpha v_{-\alpha} t_{-\alpha}) = \Gamma_1(\alpha, A_0 B_0) \tag{2.26}$$

where $\Gamma_1(\alpha, A_0B_0)$ is defined by:

$$\Gamma_1(\alpha, A_0 B_0) = \{(1 - v_\alpha[\pi_\alpha - \sigma_\alpha])^2 - \tau_\alpha^2 v_\alpha^2\}^{-1}. \tag{2.27}$$

Substituting (2.26) into (2.23) and using the "t-trick" on the A_0B_0 term, we have:

$$\langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle \cong \int_0^\infty dt_0 e^{-t_0 + \frac{1}{2}\Sigma_k \ln(1+2v_0 t_0 w_0^2(k))} \prod_{\alpha>0} \Gamma_1(\alpha, t_0) \tag{2.28}$$

or finally, taking the product over all $\alpha \neq 0$ instead of $\alpha > 0$:

$$\langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle \cong \int_0^\infty dt_0 e^{-t_0 + \frac{1}{2}\Sigma_k \ln(1+2v_0 t_0 w_0^2(k))} \cdot \exp\left\{-\tfrac{1}{2}\sum_\alpha{}' [\ln(1 - v_\alpha[\pi_\alpha - \sigma_\alpha - \tau_\alpha]) + \ln(1 - v_\alpha[\pi_\alpha - \sigma_\alpha + \tau_\alpha])]\right\}. \tag{2.29}$$

Equation (2.29) is the final expression which can be reduced further only if more details are known about the v_α and the w_α. It should be noted that π_α, σ_α and τ_α are functions of t_0 and the Σ'_α is itself an integral, thus the evaluation of $e^{-\beta\Omega_M}$ is not trivial. However, for the purpose of making a self consistent calculation, what we really need are expectation values of the one-particle and two-particle operators which occur in the Hamiltonian, and $\mathrm{Tr}(\mathscr{U} \ln \mathscr{U}) : e^{-\beta\Omega_M}$ is contained in the definitions of the expectation values, but in the derivations below, an explicit evaluation of $e^{-\beta\Omega_M}$ is not needed.

3. Expectation values of one-particle operators

The expectation value of the one-particle operator

$$J = \sum_{k,k'} J_{kk'} a_k^+ a_{k'} \tag{3.1}$$

is given by E_I 2.8:

$$\langle J\rangle = \sum_k \bar{n}_k J_{kk} + \frac{\langle 0|e^{\tilde{P}} \tilde{J} e^{\tilde{P}^+}|0\rangle}{\langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle} \tag{3.2}$$

where $\bar{n}_k$ is the average number of unpaired particles in the single particle state k, and $\tilde{J}$ is the "quenched" form of J (see § 2 of paper E_I).

A reduction of the numerator of the second term in (3.2) was carried out in paper E_{II}, the final result being (E_{II} 2.32):

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$$\langle 0|e^{\tilde{P}}\mathcal{J}e^{\tilde{P}^+}|0\rangle = \langle 0|\exp\{\tfrac{1}{2}\operatorname{Tr}\ln(1-M)\}\operatorname{Tr}\left(\frac{-M}{1-M}\mathcal{J}\right)\exp(R^+)|0\rangle. \tag{3.3}$$

Using the results of section 2, this becomes:

$$\begin{aligned}\langle 0|e^{\tilde{P}}\mathcal{J}e^{\tilde{P}^+}|0\rangle \cong \langle 0|\exp\{\tfrac{1}{2}\operatorname{Tr}\ln(1-M_0)+\sum_\alpha{}'\{(\pi_\alpha-\sigma_\alpha)v_\alpha A_\alpha B_\alpha \\ -\tfrac{1}{2}\hat{\tau}_\alpha v_\alpha(A_0^2B_\alpha B_{-\alpha}+B_0^2A_\alpha A_{-\alpha})\}\}\operatorname{Tr}\left(\frac{-M}{1-M}\mathcal{J}\right) \\ \cdot\exp\{\sum_\alpha A_\alpha^+B_\alpha^+\}|0\rangle.\end{aligned} \tag{3.4}$$

As before, we require an expansion of $-(M_0+M')/1-(M_0+M')$ to first order in v_α. To do this, we first expand $1/1-(M_0+M')$:

$$\begin{aligned}\frac{1}{1-(M_0+M')} &= 1+(M_0+M')+(M_0^2+M_0M'+M'M_0+M'^2) \\ &\quad +(M_0^3+M_0^2M'+M_0M'M_0+M'M_0^2+M_0M'^2 \\ &\quad +M'M_0M'+M'^2M_0+M'^3)+\cdots \\ &= \frac{1}{1-M_0}+\frac{1}{1-M_0}M'\frac{1}{1-M_0} \\ &\quad +\frac{1}{1-M_0}M'\frac{1}{1-M_0}M'\frac{1}{1-M_0}+\cdots.\end{aligned} \tag{3.5}$$

Then

$$\begin{aligned}\frac{-(M_0+M')}{1-(M_0+M')} &= 1-\frac{1}{1-(M_0+M')} \\ &= \frac{-M_0}{1-M_0}-\frac{1}{1-M_0}M'\frac{1}{1-M_0} \\ &\quad -\frac{1}{1-M_0}M'\frac{1}{1-M_0}M'\frac{1}{1-M_0}-\cdots.\end{aligned} \tag{3.6}$$

Neglecting terms in (3.6) of degree higher than the first in v_α we obtain for the trace of $-M/(1-M)\mathcal{J}$:

$$\begin{aligned}\operatorname{Tr}\left(\frac{-M}{1-M}\mathcal{J}\right) &\cong -\operatorname{Tr}\left(\frac{M_0}{1-M_0}\mathcal{J}\right)-\operatorname{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}\mathcal{J}\right) \\ &\quad -\operatorname{Tr}\left(\frac{1}{1-M_0}M_2\frac{1}{1-M_0}\mathcal{J}\right) \\ &\quad -\operatorname{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\frac{1}{1-M_0}\mathcal{J}\right).\end{aligned} \tag{3.7}$$

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We now note that in the exponent in (3.4) the operators A_α and B_α occur only in the products:

(3.8) $$v_\alpha A_\alpha B_\alpha,\ v_\alpha B_0^2 A_\alpha A_{-\alpha},\quad \text{and}\quad v_\alpha A_0^2 B_\alpha B_{-\alpha}$$

Thus, except for $\mathrm{Tr}(-M_0/(1-M_0)\mathcal{J})$ which equals $\sum_k h_k \mathcal{J}_{kk}$, only terms of type (3.8) in (3.7) can give non-zero contribution to (3.4).

M_1 contains $A_0 B_\alpha$ and $A_\alpha B_0$ linearly, so the second term in (3.7) contributes nothing.

In the third term, only the $\alpha = \beta$ term of M_2 can possibly give rise to anything non-zero, thus the "effective" form of $-\mathrm{Tr}((1/1-M_0)M_2 (1/1-M_0)\mathcal{J})$ equals:

(3.9)
$$\begin{aligned}
-\sum_\alpha{}' \sum_{k,k'} \frac{1}{1-\langle k|M_0|k\rangle}\, 2\langle k|q_\alpha^\alpha|k'\rangle v_\alpha A_\alpha B_\alpha \frac{1}{1-\langle k'|M_0|k'\rangle}\mathcal{J}_{k'k}
&= -\sum_\alpha{}' \sum_{k,k'} (-2\delta_{k,k'} w_\alpha^2(k-\tfrac{1}{2}K_\alpha) v_\alpha A_\alpha B_\alpha)\\
&\quad \cdot \frac{1}{(1-\langle k|M_0|k\rangle)(1-\langle k'|M_0|k'\rangle)}\mathcal{J}_{k'k}\\
&= \sum_\alpha{}' \sum_k 2(1-h_k)^2 w_\alpha^2(k-\tfrac{1}{2}K_\alpha) v_\alpha A_\alpha B_\alpha \mathcal{J}_{kk}\\
&= \sum_\alpha{}' \sum_k \tilde{\pi}_{\alpha k}\mathcal{J}_{kk}
\end{aligned}$$

where $\tilde{\pi}_{\alpha k}$ is defined by:

(3.10a) $$\tilde{\pi}_{\alpha k} = 2(1-h_k)^2 w_\alpha^2(k-\tfrac{1}{2}K_\alpha).$$

Also:

(3.11)
$$\begin{aligned}
-\mathrm{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\frac{1}{1-M_0}\mathcal{J}\right) &= \sum_{k,k',k''}\frac{1}{1-\langle k|M_0|k\rangle}\\
&\cdot \langle k|M_1|k'\rangle \frac{1}{1-\langle k'|M_0|k'\rangle}\langle k'|M_1|k''\rangle \frac{1}{1-\langle k''|M_0|k''\rangle}\mathcal{J}_{k''k}
\end{aligned}$$

and by (3.8), the "effective" form of $\langle k|M_1|k'\rangle\langle k'|M_1|k''\rangle$ (compare with (2.17)) equals:

(3.12) $$\delta_{k,k''}(\mathrm{I}+\mathrm{II}+\mathrm{III}+\mathrm{IV})$$

where I, II, III, and IV are defined by (2.18).

Substituting (3.12) into (3.11) we obtain the "effective" form of

$$-\mathrm{Tr}\left(\frac{1}{1-M_0}M_1\frac{1}{1-M_0}M_1\frac{1}{1-M_0}\mathcal{J}\right):$$

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$$
\begin{aligned}
(3.13)\quad & -4v_0 \sum_\alpha{}' \sum_k \Bigg\{\left[\frac{1}{(1+2v_0A_0B_0w_0^2(k))(1+2v_0A_0B_0w_0^2(k-K_\alpha))(1+2v_0A_0B_0w_0^2(k))}\right] \\
& \cdot [w_0^2(k-K_\alpha)w_\alpha^2(k-\tfrac{1}{2}K_\alpha)A_0B_0v_\alpha A_\alpha B_\alpha \\
& + w_0(k)w_0(k-K_\alpha)w_\alpha^2(k-\tfrac{1}{2}K_\alpha)v_\alpha A_0^2 B_\alpha B_{-\alpha}] \\
& + \left[\frac{1}{(1+2v_0A_0B_0w_0^2(k))(1+2v_0A_0B_0w_0^2(k+K_\alpha))(1+2v_0A_0B_0w_0^2(k))}\right] \\
& \cdot [w_0^2(k)w_\alpha^2(k+\tfrac{1}{2}K_\alpha)A_0B_0v_\alpha A_\alpha B_\alpha \\
& + w_0(k)w_0(k+K_\alpha)w_\alpha^2(k+\tfrac{1}{2}K_\alpha)v_\alpha B_0^2 A_\alpha A_{-\alpha}]\Bigg\} \mathcal{J}_{kk}.
\end{aligned}
$$

Combining (3.13), (3.9), and (3.7) we have finally the "effective" form of $\mathrm{Tr}(-M/(1-M)\mathcal{J})$:

$$
(3.14)\quad \sum_k \{h_k \mathcal{J}_{kk} + \sum_\alpha{}' [(\tilde{\pi}_{\alpha k} - \tilde{\sigma}_{\alpha k})v_\alpha A_\alpha B_\alpha - \tau_{\alpha k}^{(1)} v_\alpha A_0^2 B_\alpha B_{-\alpha} - \tau_{-\alpha k}^{(1)} v_\alpha B_0^2 A_\alpha A_{-\alpha}]\mathcal{J}_{kk}\}
$$

where $\tilde{\sigma}_{\alpha k}$, $\tau_{\alpha k}^{(1)}$ and $\tau_{-\alpha k}^{(1)}$ are defined by:

$$(3.10b)\quad \tilde{\sigma}_{\alpha k} = 2(1-h_k)\{h_{k-K_\alpha}(1-h_k)w_\alpha^2(k-\tfrac{1}{2}K_\alpha) + h_k(1-h_{k+K_\alpha})w_\alpha^2(k+\tfrac{1}{2}K_\alpha)\}$$

$$(3.10c)\quad \tau_{\alpha k}^{(1)} = 4v_0(1-h_k)^2(1-h_{k-K_\alpha})w_0(k)w_0(k-K_\alpha)w_\alpha^2(k-\tfrac{1}{2}K_\alpha)$$

$$(3.10d)\quad \tau_{-\alpha k}^{(1)} = 4v_0(1-h_k)^2(1-h_{k+K_\alpha})w_0(k)w_0(k+K_\alpha)w_\alpha^2(k+\tfrac{1}{2}K_\alpha).$$

We substitute (3.14) into (3.4) and observe that the "t-trick" will not work directly: we must first rewrite the α-terms as $(\alpha, -\alpha)$-terms, as before. The contribution from $\sum_k h_k \mathcal{J}_{kk}$ follows directly from (2.28): it is just

$$(3.15)\quad \sum_k \int_0^\infty dt_0 e^{-t_0+\frac{1}{2}\sum_k \ln(1+2v_0t_0w_0^2(k))} h_k \mathcal{J}_{kk} \prod_{\alpha>0} \Gamma_1(\alpha, t_0).$$

To obtain the contribution to (3.4) of the $v_\alpha A_\alpha B_\alpha$ term in (3.14) we use exactly the same procedure as we did before in going from (2.21) to (2.23) and obtain:

$$
\begin{aligned}
(3.16)\quad & \sum_{\alpha>0} (\tilde{\pi}_{\alpha k} - \tilde{\sigma}_{\alpha k})\mathcal{J}_{kk} \prod_{\substack{\beta>0\\ \beta\neq\alpha}} \langle 0|\exp[\tfrac{1}{2}\mathrm{Tr}\ln(1-M_0)](v_\alpha A_\alpha B_\alpha + v_{-\alpha}A_{-\alpha}B_{-\alpha}) \\
& \cdot F(\alpha, A_0B_0)F(\beta, A_0B_0)\exp[A_0^+B_0^+]|0\rangle
\end{aligned}
$$

where $F(\alpha, A_0B_0)$ is defined by:

$$
\begin{aligned}
(3.17)\quad F(\alpha, A_0B_0) = & \exp\{(\pi_\alpha - \sigma_\alpha)(v_\alpha A_\alpha B_\alpha + v_{-\alpha}A_{-\alpha}B_{-\alpha})\} \\
& \cdot f(\tau_\alpha^2 v_\alpha A_\alpha B_\alpha v_{-\alpha} A_{-\alpha} B_{-\alpha})\exp\{A_\alpha^+ B_\alpha^+ + A_{-\alpha}^+ B_{-\alpha}^+\}.
\end{aligned}
$$

The relevant integral for the $(\alpha, -\alpha)$ term in (3.16) is:

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$$
(3.18)\qquad \begin{aligned}&\int_0^\infty dt_\alpha \int_0^\infty dt_{-\alpha} e^{-t_\alpha - t_{-\alpha}} (v_\alpha t_\alpha + v_{-\alpha} t_{-\alpha})\\ &\qquad \cdot \exp\{(\pi_\alpha - \sigma_\alpha)(v_\alpha t_\alpha + v_{-\alpha} t_{-\alpha})\} f(\tau_\alpha^2 v_\alpha t_\alpha v_{-\alpha} t_{-\alpha})\\ &\qquad = 2v_\alpha(1 - v_\alpha[\pi_\alpha - \sigma_\alpha]) \Gamma_1^2(\alpha, A_0 B_0)\end{aligned}
$$

and the relevant integral for the $(\beta, -\beta)$ term in (3.16) is just (2.26).

For the $v_\alpha A_0^2 B_\alpha B_{-\alpha} (v_\alpha B_0^2 A_\alpha A_{-\alpha})$ term in (3.14) we use a similar procedure, but now in the expansion of

$$
\exp\{-\hat{t}_\alpha A_0^2 v_\alpha B_\alpha B_{-\alpha}\} \exp\{-\hat{t}_\alpha B_0^2 v_\alpha A_\alpha A_{-\alpha}\}
$$

the $n^{\text{th}}(n + 1^{\text{th}})$ term in the expansion of the first exponential combines with the $(n+1)^{\text{th}}$ (n^{th}) term in the expansion of the second exponential, and we obtain the contribution to (3.4):

$$
(3.19)\qquad \begin{aligned}&\sum_{\alpha>0} -\tau_{\alpha k}^{(1)} \mathcal{J}_{kk} (-\tau_{-\alpha k}^{(1)} \mathcal{J}_{kk}) \prod_{\substack{\beta>0\\ \beta\neq\alpha}} \langle 0|\exp[\tfrac{1}{2}\mathrm{Tr}\ln(1 - M_0)]\\ &\qquad \cdot 2/\hat{t}_\alpha \cdot F_1(\alpha, A_0 B_0) F(\beta, A_0 B_0) \exp[A_0^+ B_0^+]|0\rangle\end{aligned}
$$

where $F_1(\alpha, A_0 B_0)$ is defined by:

$$
(3.20)\qquad \begin{aligned}F_1(\alpha, A_0 B_0) &= \exp\{(\pi_\alpha - \sigma_\alpha)(v_\alpha A_\alpha B_\alpha + v_{-\alpha} A_{-\alpha} B_{-\alpha})\}\\ &\qquad \cdot f_1(\tau_\alpha^2 v_\alpha A_\alpha B_\alpha v_{-\alpha} A_{-\alpha} B_{-\alpha}) \exp\{A_\alpha^+ B_\alpha^+ + A_{-\alpha}^+ B_{-\alpha}^+\}\end{aligned}
$$

and

$$
(3.21)\qquad f_1(x) = -\sum_{n=0}^\infty \frac{x^{n+1}}{n!(n+1)!}
$$

and the relevant integrals are

$$
(3.22)\qquad \begin{aligned}&\frac{2}{\hat{t}_\alpha} \int_0^\infty dt_\alpha \int_0^\infty dt_{-\alpha} e^{-t_\alpha - t_{-\alpha}} \exp\{(\pi_\alpha - \sigma_\alpha)(v_\alpha t_\alpha + v_{-\alpha} t_{-\alpha})\}\\ &\qquad \cdot f_1(\tau_\alpha^2 v_\alpha t_\alpha v_{-\alpha} t_{-\alpha})\\ &\qquad = -\frac{2\tau_\alpha^2 v_\alpha^2}{\hat{t}_\alpha} \Gamma_1^2(\alpha, A_0 B_0)\end{aligned}
$$

for the $(\alpha, -\alpha)$ term, and (2.26):

$$
(3.23)\qquad \Gamma_1(\beta, A_0 B_0)
$$

for the $(\beta, -\beta)$ term.

Combining the results obtained so far and then applying the "t-trick" on the $A_0 B_0$ term, we have:

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$$\langle 0|e^{\tilde{P}}\mathcal{J}e^{\tilde{P}^+}|0\rangle \cong \sum_k \int_0^\infty dt_0 e^{-t_0+\frac{1}{2}\sum_k \ln(1+2v_0 t_0 w_0^2(k))} \tag{3.24}$$
$$\cdot \Big\{ h_k \mathcal{J}_{kk} \prod_{\alpha>0} \Gamma_1(\alpha, t_0) + \sum_{\alpha>0} \Big[(\tilde{\pi}_{\alpha k} - \tilde{\sigma}_{\alpha k}) \cdot 2v_\alpha(1 - v_\alpha[\pi_\alpha - \sigma_\alpha])\, \Gamma_1^2(\alpha, t_0)\mathcal{J}_{kk} + \tilde{\tau}_{\alpha k} \frac{2\tau_\alpha^2 v_\alpha^2}{\hat{\tau}_\alpha} \Gamma_1^2(\alpha, t_0)\mathcal{J}_{kk} \Big] \prod_{\substack{\beta>0 \\ \beta\neq\alpha}} \Gamma_1(\beta, t_0) \Big\}$$

where $\tilde{\tau}_{\alpha k}$ is defined by:

$$\tilde{\tau}_{\alpha k} = \tau_{\alpha k}^{(1)} + \tau_{-\alpha k}^{(1)}. \tag{3.25}$$

In our expression for $\langle J\rangle$ ((3.2)), we require the ratio of the integrals (3.24) and (2.28). "State 0" is the condensed state with $v_0 > 1$, so both integrals can be evaluated approximately by the saddle point method. $\Gamma_1(\alpha, t_0)$ [in (2.28)], and the terms in the curly brackets [in (3.24)] are functions of t_0; however, compared with the exponential factor, these terms are slowly varying functions of t_0; therefore, to a first approximation, the saddle point for both integrals is $t_{0\,\max}$ [2] (called t_0 henceforth). With this approximation $\langle J\rangle$ is given approximately by (taking the sum over all $\alpha \neq 0$ instead of $\alpha > 0$):

$$\langle J\rangle \cong \sum_k \tilde{n}_k J_{kk} + \mathrm{Tr}(h'\mathcal{J}) + \mathrm{Tr}(h''\mathcal{J}) \tag{3.26}$$

where h' and h'' are defined by:

$$\langle k|h'|k'\rangle = \delta_{k,k'} h_k \tag{3.27a}$$

and

$$\langle k|h''|k'\rangle = \delta_{k,k'} \sum_\alpha{}' h_{\alpha k} \tag{3.27b}$$

where

$$h_{\alpha k} = (\tilde{\pi}_{\alpha k} - \tilde{\sigma}_{\alpha k})\Gamma(\alpha, t_0) + \tilde{\tau}_{\alpha k}\Delta(\alpha, t_0) \tag{3.27c}$$

$$\Gamma(\alpha, t_0) = \frac{v_\alpha(1 - v_\alpha[\pi_\alpha - \sigma_\alpha])}{(1 - v_\alpha[\pi_\alpha - \sigma_\alpha])^2 - \tau_\alpha^2 v_\alpha^2} \tag{3.27d}$$

and

$$\Delta(\alpha, t_0) = \frac{\tau_\alpha^2 v_\alpha^2}{\hat{\tau}_\alpha\{(1 - v_\alpha[\pi_\alpha - \sigma_\alpha])^2 - \tau_\alpha^2 v_\alpha^2\}}. \tag{3.27e}$$

The terms $\sum_k \tilde{n}_k J_{kk}$, $\mathrm{Tr}(h'\mathcal{J})$ and $\mathrm{Tr}(h''\mathcal{J})$ in (3.26) can be interpreted as

[2] $\{\frac{1}{2}\sum_k \ln(1 + 2v_0 t_0 w_0^2(k)) - t_0\}$ takes its maximum value at $t_0 = t_{0\,\max} = N_0$, where N_0 is the number of Bose-condensed pairs and N_0 is proportional to the volume of the box (see paper C).

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the contributions from: (1) the unpaired particles, (2) the condensed pairs (i.e. the pairs occupying 'state 0'), and (3) the non-condensed pairs (i.e. the pairs occupying the 'states α' $\alpha \neq 0$), respectively.

We note that since a macroscopic number of particles occupy the ground state (footnote 2), we expect that the contribution from any one non-condensed state should be negligible compared with the contribution from the condensed state. A simple volume dependence check in fact shows that $h_k \sim 1$ and $h_{\alpha k} \sim 1/V$, where V is the volume of the container. However, a large number of non-condensed states ($\sim V$) contribute, so that finally the two contributions $\mathrm{Tr}(h'\mathscr{J})$ and $\mathrm{Tr}(h''\mathscr{J})$ are comparable.

Finally, for extreme condensation (i.e. all pairs occupy 'state 0'), $\mathrm{Tr}(h''\mathscr{J})$ vanishes and (3.26) reduces to $\mathrm{E_I}$ 4.24.

4. Expectation values of two-particle operators

The expectation value of the two-particle operator

(4.1)
$$K = \sum_{l,m,l',m'} K_{lml'm'} a_l^+ a_m^+ a_{m'} a_{l'}$$

is given by $\mathrm{E_I}$ 2.12:

(4.2)
$$\langle K \rangle = \sum_{l,m} (K_{lm,lm} - K_{ml,lm}) \bar{n}_l \bar{n}_m + \frac{\langle 0|e^{\tilde{P}} \tilde{K}^{(1)} e^{\tilde{P}^+}|0\rangle}{\langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle} + \frac{\langle 0|e^{\tilde{P}} \tilde{K} e^{\tilde{P}^+}|0\rangle}{\langle 0|e^{\tilde{P}} e^{\tilde{P}^+}|0\rangle}$$

where the quantities $\tilde{K}$ and $\tilde{K}^{(1)}$ are as in $\mathrm{E_I}$ ($\tilde{K}^{(1)}$ is a one-particle operator, so it is under control).

A reduction of the numerator of the last term in (4.2) was carried out in paper $\mathrm{E_{II}}$, the final result being ($\mathrm{E_{II}}$ 3.26):

(4.3)
$$\langle 0|e^{\tilde{P}} \tilde{K} e^{\tilde{P}^+}|0\rangle = \langle 0|\exp\{\tfrac{1}{2}\,\mathrm{Tr}\ln(1-M)\}[\mathrm{Tr}_2(p\tilde{K}) + \sum_{\alpha,\beta} (\psi_\alpha, \tilde{K}\psi_\beta)\sqrt{v_\alpha v_\beta} A_\alpha B_\beta] \exp(R^+)|0\rangle$$

where

(4.4a)
$$\mathrm{Tr}_2(p\tilde{K}) = \sum_{lml'm'} \langle lm|p|l'm'\rangle \tilde{K}_{l'm'lm}$$

(4.4b)
$$\langle lm|p|l'm'\rangle = \langle l\left|\frac{-M}{1-M}\right|l'\rangle \langle m\left|\frac{-M}{1-M}\right|m'\rangle - \langle l\left|\frac{-M}{1-M}\right|m'\rangle \langle m\left|\frac{-M}{1-M}\right|l'\rangle$$

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(4.4c) $$(\psi_\alpha, \tilde{K}\psi_\beta) = \sum_{lml'm'} \psi_\alpha(l, m)\tilde{K}_{lm,l'm'}\psi_\beta(l', m')$$

and

(4.4d) $$\psi_\alpha(l, m) = \sum_k 2^{-\frac{1}{2}}\left\{\langle l\left|\frac{1}{1-M}\right|k\rangle\varphi_\alpha(k, m) - \langle m\left|\frac{1}{1-M}\right|k\rangle\varphi_\alpha(k, l)\right\}.$$

Using the results of section 2 (4.3) becomes:

(4.5) $$\begin{aligned}\langle 0|e^{\hat{P}}\tilde{K}e^{\hat{P}_+}|0\rangle \cong \langle 0|\exp\{\tfrac{1}{2}\operatorname{Tr}\ln(1-M_0) + {\sum_\alpha}'\{(\pi_\alpha-\sigma_\alpha)v_\alpha A_\alpha B_\alpha \\ - \tfrac{1}{2}\hat{\tau}_\alpha v_\alpha(A_0^2 B_\alpha B_{-\alpha} + B_0^2 A_\alpha A_{-\alpha})\}\}\cdot[\operatorname{Tr}_2(p\tilde{K}) \\ + \sum_{\alpha,\beta}(\psi_\alpha, \tilde{K}\psi_\beta)\sqrt{v_\alpha v_\beta}A_\alpha B_\beta]\cdot\exp\{\sum_\alpha A_\alpha^+ B_\alpha^+\}|0\rangle.\end{aligned}$$

In keeping with our approximation we desire an expansion of:

(4.6) $$\operatorname{Tr}_2(p\tilde{K}) + \sum_{\alpha,\beta}(\psi_\alpha, \tilde{K}\psi_\beta)\sqrt{v_\alpha v_\beta}A_\alpha B_\beta$$

to first order in v_α, where again, only terms of type (3.8) in (4.6) contribute to (4.5).

For the first term in (4.6) we use the expansion (3.6) for $-M/1-M$, and (3.14); and obtain the "effective" form

(4.7) $$\begin{aligned}\sum_{lml'm'}\Big\{\delta_{l,l'}\delta_{m,m'}(h_l h_m + h_l \bar{h}_{\alpha m} + \bar{h}_{\alpha l} h_m) \\ + \langle l\left|\frac{1}{1-M_0}M_1\frac{1}{1-M_0}\right|l'\rangle \\ \cdot\langle m\left|\frac{1}{1-M_0}M_1\frac{1}{1-M_0}\right|m'\rangle - (l'\leftrightarrow m')\Big\}\tilde{K}_{l'm',lm}\end{aligned}$$

where, $\bar{h}_{\alpha l}$ is defined by:

(4.8) $$\bar{h}_{\alpha l} = (\tilde{\pi}_{\alpha l} - \tilde{\sigma}_{\alpha l})v_\alpha A_\alpha B_\alpha - \tau_{\alpha l}^{(1)}v_\alpha A_0^2 B_\alpha B_{-\alpha} - \tau_{-\alpha l}^{(1)}v_\alpha B_0^2 A_\alpha A_{-\alpha}$$

and it is understood that the second term in (4.7) in its final form will contain only terms of type (3.8).

For the second term in (4.6) we use the expansion (3.5) for $1/1-M$ in (4.4d) and obtain:

(4.9) $$\begin{aligned}\psi_\alpha(l, m) &= 2^{-\frac{1}{2}}[(1-h_l)\varphi_\alpha(l, m) - (1-h_m)\varphi_\alpha(m, l)] \\ &\quad + 2^{-\frac{1}{2}}\sum_k[(1-h_l)\langle l|M_1|k\rangle(1-h_k)\varphi_\alpha(k, m) \\ &\quad - (1-h_m)\langle m|M_1|k\rangle(1-h_k)\varphi_\alpha(k, l)] \\ &\quad + \cdots \\ &= \psi_\alpha^{(0)}(l, m) + \psi_\alpha^{(1)}(l, m) + \psi_\alpha^{(2)}(l, m) + \cdots\end{aligned}$$

where $\psi_\alpha^{(0)}$ contains no terms in v_α, $\psi_\alpha^{(1)}$ contains only term linear in $v_\alpha^{\frac{1}{2}}$, $\psi_\alpha^{(2)}$

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contains only terms linear in v_α, etc. . . . The "effective" form of the second term in (4.6) is then:

$$(4.10)\quad \begin{aligned}&(\psi_0^{(0)}, \tilde{K}\psi_0^{(0)})v_0 A_0 B_0 + \sum_\alpha{}' (\psi_\alpha^{(0)}, \tilde{K}\psi_\alpha^{(0)})v_\alpha A_\alpha B_\alpha \\ &\quad + \sum_\alpha{}' \{(\psi_0^{(0)}, \tilde{K}\psi_\alpha^{(1)})\sqrt{v_0 v_\alpha} A_0 B_\alpha + (\psi_\alpha^{(1)}, \tilde{K}\psi_0^{(0)})\sqrt{v_\alpha v_0} A_\alpha B_0 \\ &\quad + (\psi_0^{(1)}, \tilde{K}\psi_\alpha^{(0)})\sqrt{v_0 v_\alpha} A_0 B_\alpha + (\psi_\alpha^{(0)}, \tilde{K}\psi_0^{(1)})\sqrt{v_\alpha v_0} A_\alpha B_0\} \\ &\quad + (\psi_0^{(0)}, \tilde{K}\psi_0^{(2)})v_0 A_0 B_0 + (\psi_0^{(2)}, \tilde{K}\psi_0^{(0)})v_0 A_0 B_0 + (\psi_0^{(1)}, \tilde{K}\psi_0^{(1)})v_0 A_0 B_0\end{aligned}$$

where it is again understood that the last seven terms in (4.10) in their final forms will contain only terms of type (3.8).

We then substitute (4.7) and (4.10) into (4.5) and using the methods developed in section 3, we obtain finally, after an extremely tedious calculation:

$$(4.11)\quad \begin{aligned}\langle K\rangle \cong &\sum_{l,m} (K_{lm,lm} - K_{ml,lm})\tilde{n}_l \tilde{n}_m + \mathrm{Tr}(h'\tilde{K}^{(1)}) + \mathrm{Tr}_2(p'\tilde{K}) \\ &+ v_0 t_0 (\psi_0^{(0)}, \tilde{K}\psi_0^{(0)}) + \mathrm{Tr}(h''\tilde{K}^{(1)}) + \mathrm{Tr}_2(p''\tilde{K}) \\ &+ \sum_\alpha{}' \{(\psi_0^{(0)}, \tilde{K}\Psi_{\alpha\alpha}^{21}) + (\Psi_{\alpha\alpha}^{12}, \tilde{K}\psi_0^{(0)}) + (\psi_\alpha^{(0)}, \tilde{K}\Psi_{0\alpha}^{12}) \\ &+ (\Psi_{0\alpha}^{21}, \tilde{K}\psi_\alpha^{(0)}) + (q_{0\alpha}^{(1)}, \tilde{K}Q_{0\alpha}^{21}) + (q_{0\alpha}^{(2)}, \tilde{K}Q_{0\alpha}^{12})\}\end{aligned}$$

where we have used the following definitions:

$$(4.12a)\quad \langle lm|p'|l'm'\rangle = (\delta_{ll'}\delta_{mm'} - \delta_{lm'}\delta_{ml'})h_l h_m$$

$$(4.12b)\quad \langle lm|p''|l'm'\rangle = \sum_\alpha{}' (h_{\alpha lm,l'm'} - h_{\alpha lm,m'l'})$$

$$(4.12c)\quad \begin{aligned}h_{\alpha lm,l'm'} = &\{\Gamma(\alpha, t_0)t_0 p_{\alpha l}^{(1)} p_{\alpha m}^{(2)} + \Delta(\alpha, t_0) p_{\alpha l}^{(1)} p_{-\alpha m}^{(1)}\}\delta_{l',l-K_\alpha}\delta_{m',m+K_\alpha} \\ &+ \{\Gamma(\alpha, t_0)t_0 p_{\alpha l}^{(2)} p_{\alpha m}^{(1)} + \Delta(\alpha, t_0) p_{\alpha l}^{(2)} p_{-\alpha m}^{(2)}\}\delta_{l',l+K_\alpha}\delta_{m',m-K_\alpha} \\ &+ (h_l h_{\alpha m} + h_{\alpha l} h_m)\delta_{ll'}\delta_{mm'} \quad ^{3})\end{aligned}$$

$$(4.12d)\quad p_{\alpha l}^{(1)} = 2\sqrt{v_0}(1-h_l)(1-h_{l-K_\alpha})w_0(l-K_\alpha)w_\alpha(l-\tfrac{1}{2}K_\alpha)$$

$$(4.12e)\quad p_{\alpha l}^{(2)} = 2\sqrt{v_0}(1-h_l)(1-h_{l+K_\alpha})w_0(l)w_\alpha(l+\tfrac{1}{2}K_\alpha)$$

$$(4.12f)\quad \psi_0^{(0)}(l, m) = \delta_{l,-m}2^{-\frac{1}{2}}(1-h_l)w_0(l)$$

$$(4.12g)\quad \psi_\alpha^{(0)}(l, m) = \delta_{m,K_\alpha-l}2^{-\frac{1}{2}}\{(1-h_l)+(1-h_{K_\alpha-l})\}w_\alpha(l-\tfrac{1}{2}K_\alpha)$$

$$(4.12h)\quad q_{\alpha\beta}^{(2)}(l, m) = p_{\beta l}^{(2)}\varphi_\alpha(k, m)\delta_{k,l+K_\beta} - p_{\beta m}^{(2)}\varphi_\alpha(k, l)\delta_{k,m+K_\beta}$$

$$(4.12i)\quad q_{\alpha\beta}^{(1)}(l, m) = p_{\beta l}^{(1)}\varphi_\alpha(k, m)\delta_{k,l-K_\beta} - p_{\beta m}^{(1)}\varphi_\alpha(k, l)\delta_{k,m-K_\beta}$$

[3] $p_{-\alpha}$ is obtained from p_α by replacing K_α by $-K_\alpha$, and $q_{\beta,-\alpha}$ is obtained from $q_{\beta,\alpha}$ by replacing p_α by $p_{-\alpha}$ and K_α by $-K_\alpha$.

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$$\Psi^{ij}_{\beta\alpha}(l, m) = h_{\alpha l m}\delta_{\beta,\alpha} + \tfrac{1}{2}\psi^{(0)}_{\alpha}(l, m)\Gamma(\alpha, t_0)\delta_{\beta,0}$$

(4.12j) $$+ q^{(i)}_{\beta\alpha}(l, m)\sqrt{v_0}\, t_0 \Gamma(\alpha, t_0) - q^{(j)}_{\beta,-\alpha}(l, m)\sqrt{v_0}\,\Delta(\alpha, t_0) \quad (i, j = 1, 2 : \beta = 0, \alpha)$$ [3]

(4.12k) $$h_{\alpha l m} = v_0 t_0\{(\tilde{\Sigma}_{\alpha l} - \tilde{\Pi}_{\alpha l})\Gamma(\alpha, t_0) + \tilde{T}_{\alpha l}\Delta(a, t_0)\}\delta_{l,-m}$$

(4.12l) $$\tilde{\Sigma}_{\alpha l} = 2^{-\frac{1}{2}}(\tilde{\sigma}_{\alpha l} + \tilde{\sigma}_{\alpha,-l})w_0(l)$$

(4.12m) $$\tilde{\Pi}_{\alpha l} = 2^{-\frac{1}{2}}(\tilde{\pi}_{\alpha l} + \tilde{\pi}_{\alpha,-l})w_0(l)$$

(4.12n) $$\tilde{T}_{\alpha l} = 2^{-\frac{1}{2}}(\tilde{\tau}_{\alpha l} + \tilde{\tau}_{\alpha,-l})w_0(l)$$

(4.12o) $$Q^{ij}_{0\alpha}(l, m) = v_0 t_0\{q^{(i)}_{0\alpha}(l, m)\Gamma(\alpha, t_0)t_0 + q^{(j)}_{0,-\alpha}(l, m)\Delta(\alpha, t_0)\} \quad (i, j = 1, 2)$$ [3]

The terms of (4.11) can be interpreted as follows (E_I): The first term is the conventional Hartree-Fock expectation value over the single particle distribution; the second and fifth terms arise from the interactions between single particles and particles within condensed correlated pairs, and between single particles and particles within non-condensed correlated pairs respectively; the third and fourth, and the sixth and seventh terms arise from the interaction between particles, both of which are members of, condensed correlated pairs, and non-condensed correlated pairs respectively.

Again, a simple volume dependence check shows that the contribution from any one non-condensed state is negligible compared with the contribution from the condensed state, but that finally, all terms in (4.11) are comparable.

Further, for extreme condensation, the fifth, sixth and seventh terms of (4.11) vanish and we are left with E_I 5.27 [4] as required.

5. Discussion

We start by considering a special case of (3.1), namely, $J_{kk'} = \delta_{kk'}$: i.e. the number operator:

(5.1) $$\mathcal{N} = \sum_k a_k^+ a_k$$

(3.26) then gives the expectation value:

(5.2) $$\langle\mathcal{N}\rangle \cong \sum_k h_k + \sum_\alpha{}' \sum_k h_{\alpha k}$$

and we can interpret

[3] See footnote on the preceding page.

[4] ψ in paper E_I (E_I 5.19) is related to $\psi_0^{(0)}$ through $\psi = \sqrt{v_0 t_0}\,\psi_0^{(0)}$.

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$$N_\alpha = \sum_k h_{\alpha k} \tag{5.3}$$

as the number of non-condensed pairs in state α. We point out that

$$N_\alpha \neq 2v_\alpha \frac{\partial}{\partial v_\alpha} (-\beta\Omega_M), \quad ^{5)} \tag{5.4}$$

in disagreement with remarks made in paper E_{II}. However, the disagreement is not the result of any error in calculation but is, rather, an immediate consequence of the fact that v_0 was treated differently from v_α in our approximation procedure. The interpretation (5.3) is nonetheless reasonable — there is still condensation and each non-condensed pair state still contributes an amount of relative order $1/V$ (see the remarks following (3.26) and (4.11)) as required.

Interpreting our results within the framework of Bogoliubov's theory [8] we observe that the non-condensed pairs are different from Bogoliubov's "elementary excitations" (which are similar to our unpaired particles), but are analogous to his "collective excitations". The "collective excitations" in Bogoliubov's original theory were found necessary to establish a gauge-invariant Meissner effect ([9]); in the quasi-chemical equilibrium theory, as well as in a later version of Bogoliubov's theory, the condensed pairs alone suffice ([10]).

The assumption of complete condensation is applicable only in the limit of zero temperature. At any finite temperature, we expect to find some 'normal' pairs, as well as some unpaired particles. This paper is a step towards the practical evaluation of the formalism for non-zero temperatures. The most restrictive assumption in the present paper is that of "simple pairs", (1.1). Although this assumption is awkward, it now turns out to be less seriously restrictive than was supposed earlier ([10]). Zumino [11] has proved a theorem to the effect that an arbitrary pair wave function $\phi(k_1, k_2)$ can be transformed into a "simple pair" form by introducing transformed single-particle states $|m\rangle$ which are linear combinations of the states $|k\rangle$. *If* the same transformation can also be used for the unpaired particles, simple pairing becomes an acceptable assumption. In particular, a simple pairing calculation *can* be gauge-invariant, provided we make the appropriate gauge transformation on the single-particle states $|k\rangle$.

The practical evaluation of the formalism for non-zero temperatures must be done in a self-consistent fashion, and for this we require not only expecta-

[5] It is easy to show that

$$N_\alpha = \left[2v_\alpha \frac{\partial}{\partial v_\alpha} + \left(2v_0 \frac{\partial}{\partial v_0}\right)_{\alpha\text{-term}}\right] (-\beta\Omega_M)$$

within our approximation.

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tion values of one-particle and two-particle operators over the density matrix $\mathscr{U}$, but also the value of $\mathrm{Tr}(\mathscr{U} \ln \mathscr{U})$. The former have been evaluated for the general case in paper E_{II}, and more specific expressions have been obtained in the present paper. But the calculation of $\mathrm{Tr}(\mathscr{U} \ln \mathscr{U})$ has not yet been completed. It is hoped that we will be able to report on this problem at a later date.

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https://doi.org/10.1017/S1446788700028342 Published online by Cambridge University Press