

ZUMINO'S THEOREM IN THE QUASI-CHEMICAL EQUILIBRIUM THEORY

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Abstract

A theorem on the canonical form of an antisymmetric matrix, which we attribute to Zumino, is used to show how the derivations of the results of two earlier papers by Blatt on expectation values of operators can be considerably simplified.

1. Introduction

The quasi-chemical equilibrium approximation to statistical mechanics, first expounded in 1957 [1], has been shown recently ([2] and [3], called E_I and E_{II} henceforth, and references quoted there) to be particularly applicable to the phenomenon of superconductivity. The comparatively slow development of the theory was due mainly to the absence of expressions for expectation values of operators; since for any approximation to statistical mechanics to be useful, one at least requires a method for evaluating expectation values of operators which enter into the Hamiltonian of the system. It was not until 1960 [2], that any progress in the desired direction was made; even then, closed expressions for the expectation values of one and two particle operators were obtained only after a drastic simplification (viz. the assumption of one pair state only) of the problem, and the use of a rather specialized mathematical technique which could not be generalized¹. Consequently, there was another time lapse before general expressions (for the case of many pair states) were obtained [3]; again with the help of a rather abstruse formalism¹. It is the purpose of the present paper to show, using a theorem which we attribute to Zumino [4], how the derivations of the results of papers E_I and E_{II} can be considerably simplified.

Since the difficulties encountered in E_I and especially in E_{II} , resulted from the use of formal labelling operators in the original Ansatz, it is clearly desirable to eliminate these operators in the beginning; this is done in section 2. The new expression for the density matrix, together with

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¹ The reader is referred to papers E_I and E_{II} for details.

Zumino's theorem, as stated in section 2, is used in sections 3 and 4 to rederive expectation values of one and two particle operators.

2. Formalism and Preliminaries

The density matrix $\hat{\mathcal{U}}$ in the quasi-chemical equilibrium theory is (equation (2.12) of reference [5]):

$$(2.1) \quad \hat{\mathcal{U}} = \omega \exp(Q^\dagger) \mathcal{V} \exp(Q) \omega$$

where

$$(2.2a) \quad Q = \sum_{\alpha} W_{\alpha} A_{\alpha}^{\dagger}$$

$$(2.2b) \quad \mathcal{V} = \prod_k (u_k)^{a_k^{\dagger} a_k}$$

and

$$(2.2c) \quad W_{\alpha} = 2^{-\frac{1}{2}} \sum_{k_1, k_2} w_{\alpha}(k_1, k_2) a_{k_1} a_{k_2}.$$

The $w_{\alpha}(k_1, k_2)$ are related to the eigenfunctions $\varphi_{\alpha}(k_1, k_2)$ and the eigenvalues v_{α} of the pair correlation matrix through:

$$(2.2d) \quad w_{\alpha}(k_1, k_2) = v_{\alpha}^{\frac{1}{2}} (1 + u_{k_1}) \varphi_{\alpha}(k_1, k_2) (1 + u_{k_2})^{\frac{1}{2}}.$$

The operator \mathcal{V} describes the statistical behaviour of single particles, and both $\exp(Q^\dagger)$ and $\exp(Q)$ describe that of correlated pairs. The a_k, a_k^{\dagger} are Fermi destruction and creation operators respectively and satisfy the anti-commutation relations;

$$(2.2e) \quad [a_k, a_k^{\dagger}]_{+} = \delta_{kk'}; [a_k, a_{k'}]_{+} = [a_k^{\dagger}, a_{k'}^{\dagger}]_{+} = 0$$

the $A_{\alpha}, A_{\alpha}^{\dagger}$ are formal "labelling operators" (introduced to make $\hat{\mathcal{U}}$ commute with the number operator $\mathcal{N} = \sum_k a_k^{\dagger} a_k$) which satisfy the Bose-Einstein commutation relations;

$$(2.2f) \quad [A_{\alpha}, A_{\beta}^{\dagger}]_{-} = \delta_{\alpha\beta}; [A_{\alpha}, A_{\beta}]_{-} = [A_{\alpha}^{\dagger}, A_{\beta}^{\dagger}]_{-} = 0$$

and ω is the projection operator onto the formal vacuum state; i.e., the state for which the eigenvalues of $A_{\alpha}^{\dagger} A_{\alpha}$ are zero for all α .

An expression for $\hat{\mathcal{U}}$ which contains no labelling operators, we assert, is the following:

$$(2.3) \quad \hat{\mathcal{U}} = \int_{\mathcal{T}} d\tau \prod_{\alpha} e^{-\tau_{\alpha}} \int_R d\mu e^{\mathcal{P}^{\dagger}} \mathcal{V} e^{\mathcal{P}}$$

where ²

² \prod denotes direct product.

$$(2.4a) \quad P \equiv \sum_{\alpha} W_{\alpha} z_{\alpha}^{*}$$

$$(2.4b) \quad z_{\alpha} = (t_{\alpha})^{\frac{1}{2}} e^{i\nu_{\alpha}}$$

$$(2.4c) \quad \tau = \prod_{\alpha} t_{\alpha} \quad \text{and} \quad \mu = \prod_{\alpha} \left(\frac{\nu_{\alpha}}{2\pi} \right)$$

$$(2.4d) \quad T = \prod_{\alpha} T_{\alpha} \quad \text{and} \quad R = \prod_{\alpha} R_{\alpha}$$

and

$$(2.4e) \quad T_{\alpha} = \{x : x \text{ real}, x > 0\} \quad \text{and} \quad R_{\alpha} = \{x : x \text{ real}, -\pi < x < \pi\} \quad \text{for all } \alpha.$$

To prove this assertion, we first consider the special case in which the sum (2.2a) reduced to one term (i.e. there is only one pair state). We therefore drop the index α . Expanding the exponentials in (2.1) and using the identity (which follows from (2.2f))

$$(2.5) \quad \omega(A)^N (A^{\dagger})^M \omega = \omega \delta_{N,M} N!$$

we get ³

$$(2.6) \quad \hat{Q} = \sum_{N=0}^{\infty} (N!)^{-1} (W^{\dagger})^N \mathcal{V} (W)^N.$$

Now for the special case under consideration, (2.3) becomes

$$(2.7) \quad \hat{Q} = \int_0^{\infty} dt e^{-t} \int_{-\pi}^{\pi} \frac{d\nu}{2\pi} e^{it\nu} W^{\dagger} \mathcal{V} e^{it\nu} W$$

and since

$$(2.8a) \quad \int_{-\pi}^{\pi} \frac{d\nu}{2\pi} e^{it\nu(M-N)} = \delta_{N,M}$$

and

$$(2.8b) \quad \int_0^{\infty} dt e^{-t} t^N = N!$$

the expanded form of (2.7) is identical with (2.6). This completes the proof for the special case.

For the general case, we first note that the identity corresponding to (2.5) is

$$(2.5a) \quad \omega \prod_{\alpha} (A_{\alpha})^{N_{\alpha}} \prod_{\beta} (A_{\beta}^{\dagger})^{M_{\beta}} \omega = \omega \prod_{\alpha} \delta_{N_{\alpha}, M_{\alpha}} (N_{\alpha})!$$

and since we can obtain the same result (again ignoring the ω) by replacing A_{α} by z_{α} and integrating (c.f. (2.8)) viz.:

³ If we are content to use the expanded form we may neglect the projection operator ω .

$$(2.8c) \quad \int_T d\tau \prod_{\alpha} e^{-i\tau} \int_R d\mu \prod_{\alpha} (z_{\alpha})^{N_{\alpha}} \prod_{\beta} (z_{\beta}^*)^{M_{\beta}} = \prod_{\alpha} \delta_{N_{\alpha}, M_{\alpha}} (N_{\alpha})!$$

it is clear that the proof for the general case goes through in an entirely analogous way to the above. This completes the proof of the assertion.

A theorem which will be of major importance in the remainder of this work is

THEOREM (Zumino). *If Y is a complex anti-symmetric matrix, then there exists a unitary matrix U such that*⁴

$$U^T Y U = X$$

where X has a normal form, i.e.

$$X(k, k') = 0 \quad \text{unless} \quad k' = \bar{k}$$

and

$$X(k, \bar{k}) = -X(\bar{k}, k).$$

A proof of this theorem may be found in reference [4].

In the statement of the Z -theorem above, the "conjugate" of k , denoted by \bar{k} and satisfying $(\bar{\bar{k}}) = k$, is used to indicate a pairing (k, \bar{k}) of the index parameters $\{k\}$ ⁵. For finite dimensional matrices, the dimension must be even for the pairing process to be exhaustive. In this case, the canonical form of Y consists of "boxes" down the diagonal of the form

$$\begin{pmatrix} 0 & X(k, \bar{k}) \\ -X(k, \bar{k}) & 0 \end{pmatrix}$$

and zeros elsewhere. (The possibility of some $X(k, \bar{k})$'s being zero is not excluded.) When the dimension is odd, there will be an index remaining: this merely gives rise to a "diagonal box" of one element, which is zero.

The applications of the Z -theorem in the present paper will be to "infinite dimensional" matrices, so that a pairing (k, \bar{k}) of the index parameters will always be possible. Moreover, in the work to follow, we will find it convenient to decompose the index set into a union of a set \mathcal{S} and its conjugate $\bar{\mathcal{S}}$ defined by $\bar{\mathcal{S}} = \{\bar{k} : k \in \mathcal{S}\}$.

To demonstrate the applicability of the Z -theorem to our theory, as well as to provide us with a result that will be needed in the following sections, we devote the remainder of this section to an evaluation of $\text{Tr}(\hat{\mathcal{U}})$.

As a first step we write (2.3) in the form

⁴ T denotes transpose.

⁵ Normally, the index parameters are the states $k = (\vec{k}, s)$, \vec{k} denoting wave vector and s spin. In this case it is usual to take \bar{k} as the time reversed state to k , i.e. $\bar{k} = (-\vec{k}, -s)$. However, since in the present work we will find it convenient not to specify our index parameters, the normal convention will not be adopted.

$$(2.9) \quad \hat{U} = \int_T d\tau \prod_{\alpha} e^{-i\tau} \int_R d\mu \hat{U}(\nu, t)$$

with

$$\nu \equiv \{\nu_{\alpha}\}, \quad t = \{t_{\alpha}\}$$

and

$$(2.10) \quad \mathcal{U}(\nu, t) \equiv e^{P^{\dagger} \mathcal{V}} e^P$$

The problem then reduces to calculating $\text{Tr}(\hat{U}(\nu, t))$.

Using the cyclic property of the trace, we may write

$$(2.11) \quad \text{Tr}(\hat{U}(\nu, t)) = \text{Tr}(\mathcal{V} e^P e^{P^{\dagger}})$$

(2.11) can be simplified using the ‘‘quenching identity’’ of reference [5]: Let $F(a \cdots)$ be an operator containing only destruction operators and let $G(a^{\dagger} \cdots)$ be an operator containing only creation operators, then

$$(2.12) \quad \text{Tr}(\mathcal{V} F G) = \text{Tr}(\mathcal{V}) \langle 0 | \tilde{F} \tilde{G} | 0 \rangle$$

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

$$(2.13a) \quad a_k \rightarrow \tilde{a}_k = (1 + u_k)^{-\frac{1}{2}} a_k$$

$$(2.13b) \quad a_k^{\dagger} \rightarrow \tilde{a}_k^{\dagger} = (1 + u_k)^{-\frac{1}{2}} a_k^{\dagger}$$

and $|0\rangle$ is the vacuum state defined by

$$(2.13c) \quad a_k |0\rangle = 0 \quad \text{all } k.$$

Thus

$$(2.14) \quad \text{Tr}(\hat{U}(\nu, t)) = \text{Tr}(\mathcal{V}) \langle 0 | e^{\tilde{P}} e^{\tilde{P}^{\dagger}} | 0 \rangle$$

where from (2.13), (2.4a), (2.2d) and (2.2c)

$$(2.15) \quad \tilde{P} = \sum_{k_1 k_2} Y(k_1, k_2) a_{k_1} a_{k_2}$$

$Y(k_1, k_2)$ being defined by

$$(2.16) \quad Y(k_1, k_2) = 2^{-\frac{1}{2}} \sum_{\alpha} v_{\alpha}^{\frac{1}{2}} z_{\alpha}^* \varphi_{\alpha}^*(k_1, k_2).$$

Now since the $\varphi_{\alpha}^*(k_1, k_2)$ are anti-symmetric, ($Y(k_1, k_2)$) is antisymmetric, so we may employ the Z -theorem:

We first define new Fermi destruction and creation operators α_{λ} and $\alpha_{\lambda}^{\dagger}$ respectively, through ⁶:

⁶ Note that the transformation (2.17) preserves the Fermi anti-commutation relations (2.2e).

$$(2.17) \quad \begin{aligned} a_k &= \sum_{\lambda} U_{k\lambda} \alpha_{\lambda} \\ a_k^{\dagger} &= \sum_{\lambda} U_{k\lambda}^* \alpha_{\lambda}^{\dagger} \end{aligned}$$

and choose the unitary matrix U such that

$$(2.18) \quad X = U^T Y U$$

is in canonical form. (The transformation 2.17—18 will be known henceforth as the Z -transformation.)

Substitution in (2.15) then yields ⁷

$$(2.19) \quad \tilde{P} = \sum'_{\lambda} x(\lambda) \beta_{\lambda}$$

where

$$(2.20) \quad \left. \begin{aligned} x(\lambda) &\equiv 2X(\lambda, \bar{\lambda}) \\ x(\bar{\lambda}) &= -x(\lambda) \end{aligned} \right\} \lambda \in \mathcal{S}$$

and

$$(2.21) \quad \left. \begin{aligned} \beta_{\lambda} &\equiv \alpha_{\lambda} \alpha_{\bar{\lambda}} \\ \beta_{\bar{\lambda}} &= -\beta_{\lambda} \end{aligned} \right\} \lambda \in \mathcal{S}.$$

To complete the calculation we require a method for evaluating vacuum expectation values. One method is as follows: In an expression of the form $\langle 0|F(a_k, a_k^{\dagger})|0\rangle$ we use the Fermi anticommutation relations (2.2e) to move destruction operators to the right then use the identity $a_k|0\rangle = 0$ all k (or perhaps $\langle 0|a_k^{\dagger} = 0$ all k).

Applying this procedure to the vacuum expectation value in (2.14), noting, from (2.2e) that

$$(2.22a) \quad e^{\sum'_{\lambda} x(\lambda) \beta_{\lambda}} e^{\sum'_{\lambda} x^*(\lambda) \beta_{\lambda}^{\dagger}} = \prod'_{\lambda} e^{x(\lambda) \beta_{\lambda}} e^{x^*(\lambda) \beta_{\lambda}^{\dagger}}$$

and

$$(2.22b) \quad (\beta_{\lambda})^2 = (\beta_{\lambda}^{\dagger})^2 = 0$$

one has

$$\begin{aligned} \langle 0|e^{\tilde{P}} e^{\tilde{P}^{\dagger}}|0\rangle &= \prod'_{\lambda} \langle 0|(1+x(\lambda)\beta_{\lambda})(1+x^*(\lambda)\beta_{\lambda}^{\dagger})|0\rangle \\ &= \prod'_{\lambda} (1+|x(\lambda)|^2) \\ &= \exp \left[\sum'_{\lambda} \ln (1+|x(\lambda)|^2) \right] \end{aligned}$$

or, in terms of the X operator (2.20)

$$(2.23) \quad = \exp \left[\frac{1}{2} \text{Tr} \ln (1-4X^* X) \right]$$

⁷ Primed sums and products will denote sums and products over the set \mathcal{S} .

Now from (2.18)

$$(2.24) \quad X^* X = U^\dagger Y^* Y U$$

and since (U is unitary)

$$(2.25) \quad \text{Tr} (U^\dagger A U) = \text{Tr} (A)$$

$$(2.26) \quad \langle 0 | e^{\mathcal{P}} e^{\mathcal{P}^\dagger} | 0 \rangle = \exp \left[\frac{1}{2} \text{Tr} \ln (1 - M) \right]$$

where

$$(2.27) \quad M \equiv 4 Y^* Y = 2 \sum_{\alpha\beta} (v_\alpha v_\beta)^{\frac{1}{2}} q_\beta^\alpha z_\alpha z_\beta^*$$

and

$$(2.28) \quad \langle k | q_\beta^\alpha | k' \rangle \equiv \sum_{k''} \varphi_\alpha (k, k'') \varphi_\beta^* (k'', k').$$

Finally, we combine (2.26), (2.14) and (2.9) to get

$$(2.29) \quad \text{Tr} (\hat{\mathcal{Q}}) = \text{Tr} (\mathcal{V}) \int_{\mathcal{T}} d\tau \prod_\alpha e^{-t_\alpha} \int_R d\mu \exp \left[\frac{1}{2} \text{Tr} \ln (1 - M) \right].$$

For the case of one pair state only, noting that M is independent of ν (2.29) reduces to the result given in E_1 .

$$(2.30) \quad \text{Tr} (\hat{\mathcal{Q}}) = \text{Tr} (\mathcal{V}) \int_0^\infty dt e^{-t} \exp \left[\frac{1}{2} \text{Tr} \ln (1 - 2vtq) \right]$$

with

$$(2.31) \quad \langle k | q | k' \rangle \equiv \sum_{k''} \varphi (k, k'') \varphi^* (k'', k')$$

The equivalence of (2.29), in its full generality, and ([6], 2.25) can be easily established by inverting the process indicated in the arguments from (2.3—8).

In the work to follow, we will be required to evaluate expressions of the form

$$(2.32) \quad \int_{\mathcal{T}} d\tau \prod_\alpha e^{-t_\alpha} \int_R d\mu \langle 0 | e^{\mathcal{P}} A e^{\mathcal{P}^\dagger} | 0 \rangle / \int_{\mathcal{T}} d\tau \int_R d\mu C(\nu, \mathbf{t})$$

with

$$(2.33) \quad C(\nu, \mathbf{t}) \equiv \prod_\alpha e^{-t_\alpha} \exp \left[\frac{1}{2} \text{Tr} \ln (1 - M) \right]$$

and A some operator.

For convenience we introduce the following notation

$$\langle\langle A \rangle\rangle = \langle 0 | e^{\mathcal{P}} A e^{\mathcal{P}^\dagger} | 0 \rangle / \exp \left[\frac{1}{2} \text{Tr} \ln (1 - M) \right]$$

and the weight function $p(\nu, \mathbf{t})$ defined by

$$(2.35) \quad \rho(\nu, t) = C(\nu, t) / \int_{\mathcal{T}} d\tau \int_{\mathcal{R}} d\mu C(\nu, t).$$

With this notation, (2.32) can be written in the form

$$(2.36) \quad \int_{\mathcal{T}} d\tau \int_{\mathcal{R}} d\mu \rho(\nu, t) \ll A \gg.$$

3. Expectation values of one-particle operators

The expectation value of a typical one-particle operator

$$(3.1) \quad J = \sum_{kk'} J_{kk'} a_k^\dagger a_{k'}$$

is defined by

$$(3.2) \quad \langle J \rangle = \text{Tr} (J\mathcal{U})$$

where

$$(3.3) \quad \mathcal{U} \equiv \hat{\mathcal{U}} [\text{Tr} (\hat{\mathcal{U}})]^{-1}.$$

The reduction of (3.2) was carried out in E_I (E_I 2.8) using the quenching identity (2.12). In the notation of section 2, E_I 2.8 reads

$$(3.4) \quad \langle J \rangle = \sum_k \bar{n}_k J_{kk} + \int_{\mathcal{T}} d\tau \int_{\mathcal{R}} d\mu \rho(\nu, t) \ll \mathcal{J} \gg$$

with

$$(3.5a) \quad \bar{n}_k = u_k(1+u_k)^{-1}$$

and

$$(3.5b) \quad \mathcal{J} = \sum_{kk'} (1+u_k)^{-\frac{1}{2}} J_{kk'} (1+u_{k'})^{-\frac{1}{2}} a_k^\dagger a_{k'} = \sum_{kk'} J_{kk'} a_k^\dagger a_{k'}$$

To evaluate the quantity in (3.4) under the integrals, we employ the Z -transformation (2.17—18) and the method of section 2; thus:

$$(3.6) \quad \ll \mathcal{J} \gg = \sum_{\lambda\mu} \mathcal{J}(\lambda, \mu) \ll \alpha_\lambda^\dagger \alpha_\mu \gg$$

where

$$(3.7) \quad \mathcal{J} \equiv U^\dagger J U$$

$$(3.8) \quad \begin{aligned} \ll \alpha_\lambda^\dagger \alpha_\mu \gg &= \delta_{\lambda\mu} \langle 0 | (1+x(\lambda)\beta_\lambda) \alpha_\lambda^\dagger \alpha_\lambda (1+x^*(\lambda)\beta_\lambda^\dagger) | 0 \rangle / (1+|x(\lambda)|^2) \\ &= \delta_{\lambda\mu} |x(\lambda)|^2 / (1+|x(\lambda)|^2) \\ &\equiv \delta_{\lambda\mu} I(\lambda) \quad \lambda \in \mathcal{S} \end{aligned}$$

and

$$(3.9) \quad \ll \alpha_\lambda^\dagger \alpha_\lambda \gg = \ll \alpha_\lambda^\dagger \alpha_\lambda \gg \quad \lambda \in \mathcal{S}.$$

If we now define an operator H by

$$(3.10) \quad H = -4X^*X(1-4X^*X)^{-1}$$

it follows from (2.20) and (3.8) that

$$(3.11) \quad \begin{aligned} H(\lambda, \lambda') &= \delta_{\lambda', \lambda} I(\lambda) \\ H(\lambda, \bar{\lambda}) &= H(\bar{\lambda}, \lambda) \quad \lambda \in \mathcal{S} \end{aligned}$$

so (3.6) can be expressed in the following way:

$$(3.12) \quad \langle\langle J \rangle\rangle = \sum_{\lambda, \lambda'} \mathcal{J}(\lambda, \lambda') H(\lambda', \lambda) \equiv \text{Tr}_1(\mathcal{J}H).$$

We now substitute (3.7) in (3.12), noting that (c.f. 2.24–28)

$$(3.13) \quad UHU^\dagger = -M(1-M)^{-1} \equiv h$$

to get

$$(3.14) \quad \langle\langle J \rangle\rangle = \text{Tr}_1(\mathcal{J}h).$$

Combining (3.14) and (3.4) we obtain finally:

$$(3.15) \quad \langle J \rangle = \sum_k \bar{n}_k J_{kk} + \int_T d\tau \int_R d\mu \rho(\nu, t) \text{Tr}_1(\mathcal{J}h).$$

It should be noted that in general, h is a function of the z_α ; though for the special case of only one pair state, it is a function only of t : indeed, for this case

$$(3.16) \quad h = -2vtq(1-2vtq)^{-1}$$

and (3.15) reduces to the result given in E_I . The equivalence of (3.15) and the general expression given in E_{II} can be easily established by the process indicated in section 2.

4. Expectation values of two-particle operators

The reduction of the expectation value

$$(4.1) \quad \langle K \rangle = \text{Tr}(K\mathcal{Q})$$

of a typical two-particle operator

$$(4.2) \quad K = \sum_{k\ell, k'\ell'} K_{k\ell, k'\ell'} a_k^\dagger a_\ell^\dagger a_{\ell'} a_{k'}$$

has been again carried out in E_I (E_I 2.12) using the quenching identity. In our notation, E_I 2.12 reads

$$(4.3) \quad \langle K \rangle = \sum_{kl} (K_{kl,kl} - K_{kl,lk}) \bar{n}_k \bar{n}_l + \int_T d\tau \int_R d\mu \phi(\nu, \mathbf{t}) \ll \tilde{K}^{(1)} \gg + \int_T d\tau \int_R d\mu \phi(\nu, \mathbf{t}) \ll \tilde{K} \gg$$

where

$$(4.4) \quad \bar{n}_k = u_k(1+u_k)^{-1}$$

is the average number of particles in the single particle state k , and the one-particle operator $\tilde{K}^{(1)}$ and the two-particle operator \tilde{K} are defined by

$$(4.5a) \quad \tilde{K}^{(1)} = \sum_{kk'} \tilde{K}_{kk'}^{(1)} a_k^\dagger a_{k'}$$

$$(4.5b) \quad \tilde{K}_{kk'}^{(1)} = \sum_m \bar{n}_m (1+u_k)^{-\frac{1}{2}} (K_{mk,mk'} + K_{km,k'm} - K_{km,mk'} - K_{mk,k'm}) (1+u_{k'})^{-\frac{1}{2}}$$

and

$$(4.6a) \quad \tilde{K} = \sum_{kl,k'l'} \tilde{K}_{kl,k'l'} a_k^\dagger a_l^\dagger a_{l'} a_{k'}$$

$$(4.6b) \quad \tilde{K}_{kl,k'l'} = \{(1+u_k)(1+u_l)\}^{-\frac{1}{2}} K_{kl,k'l'} \{(1+u_{k'})(1+u_{l'})\}^{-\frac{1}{2}}$$

respectively.

Since $\tilde{K}^{(1)}$ is a one-particle operator, the second term in (4.3) becomes, using the results of section 3

$$(4.7) \quad \int_T d\tau \int_R d\mu \phi(\nu, \mathbf{t}) \text{Tr}_1(\tilde{K}^{(1)} h).$$

The term remaining in (4.3) can be evaluated, again with the help of the Z -theorem, in the following way:

We first apply the Z -transformation (2.17—18) to get

$$(4.8) \quad \ll \tilde{K} \gg = \sum_{\lambda\mu,\lambda'\mu'} \mathcal{H}(\lambda\mu, \lambda'\mu') \ll \alpha_\lambda^\dagger \alpha_\mu^\dagger \alpha_{\mu'} \alpha_{\lambda'} \gg$$

where

$$(4.9) \quad \mathcal{H}(\lambda\mu, \lambda'\mu') \equiv \sum_{kl,k'l'} U_{\lambda k}^\dagger U_{\mu l}^\dagger \tilde{K}_{kl,k'l'} U_{k'l'} U_{\lambda'\mu'}$$

then observe that $\ll \alpha_\lambda^\dagger \alpha_\mu^\dagger \alpha_{\mu'} \alpha_{\lambda'} \gg$ vanishes unless either

- 1) $\mu' = \lambda$ and $\lambda' = \mu$, or $\mu' = \mu$ and $\lambda' = \lambda$; or
- 2) $\mu = \bar{\lambda}$ and $\mu' = \bar{\lambda}'$.

That is:

$$(4.10) \quad \ll \tilde{K} \gg = \sum_{\lambda \neq \mu} \mathcal{M}(\lambda, \mu) \ll \alpha_\lambda^\dagger \alpha_\mu^\dagger \alpha_\mu \alpha_\lambda \gg + \sum_{\lambda \neq \mu} \mathcal{L}(\lambda, \mu) \ll \beta_\lambda^\dagger \beta_\mu \gg$$

where

$$(4.11a) \quad \mathcal{M}(\lambda, \mu) \equiv \mathcal{K}(\lambda\mu, \lambda\mu) - \mathcal{K}(\lambda\mu, \mu\lambda) + [(\lambda, \mu) \leftrightarrow (\bar{\lambda}, \bar{\mu})] \quad \lambda, \mu \in \mathcal{S}$$

and

$$(4.11b) \quad \mathcal{L}(\lambda, \mu) \equiv \mathcal{K}(\lambda\bar{\lambda}, \mu\bar{\mu}) - \mathcal{K}(\bar{\lambda}, \lambda, \mu\bar{\mu}) - [\mu \leftrightarrow \bar{\mu}] \quad \lambda, \mu \in \mathcal{S}.$$

Now, using the methods of sections 2 and 3, noting that $\lambda \neq \mu$, we have

$$(4.12a) \quad \begin{aligned} \langle\langle \beta_\lambda^\dagger \rangle\rangle &= \langle 0 | (1 + x(\lambda)\beta_\lambda)\beta_\lambda^\dagger(1 + x^*(\lambda)\beta_\lambda^\dagger) | 0 \rangle / (1 + |x(\lambda)|^2) \\ &= x(\lambda) (1 + |x(\lambda)|^2)^{-1} \\ &\equiv \Phi(\lambda) \quad \lambda \in \mathcal{S} \end{aligned}$$

$$(4.12b) \quad \langle\langle \beta_\lambda^\dagger \rangle\rangle = -\langle\langle \beta_\lambda^\dagger \rangle\rangle \quad \lambda \in \mathcal{S}$$

$$(4.12c) \quad \langle\langle \beta_\mu \rangle\rangle = \Phi^*(\mu) = -\langle\langle \beta_{\bar{\mu}} \rangle\rangle \quad \mu \in \mathcal{S}$$

and

$$(4.13) \quad \langle\langle \beta_\lambda^\dagger \beta_\mu \rangle\rangle = \Phi(\lambda)\Phi^*(\mu) \quad \lambda, \mu \in \mathcal{S}$$

and also, from (3.8)

$$(4.14) \quad \langle\langle \alpha_\lambda^\dagger \alpha_\lambda \alpha_\mu^\dagger \alpha_\mu \rangle\rangle = I(\lambda)I(\mu) \quad \lambda, \mu \in \mathcal{S}.$$

Next, we define an operator Ψ by

$$(4.15) \quad \Psi = \{(1 - 4X^*X)^{-1}X - [(1 - 4X^*X)^{-1}X]^T\}$$

and observe that (c.f. (2.20))

$$\left. \begin{aligned} (4.16a) \quad &\Psi(\lambda, \lambda') = \delta_{\lambda'\lambda} \Phi(\lambda) \\ (4.16b) \quad &\Psi(\lambda, \bar{\lambda}) = -\Psi(\bar{\lambda}, \lambda) \end{aligned} \right\} \lambda \in \mathcal{S}$$

so on combining (4.10), (4.13), (4.15) and (3.10) we have

$$(4.17) \quad \begin{aligned} \langle\langle \hat{K} \rangle\rangle &= \sum_{\lambda\mu, \lambda'\mu'} \mathcal{K}(\lambda\mu, \lambda'\mu') \langle \lambda'\mu' | P | \lambda\mu \rangle \\ &\quad + \sum_{\lambda\mu, \lambda'\mu'} \Psi^*(\lambda, \mu) \mathcal{K}(\lambda\mu, \lambda'\mu') \Psi(\lambda', \mu') \\ &\equiv \text{Tr}_2(\mathcal{K}P) + \langle \Psi | \mathcal{K} | \Psi \rangle \end{aligned}$$

with

$$(4.18) \quad \langle \lambda\mu | P | \lambda'\mu' \rangle \equiv H(\lambda, \lambda')H(\mu, \mu') - H(\lambda, \mu')H(\mu, \lambda').$$

To obtain a result in terms of our original quantities, we simply substitute (4.9) in (4.17), using (3.13) and (c.f. (2.18) and (2.24–28))

$$(4.19) \quad U\Psi U^\dagger = \{(1 - M)^{-1}Y - [(1 - M)^{-1}Y]^T\} \equiv \psi$$

to get

$$(4.20) \quad \langle\langle \tilde{K} \rangle\rangle = \text{Tr}_2(\tilde{K}\rho) + \langle\psi|\tilde{K}|\psi\rangle$$

where

$$(4.21) \quad \langle k'l|\rho|k'l'\rangle = \langle k|h|k'\rangle\langle l|h|l'\rangle - \langle k|h|l'\rangle\langle l|h|k'\rangle$$

and, in expanded form

$$(4.22a) \quad \psi(k, k') = \sum_{\alpha} \psi_{\alpha}(k, k')$$

$$(4.22b) \quad \psi_{\alpha}(k, k') = \left(\frac{v_{\alpha}}{2}\right)^{\frac{1}{2}} z_{\alpha} \sum_{k''} \{ \langle k|(1-M)^{-1}|k''\rangle \varphi_{\alpha}(k'', k') \\ - \langle k'|(1-M)^{-1}|k''\rangle \varphi_{\alpha}(k'', k) \}.$$

Combining (4.20), (4.7) and (4.3) we have, finally

$$(4.23) \quad \langle K \rangle = \sum_{ki} (K_{ki,ki} - K_{ki,ik}) \bar{n}_k \bar{n}_i \\ + \int_{\mathcal{T}} d\tau \int_{\mathcal{R}} d\mu \rho(\nu, \boldsymbol{\epsilon}) \{ \text{Tr}_1(\tilde{K}^{(1)}h) + \text{Tr}_2(\tilde{K}\rho) + \langle\psi|\tilde{K}|\psi\rangle \}.$$

Again it is an easy matter to show that (4.23) is equivalent, in its full generality, to the result given in E_{II} , and of course, in the special case of only one pair state, to the result given in E_I .

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