On the Propagator Form of Thermodynamic Perturbation Theory

by **Charles P. Enz**
Institut de Physique Théorique, Université de Genève

E. C. G. STUECKELBERG zum 60. Geburtstag

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Zusammenfassung. Die Schwierigkeit bei der Entwicklung der Propagator-Version der thermodynamischen Störungstheorie liegt darin, dass die Mittelwerte von Normal ($\mathfrak{N}$-) Produkten nicht verschwinden. In MATSUBARA's Methode wird sie durch den Kunstgriff einer Aufspaltung der Feldoperatoren umgangen, die nicht der physikalischen Aufspaltung in Emissions- und Absorptions-Teile entspricht. Hier wird gezeigt, dass die letztere zu denselben Resultaten führt. Insbesondere wird eine allgemeine Reduktionsformel für Mittelwerte von $\mathfrak{N}$-Produkten hergeleitet. Ferner wird gezeigt, dass diese einen typischen Beitrag, proportional zur Verteilungsfunktion, zu den thermodynamischen Propagatoren liefern. Explizite Ausdrücke für allgemeine freie Propagatoren werden angegeben.

1. Introduction

In the application of field theoretical methods to statistical mechanics the development of a propagator technique, i.e. of a reduction formula for temperature ordered (or $\mathfrak{T}$-)products, was an important and not quite trivial step. For, whereas in field theory all averages (vacuum expectation values) of normal (or $\mathfrak{N}$-)products of field operators vanish by definition this is not so with statistical averages (taken over a grand canonical ensemble). And hence it is not immediately obvious how to obtain a resolution of perturbation theoretical expressions into the analogue of the celebrated causal Green's functions pioneered by STUECKELBERG[1]).

In statistical mechanics the pioneering contribution came from MATSUBARA[2]) who observed that by a suitable redefinition of "positive" and "negative" parts of field operators (as implied in the definition of $\mathfrak{N}$-products) the averages of $\mathfrak{N}$-products could be made to vanish. Together with the general proof of this given by THOULESS[3]) MATSUBARA's procedure forms the basis for the propagator technique of modern thermodynamic perturbation theory[4]).

A disadvantage of MATSUBARA's method is the fact that in his definition the positive and negative parts of field operators have lost their physical meaning of emission and absorption parts. In the present paper identical results are obtained without giving

up this natural division of field operators. In particular we derive a general reduction formula for averages of $\mathfrak{N}$-products (for bosons it had been indicated without proof in reference 3). For systems without a condensed phase non-vanishing averages of $\mathfrak{N}$-products are characteristic of *finite* temperatures and contribute typically to the thermodynamical propagators. In fact, the latter fall naturally into two parts for which the designation "spontaneous" and "induced" are appropriate, in analogy with EINSTEIN's probabilities of black body radiation.

The spontaneous part is due to the contractions in the $\mathfrak{N}$-products and hence is independent of the statistical average (distribution function) and, consequently, independent of temperature. The induced part comes from the statistical average of $\mathfrak{N}$-products, it is proportional to the distribution function and hence disappears at zero temperature.

Since the emission and absorption parts of field operators are in direct relation with the definition of the groundstate (vacuum), MATSUBARA's method could be characterized as using an unphysical ground state. Now it is well known that for systems with a condensed phase (superfluids, superconductors) the ground state plays a very particular role, in that for this state $\mathfrak{N}$-product averages do not vanish, even not at zero temperature[5]). It is clear that MATSUBARA's method does not apply to this situation, as is emphasized in reference 4, page 32. On the other hand bose condensation might be an interesting application of our reduction formula for $\mathfrak{N}$-product averages. *)

In order to facilitate the application of the reduction formulas for $\mathfrak{N}$- and $\mathfrak{T}$-products derived here to any type of "vertices" of "fields" and "particles" the following terminology is used for convenience: A field operator (defined as a linear combination of emission and absorption operators **) has the appearance of a "field" if it contains emission and absorption parts in equal proportion, it has the appearance of a "particle" if it consists of an emission or an absorption part only. The "field" case is realized throughout in field theoretical interaction hamiltonians but also in all the couplings of phonons, which justifies the designation phonon field***) [6][7]).

The "particle" case is realized in all the two-body interactions of many-body theory because of the very form of two-body operators in second quantization[7]). Clearly, this case also occurs in the operators that build up many particle states both in field theory and in many-body theory.

The "vertices" are characterized by the number of field operators ("branches") united by the same temperature argument, and by a coefficient (matrix element). In this terminology the simplest vertex is one with one branch, representing e.g. the

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*) A quite different but very simple application are GLAUBER's correlation functions of higher order for black body radiation; see R.J. GLAUBER, Phys. Rev. *131*, 2766 (1963); C.L. MEHTA and E. WOLF, Phys. Rev. *134*, A1149 (1964).

**) Note that this linearity is a property reflecting in second quantization the superposition principle of first quantization or of classical fields.

***) Spin waves are similar to bosons, however, their commutators are not c-numbers. As a consequence WICK's theorem is a relatively complicated problem which has been solved only recently[6]). From another point of view, related to the mass carried by excitations in solids, spin waves (magnons) have an intimate analogy to phonons and have therefore both been called "fields" elsewhere[7]).

operator of a one-particle state. Vertices with two branches are realized in couplings to external (i.e. non-quantized) fields or, more generally, in density operators. The latter are of particular importance in calculations of transport coefficients with Kubo-type formulas[8]). Whereas conventional field theoretic and many-body interactions are characterized by vertices with 3 or 4 branches, the phonon-phonon interaction (describing anharmonic effects in crystals) has in addition vertices with 5, 6,... branches. The technique developed in this paper is general enough to handle this case, in which all kinds of vertices may be mixed together. It also includes a general and concise proof of the well known theorem concerning connected graphs[9]). The results will be used in a forthcoming work[10]) to evaluate the energy density correlation function of a phonon system with the hope to gain some insight into the question of second sound in dielectric crystals[11]).

In connection with the last mentioned work an additional remark may be made in support of the terminology field-particle used here. It has recently been noticed by several people[12]) that the construction of density operators for a phonon system is not trivial. In reference 10 it will be shown that this construction is quite different from the analogous problem in many-body systems. The reason is that many-body theory applies only to the ions of the lattice but not to their phonon excitations, which, particularly from this point if view, are very analogous to the electromagnetic field.

One difficulty with the correlation functions used in transport theory is that they depend both on temperature and time so that the orderings with respect to these two variables in perturbation expansions interfere. Except for special cases there does not yet exist a method to handle this problem[13]). In some applications, however, the knowledge of these correlation functions in the neighbourhood of zero time is sufficient[10]). Here we give explicit expressions for the temperature and time dependent free propagators for arbitrary field operators as well as rules for their evaluation in the cases of interest.

2. General Perturbation Expression

Each species (bosons or fermions) of field operators may be linearly built up from operators of the form

$$A_k = \alpha_k a_k + \alpha'_k a^+_{-k} , \tag{1}$$

where $\pm k$ labels the momentum $\pm \boldsymbol{k}$ and any other variables necessary to characterize a one-particle state, such as polarization and mode. a^+_k and a_k are the emission and absorption operators; they are the basic operators in "particle" couplings. The "positive" and "negative" parts of A_k are

$$A^{(+)}_k = \alpha'_k a^+_{-k} ; \quad A^{(-}_k = \alpha_k a_k . \tag{2}$$

In "field" couplings the basic operators are of the form

$$P_{-k} = P^+_k = \frac{-i}{\sqrt{2\gamma_k}} (a_k - \gamma_k a^+_{-k}) \qquad Q_k = Q^+_{-k} = \frac{1}{\sqrt{2\gamma_k}} (a_k + \gamma_k a^+_{-k}) , \tag{3}$$

where γ_k is an arbitrary phase factor satisfying

$$\gamma_{-k} = \gamma_k . \tag{3'}$$

A pair of canonically conjugate field operators may be written as

$$\Pi_i(\boldsymbol{r}, t) = \sum_k e_{ik} \sqrt{\omega_k}\, P_k(t)\, e^{i\boldsymbol{k}\boldsymbol{r}} \qquad \Phi_i(\boldsymbol{r}, t) = \sum_k e_{ik} \frac{1}{\sqrt{\omega_k}}\, Q_k(t)\, e^{i\boldsymbol{k}\boldsymbol{r}} \tag{4}$$

where the time dependence is given by (free fields)

$$a_k^+(t) \equiv e^{iH_0 t}\, a_k^+\, e^{-iH_0 t} = a_k^+\, e^{i\omega_k t}\ ;\ a_k(t) \equiv e^{iH_0 t}\, a_k\, e^{-iH_0 t} = a_k\, e^{-i\omega_k t}\,. \tag{5}$$

With appropriate identification of coefficients and labels (4) is the standard form both in field theory and in many-body theory. Thus (1) has the generality necessary to describe any type of vertices and propagators.

A general term of a thermodynamic perturbation expression is an averaged temperature ordered product of vertex terms V_i with reciprocal temperature argument λ_i (we use units such that $\hbar = k_B = 1$, where k_B is BOLTZMANN's constant),

$$\left\langle \mathfrak{T}\left(\prod_i V_i[\lambda_i]\right)\right\rangle_0\,, \tag{6}$$

$\mathfrak{T}$ is WICK's time (here temperature) ordering operator[14]), the temperature dependence being that of the interaction representation as defined for any operator O by

$$O[\lambda] \equiv e^{\lambda K_0}\, O\, e^{-\lambda K_0}\,. \tag{7}$$

In particular

$$a_k^+[\lambda] = a_k^+\, e^{\lambda\varepsilon_k}\ ;\ a_k[\lambda] = a_k\, e^{-\lambda\varepsilon_k}\ , \tag{7'}$$

K_0 is the sum of the unperturbed hamiltonian

$$H_0 = \sum \omega_k\, a_k^+\, a_k + \cdots \tag{8}$$

and the chemical potential term $-\mu \sum a_k^+\, a_k \ldots$ of the grand canonical ensemble,

$$K_0 = \sum \varepsilon_k\, a_k^+\, a_k + \cdots\ ;\ \varepsilon_k = \varepsilon_{-k} = \omega_k - \mu\,. \tag{8'}$$

Here and in the following the dots indicate similar expressions for all the other species of field operators occurring in the theory.

A vertex V_i has the general form

$$V_i = \sum_{(k\cdots)} \Gamma^{(i)}_{(k\cdots)} \times \prod_{r=1}^{n_i} A_{rk_r} \times \cdots\,, \tag{10}$$

where n_i is the number of branches of the A-species and A_{rk} is of the form (1) with parameters α_{rk}, α'_{rk}. $\Gamma^{(i)}_{(k\ldots)}$ is the matrix element. In (6) some of the vertices may represent the operators of state vectors and density operators, the remaining V_i come from the expansion of the operator

$$S(\beta) \equiv e^{\beta K_0}\, e^{-\beta(K_0+H')} = \mathfrak{T} \exp\left(-\int_0^\beta d\lambda\, H'[\lambda]\right), \tag{11}$$

which makes the transition from the exact density matrix const. $\times \exp(-\beta(K_0 + H'))$ to the unperturbed one. The latter defines the average occurring in Equation (6),

$$\langle O \rangle_0 \equiv \frac{Tr\,(e^{-\beta K_0} O)}{Tr\,(e^{-\beta K_0})} . \tag{12}$$

H' is the sum of all types of interaction terms.

Since different species of field operators in (6) factor out (statistical independence) one is left with expressions of the form

$$\left\langle \mathfrak{T}\left(\prod_{(s)} A_s\right)\right\rangle_0 ; \quad A_s \equiv A_{\nu_s k_s}[\lambda_{i_s}] , \tag{13}$$

where a relabeling of indices has been introduced such that factors in the product are distinguished by the set of numbers $s = 1, 2, \ldots$.

3. Reduction of $\mathfrak{N}$-Product Averages

As in field theory the evaluation of expressions like (13) proceeds via $\mathfrak{N}$-products. Their definition is

$$\mathfrak{N}\left(\prod_{(s)} A_s\right) \equiv \sum_{(t/s)} (\pm 1)^{\sigma(t/s)} \prod_{(t)} A_t^{(+)} \prod_{(\bar{t})} A_{\bar{t}}^{(-)} . \tag{14}$$

Here and in the following the upper sign is for bosons, the lower for fermions. (t) is an ordered subset $t_1 < t_2 < \ldots$ of the set (s) and $(\bar{t})$ the complement $(s) - (t)$. (t/s) are all the subdivisions; their number is

$$N\,(t/s) = \sum_{n=0}^{N(s)} \frac{N(s)!}{n!\,(N(s)-n)!} = 2^{N(s)} ,$$

$N(s)$ being the number of elements in the set (s). $\sigma(t/s)$ is the number of transpositions of adjacent numbers necessary to separate the subsets (t) and $(\bar{t})$.

The result to be derived is a resolution of the average of (14) into factors

$$\underbrace{A_s\, A_t} \equiv \langle A_s^{(+)}\, A_t^{(-)} \rangle_0 . \tag{15}$$

It is based on the following formula (see appendix) which for bosons has been derived independently by Bloch and de Dominicis[15]) and by Thouless[3]) whereas it is trivial for fermions since $(a_k^+)^n = (a_k)^n = 0$ for $n \geqslant 2$ (Pauli principle):

$$\langle (a_k^+)^n\, (a_k)^n \rangle_0 = n!\, f_k^n ; \quad \begin{cases} \text{bosons:} & n = 0, 1, 2, \cdots \\ \text{fermions:} & n = 0, 1 \end{cases} \tag{16}$$

Here

$$f_k \equiv \langle a_k^+\, a_k \rangle_0 = (e^{\beta \varepsilon_k} \mp 1)^{-1} \tag{17}$$

is the unperturbed one-particle distribution function. This formula will now be generalized in several steps. First it is evident that

$$\langle (a_k^+)^n\, (a_{k'})^{n'} \rangle_0 = \delta_{nn'}\, n!\, (\langle a_k^+\, a_{k'} \rangle_0)^n \sim \delta_{kk'} ,$$

so that with Equation (2)

$$\left\langle \prod_{(s)} A_{\nu_s k}^{(+)}\,[\lambda_{i_s}] \prod_{(t)} A_{\nu_t k'}^{(-)}\,[\lambda_{i_t}] \right\rangle_0 = \delta_{N(s),\,N(t)} \prod_{(s)} \alpha'_{\nu_s k}\, e^{i\lambda_{i_s}\varepsilon_k} \prod_{(t)} \alpha_{\nu_t k'}\, e^{-i\lambda_{i_t}\varepsilon_{k'}} \times$$
$$\times\, N(s)!\, (\langle a_{-k}^+\, a_{k'} \rangle_0)^{N(s)}$$

(for fermions $N(s) = 0$ or 1). Now for $N(s) = N(t)$ the sets (s) and (t) can be grouped into pairs (s, t) and this can be done in $N(s)!$ ways by permutations, $P(t)$, of the set (t). Hence, making use again of Equation (2),

$$\left\langle \prod_{(s)} A^{(+)}_{\nu_s k}[\lambda_{i_s}] \prod_{(t)} A^{(-)}_{\nu_t k'}[\lambda_{i_t}] \right\rangle_0 = \delta_{N(s),\,N(t)} \sum_{P(t)} \prod_{(s)} \left\langle A^{(+)}_{\nu_s k}[\lambda_{i_s}]\; A^{(-)}_{\nu_t k'}[\lambda_{i_t}] \right\rangle_0 . \tag{18}$$

Next we remark that this equation is still correct if we assign to each t of the set (t) an individual label k_t. In fact, (18) is identically zero unless all k_t equal k. Now take a product of expressions of the form of the left hand side of (18) each factor with a different value of k. Because of the statistical independence of factors with different k the product may again be written as a single expression of the same form but with individual labels k_s. Making use of the contraction symbol (15) and of the abbreviated notation (13) we have

$$\left\langle \prod_{(s)} A^{(+)}_s \prod_{(t)} A^{(-)}_t \right\rangle_0 = \delta_{N(s),\,N(t)} \sum_{P(t)} (\pm 1)^{1/2\, N(s)\,(N(s)-1)+\sigma_{P(t)}} \prod_{(s)} \underbrace{A_s\, A_t} , \tag{19}$$

$\sigma_{P(t)}$ is the number of transpositions of adjacent numbers from which the permutation $P(t)$ can be built up.

At this point a more careful consideration of the fermion case is necessary. First the k_s in Equation (19) are all different by construction, and their number, $N(s)$, may now be any integer. Next we assert that the condition of different k_s may actually be droped since coincidence of some k_s values makes Equation (19) vanish identically. This is trivial for the left hand side. For the right hand side it is a consequence of the anticommutativity combined with taking the sum over permutations $P(t)$. Indeed, suppose $A^{(+)}_{s_1} \ldots A^{(+)}_{s_d}$ are degenerate in k_s ($k_{s_1} = k_{s_2} = \ldots = k_{s_d}$; $d \geqslant 2$). Now consider among all $P(t)$ the $d!$ permutations which act only on a given subset $t_1 \ldots t_d$ which is paired with the set $s_1 \ldots s_d$. It is easily seen that even and odd permutations just compensate each other, which proves the assertion. Hence Equation (19) is valid without restriction also for the fermion case. In other words *the pairings may be made irrespective of the* PAULI *principle*, a fact which in other contexts of perturbation theory is well known[16]) and follows here for $\mathfrak{N}$-products in an explicit and direct way.

Combining the result (19) with the definition (14) one obtains

$$\left\langle \mathfrak{N}\left(\prod_{(s)} A_s \right) \right\rangle_0 = \sum_{(t/s)} (\pm 1)^{\sigma(t,\bar{t})} \sum_{P(\bar{t})} \prod_{(t)} \underbrace{A_t\, A_{\bar{t}}} \tag{20}$$

where $\sigma(t, \bar{t}) \equiv \sigma(t/s) + \sigma_{P(\bar{t})}$. (20) vanishes unless $N(s)$ is even,

$$N(s) = 2\,N . \tag{20'}$$

The number of terms in the double sum is

$$\frac{(2\,N)!}{(N!)^2}\, N! = (2\,N)\,(2\,N-1) \cdots (N+1) = 2^N (2\,N-1)!! \tag{20''}$$

Another way of writing (20) is

$$\left\langle \mathfrak{N}\left(\prod_{(s)} A_s \right) \right\rangle_0 = \frac{1}{N!} \sum_{P(s)} (\pm 1)^{\sigma_{P(s)}} \underbrace{A_{s_1} A_{s_2}}\, \underbrace{A_{s_3} A_{s_4}} \cdots \underbrace{A_{s_{2N-1}} A_{s_{2N}}} . \tag{21}$$

Here the factor $1/N!$ corrects for the repetitions due to the commutability of contracted pairs within the product.

The sum over $P(s)$ contains in particular the sum (with appropriate sign) over transpositions within each contracted pair, the result of which are symmetrized (antisymmetrized) contractions

$$\overbrace{A_s A_t} \equiv \underbrace{A_s A_t} \pm \underbrace{A_t A_s} = \langle \mathfrak{N}(A_s A_t) \rangle_0 . \tag{22}$$

Hence Equation (21) may also be written as

$$\left\langle \mathfrak{N}\Big(\prod_{(s)} A_s\Big)\right\rangle_0 = \frac{1}{2^N N!} \sum_{P(s)} (\pm 1)^{\sigma P(s)} \overbrace{A_{s_1} A_{s_2}} \overbrace{A_{s_3} A_{s_4}} \cdots \overbrace{A_{s_{2N-1}} A_{s_{2N}}} =$$

$$= \sum_{\text{all pairings}} (\pm 1)^{\sigma(t,\bar{t})} \prod_{(t)} \overbrace{A_t A_{\bar{t}}} , \tag{23}$$

where the last sum, according to (20″), has $(2N-1)!!$ terms. This is the fundamental reduction formula.

4. Reduction of $\mathfrak{T}$-Product Averages

WICK's definition of the $\mathfrak{T}$-product[14]) is

$$\mathfrak{T}\Big(\prod_{(s)} A_s[\beta_s]\Big) \equiv \sum_{P(s)} (\pm 1)^{\sigma P(s)} \prod_{j=1}^{N(s)-1} \theta(\beta_{s_{j+1}} - \beta_{s_j}) \prod_{(s)} A_s[\beta_s] . \tag{24}$$

Here the arguments are reciprocal temperatures β_s which are ordered with the help of the step functions,

$$\theta(\beta) = \begin{cases} 1; \beta > 0 \\ 0; \beta < 0. \end{cases}$$

The important step in the reduction of $\mathfrak{T}$-products is contained in WICK's theorem[14]) giving the resolution of $\mathfrak{T}$-products into $\mathfrak{N}$-products, plus contractions of the form

$$\overbrace{A_s[\lambda] A_t[\lambda']} \equiv \theta(\lambda - \lambda') \underbrace{A_s[\lambda] A_t[\lambda']} \pm \theta(\lambda' - \lambda) \underbrace{A_t[\lambda'] A_s[\lambda]} . \tag{25}$$

Here it is of course assumed that the commutators (anticommutators)

$$\underbrace{A_s A_t} \equiv [A_s^{(-)} A_t^{(+)}]_{\mp} \tag{25'}$$

are c-numbers, which excludes the magnon case*). WICK's theorem now reads

$$\mathfrak{T}\Big(\prod_{(s)} A_s[\lambda_{i_s}]\Big) = \mathfrak{N}\Big(\prod_{(s)} A_s\Big) + \sum_{t<t'} (\pm 1)^{\sigma_t + \sigma_{t'}} \overbrace{A_t A_{t'}} \mathfrak{N}\Big(\prod_{(s)-t-t'} A_s\Big) +$$

$$+ \sum_{\substack{t_1<t_1' \\ (t_1<t_2)}} \sum_{t_2<t_2'} (\pm 1)^{\sigma_{t_1} + \sigma_{t_1'} + \sigma_{t_2} + \sigma_{t_2'}} \overbrace{A_{t_1} A_{t_1'}} \overbrace{A_{t_2} A_{t_2'}} \mathfrak{N}\left(\prod_{\substack{(s)-t_1-t_1' \\ -t_2-t_2'}} A_s\right) + \cdots , \tag{26}$$

*) See footnote ***) on page 151.

where σ_t is the number of transpositions necessary to bring t in front of the set (s). Because of the symmetry (antisymmetry) of $\mathfrak{N}$- and $\mathfrak{T}$-products and of the contraction (25) Equation (26) can be written

$$\mathfrak{T}\Big(\prod_{(s)} A_s[\lambda_{i_s}]\Big) = \sum_{n=0}^{N} \frac{1}{2^n\, n!}\, \frac{1}{(2(N-n))!} \sum_{P(s)} (\pm 1)^{\sigma_{P(s)}}\, \overbrace{A_{s_1} A_{s_2}} \times$$

$$\times \cdots \overbrace{A_{s_{2n-1}} A_{s_{2n}}}\, \mathfrak{N}\big(A_{s_{2n+1}} \cdots A_{s_{2N}}\big)\,. \tag{27}$$

Here the factor $1/(2^n\, n!)$ has the same origin and significance as in Equation (23). The factor $1/(2\,(N-n))!$ corrects for the repetitions in the sum over $P(s)$ due to the symmetry (antisymmetry) of the $\mathfrak{N}$-product. Combining Equation (27) with the basic formula (23) leads to the reduction formula for $\mathfrak{T}$-product averages:

$$\Big\langle \mathfrak{T}\Big(\prod_{(s)} A_s[\lambda_{i_s}]\Big)\Big\rangle_0 = \sum_{n=0}^{N} \frac{1}{2^n\, n!}\, \frac{1}{(2(N-n))!} \sum_{P(s)} (\pm 1)^{\sigma_{P(s)}}\, \overbrace{A_{s_1} A_{s_2}} \times$$

$$\times \cdots \overbrace{A_{s_{2n-1}} A_{s_{2n}}}\, \frac{1}{2^{N-n}\,(N-n)!} \sum_{P(s_{2n+1} \cdots s_{2N})} \overbrace{A_{s_{2n+1}} A_{s_{2n+2}}} \cdots \overbrace{A_{s_{2N-1}} A_{s_{2N}}}\,.$$

Now the sum over the $(2\,(N-n))!$ permutations $P(s_{2n+1} \ldots s_{2N})$ is already contained in the sum over $P(s)$, so that it may be canceled against the factor $1/(2\,(N-n))!$. The sum over n is then simply a binomial sum over $\overbrace{\quad}$- and $\overbrace{\quad}$-contractions. Thus we may write symbolically

$$\Big\langle \mathfrak{T}\Big(\prod_{(s)} A_s[\lambda_{i_s}]\Big)\Big\rangle_0 = \frac{1}{2^n\, N!} \sum_{P(s)} (\pm 1)^{\sigma_{P(s)}} \sum_{n=0}^{N} \frac{N!}{n!\,(N-n)!} \times$$

$$\times\, (\overbrace{\quad})^n\, (\overbrace{\quad})^{N-n} \prod_{(s)} A_s = \frac{1}{2^N\, N!} \sum_{P(s)} (\pm 1)^{\sigma_{P(s)}}\, (\overbrace{\quad} + \overbrace{\quad})^N \prod_{(s)} A_s\,. \tag{28}$$

The new contraction $\overbrace{\quad} + \overbrace{\quad}$ occurring in the second line is now just the propagator, as is easily seen by taking $N = 1$ in Equation (28), or by direct verification with the help of the definitions (15), (22), (24), (25):

$$g_{A_s A_t}(\lambda - \lambda') \equiv \big\langle \mathfrak{T}(A_s[\lambda]\, A_t[\lambda'])\big\rangle_0 = \overbrace{A_s A_t} + \overbrace{A_s A_t}\,. \tag{29}$$

Thus (28) takes the final form analogous to (23)

$$\Big\langle \mathfrak{T}\Big(\prod_{(s)} A_s[\lambda_{i_s}]\Big)\Big\rangle_0 = \frac{1}{2^N\, N!} \sum_{P(s)} (\pm 1)^{\sigma_{P(s)}}\, g_{A_{s_1} A_{s_2}} \cdots g_{A_{s_{2N-1}} A_{s_{2N}}}\,. \tag{30}$$

The graphical representation of this formula is as usual: Each vertex of the left hand side is drawn with the appropriate number of branches. The latter are connected in pairs according to the contractions of the right hand side, except for those branches representing incoming and outgoing particles which stay free.

In order to complete this discussion we briefly derive a general formula concerning connected diagrams which includes the possibility that the interaction H' may consist of many different types of vertices. For this purpose we rewrite the general perturbation term (6) more specifically with the use of (11)*),

*) Note that $\mathfrak{T}^2 = \mathfrak{T}$, so that the double application of $\mathfrak{T}$ in $S(\beta)$ implied by (31) is alright.

$$T = \left\langle \mathfrak{T}\left(S(\beta) \prod_i V_i[\lambda_i] \right) \right\rangle_0 , \tag{31}$$

where all the vertices indicated explicitely are of dynamical origin, i.e. come from operators in state vectors and from density operators. The general term of the power series expansion of $S(\beta)$,

$$S_n(\beta) = \frac{1}{n!} \mathfrak{T}(W(\beta))^n , \tag{32}$$

where

$$W(\beta) \equiv - \int_0^\beta d\lambda \, H'[\lambda] , \tag{32'}$$

contributes to T the term

$$T_n = \frac{1}{n!} \left\langle \mathfrak{T}\left((W(\beta))^n \prod_i V_i[\lambda_i] \right) \right\rangle_0 . \tag{33}$$

According to the reduction formula (30) some of the dynamical vertices V_i and of the vertices in S_n are linked by a propagator contraction (29). Now we order the contributions to T_n according to the number of factors $W(\beta)$ of S_n that are linked to $\prod_i V_i$. The number of ways $\prod_i V_i$ can be linked to a group of k out of n factors W is $n!/(k!\,(n-k)!)$. Hence, if we denote the terms in which there are no disconnected parts between $\prod_i V_i$ and the W's by an index "c" (connected) and define

$$\left\langle \mathfrak{T}\left(\prod_i V_i \right) \right\rangle_{0c} \equiv \left\langle \mathfrak{T}\left(\prod_i V_i \right) \right\rangle_0 \tag{34}$$

(which does not necessarily mean that all the V_i must be linked together, although this is the case in most applications), then

$$\left\langle \mathfrak{T}\left(W^n \prod_i V_i \right) \right\rangle_0 = \sum_{k=0}^{n} \frac{n!}{k!\,(n-k)!} \left\langle \mathfrak{T}\left(W^k \prod_i V_i \right) \right\rangle_{0c} \left\langle \mathfrak{T}\, W^{n-k} \right\rangle_0 . \tag{35}$$

With (32), (32') and (33) Equation (35) can be written, after division by $n!$,

$$T_n = \sum_{k=0}^{n} \left\langle \mathfrak{T}\left(S_k \prod_i V_i \right) \right\rangle_{0c} \left\langle S_{n-k} \right\rangle_0 . \tag{36}$$

Hence

$$T = \sum_{n=0}^{\infty} T_n = \sum_{n=0}^{\infty} \sum_{k=0}^{n} \left\langle \mathfrak{T}\left(S_k \prod_i V_i \right) \right\rangle_{0c} \left\langle S_{n-k} \right\rangle_0 = \sum_{k=0}^{\infty} \sum_{n=k}^{\infty} \left\langle \mathfrak{T}\left(S_k \prod_i V_i \right) \right\rangle_{0c} \left\langle S_{n-k} \right\rangle_0$$

or finally

$$\left\langle \mathfrak{T}\left(S(\beta) \prod_j V_i[\lambda_i] \right) \right\rangle_0 = \left\langle \mathfrak{T}\left(S(\beta) \prod_j V_i[\lambda_i] \right) \right\rangle_{0c} \left\langle S(\beta) \right\rangle_0 . \tag{37}$$

Note that here connectedness "c" refers to the factors in S, and to the product $\prod_i V_i$ as a whole (some of the factors V_i may still be disconnected).

As an application consider the sum of Equation (37) for all vertices occurring in H', so that

$$\langle \mathfrak{T}(S(\beta)\, H'[\beta]) \rangle_0 = \langle \mathfrak{T}(S(\beta)\, H'[\beta]) \rangle_{0c}\, \langle S(\beta) \rangle_0 . \tag{37'}$$

Now from the definition (11) follows

$$\frac{dS(\beta)}{d\beta} = - H'[\beta]\, S(\beta) .$$

Hence

$$\frac{1}{\langle S(\beta) \rangle_0} \frac{d}{d\beta} \langle S(\beta) \rangle_0 = \frac{d}{d\beta} \langle S(\beta) \rangle_{0c}$$

or integrated, remembering that $S(0) = 1$,

$$\langle S(\beta) \rangle_0 = e^{\langle S(\beta) - 1 \rangle_{0c}} . \tag{38}$$

At zero temperature ($\beta = \infty$) this leads to the well known BRUECKNER-GOLDSTONE formula for the ground state energy[17]) (generalized to an interaction consisting of an arbitrary number of different types of vertices).

5. Propagators

According to the definition (29) the propagator $g_{A_s A_t}$ is the sum of the two contractions (25) and (22). The first is independent of statistics and may therefore be called the "spontaneous" part,

$$g^{sp}_{A_{sk} A_{tk'}}(\lambda - \lambda') \equiv \overline{A_{sk}[\lambda]\, A_{tk'}}\,[\lambda'] = \{\theta(\lambda - \lambda')\, \alpha_{sk}\, \alpha'_{t-k} \times$$
$$\times\, e^{-(\lambda - \lambda')\varepsilon_k} \pm \theta(\lambda' - \lambda)\, \alpha'_{sk}\, \alpha_{t-k}\, e^{(\lambda - \lambda')\varepsilon_k}\} \delta_{k,-k'} . \tag{39}$$

In particular ($\alpha_{1k} = 1$, $\alpha'_{1k} = 0$, $\alpha_{2k} = 0$, $\alpha'_{2k} = 1$),

$$g^{sp}_{a_k a_k^+}(\lambda) = \theta(\lambda)\, e^{-\lambda\varepsilon_k};\quad g^{sp}_{a_k^+ a_k}(\lambda) = \pm\, \theta(-\lambda)\, e^{\lambda\varepsilon_k} . \tag{39'}$$

The second contraction is proportional to the one-particle distribution function f_k suggesting the designation "induced" part,

$$g^{ind}_{A_{sk} A_{tk'}}(\lambda - \lambda') \equiv \overbrace{A_{sk}[\lambda]\, A_{tk'}}[\lambda'] = \{\alpha'_{sk}\, \alpha_{t-k} \times$$
$$\times\, e^{(\lambda - \lambda')\varepsilon_k} \pm \alpha_{sk}\, \alpha'_{t-k}\, e^{-(\lambda - \lambda')\varepsilon_k}\} f_k\, \delta_{k,-k'} . \tag{40}$$

In particular

$$g^{ind}_{a_k a_k^+}(\lambda) = \pm\, e^{-\lambda\varepsilon_k} f_k;\quad g^{ind}_{a_k^+ a_k}(\lambda) = e^{\lambda\varepsilon_k} f_k . \tag{40'}$$

Hence

$$g_{A_{sk}A_{tk'}}(\lambda) = g^{sp}_{A_{sk}A_{tk'}}(\lambda) + g^{ind}_{A_{sk}A_{tk'}}(\lambda) = \{\alpha'_{sk}\,\alpha_{t-k} \times$$
$$\times \left(f_k \pm \theta(-\lambda)\right) e^{\lambda\varepsilon_k} \pm \alpha_{sk}\,\alpha'_{t-k}\left(f_k \pm \theta(\lambda)\right) e^{-\lambda\varepsilon_k}\}\,\delta_{k,-k'}\,, \tag{41}$$

which is a generalization of Equation (I), appendix 2, of reference 4. (39), (40) and (41) all have the property

$$g^{()}_{AB}(\lambda) = \pm\, g^{()}_{BA}(-\lambda)\,. \tag{42}$$

Another important property of the propagator is obtained from the identity

$$\left\langle A[\lambda+\beta]\,B\right\rangle_0 = \left\langle B\,A[\lambda]\right\rangle_0 \tag{43}$$

by writing

$$\theta(-\lambda)\,\theta(\lambda+\beta)\,g_{AB}(\lambda+\beta) = \theta(-\lambda)\,\theta(\lambda+\beta)\,\langle A[\lambda+\beta]\,B\rangle_0 =$$
$$= \theta(-\lambda)\,\theta(\lambda+\beta)\,\langle B\,A[\lambda]\rangle_0 = \pm\,\theta(-\lambda)\,\theta(\lambda+\beta)\,g_{AB}(\lambda)\,.$$

This is the well known periodicity (antiperiodicity)

$$g_{AB}(\lambda+\beta) = \pm\, g_{AB}(\lambda);\ 0 > \lambda > -\beta \tag{44}$$

(see e.g. reference 4).

Combining (43) and (44) for $\lambda = \beta/2$ gives

$$g_{AB}\left(\frac{\beta}{2}\right) = g_{BA}\left(\frac{\beta}{2}\right). \tag{45}$$

In particular

$$g^{sp}_{a_k a_k}\left(\frac{\beta}{2}\right) + g^{ind}_{a_k\,a^+_k}\left(\frac{\beta}{2}\right) = g^{sp}_{a^+_k\,a_k}\left(\frac{\beta}{2}\right) + g^{ind}_{a^+_k\,a_k}\left(\frac{\beta}{2}\right) \tag{45'}$$

(the first term on the right is zero) or with (39'), (40')

$$(1 \pm f_k)\,e^{-(\beta/2)\,\varepsilon_k} = f_k\,e^{+(\beta/2)\,\varepsilon_k}$$

and solving for f_k

$$f_k = \frac{1}{e^{\beta\varepsilon_k} \mp 1}\,,$$

which is Equation (17). This determination of f_k is noteworthy because of its close analogy with the derivation of PLANCK's radiation law by EINSTEIN.

The property (44) suggests a Fourier representation

$$g_{AB}(\lambda) = \sum_{r=-\infty}^{+\infty} \tilde{g}_{AB}(\sigma_r)\,e^{i\sigma_r\lambda} \tag{46}$$

in which the condition on σ_r is

$$e^{i\sigma_r\beta} = \pm 1\,;\quad \sigma_r = \frac{2\pi}{\beta}\begin{cases} r \\ (r+1/2) \end{cases}. \tag{46'}$$

Because of the orthogonality

$$\frac{1}{\beta}\int_0^\beta d\lambda\, e^{i(\sigma_r \pm \sigma_s)\lambda} = \delta_{r\pm s,0} \tag{47}$$

one has

$$\tilde{g}_{AB}(\sigma_r) = \frac{1}{\beta}\int_0^\beta d\lambda\, g_{AB}(\lambda)\, e^{-i\sigma_r\lambda} = \frac{1}{\beta}\int_0^\beta d\lambda\, \langle A[\lambda]\, B\rangle_0\, e^{-i\sigma_r\lambda}\,. \tag{48}$$

With (7′), (17) and (46′) integration of (48) for the case $A = a_k^+$, $B = a_{k'}$, and vice versa, yields

$$\tilde{g}_{a_k a_{k'}^+}(\sigma_r) = \frac{1}{\beta}\frac{1}{\varepsilon_k + i\,\sigma_r}\delta_{kk'};\quad g_{a_k^+ a_{k'}}(\sigma_r) = \pm\frac{1}{\beta}\frac{1}{\varepsilon_k - i\,\sigma_r}\delta_{kk'};\quad g_{a_k^+ a_{k'}^+} = g_{a_k a_{k'}} = 0\,. \tag{49}$$

With (1) the general propagator has the Fourier representation

$$\tilde{g}_{A_{sk}A_{tk'}}(\sigma_r) = \frac{1}{\beta}\left\{\frac{\alpha_{sk}\,\alpha'_{t-k}}{\varepsilon_k + i\,\sigma_r} \pm \frac{\alpha'_{sk}\,\alpha_{t-k}}{\varepsilon_k - i\,\sigma_r}\right\}\delta_{k,-k'}\,. \tag{50}$$

For the operators P_k, Q_k, Equation (3), one has

$$\begin{aligned}
\tilde{g}_{Q_k Q_{k'}}(\sigma_r) &= \tilde{g}_{P_k P_{k'}}(\sigma_r) = \frac{1}{\beta}\frac{1}{\varepsilon_k^2 + \sigma_r^2}\delta_{k,-k'} \times \begin{cases} \varepsilon_k \\ (-i\,\sigma_r) \end{cases}, \\
g_{Q_k P_{k'}}(\sigma_r) &= -\,g_{P_k Q_{k'}}(\sigma_r) = \frac{1}{\beta}\frac{1}{\varepsilon_k^2 + \sigma_r^2}\delta_{k,-k'} \times \begin{cases} (-\sigma_r) \\ i\,\varepsilon_k \end{cases}.
\end{aligned} \tag{51}$$

In some applications propagators with mixed temperature and time dependence are of interest[10]), where as before the $\mathfrak{T}$-ordering refers to the variable λ.

$$g_{AB}(\lambda; t) \equiv \langle \mathfrak{T}(A([\lambda]; t)\, B)\rangle_0\,. \tag{52}$$

Here

$$A([\lambda]; t) \equiv e^{iH_0 t}\, A[\lambda]\, e^{-iH_0 t}\,, \tag{52′}$$

or with (5), noting that according to (8), (8′) H_0 and K_0 commute,

$$A([\lambda]; t) = A^{(+)}[\lambda]\, e^{+i\omega_k t} + A^{(-)}[\lambda]\, e^{-i\omega_k t}\,. \tag{52″}$$

With (2) and (49) we then obtain the general result

$$\tilde{g}_{A_{sk}A_{tk'}}(\sigma_r; t) = \frac{1}{\beta}\left\{\frac{\alpha_{sk}\,\alpha'_{t-k}\,e^{-i\omega_k t}}{\varepsilon_k + i\,\sigma_r} \pm \frac{\alpha'_{sk}\,\alpha_{t-k}\,e^{+i\omega_k t}}{\varepsilon_k - i\,\sigma_r}\right\}\delta_{k,-k'}\,. \tag{53}$$

We close this paper with some rules to evaluate the Fourier sums (see reference 4, appendix 2; LUTTINGER and WARD, reference 17). By definition

$$g_{AB}(+0) = \langle A\, B\rangle_0\,;\quad g_{AB}(-0) = \pm\langle B\, A\rangle_0$$

so that from (46), (49)

$$1 \pm f_k = g_{a_k a_k^+}(+0) = \frac{1}{\beta} \sum_r \frac{1}{\varepsilon_k + i\,\sigma_r} e^{i\sigma_r(+0)}$$

$$f_k = g_{a_k^+ a_k}(+0) = \pm \frac{1}{\beta} \sum_r \frac{1}{\varepsilon_k - i\,\sigma_r} e^{i\sigma_r(+0)} \quad . \tag{54}$$

Hence

$$\sum_r \frac{1}{\varepsilon_k + i\,\sigma_r} \frac{1}{\varepsilon_{k'} + i\,\sigma_r} = \sum_r \frac{1}{\varepsilon_{k'} - \varepsilon_k} \left(\frac{1}{\varepsilon_k + i\,\sigma_r} - \frac{1}{\varepsilon_{k'} + i\,\sigma_r} \right) = \mp \beta \frac{f_{k'} - f_k}{\varepsilon_{k'} - \varepsilon_k}$$

$$\sum_r \frac{1}{\varepsilon_k - i\,\sigma_r} \frac{1}{\varepsilon_{k'} + i\,\sigma_r} = \sum_r \frac{1}{\varepsilon_{k'} + \varepsilon_k} \left(\frac{1}{\varepsilon_k - i\,\sigma_r} + \frac{1}{\varepsilon_{k'} + i\,\sigma_r} \right) = \beta \frac{1 \pm f_{k'} \pm f_k}{\varepsilon_{k'} + \varepsilon_k} . \tag{55}$$

The first equation also exists for $k = k'$ and reads

$$\sum_r \frac{1}{(\varepsilon_k + i\,\sigma_r)^2} = \mp \beta \frac{\partial f_k}{\partial \varepsilon_k} = \beta^2 f_k (f_k \pm 1) \quad . \tag{55'}$$

More complicated expressions can be summed by the same method.

Appendix

A simple derivation of formula (16) for bosons is obtained with the help of the following generating function:

$$G(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} c_n$$

with

$$c_n \equiv \sum_{m=0}^{\infty} \langle m | (a_k^+)^n (a_k)^n | m \rangle \; w^m \quad .$$

Now

$$\langle m | (a_k^+)^n (a_k)^n | m \rangle = \frac{m!}{(m-n)!}$$

which vanishes automatically for $n > m$. Hence interchange of the n- and m-summations yields

$$G(x) = \sum_{m=0}^{\infty} w^m \sum_{n=0}^{\infty} \frac{m!}{n!\,(m-n)!} x^n = \sum_{m=0}^{\infty} w^m (1+x)^m =$$

$$= \frac{1}{1 - w\,(1+x)} = \frac{1}{1-w} \sum_{n=0}^{\infty} \left(\frac{w}{1-w} \right)^n x^n$$

or

$$c_n = \frac{1}{1-w}\left(\frac{w}{1-w}\right)^n n!$$

But with $w = e^{-\beta\varepsilon_k}$

$$\left\langle (a_k^+)^n (a_k)^n \right\rangle_0 = c_n/c_0 = n! \left(\frac{w}{1-w}\right)^n$$

which is Equation (16).

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