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Perturbation Expansions in Quantum Statistical Mechanics

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Abstract. The perturbation expansion introduced by C. Bloch and C. de Dominicis [1, 2] for the reduced density matrix (RDM) is investigated for multi-time-temperature complex variables for $T > 0$. A uniform upper bound is found for the truncated RDM, and in the Euclidean case lower bounds are derived for potentials of one sign. It is found that, for a bounded number of particles in any intermediate state, the partial expansion defines an entire function of the coupling constant. At least in the case of bosons, however, the complete expansion diverges.

Introduction

We investigate, in this paper, thermodynamic perturbation expansions in quantum statistical mechanics for finite non-zero temperatures. More precisely, we study such expansions in the form introduced by C. Bloch and C. de Dominicis [1, 2].

We consider a system of identical, spinless, non-relativistic particles, interacting through a two-body potential in a cube of volume $V = L^3$. We set $m = 1/2$, $\hbar = 1$. The particles are either bosons or fermions with $c_V(\mathbf{k})$ as the annihilation operator for a particle of momentum $\mathbf{k}$, and with $c_V^*(\mathbf{k})$ as the respective creation operator. These operators satisfy the usual commutation relations. The Hamiltonian of the system is given by

$$H_V = H_V^0 + U_V, \tag{I.1}$$

where

$$H_V^0 = \sum_{\mathbf{k}} \mathrm{E}_{\mathbf{k}}\, c_V^*(\mathbf{k})\, c_V(\mathbf{k}) \tag{I.2}$$

is the free particle Hamiltonian and

$$U_V = \frac{1}{2V} \sum_{\mathbf{k}_1, \dots, \mathbf{k}_4} (\mathbf{k}_1 \mathbf{k}_2 | U | \mathbf{k}_3 \mathbf{k}_4)\, c_V^*(\mathbf{k}_1)\, c_V^*(\mathbf{k}_2)\, c_V(\mathbf{k}_4)\, c_V(\mathbf{k}_3) \tag{I.3}$$

describes the interaction. The momenta in these sums run over the allowed values in a box $V = L^3$, and $\mathrm{E}_{\mathbf{k}} = \mathbf{k}^2$ is the energy of a particle of momentum $\mathbf{k}$. The potential

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function in (I.3) satisfies

$$(\mathbf{k}_1\mathbf{k}_2|U|\mathbf{k}_3\mathbf{k}_4) = (\mathbf{k}_2\mathbf{k}_1|U|\mathbf{k}_4\mathbf{k}_3) = U(\mathbf{k}_1 - \mathbf{k}_4)\,\delta(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4), \tag{I.4}$$

$$U(\mathbf{k}) = U(-\mathbf{k}) = U^*(\mathbf{k}), \tag{I.4a}$$

where the Kronecker δ expresses the conservation of momentum.

We investigate the Bloch perturbation expansion for the reduced density matrix (RDM), which is defined as the thermodynamic expectation value in the grand canonical ensemble

$$P_V = \exp[\beta(R_V - H_V + \mu N_V)] \tag{I.5}$$

of a product of operators (I.7) given below. Here $\beta = 1/kT$ is the inverse temperature (T = temperature, k = Boltzmann constant) of the system, μ the chemical potential, N_V the particle number operator, and the thermodynamic potential R_V is determined from condition $\mathrm{Tr}\,P_V = 1$. We choose as fixed thermodynamic parameters β and μ, restricted to values $0 < \beta < \infty$, $-\infty < \mu < +\infty$ for fermions and $\mu < 0$ for bosons.

Let $\tau_1, \tau_2, \ldots, \tau_{2n}$ be a set of complex quantities ($\mathrm{Re}\,\tau$ = inverse temperature and $\mathrm{Im}\,\tau$ = time) satisfying

$$\mathrm{Re}\,\tau_1 \geqslant \cdots \geqslant \mathrm{Re}\,\tau_{2n}; \quad \mathrm{Re}(\tau_1 - \tau_{2n}) \leqslant \beta. \tag{I.6}$$

Define operators

$$c_V^{\#}(\mathbf{k}_i, \tau_i) = \exp[\tau_i(H_V - \mu N_V)]\, c_V^{\#}(\mathbf{k}_i)\exp[-\tau_i(H_V - \mu N_V)], \tag{I.7}$$

where symbol $\#$ in $c_V^{\#}(\mathbf{k}_i)$ means that it can be either a creation or an annihilation operator. Then the RDM is defined as

$$\mathrm{RDM} = V^n \langle\!\langle c_V^{\#}(\mathbf{k}_1, \tau_1)\cdots c_V^{\#}(\mathbf{k}_{2n}, \tau_{2n})\rangle\!\rangle_V, \tag{I.8}$$

where $\langle\!\langle A\rangle\!\rangle_V = \mathrm{Tr}(AP_V)$. In order that (I.8) be non-trivial, it must contain n creators and n annihilators.

To obtain the Bloch perturbation expansion for (I.8), one considers [2] the 'time' evolution operator

$$\mathrm{U}(\tau, \tau') = \exp(\tau H_V^0)\exp[-(\tau - \tau')\,H_V]\exp(-\tau H_V^0) \tag{I.9}$$

with complex τ as described above. This quantity satisfies the Bloch equation, which for $\mathrm{Re}\,\tau = 0$ is identical with the equation of motion in the interaction picture. Consequently, the Bloch equation can be treated formally as in ordinary quantum mechanics. This leads to the Dyson expansion for $\mathrm{U}(\tau, \tau')$, which is then used in (I.8) to obtain a perturbation expansion. This expansion is discussed further in Section 1, where we write down the final perturbation expansion for the truncated RDM.

In Section 2 we prove three theorems. In Theorem 2.1 we find a majorization for our expansion, and Theorems 2.2 and 2.3 give minorizations for the Euclidean truncated RDM.

In Section 3 we turn to convergence questions. We find that for potential U_1 (given by (2.1) below) the partial sum over graphs with less than N (a finite integer) particles in any intermediate state yields an entire function in the coupling constant λ. In Theorems 3.2 and 3.3 we find that, for potentials U_2 and U_3 (given by (2.2) and (2.3) below), the truncated RDM expansion is not analytic in λ at $\lambda = 0$. The expansion clearly diverges, at least in the case of bosons.

1. The Perturbation Expansion

In this section we shall write down the Bloch interaction expansion for the truncated RDM.

As explained in the Introduction, one uses the Dyson expansion for $U(\tau,\tau')$ to get a perturbation expansion for (I.8). The expansion thus obtained is then developed further with the aid of the Wick–Bloch–de Dominicis Theorem [1–5] to obtain the expansion in a form in which each term corresponds to a graph. The Linked Cluster Theorem [6, 7] yields then the result

$$\mathrm{RDM} = \sum_A G_{l_1}\cdot G_{l_2}\cdots G_{l_r}, \tag{1.1}$$

in which $G_{l_i}(i=1,\ldots,r)$ are connected graphs each containing at least one pair of external vertices; each external vertex appears in one and only one G_{l_i}. The sum is over all possible products with $1 \leqslant r \leqslant n$. The procedure to arrive at (1.1) is well known; we refer to the book by Mills [8], in which this derivation is given in detail for $n=1$.

We now define recursively [9] a truncated RDM, which we denote by the superscript T

$$\langle\!\langle c_V^{\#}(\mathbf{k}_1,\tau_1)\, c_V^{\#}(\mathbf{k}_2,\tau_2)\rangle\!\rangle_V^T = \langle\!\langle c_V^{\#}(\mathbf{k}_1,\tau_1)\, c_V^{\#}(\mathbf{k}_2,\tau_2)\rangle\!\rangle_V$$

$$\langle\!\langle c_1^{\#}\, c_2^{\#}\cdots c_{2n}^{\#}\rangle\!\rangle_V^T = \langle\!\langle c_1^{\#}\, c_2^{\#}\cdots c_{2n}^{\#}\rangle\!\rangle_V - \sum_{\mathrm{Part}} \epsilon^P \langle\!\langle c_{P_{11}}^{\#} c_{P_{12}}^{\#}\cdots c_{P_{1s(1)}}^{\#}\rangle\!\rangle_V^T \cdots \langle\!\langle c_{P_{r1}}^{\#} c_{P_{r2}}^{\#}\cdots c_{P_{rs(r)}}^{\#}\rangle\!\rangle_V^T, \tag{1.2}$$

where $\sum_{\mathrm{Part}}$ extends over all partitions

$$\{P_{11}, P_{12},\ldots, P_{1s(1)}\}\{P_{21}, P_{22},\ldots, P_{2s(2)}\}\ldots\{P_{r1}, P_{r2},\ldots, P_{rs(r)}\}$$

of $\{1,2,\ldots,2n\}$ with $r>1$ and

$$P_{11} < P_{12} < \cdots < P_{1s(1)};\ldots; P_{r1} < P_{r2} < \cdots < P_{rs(r)}.$$

$\epsilon = 1$ for bosons and $\epsilon = -1$ for fermions. In ϵ^P we have $P=0$ for an even and $P=1$ for an odd permutation from $1, 2, \ldots, 2n$ to $P_{11}, P_{12}, \ldots, P_{rs(r)}$. With this definition we arrive at

$$V^n \langle\!\langle c_V^{\#}(\mathbf{k}_1,\tau_1)\ldots c_V^{\#}(\mathbf{k}_{2n},\tau_{2n})\rangle\!\rangle_V^T = \sum_{m=n-1}^{\infty}\sum_{r=1}^{r(m)} G_r^{(m)}(\mathbf{k}_1^{\#},\tau_1;\ldots;\mathbf{k}_{2n}^{\#},\tau_{2n})_V \tag{1.3}$$

which is a sum over all connected graphs containing all external vertices. For each graph we have two indices, m and r. m is the number of interaction lines in the graph

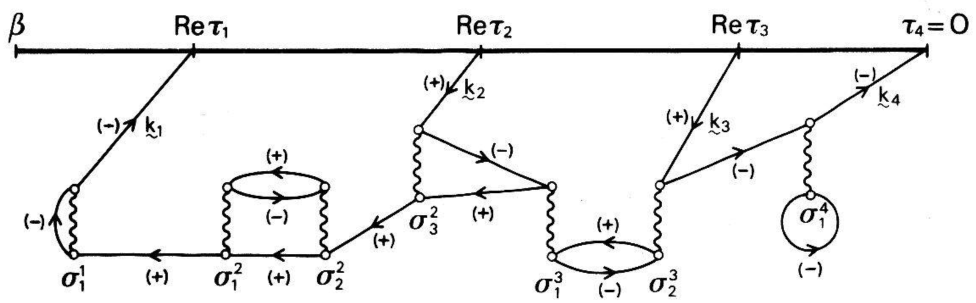

Figure 1.1

and is called the *order* of the graph. There are, in general, a large number of different graphs having the same order. These we have distinguished with the additional index r. The analytic expression corresponding to a graph $G_r^{(m)}$ is

$$G_r^{(m)} = (-1)^m \epsilon^{L+S+C} \prod_{i=1}^{2n} \left(\int_{\tau_i}^{\tau_{i-1}} d\sigma_1^i \int_{\tau_i}^{\sigma_1^i} d\sigma_2^i \cdots \int_{\tau_i}^{\sigma_{m_i-1}^i} d\sigma_{m_i}^i \right) .$$

$$V^{n-m} \sum_{\mathbf{k}_{11}^1, \ldots, \mathbf{k}_{m_{2n}4}^{2n}} \left[\prod_{i=1}^{2n} \exp[\pm\tau_i(\mathrm{E}_i - \mu)] \prod_{j=1}^{m_i} (\mathbf{k}_{j1}^i \, \mathbf{k}_{j2}^i | U | \mathbf{k}_{j3}^i \, \mathbf{k}_{j4}^i) \right.$$

$$\left. \exp[\sigma_j^i(\mathrm{E}_{j1}^i + \mathrm{E}_{j2}^i - \mathrm{E}_{j3}^i - \mathrm{E}_{j4}^i)] \prod_{\nu=1}^{2m+n} \delta(\mathbf{1}_\nu, \mathbf{1}_\nu^*) f_\varepsilon^\pm(\mathbf{1}_\nu) \right] . \tag{1.4}$$

An example of a graph is given in Figure 1.1. At each interaction line we have two incoming and two outgoing particle lines as shown in Figure 1.2. The integration path in (1.4) for the complex σ-integrals must be chosen so that $\mathrm{Re}\,\sigma$ increases along the

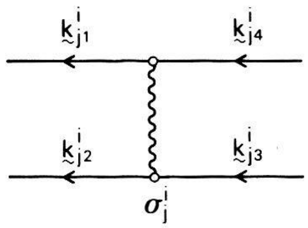

Figure 1.2

path of integration [2]. In $\exp[\pm\tau_i(\mathrm{E}_i - \mu)]$ we have (+)-sign for a created and (—)-sign for an annihilated external particle. The integer m_i gives the number of interaction lines in interval (τ_{i-1}, τ_i). We have $\sum m_i = m$. Further we have denoted $\mathrm{E}_{js}^i = (\mathbf{k}_{js}^i)^2$. In the last product in (1.4) $\mathbf{1}_\nu$ and $\mathbf{1}_\nu^*$ are the incoming and outgoing particle lines, which are connected to produce particle line $\mathbf{1}_\nu$ in the graph. Each particle line in the graph gives rise to a factor $f_\varepsilon^\pm(\mathbf{1}_\nu)$, where

$$f_\varepsilon^+(\mathbf{1}_\nu) = \frac{1}{1 - \epsilon \exp[\beta(\mu - \mathbf{1}_\nu^2)]} \tag{1.5}$$

corresponds to a particle line going from right to left, and

$$f_\varepsilon^-(\mathbf{1}_\nu) = \frac{1}{\exp[\beta(\mathbf{1}_\nu^2 - \mu)] - \epsilon} \tag{1.6}$$

corresponds to a particle line going from left to right. The former are called (+)-lines and the latter (—)-lines. $\epsilon = 1$ for bosons and $\epsilon = -1$ for fermions.

Then we still have the sign factor in front of (1.4). To find the sign of the graph in the case of fermions, we proceed as follows. We complete the graph with extra particle lines connecting the external vertices pairwise with dotted lines as indicated in the special example shown in Fig. 1.3. L is then the number of closed loops and S the number of (—)-lines in the completed graph. C is the number of crossings among the completion lines. In Figure 1.3 we have $L = 3$, $S = 5$ and $C = 1$.

There are m δ-functions in (1.4) coming from (I.4) and $2m + n$ δ-functions appearing in the last product. These reduce the number of independent momenta. One of the former δ-functions reduces to $\delta(\Sigma \pm \mathbf{k}_i)$, in which created and annihilated particles appear with opposite signs. Thus we have $m - n + 1$ independent momenta. If we write

$$G_r^{(m)}(\mathbf{k}^\#, \tau)_V = V\delta(\sum \pm \mathbf{k}_i)\, \bar{G}_r^{(m)}(\mathbf{k}^\#, \tau)_V, \tag{1.7}$$

then $\bar{G}_r^{(m)}$ is independent of volume in the limit $V \to \infty$.

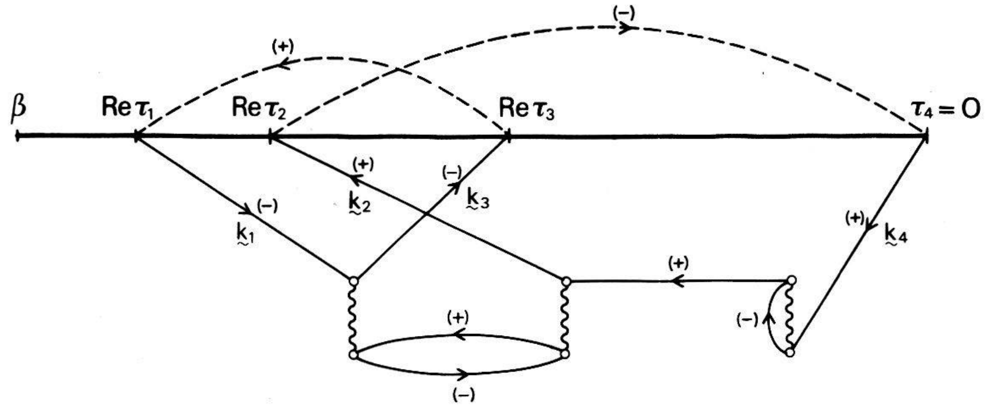

Figure 1.3

The grand partition function can be obtained as a special case of the RDM, and it is given by [2]

$$\log Z_V = \log Z_V^0 + \sum_{k=1}^{\infty} \frac{1}{S_k} G_k, \tag{1.8}$$

where Z_V^0 is for non-interacting system, S_k is the symmetry number of graph G_k, and the sum runs over all connected graphs containing no external vertices. The pressure is then given by

$$P_V = -\frac{1}{V} R_V = \frac{1}{\beta V} \log Z_V. \tag{1.9}$$

The thermodynamic limit exists also for pressure.

Our description differs somewhat from the conventional one (see, for instance [6, 8]). We have definite signs for the particle lines in the graph. This is not the case in the description normally used. One usually takes the σ-integrals from 0 to β and replaces the last product in (1.4) by a more complicated expression

$$\prod_{\nu=1}^{2m+n} \delta(\mathbf{1}_\nu, \mathbf{1}'_\nu)\,[\Theta(\sigma'_\nu - \sigma_\nu) f_\varepsilon^+(\mathbf{1}_\nu) + \epsilon\Theta(\sigma_\nu - \sigma'_\nu) f_\varepsilon^-(\mathbf{1}_\nu)] \tag{1.10}$$

to take care of the different possibilities for (+)- and (–)-particle-lines. Here

$$\Theta(\sigma) = \begin{cases} +1 & \text{for } \sigma > 0 \\ 0 & \text{for } \sigma < 0 \end{cases} \tag{1.11}$$

σ_ν is the complex 'time' at which $\mathbf{l}_\nu$ is annihilated and σ'_ν is that for the creation of $\mathbf{l}'_\nu$. Thus in the usual description all such graphs are identical, in which only the directions of the particle lines are varied. If we expand the analytical expression of such graph by taking explicitly account of the Θ-functions in the σ-integrals, we get a sum of terms in which each term corresponds to a distinct graph in our representation.

2. Uniform Bounds for Diagrams at $T > 0$

We consider the thermodynamic perturbation expansion for grand canonical pressure and multi-time-temperature RDM at $T > 0$. In this section we shall derive uniform upper bounds for every term (characterized by a diagram) in such expansions. Uniform lower bounds will then be established for positive (or negative) potentials for the pressure and the Euclidean RDM.

Without striving at the utmost generality we investigate a system of identical non-relativistic spinless particles with mass 1/2, interacting through a two-body potential $U(\mathbf{x})$ in three-dimensional space. We set $\hbar = 1$. Let $V = L^3$ be a cube

$$\{\mathbf{x} \in \mathbb{R}^3;\ |\mathbf{x}_i| < L/2\}$$

and $\Gamma = \Gamma(V)$ the set of lattice points $\mathbf{k} = 2\pi\mathbf{n}/L$ with $\mathbf{n} \in \mathbb{Z}^3$. The two-body potentials $U(\mathbf{x})$ with Fourier transform $U(\mathbf{k})$ are assumed to belong to one of the following classes:

U_1: The potential function is continuous and satisfies

$$U(\mathbf{k}) = U(-\mathbf{k}) = U^*(\mathbf{k}),$$

$$\|U\|_\infty = \sup_{\mathbf{k}} |U(\mathbf{k})| < \infty,$$

$$\|U\|_{\bar{1}} = \sup_L \frac{1}{V} \sum_{\mathbf{k}\in\Gamma} |U(k)| = \sup_L \|U\|_{1,L} < \infty. \tag{2.1}$$

U_2:

$$U \in U_1, \quad U(\mathbf{k}) \geqslant 0, \quad U(0) > 0. \tag{2.2}$$

U_3:

$$U \in U_1, \quad U(\mathbf{k}) \geqslant a\,\mathrm{e}^{-bk^2} \text{ for some } a > 0, b < \infty. \tag{2.3}$$

Obviously $U(\mathbf{x}) \in L^2(\mathbb{R}^3)$, if $U \in U_1$.

Theorem 2.1: Assume $U \in U_1$, $0 < \beta < \infty$, $\mu \in \mathbb{R}^1 (\mu < 0$ for bosons) and $n = 0, 1, 2, \ldots$. Then there exist constants A, $B < \infty$ such that every term in expansion (1.3) with (1.7) satisfies

$$|\bar{G}_r^{(m)}(\mathbf{k}_1^\#, \tau_1; \ldots; \mathbf{k}_{2n}, \tau_{2n})_V| < AB^m \prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!} \tag{2.4}$$

where the τ's satisfy (I.6), $\tau_0 = \beta$, $\tau_{2n} = 0$, $0 < V < \infty$ and $\sum \pm \mathbf{k}_i = 0$.

Proof: The whole σ- and τ-dependence of $G_r^{(m)}(\mathbf{k}^\#, \tau)_V$ is in the exponent of (1.4) and can be easily estimated. We write

$$\mathrm{E}_j^i = \mathrm{E}_{j3}^i + \mathrm{E}_{j4}^i - \mathrm{E}_{j1}^i - \mathrm{E}_{j2}^i \tag{2.5}$$

and obtain

$$\exp\left\{-\sum_{i=1}^{2n}[\sigma_j^i \mathrm{E}_j^i \mp \tau_i \mathrm{E}_i]\right.$$

$$= \exp\left\{-\sum_{i=1}^{2n}\left[(\tau_{i-1}-\sigma_1^i)\mathscr{E}_0^i + \sum_{j=1}^{m_i-1}(\sigma_j^i-\sigma_{j+1}^i)\mathscr{E}_j^i + (\sigma_{m_i}^i-\tau_i)\mathscr{E}_{m_i}^i\right]\right\}, \tag{2.6}$$

$$\begin{cases} \mathscr{E}_0^i = \sum_{a=1}^{i-1}\left[\mp \mathrm{E}_a + \sum_{b=1}^{m_a}\mathrm{E}_b^a\right], \\ \mathscr{E}_j^i = \mathscr{E}_0^i + \sum_{b=1}^{j}\mathrm{E}_b^i, \end{cases} \tag{2.7}$$

where E_a appears with a (–)-sign for a created and with a (+)-sign for an annihilated external particle. The energies $\mathscr{E}_j^i$ can be read off directly from the graph: for $\mathscr{E}_0^i$ one has to cut the graph vertically between τ_{i-1} and σ_1^i, and for $\mathscr{E}_j^i (j \geqslant 1)$ a similar cut after σ_j^i. Then $\mathscr{E}_j^i$ is the sum of the energies of the cut (+)-lines minus the sum of the energies of the cut (–)-lines. The cut (+)-lines and (–)-lines define an 'intermediate state' of the graph.

The absolute value of (2.6) is smaller than

$$\exp\left\{-\min_{i,j}(\mathscr{E}_j^i)\,\beta\right\} \leqslant \sum_{i=1}^{2n}\sum_{j=0}^{m_i}\exp\{-\mathscr{E}_j^i\beta\}, \tag{2.8}$$

since

$$\mathrm{Re}\sum_{i=1}^{2n}\left[(\tau_{i-1}-\sigma_1^i) + \sum_{j=1}^{m_i-1}(\sigma_j^i-\sigma_{j+1}^i) + (\sigma_{m_i}^i-\tau_i)\right] = \beta.$$

When $0 < \beta < \infty$, $\mu \in \mathbb{R}^1$ and $\mathbf{k} \in \mathbb{R}^3$, we have from (1.5) for bosons

$$1 < f^+(\mathbf{k}) < \frac{1}{1-\exp(-\beta|\mu|)} \quad (\mu < 0)$$

and for fermions

$$0 < f^+(\mathbf{k}) < 1.$$

Consequently,

$$0 < f_\varepsilon^-(\mathbf{k}) < C\exp[-\beta(\mathbf{k}^2-\mu)],$$

where the constant satisfies $C > 1$ for bosons and $C = 1$ for fermions. Thus the absolute value of $G_r^{(m)}(\mathbf{k}^\#, \tau)_V$ $(V \leqslant \infty)$ is smaller than

$$V^{n-m}C^{2m+n}\prod_{i=1}^{2n}\frac{|\tau_{i-1}-\tau_i|^{m_i}}{m_i!}\sum_{\mathbf{k}_{11}^1,\ldots,\mathbf{k}_{m_{2n}4}^{2n}}\prod_{i=1}^{2n}\prod_{j=1}^{m_i}|(\mathbf{k}_{j1}^i\mathbf{k}_{j2}^i|U|\mathbf{k}_{j3}^i\mathbf{k}_{j4}^i)|.$$

$$\prod_{i=1}^{2m+n}\delta(\mathbf{1}_i^*, \mathbf{1}_i)\sum_{i=1}^{2n}\sum_{j=0}^{m_i}\exp\left\{-\beta\left[\mathscr{E}_j^i + \sum_{-}(\mathbf{1}_\nu^2-\mu)\right]\right\}, \tag{2.9}$$

where $\sum_-$ extends only over the (–)-lines in the graph; $\mathbf{l}_i^*$ and $\mathbf{l}_i$ are the outgoing and incoming momentum belonging to the same particle line. The energy $(\mathscr{E}_j^i + \sum_- \mathbf{l}_\nu^2)$ can again be read off from the graph: at the appropriate cut it is the sum over the energies of all cut (+)-lines and uncut (–)-lines. This factor, together with the potentials

$$\prod |(\mathbf{k}_{j1}^i \mathbf{k}_{j2}^i | U | \mathbf{k}_{j3}^i \mathbf{k}_{j4}^i)| \sim \prod |U(\mathbf{k}_{j1}^i - \mathbf{k}_{j4}^i)|,$$

will provide a uniform majorization for the sum (integral) over the $m + 1 - n$ independent loop momenta, after the complete use of the δ-functions.

Consider one of the $m + 2n - 1$ cuts, which gives rise to factor

$$\exp\left[-\beta\left(\mathscr{E}_j^i + \sum_- \mathbf{l}_\nu^2\right)\right].$$

Those closed loops which are crossed by this line contain at least one (+)-line which is cut. Those loops which are not cut contain at least one (–)-line each. Denote these distinguished particle lines by $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_L$. The remaining $m + 1 - n - L$ independent loop momenta are labelled according to the following algorithm. Start at any open orbit at one end or at any closed orbit at the distinguished particle line in the direction of the arrow. Denote by $\mathbf{p}_{L+1}$ the first internal momentum, which is not determined (via the δ-functions) by $\mathbf{k}_1, \ldots, \mathbf{k}_{2n}, \mathbf{p}_1, \ldots, \mathbf{p}_L$. If there is none, proceed to the next orbit. The subsequent particle line is either independent or a linear combination of $\mathbf{k}_1, \ldots, \mathbf{k}_{2n}, \mathbf{p}_1, \ldots, \mathbf{p}_{L+1}$. If it is independent, denote it by $\mathbf{p}_{L+2}$. The next particle line is again either independent, when it is denoted by $\mathbf{p}_{L+3}$, or it is a linear combination of $\mathbf{k}_1, \ldots, \mathbf{k}_{2n}, \mathbf{p}_1, \ldots, \mathbf{p}_{L+2}$. We proceed in this manner, until all particle lines are labelled. After this we write down the potentials corresponding to the interaction lines in the graph in the same order as the labelling was performed. Each potential is written down when it appears for the first time in our path. In this way we obtain the following product of potentials

$$\begin{aligned} &U(\mathbf{q}_0^1)\, U(\mathbf{q}_0^2) \ldots U(\mathbf{q}_0^{\nu_1})\, U(\mathbf{q}_0 - \mathbf{p}_{L+1})\, U(\mathbf{q}_1 - \mathbf{p}_{L+2}) \ldots U(\mathbf{q}_{\mu_1 - 1} - \mathbf{p}_{L+\mu_1}) \\ &U(\mathbf{q}_{\mu_1}^1)\, U(\mathbf{q}_{\mu_1}^2) \ldots U(\mathbf{q}_{\mu_1}^{\nu_2})\, U(\mathbf{q}_{\mu_1} - \mathbf{p}_{L+\mu_1+1})\, U(\mathbf{q}_{\mu_1+1} - \mathbf{p}_{L+\mu_1+2}) \ldots \\ &U(\mathbf{q}_{\mu_2 - 1} - \mathbf{p}_{L+\mu_2})\, U(\mathbf{q}_{\mu_2}^1)\, U(\mathbf{q}_{\mu_2}^2) \ldots U(\mathbf{q}_{m+1-n}^1)\, U(\mathbf{q}_{m+1-n}^2) \ldots U(\mathbf{q}_{m+1-n}^{\nu r}), \end{aligned} \tag{2.10}$$

where $\mathbf{q}_\mu^\nu$ (with or without superscript ν) is a linear combination of $\mathbf{k}_1, \ldots, \mathbf{k}_{2n}, \mathbf{p}_1, \ldots, \mathbf{p}_{L+\mu}$. There appears in (2.10) chains of potentials

$$\begin{aligned} &U(\mathbf{q}_0 - \mathbf{p}_{L+1})\, U(\mathbf{q}_1 - \mathbf{p}_{L+2}) \ldots U(\mathbf{q}_{\mu_1-1} - \mathbf{p}_{L+\mu_1}); \\ &U(\mathbf{q}_{\mu_1} - \mathbf{p}_{L+\mu_1+1})\, U(\mathbf{q}_{\mu_1+1} - \mathbf{p}_{L+\mu_1+2}) \ldots U(\mathbf{q}_{\mu_2-1} - \mathbf{p}_{L+\mu_2}); \ \ldots \end{aligned} \tag{2.11}$$

corresponding to chains of independent momenta:

$$\begin{aligned} &\mathbf{p}_{L+1}, \mathbf{p}_{L+2}, \ldots, \mathbf{p}_{L+\mu_1}; \\ &\mathbf{p}_{L+\mu_1+1}, \mathbf{p}_{L+\mu_1+2}, \ldots, \mathbf{p}_{L+\mu_2}; \ \ldots \end{aligned} \tag{2.12}$$

on various orbits. We split the product of sums (integrals) over the independent momenta to two independent sums (integrals)

$$\frac{1}{V^L} \sum_{\mathbf{p}_1, \ldots, \mathbf{p}_L} \cdot \frac{1}{V^{m-n+1-L}} \sum_{\mathbf{p}_{L+1}, \ldots, \mathbf{p}_{m-n+1}}$$

as follows. We replace the product $U(\mathbf{q}_\mu^1)\, U(\mathbf{q}_\mu^2) \ldots U(\mathbf{q}_\mu^\nu)$ by $[\|U\|_\infty]^\nu$. In place of (2.12) we introduce new variables of integration

$$\mathbf{p}'_{L+\mu} = \mathbf{q}_{\mu-1} - \mathbf{p}_{L+\mu}$$

The momenta in $[\mathscr{E}_j^i + \sum_- \mathbf{l}_\nu^2]$ different from $\mathbf{p}_1, \ldots, \mathbf{p}_L$ are replaced by zero. We thus get for $\bar{G}_r^{(m)}(\mathbf{k}^\#, \tau)_V$ the following majorization, when $\mu < 0$

$$C^{2m+n} \prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!} (\|U\|_\infty)^{n+L-1} \prod_{\mu=1}^{m+1-n-L} \left(\frac{1}{V} \sum_{\mathbf{p}'_{L+\mu}} |U(\mathbf{p}'_{L+\mu})| \right)$$

$$\exp(-L\beta|\mu|) \prod_{\nu=1}^{L} \left(\frac{1}{V} \sum_{\mathbf{p}_\nu} \exp(-\beta \mathbf{p}_\nu^2) \right) \sum_{i=1}^{2n} (m_i + 1)$$

or

$$C^{2m+n} \prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!} (\|U\|_\infty)^{n+L-1} (\|U\|_{\bar{1}})^{m+1-n-L}$$

$$\exp(-L\beta|\mu|)\, d^L(m + 2n), \tag{2.13}$$

where

$$d = \sup_V \frac{1}{V} \sum_{\mathbf{p} \in \Gamma} \exp(-\beta \mathbf{p}^2) \tag{2.14}$$

In the case of positive chemical potential (fermions only) the factor $\exp(-L\beta|\mu|)$ is to be replaced by $\exp[(2m + n)\, \beta\mu]$. For bosons $C > 1$ and for fermions $C = 1$.

Expression (2.13) can be brought into the form of the right-hand side of (2.4).

QED

Theorem 2.2: Let $U \in U_2$, $0 < \beta < \infty$, $\mu \in \mathbb{R}^1$ ($\mu < 0$ for bosons), and $0 < V < \infty$. Then every graph for the pressure or the truncated Euclidean RDM

$$(\operatorname{Im} \tau_1 = \cdots = \operatorname{Im} \tau_{2n} = 0)$$

satisfies

$$|\bar{G}_r^{(m)}(\mathbf{0}^\#, \tau_1; \ldots; \mathbf{0}^\#, \tau_{2n})_V| \geqslant \frac{U(\mathbf{0})^m}{V^{m-n+1}} \exp(\sum \pm \tau_i \mu) \prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!} f^{2m+n}, \tag{2.15}$$

where $f = \min\{f_\varepsilon^\pm(\mathbf{0})\}$.

Proof: We observe, that for potentials of uniform sign and real temperatures τ_i, $G_r^{(m)}(\mathbf{k}^\#, \tau)_V$ is a sum over a function of uniform sign. As lower bound for $|\bar{G}_r^{(m)}(\mathbf{0}, \tau)_V|$ we restrict the $\mathbf{k}$-summation to the contribution with $\mathbf{k}_{11}^1 = \cdots = \mathbf{k}_{m_{2n}4}^{2n} = 0$, which is consistent with the δ-functions. This leads to (2.15).

For $V \to \infty$ estimate (2.15) breaks down. For convenience we shall then restrict our discussion to a class of potentials, to which the techniques of Feynman integrals can be applied.

Theorem 2.3: Let $U \in U_3$, $0 < \beta < \infty$, $\mu \in \mathbb{R}^1$ ($\mu < 0$ for bosons), and $\operatorname{Im} \tau_1 = \cdots = \operatorname{Im} \tau_{2n} = 0$. There exist constants $A > 0, B > 0, C < \infty$ such that every graph $G_r^{(m)}(\mathbf{k}^\#, \tau)_\infty$ of order m for the pressure or the truncated Euclidean RDM satisfies

$$|\bar{G}_r^{(m)}(\mathbf{k}_1^\#, \tau_1; \ldots; \mathbf{k}_{2n}^\#, \tau_{2n})_\infty| \geqslant AB^m \prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!} \left(\exp\left[-C \sum_{i=1}^{2n} \mathbf{k}_i^2\right]\right)^m. \tag{2.16}$$

Proof: From (1.5) and (1.6) one finds lower bounds

$$f_\varepsilon^\pm(\mathbf{k}) \geqslant c \exp(-\beta \mathbf{k}^2), \tag{2.17a}$$

where

$$0 < c \leqslant \frac{1}{1 + \exp(\beta|\mu|)}.$$

Further we have

$$U(\mathbf{k} - \mathbf{l}) \geqslant a \exp[-b(\mathbf{k} - \mathbf{l})^2] \geqslant a \exp[-2b(\mathbf{k}^2 + \mathbf{l}^2)], \tag{2.17b}$$

$$\exp[\sigma_j^i(\mathrm{E}_{j1}^i + \mathrm{E}_{j2}^i - \mathrm{E}_{j3}^i - \mathrm{E}_{j4}^i)] \geqslant \exp\left[-\beta \sum_{\nu=1}^{4} \mathrm{E}_{j\nu}^i\right] \tag{2.17c}$$

and

$$\exp[\pm\tau_i \mathrm{E}_i] \geqslant \exp[-\beta \mathrm{E}_i] \tag{2.17d}$$

Using these lower bounds and the fact that the integrand of $G_r^{(m)}(\mathbf{k}^\#, \tau)_\infty$ has a uniform sign, we get according to (I.4), (1.4) and (1.7) in the limit $V \to \infty$

$$|\bar{G}_r^{(m)}(\mathbf{k}_1^\#, \tau_1; \cdots; \mathbf{k}_{2n}^\#, \tau_{2n})_\infty| \geqslant [\delta(\textstyle\sum \pm \mathbf{k}_i)]^{-1} \displaystyle\prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!} \exp\left(-\beta \sum_{i=1}^{2n} \mathbf{k}_i^2\right)$$

$$\times \frac{1}{(2\pi)^{3(m-n+1)}} \int d_{p_1}^3 \cdots \int d^3 p_{2m-n}\, a^m \prod_{j=1}^{m} \exp[-b(\mathbf{q}_1^j - \mathbf{q}_2^j)^2] \prod_{\nu=1}^{m} \delta(\mathbf{q}\nu)$$

$$\times \prod_{i=1}^{2n} \prod_{j=1}^{m_i} \exp\left(-\beta \sum_{r=1}^{4} \mathrm{E}_{jr}^i\right) c^{2m+n} \exp\left(-\beta \sum_{i=1}^{2n} \mathbf{k}_i^2\right) \exp\left(-\beta \sum_{\nu=1}^{2m-n} \mathbf{p}_\nu^2\right), \tag{2.18}$$

where $\mathbf{q}_1^j - \mathbf{q}_2^j$ is the momentum transfer at jth vertex and $\delta(\mathbf{q}_\nu)$ expresses the conservation of momentum at the νth interaction line;

$$\mathbf{q}_1^j, \mathbf{q}_2^j \in \left(\bigcup_{\nu=1}^{2m-n} \mathbf{p}_\nu\right) \cup \left(\bigcup_{i=1}^{2n} \mathbf{k}_i\right)$$

and $\mathbf{q}_\nu$ is a linear combination of vectors belonging to the same set. The same momentum $\mathbf{p}_\nu$ belongs to two different vertices and each $\mathbf{k}_i$ belongs to just one vertex. The energies E_{jr}^i are either $\mathbf{p}_\nu^2$ or $\mathbf{k}_i^2$ ($\nu = 1, 2, \ldots, 2m - n; i = 1, 2, \ldots, 2n$): each $\mathbf{p}_\nu^2$ appears twice and each $\mathbf{k}_i^2$ only once in the sum

$$\sum_{i=1}^{2n} \sum_{j=1}^{m_i} \sum_{s=1}^{4} \mathrm{E}_{js}^{i}.$$

From (2.18) follows

$$|\bar{G}_r^{(m)}(\mathbf{k}_1^{\#}, \tau_1; \ldots; \mathbf{k}_{2n}^{\#}, \tau_{2n})_\infty| \geqslant [\delta(\sum \pm \mathbf{k}_i)]^{-1} \frac{a^m c^{2m+n}}{(2\pi)^{3(m-n+1)}} \prod_{i=1}^{2n} \frac{|\tau_{i-1} - \tau_i|^{m_i}}{m_i!}$$

$$\times \int d^3p_1 \cdots \int d^3p_{2m-n} \prod_{\nu=1}^{m} \delta(\mathbf{q}_\nu) \exp\left\{-g\left[\sum_{i=1}^{2n} \mathbf{k}_i^2 + \sum_{j=1}^{2m-n} \mathbf{p}_j^2\right]\right\}, \tag{2.19}$$

where a, c and g are constants independent of the graph. The Gaussian integral in (2.19) can be obtained from a calculation given by Symanzik [10] (or use [11]). The result is

$$\int d^3p_1 \cdots \int d^3p_{2m-n} \prod_{\nu=1}^{m} \delta(\mathbf{q}_\nu) \exp\left\{-g\left[\sum_{i=1}^{2n} \mathbf{k}_i^2 + \sum_{j=1}^{2m-n} \mathbf{p}_j^2\right]\right\}$$

$$= \left(\frac{\pi}{g}\right)^{(3/2)(m-n+1)} \delta(\sum \pm \mathbf{k}_i)\,[T(G_r^{(m)})]^{-3/2} \exp\left\{-\sum_{i,j=1}^{2n} A_{ij}^G(g)\, \mathbf{k}_i \cdot \mathbf{k}_j\right\} \tag{2.20}$$

where $T(G_r^{(m)})$ is the number of trees in graph $G_r^{(m)}$. It can be shown that $\sum A_{ij}^G \cdot \mathbf{k}_i \cdot \mathbf{k}_j$ is a positive definite quadratic form of the $\mathbf{k}_i$'s. The proof for this is the same as given in the book by Bogoliubov and Shirkov [12] on pp. 324–6 for an analogous problem. According to this same source

$$0 \leqslant \sum_{i,j=1}^{2n} A_{ij}^G \mathbf{k}_i \cdot \mathbf{k}_j \leqslant \sum_{i,j=1}^{2n} A_{ij}^{G'}(g)\, \mathbf{k}_i \cdot \mathbf{k}_j, \tag{2.21}$$

if G' is any tree of G. For tree G' with $m - 1$ internal lines the momenta $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_{m-1}$ are linear combinations of $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_{2n}$ with coefficients ± 1 or 0 satisfying $\mathbf{p}_j^2 \leqslant 2n \sum_{i=1}^{2n} \mathbf{k}_i^2$. Hence

$$\sum_{i,j=1}^{2n} A_{ij}^{G'}(g)\, \mathbf{k}_i \cdot \mathbf{k}_j = \sum_{i=1}^{2n} g\, \mathbf{k}_i^2 + \sum_{j=1}^{m-1} g\, \mathbf{p}_j^2 < 2\, gmn \sum_{i=1}^{2n} \mathbf{k}_i^2. \tag{2.22}$$

Finally, we find an upper estimate for the number of trees of a graph of order m. The number of internal lines is $2m - n$, and each tree contains $m - 1$ particle lines. Thus the number of trees is smaller or equal to $\binom{2m-n}{m-1}$. For $m - n \gg 1$ we can use Stirlings formula $x! \approx (2\pi x)^{1/2} x^x e^{-x}$, which is good for $x \gg 1$. From this one finds that the number of trees is at most $(\pi m)^{-1/2} 2^{2m-n}$. These minorizations can be combined into form (2.16).

3. Partial Summations for $T > 0$

In this section we shall apply Theorems 2.1–2.3 to investigate the convergence properties of the perturbation expansion in quantum statistical mechanics. The systems considered interact through two-body potentials λU, where $\lambda \in \mathbb{R}^1$ and $U \in U_i$ ($i = 1,2,3$). We ask for analyticity properties at $\lambda = 0$.

Theorem 3.1: Let $U \in U_1$, $0 < \beta < \infty$, $\mu \in \mathbb{R}^1$ ($\mu < 0$ for bosons), N a fixed integer, and $0 \leqslant V \leqslant \infty$. When $\Sigma \pm \mathbf{k}_i = 0$ and $\{\tau\}$ satisfies (I.6), then the partial sum over all graphs $G_r^{(m)}(\mathbf{k}_1^\#, \tau_1; \ldots; \mathbf{k}_{2n}^\#, \tau_{2n})_V$ in the truncated RDM with less than N intermediate particles is an entire function of λ, which is continuous in $\{\tau\}$ (and continuous in $(\mathbf{k})$ for $V = \infty$) and uniformly bounded for $\{\tau\}$ varying over a bounded region satisfying (I.6).

Proof: We apply Theorem 2.1 to prove absolute and uniform convergence. We only need a bound on the number of graphs contributing to the truncated RDM, when the number of particle lines in every intermediate state is bounded by N. It is not difficult to see that there exists a constant $M = M(N)$ which gives the maximum number of different choices for the next interaction after a certain intermediate state. Thus the subclass of graphs of order m contains $\leqslant CM^m$ graphs where $C < \infty$. Now it follows immediately from Theorem 2.1 that our partial sum represents an entire function of λ.

QED

A uniform bound N of the number of intermediate particles is obtained, if one requires that the number of (+)- or (−)-lines in an intermediate state is bounded by K. Thus those Brueckner–Goldstone and Bethe–Faddeev ladder expansions which fulfil this requirement always converge. This is true for attractive or repulsive potentials both for bosons and for fermions. The ladder expansions which do not satisfy this requirement may converge or diverge. As an example of this we refer to the zig-zag expansion treated in [13] for which both convergence and divergence can occur.

The above results hold for $T > 0$. When $T \to 0$, expansions which converged for $T > 0$, may become divergent. Finally we remark that C. Gruber [14] has proved the analyticity of the Euclidean Green's function at $\lambda = 0$ with $V < \infty$ for fermion systems with $0 < \beta < \infty$, $\mu \in \mathbb{R}^1$, and $\|U\| < \infty$.

Since $\epsilon = +1$ for bosons, no cancellations between contributions of diagrams of the same order occur for boson systems if $U \in U_2$ or U_3. Therefore, as in quantum field theory [15], sufficiently strong lower estimates on the contributions of individual graphs lead immediately to:

Theorem 3.2: Let $U \in U_2$, $0 < \beta < \infty$, $\mu < 0$ and $V < \infty$. Then for a boson system the interaction expansion of the truncated RDM is not analytic at $\lambda = 0$, if $\operatorname{Im} \tau_1 = \cdots = \operatorname{Im} \tau_{2n} = 0$.

and

Theorem 3.3: Let $U \in U_3$, $0 < \beta < \infty$, $\mu < 0$ and $V = \infty$. Then, for a boson system, the interaction expansion for the truncated RDM is not analytic at $\lambda = 0$ if $\operatorname{Im} \tau_1 = \cdots = \operatorname{Im} \tau_{2n} = 0$.

Proof: A necessary condition for a series $\sum_{m=0}^{\infty} a_m \lambda^m$ to define a holomorphic function at $\lambda = 0$ is that $\sum |a_m| r^m$ converges for some $r > 0$. This can be easily disproved for the interaction expansion using the violent increase of the number of graphs $G_r^{(m)}$ with the order m together with Theorems 2.2 and 2.3. Consider the set of connected graphs of order m. Connect first the m lower vertices of the interaction lines by one closed orbit ($(m-1)!$ different possibilities). Select among the m upper vertices n vertices, and attach to each of those an incoming and an outgoing external line $\left(\binom{m}{n}\cdot(n!)^2 \text{ different possibilities}\right)$. Connect the remaining $m-n$ upper vertices in any way ($(m-n)!$ different possibilities). We obtain $\geqslant(m-1)!\,m!$ connected diagrams, which produce for the interaction expansion a divergence at least as $\sum r^m m!$, when (2.15) or (2.16) is used.

QED

We remark that the divergence of the interaction expansion for bosons has nothing to do with the Bose–Einstein condensation, since it occurs at all temperatures.

The work of Ginibre [16] and Gruber [14] has shown that, for positive Gaussian potentials, the Euclidean Green's functions exist for $V \leqslant \infty$, $\mu < 0$, and for sufficiently small values of the activity $z = e^{\beta\mu}$ (no phase transition at this temperature and small densities), and are analytic in z around $z = 0$.

For 1-dimensional quantum lattice, H. Araki [17] has proved analyticity at $\lambda = 0$ of the pressure and the RDM, while our divergence proof for bosons systems also holds in one dimension.

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