A SIMPLE PROOF OF THE LINKED CLUSTER EXPANSION THEOREM IN THE MANY-BODY PROBLEM

By M. Matlak and A. Pawlikowski

Silesian University, Katowice*

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A proof of the Linked Cluster Expansion Theorem for the Green functions is given. The use of cumulant averages developed by Kubo and of a generating functional makes this proof very simple. The proof is quite general and is valid for the temperature $T \neq 0$ as well as for $T = 0$ (ground state).

1. *Introduction*

In the last two decades methods of quantum theory were succesfully applied to the many-body problem in solid state and nuclear physics [1], [2]. By "many-body" we mean here both many particles and many spins. The mentioned methods consist, *inter alia*, of the use graph techniques in the perturbation theory. One obtains unperturbed averages of products of several annihilation and creation (or spin) operators. Applying some reduction formulae (generalized Wick's theorems) we can represent each of the averages of n operators by averages of m operatos, where $m < n$. This makes it possible to obtain a one to one correspondence between terms of the perturbation series and graphs. To every graph[1] there corresponds an expression named the contribution from this graph which is equal to a particular perturbation term (multiplied by $n!$, where n is equal to the order of this term[2]).

In the many-body problem one considers perturbation series for the free energy and the Green functions (perturbed averages of the ordered operators). The graph for the free energy or for the Green function is called unlinked (unconnected) if the contribution from it is equal to a contribution from a graph of a lower order for the same quantity (for the free energy or for the Green function) multiplied by a product of contributions from graph of lower order for the free energy. Otherwise it is called linked (or connected). A linked graph for the Green function is called weakly linked if the contribution from it is equal to a product of contributions from graphs for lower order Green functions[3]. Otherwise this linked graph is called strongly linked.

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* Address: Instytut Fizyki Uniwersytetu Śląskiego, Katowice, Bankowa 12, Polska.

[1] Drawn in accordance with conservation laws.

[2] We consider labeled graps.

[3] The order of a Green functions is equal to the number of perturbed averaged operators entering it

The Linked Cluster Expansion (LCE) theorem states that both the free energy and the Green functions are represented by linked graphs only.

There are many proofs of this theorem in the literature, but almost all of them depend on the concrete form of the Hamiltonian. To the authors' knowledge there are only three methods with help of which the LCE theorem can be proved for arbitrary many-body Hamiltonian. The first method based on the Uhlenbeck's theorem (see [3], p. 132) and the second one given in a paper of Kubo [4] can serve to proving the LCE for the free energy while the third method given by Watanabe [5] can be used for proving the LCE tor the free energy as well as for the Green functions (ses *e. g.* [1]).

The aim of this paper is to give another simple proof of the LCE for Green functions holding for arbitrary Hamiltonian. We exploit the very important and useful concept of cumulant averages as it suggested Kubo [4]. In passing we outline Kubo's proof of LCE for free energy.

In § *2* we define some basic concepts of cumulants (semiinvariants) related to the β-ordered products of some operators. We give the proof of an important theorem about cumulant averages.

In § *3* we recall some well known formulae from the statistical perturbation theory.

In § *4* we give a simple proof of the LCE theorem for free energy and for the Green functions.

2. Green functions and cumulant Green functions

Let A be a random variable and $\langle A\rangle$ its average value. It is very well known in the probability theory that the cumulants are defined by means of their generating function

$$K[\xi] = \ln \langle e^{\xi A}\rangle = \sum_{n=1}^{\infty} \frac{\xi^n}{n!} \langle A^n\rangle_c \equiv \langle \exp \xi A - 1\rangle_c, \tag{2.1}$$

where by $\langle A\rangle_c$ we have denoted just the cumulant average.

Because in the many-body theory we deal with random variables A_α depending on some continuous parameter β ($\beta = 1/kT$, k-Boltzmann constant) and operators representing these random variables are often β-ordered, we concern ourselves with the generalization of cumulant averages to this subject.

We consider the functional

$$M[\xi] = \langle T \exp \int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\xi_\alpha(\beta')\rangle, \tag{2.2}$$

where A_α's are some operators,

$$\langle\ldots\rangle = \frac{\mathrm{Tr}\,\{e^{-\beta H}\ldots\}}{\mathrm{Tr}\, e^{-\beta H}}, \tag{2.3}$$

$$A_\alpha(\beta) = e^{\beta H} A_\alpha e^{-\beta H},$$

H is the time-dependent Hamiltonian, ξ_α's are c-numbers, and T denotes the β-ordering operator defined as follows[4]

$$T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2)\dots A_{\alpha m}(\beta_m)) = A_{\alpha_{\gamma_1}}(\beta_{\gamma_1})A_{\alpha_{\gamma_2}}(\beta_{\gamma_2})\dots A_{\alpha_{\gamma m}}(\beta_{\gamma_m}) \tag{2.4}$$

with

$$\beta_{\gamma_1} > \beta_{\gamma_2} \dots > \beta_{\gamma m}.$$

The expansion of the functional $M[\xi]$ into the functional Volterra series gives

$$M[\xi] = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\beta d\beta_1' \dots \int_0^\beta d\beta_n' \sum_{\alpha_1} \dots \sum_{\alpha_n} \langle T \prod_{j=1}^{n} A_{\alpha_j}(\beta_j') \rangle \prod_{k=1}^{n} \xi_{\alpha_k}(\beta_k'). \tag{2.5}$$

Thus, $M[\xi]$ is the generating functional for β-ordered averages which we shall also call the Green functions[5]

$$\langle T \prod_{j=1}^{m} A_{\alpha_j}(\beta_j) \rangle = G_m(\alpha_1, \beta_1; \dots; \alpha_m, \beta_m), \tag{2.6}$$

i.e.

$$G_m(\alpha_1, \beta_1; \dots; \alpha_m, \beta_m) = \left. \frac{\delta^m}{\delta\xi_{\alpha_1}(\beta_1) \dots \delta\xi_{\alpha_m}(\beta_m)} M[\xi]. \right|_{\xi=0} \tag{2.7}$$

Let us first note that the Green function of the first order (*i.e.* for $m = 1$) is simply equal to the average of an operator A_1. Now we consider another functional

$$K[\xi] = \ln M[\xi]. \tag{2.8}$$

We define the cumulant β-ordered averages, which we shall call also the cumulant Green functions [6], and denote by

$$\langle T \prod_{j=1}^{m} A_{\alpha_j}(\beta_j) \rangle_c = C_m(\alpha_1, \beta_1; \dots; \alpha_m, \beta_m), \tag{2.9}$$

assuming that the functional $K[\xi]$ is their generating functional, *i.e.*

$$C_m(\alpha_1, \beta_1; \dots; \alpha_m, \beta_m) = \left. \frac{\delta^m}{\delta\xi_{\alpha_1}(\beta_1) \dots \delta\xi_{\alpha_m}(\beta_m)} K[\xi]. \right|_{\xi=0} \tag{2.10}$$

Taking (2.8), (2.9) and (2.10) into account we can write[6]

$$\begin{aligned} K[\xi] &= \ln \langle T \exp \int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\xi_\alpha(\beta') \rangle \\ &= \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^\beta d\beta_1' \dots \int_0^\beta d\beta_n \sum_{\alpha_1} \dots \sum_{\alpha n} \langle T \prod_{j=1}^{n} A_{\alpha_j}(\beta') \rangle_c \prod_{k=1}^{n} \xi_{\alpha_k}(\beta_k') \\ &= \langle T \exp \int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\xi_\alpha(\beta') - 1 \rangle_c. \end{aligned} \tag{2.11}$$

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[4] For the sake of simplicity we do not consider the case when the operators A_α are the fermion annihilation and creation operators. In this case we should insert in many places the factor ± 1.

[5] This definition coincides with the common definition of the statistical causal Green function [1].

[6] Kubo considers (2.11) as a theorem. In our opinion (2.11) should be treated rather as a definition of β-ordered averages. Kubo's proof of (2.11) from [4] is in fact a proof of the expansion of a functional into a Volterra series.

From (2.7), (2.8), (2.10) we obtain relations between Green functions and cumulant Green functions. The Green function can be explicitly represented only by lower (not higher) order cumulant Green functions and vice versa. For example

$$\langle A_\alpha(\beta)\rangle = \langle A_\alpha(\beta)\rangle_c$$

$$\langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2))\rangle = \langle A_{\alpha_1}(\beta_1)\rangle_c \langle A_{\alpha_2}(\beta_2)\rangle_c + \langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2))\rangle_c$$

$$\langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2)A_{\alpha_3}(\beta_3))\rangle = \langle A_{\alpha_1}(\beta_1)\rangle_c A_{\alpha_2}(\beta_2)\rangle_c \langle A_{\alpha_3}(\beta_3))\rangle_c +$$

$$+\langle A_{\alpha_1}(\beta_1)\rangle_c \langle T(A_{\alpha_2}(\beta_2)A_{\alpha_3}(\beta_3))\rangle_c + \rangle A_{\alpha_2}(\beta_2)\rangle_c \langle T(A_{\alpha_1}(\beta_1)A_{\alpha_3}(\beta_3))\rangle_c +$$

$$+\langle A_{\alpha_3}(\beta_3)\rangle_c \langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2))\rangle_c + \langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2)A_{\alpha_3}(\beta_3))\rangle_c \tag{2.12}$$

and so on.

From the second equation in (2.12) we easily see that the cumulant Green function $\langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2))\rangle_c$ is zero if the random variables $A_{\alpha_1}(\beta_1)$, $A_{\alpha_2}(\beta_2)$ are statisticaly independent, that is if

$$\langle T(A_{\alpha_1}(\beta_1)A_{\alpha_2}(\beta_2))\rangle = \langle A_{\alpha_1}(\beta_1)\rangle\langle A_{\alpha_2}(\beta_2)\rangle.$$

In general we have the following theorem[7]: A cumulant Green function $\langle T(A_iA_j\ldots)\rangle_c$ is Iero if variables $\{A_i, A_j\ldots\}$ are divided into two or more groups which are statistically zndependent.

Proof:

if the variables $\{A_i, A_j, \ldots\}$ are divided into two groups, *i.e.* if

$$\{A\} = \{A'\} + \{A''\}$$

which are statistically independent, the generating functional (2.2) is factorized as

$$e^{K[\xi]} = \langle T\exp\int_0^\beta d\beta' \sum A(\beta')\xi(\beta')\rangle$$

$$= \langle T\exp\int_0^\beta d\beta' \sum A'(\beta')\xi(\beta')\rangle\langle T\exp\int_0^\beta d\beta' \sum A''(\beta')\xi''(\beta')\rangle$$

$$= \exp\langle T\exp\int_0^\beta d\beta' \sum A'(\beta')\xi'(\beta') - 1\rangle_c \exp\langle T\exp\int_0^\beta d\beta' \sum A''(\beta')\xi''(\beta') - 1\rangle_c$$

$$= e^{K[\xi']}\cdot e^{K[\xi'']}. \tag{2.13}$$

Thus we see, that

$$K[\xi] = K[\xi'] + K[\xi'']$$

and power series of ξ' and ξ'' will never mix in the functional if the sets $\{A'\}$ and $\{A''\}$ are unconnected. This implies from (2.9) and (2.10) that any cumulant Green function in which the variables from two groups appear does vanish identically. In other words the theorem states that the variables in each cumulant Green function must be statistically connected or linked. Otherwise it vanishes.

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[7] This theorem is, in fact, a theorem from [4] slightly modified for our purposes.

3. *Summary of useful formulae*

In this paragraph we recall some fundamental formulae from many-body perturbation theory. The Hamiltonian is written in the form

$$H = H_0 + V, \tag{3.1}$$

where H_0 is the unperturbed Hamiltonian and V is the perturbation. For perturbative calculations it is convenient to write

$$e^{-\beta H} = e^{-\beta H_0}\,\sigma(\beta) \tag{3.2}$$

where

$$\sigma(\beta) = e^{\beta H_0} \cdot e^{-\beta H}. \tag{3.3}$$

This last quantity satisfies the equation

$$\frac{d\sigma(\beta)}{d\beta} = -\tilde{V}(\beta)\sigma(\beta), \tag{3.4}$$

where

$$\tilde{V}(\beta) = e^{\beta H_0} V e^{-\beta H_0}$$

and the initial condition

$$\sigma(0) = 1. \tag{3.5}$$

The iterative solution of the equation (3.4) with the condition (3.5) is

$$\sigma(\beta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\beta_1 \ldots \int_0^\beta d\beta_n T\Big(\prod_{i=1}^{n} \tilde{V}(\beta_i)\Big) = T e^{-\int_0^\beta \tilde{V}(\beta')d\beta'} . \tag{3.6}$$

The logarithm of the trace of $e^{-\beta H}$ multiplied by $-\frac{1}{\beta}$ gives us the free energy[8]. Therefore

$$F = -\frac{1}{\beta} \ln \operatorname{Tr} e^{-\beta H} = -\frac{1}{\beta} \ln \left\{ \operatorname{Tr} e^{-\beta H_0}\sigma(\beta) \cdot \frac{\operatorname{Tr} e^{-\beta H_0}}{\operatorname{Tr} e^{-\beta H_0}} \right\} = F_0 + F_1, \tag{3.7}$$

where

$$F_0 = -\frac{1}{\beta} \ln \operatorname{Tr} e^{-\beta H_0}, \tag{3.8}$$

$$F_1 = -\frac{1}{\beta} \ln \langle \sigma(\beta) \rangle_0 \tag{3.9}$$

$$\langle \ldots \rangle_0 = \frac{\operatorname{Tr}\{e^{-\beta H_0} \ldots\}}{\operatorname{Tr} e^{-\beta H_0}} . \tag{3.10}$$

After substituting (3.6) into (3.9) we get perturbation series for the free energy.

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[8] Our considerations can be applied as well to the great canonical ensemble. It is enough to substitute $H \rightarrow H - \mu N$ and to include in the trace calculations the summation over particle numbers.

Let us now see what form does the functional $M[\xi]$ take in perturbation theory. Similarly to the above we write

$$M[\xi] = \langle T \exp \int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\, \xi_\alpha(\beta')\rangle$$
$$= \frac{\mathrm{Tr}\,\{e^{-\beta H}\, T \exp\,[\int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\, \xi_\alpha(\beta')]\}}{\mathrm{Tr}\,\{e^{-\beta H}\}}$$
$$= \frac{\mathrm{Tr}\,\{e^{-\beta H_0}\sigma(\beta)\, T \exp\,[\int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\xi_\alpha(\beta')]\}}{\mathrm{Tr}\,\{e^{-\beta H_0}\sigma(\beta)\}}\ \frac{\mathrm{Tr}\, e^{-\beta H_0}}{\mathrm{Tr}\, e^{-\beta H_0}}$$
$$= \frac{\langle \sigma(\beta)\, T \exp \int_0^\beta d\beta' \sum_\alpha A_\alpha(\beta')\xi_\alpha(\beta')\rangle_0}{\langle\sigma(\beta)\rangle_0}$$
$$= \frac{\langle T\{\sigma(\beta) \exp \int_0^\beta d\beta' \sum_\alpha \tilde{A}_\alpha(\beta')\xi_\alpha(\beta')\}\rangle_0}{\langle\sigma(\beta)\rangle_0}, \tag{3.11}$$

where

$$\tilde{A}_\alpha = e^{\beta H_0} A_\alpha e^{-\beta H_0}. \tag{3.12}$$

Differentiating the r.h.s. of (3.11)(or the log of the r.h.s. of (3.11)) with respect to ξ_α, putting $\xi_\alpha = 0$ and substituting (3.6) into the results we obtain perturbation expressions for Green functions (cumulant Green functions).

4. The proof of the LCE Theorem

Let us note that $\langle\sigma(\beta)\rangle_0$(3.6), (3.10)) is very similar to (2.2). We can say the same about the numerator of (3.11) when we write it as

$$\langle T \exp\,\{-\int_0^\beta d\beta'(\tilde{V}(\beta') - \sum_\alpha \tilde{A}_\alpha(\beta')\xi_\alpha(\beta'))\}\rangle_0. \tag{4.1}$$

The more difference consists in replacing perturbed averages $\langle\ldots\rangle$ by unperturbed ones $\langle\ldots\rangle_0$. Having unperturbed averages of β-ordered exponentials we can apply to all of them the considerations of § 2.[9] Analogously to the perturbed β-ordered cumulant averages $\langle\ldots\rangle_c$ defined there we now shall have unperturbed ones $\langle\ldots\rangle_{0c}$.

Namely, from (3.9), (3.11) and (2.11) we can write:

1) for the free energy

$$F_1 = F - F_0 = -\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\beta_1' \ldots \int_0^\beta d\beta_n' \langle T(\tilde{V}(\beta_1')\ldots\tilde{V}(\beta_n'))\rangle_{0c}$$
$$= -\frac{1}{\beta}\left\langle T \exp\left\{-\int_0^\beta d\beta' \tilde{V}(\beta')\right\} - 1\right\rangle_{0c} \tag{4.2}$$

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[9] Here as the operators A_α from §2 we must take both $\tilde{A}_\alpha$'s and $\tilde{V}$'s.

and *2*) for the functional $K[\xi]$

$$K[\xi]=\langle T\exp\{-\int_0^\beta d\beta'(\tilde V(\beta')-\sum_\alpha \tilde A_\alpha(\beta')\xi_\alpha(\beta')\}-1\rangle_{0c}-\langle\sigma(\beta)-1\rangle_{0c}$$

$$=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\beta_1'\ldots\int_0^\beta d\beta_n'\langle T\prod_{j=1}^{n}(\tilde V(\beta_j')-\sum_\alpha \tilde A_\alpha(\beta_j')\xi_\alpha(\beta_j'))\rangle_{0c}-\langle\sigma(\beta)-1\rangle_{0c}. \quad (4.3)$$

From (4.2), (4.3) and (2.10) we see that we have expressed the free energy and the cumulant Green functions by the unperturbed β-ordered cumulant averages only. The latter in turn correspond to linked graphs in the case of the free energy and to strongly linked graphs in the case of Green function, as we can see from the definition of linked graphs and from the theorem of § 2. Therefore we have proved that the free energy (the cumulant Green function) is expressed by linked (strongly linked) graphs only. Having proved the LCE for cumulant Green functions we get the proof of LCE theorem for ordinary Green functions (2.6) using (2.12). By taking into account the limit $\beta\to\infty$ we obtain the LCE for corresponding quantities related to the ground state.

5. *Conclusions*

We have proved the LCE theorem for the Green functions using the concept of cumulant averages. The proof is quite general and we had not assumed anywhere any concrete form of the Hamiltonian. The proof which is done for temperature T holds in the case $T=0$ (ground state) as well.

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