Deviations from Wick’s theorem in the canonical ensemble

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(Dated: April 11, 2018)

Wick’s theorem for the expectation values of products of field operators for a system of noninteracting fermions or bosons plays an important role in the perturbative approach to the quantum many-body problem. A finite temperature version holds in the framework of the grand canonical ensemble but not for the canonical ensemble appropriate for systems with fixed particle number like ultracold quantum gases in optical lattices. Here we present new formulas for expectation values of products of field operators in the canonical ensemble using a method in the spirit of Gaudin’s proof of Wick’s theorem for the grand canonical case. The deviations from Wick’s theorem are examined quantitatively for two simple models of noninteracting fermions.

I. INTRODUCTION

Properties of a large system of noninteracting fermions or bosons in thermal equilibrium are usually described using the grand canonical ensemble with variable particle number. For a system of fixed number $N$ of fermions in a closed box this provides an excellent approximation for large enough $N$. An exception is provided by the ideal Bose gas, where the probability distribution for the particle number from one to $N$, which are numerically unstable for large values of $N$. For fermions the occupation numbers and products of them are discussed. Here a different approach in the spirit of Gaudin’s proof is presented.

In a recent publication a new formula for the $n$-particle density matrices in the canonical ensemble was presented. In contrast to Wick’s theorem for the grand canonical ensemble the higher order reduced density matrices cannot be expressed in terms of the one-particle function. Here a different approach in the spirit of Gaudin’s proof of Wick’s theorem for the grand canonical ensemble is presented.

In section II earlier results for expectation values of occupation numbers and products of them are discussed. In contrast to the grand canonical ensemble no simple factorization of the expectation values of products of occupation number operators occurs when the canonical ensemble is used. The formulas presented earlier involve a summation which involves all partition functions for particle number from one to $N$, which are numerically rather unstable for large values of $N$.

In section III new formulas are derived in which expectation values of $m$-particle operators are expressed in terms of the mean occupation numbers. For simple models like one-dimensional fermions in a harmonic trap and a zero bandwidth semiconductor explicit results are presented and the deviations from Wick’s theorem are elucidated quantitatively in section IV. Analytical expressions for the deviation from Wick’s theorem are presented.

II. KNOWN RESULTS FOR NONINTERACTING FERMIONS IN THE CANONICAL AND GRAND CANONICAL ENSEMBLE

An $N$-particle system with Hamiltonian $H_N$ in thermal equilibrium at temperature $T$ is described by the canonical statistical operator

$$\rho_c = e^{-\beta H_N} / Z_N, \quad Z_N = \text{Tr}_N e^{-\beta H_N},$$

where $\beta = 1/(k_B T)$ with $k_B$ Boltzmann’s constant and $\text{Tr}_N$ the trace over the $N$-particle Hilbert space. The expectation value of an observable $A$ is given by

$$\langle A \rangle_c = \text{Tr}_N A e^{-\beta H_N} / Z_N.$$  

In this paper systems of $N$ noninteracting fermions with $H_N = \sum_{\alpha=1}^N h_\alpha$ are considered. The eigenstates of such a system can be expressed as a determinant of the single particle eigenstates obeying the single particle Schrödinger equation $h(\epsilon_i) = \epsilon_i |\epsilon_i\rangle$. A convenient way to express the $N$-particle eigenstates is by the list of occupation numbers $\{n\}$ of these one-particle states leading to

$$H_N |\{n\}\rangle_N = \sum_i \epsilon_i n_i |\{n\}\rangle_N$$

with $\sum_i n_i = N$. For fermions the occupation numbers $n_i$ can take the values 0 and 1. The canonical partition function is given by

$$Z_N(\beta) = \sum_{\{n\}} e^{-\beta \sum_i \epsilon_i n_i} \delta_N, \sum_j n_j$$

The Kronecker delta restricting the occupation number sums makes a closed evaluation of $Z_N$ generally difficult. Therefore for large particle number $N$ the grand canonical statistical operator $\rho_{gc}$ with varying particle number is often used. It acts in Fock space which is the direct sum over all $N$ from zero to infinity of the Hilbert spaces of totally antisymmetric $N$-particle states. In this context it is appropriate to use second quantization by introducing the creation and annihilation operators $c_i^\dagger$ and...
leading to system with fixed particle number is often used as an approximate description for a different occupation number operators is obvious. It is

c creates a fermion in the energy eigenstate |\epsilon_i\rangle. The n_i = c_i^\dagger c_i are the occupation number operators. The corresponding grand canonical statistical operator reads

\[ \rho_{gc}^{(0)} = \frac{e^{-\beta H_0}}{Z}, \hspace{1cm} Z = Tr e^{-\beta H_0}, \]

where \( \tilde{H}_0 \equiv H_0 - \mu N \) with \( N = \sum_i n_i \) the particle number operator expressed in terms of the occupation number operators and \( \mu \) the chemical potential. Because it simplifies the calculations the grand canonical ensemble is often used as an approximate description for a system with fixed particle number \( N \), using \( \langle N \rangle_{gc} = N \) to fix the chemical potential.

In the rest of this section we discuss known results for the expectation values \( \langle n_i \rangle \) and \( \langle n_i n_j \rangle \) with \( i \neq j \) for both ensembles. We begin with the much simpler case of the grand canonical ensemble. The statistical operator \( \rho_{gc}^{(0)} \) factorizes

\[ \rho_{gc}^{(0)} = \prod_i e^{-\beta \epsilon_i n_i / z_i} \equiv \prod_i \rho_i^{(0)} \]

with \( \tilde{\epsilon}_i = \epsilon_i - \mu \) and \( z_i = 1 + e^{-\beta \epsilon_i} \). This leads to \( \langle n_i \rangle_{gc} = e^{-\beta \epsilon_i / z_i} \) and one obtains the Fermi function

\[ \langle n_i \rangle_{gc} = \frac{1}{e^{\beta \epsilon_i} + 1} \equiv f(\tilde{\epsilon}_i). \]

Because of the factorization of \( \rho_{gc}^{(0)} \) the factorization for the expectation value of two different occupation number operators easily follows

\[ \langle n_i n_j \rangle_{gc} = \langle n_i \rangle_{gc} \langle n_j \rangle_{gc}. \]

This is the simplest version of Wick’s theorem. The total factorization of a product of an arbitrary number of different occupation number operators is obvious. It is discussed in more detail in the next section.

With Eqs. 8 and 9 a simple expression for the mean square deviation of the total particle number can be given. With \( n_i^2 = n_i \) one obtains

\[ \langle N^2 \rangle_{gc} = \sum_{i \neq j} \langle n_i n_j \rangle_{gc} + \sum_i \langle n_i \rangle_{gc} \]

leading to

\[ \langle N^2 \rangle_{gc} - \langle N \rangle_{gc}^2 = \sum_i \langle n_i \rangle_{gc} (1 - \langle n_i \rangle_{gc}). \]

As the right hand side of this equation is of order \( N \) (see section III for explicit examples), the relative width of the particle number distribution in the grand canonical ensemble decreases like \( 1/\sqrt{N} \) in the large \( N \) limit.

For the canonical ensemble the mean occupation numbers \( \langle n_i \rangle_N \)

\[ \langle n_i \rangle_{N,c} = \frac{1}{Z_N} \sum_{\{n\}} n_i e^{-\beta \sum_i \epsilon_i n_i} \delta_{N,n} \]

were early studied by Schmidt. He derived a simple relation between \( \langle n_i \rangle_N \) and \( \langle n_i \rangle_{N-1} \) (we suppress the index “c” for the rest of this section)

\[ \langle n_i \rangle_N = e^{-\beta \epsilon_i} Z_{N-1}/Z_N (1 - \langle n_i \rangle_{N-1}) \]

by performing the \( n_i \) sum and introducing the factor \( 1 - n_i \) in order to return to the complete sum over \( \{n\} \) with \( N \) replaced by \( N-1 \) in the Kronecker delta. In the large \( N \) limit \( \langle n_i \rangle_N \approx \langle n_i \rangle_{N-1} \) and \( Z_{N-1}/Z_N = e^{\beta (F_N - F_{N-1})} \approx e^{\beta \mu} \) with \( F_N \) the free energy and \( \mu \) the chemical potential holds, leading to the Fermi function

\[ \langle n_i \rangle_N \approx (e^{\beta (\epsilon_i - \mu)} + 1)^{-1} = f(\epsilon_i). \]

For arbitrary values of \( N \) the recursion relation in Eq. 13 can be used. With the initial value \( \langle n_i \rangle_0 = 0 \) one obtains in the first step \( \langle n_i \rangle_1 = e^{-\beta \epsilon_i} / Z_N \) and easily proves by induction

\[ \langle n_i \rangle_N = \frac{1}{Z_N} \sum_{k=1}^N (-1)^{k-1} e^{-\beta \epsilon_i} Z_{N-k}(\beta). \]

The summation over all \( i \) yields \( N \) on the left hand side leading to

\[ Z_N(\beta) = \frac{1}{N} \sum_{k=1}^N (-1)^{k-1} Z_{N-k}(\beta) Z_1(\beta) \]

with \( Z_1(\beta) = \sum_i e^{-\beta \epsilon_i} \). There are also other ways to derive this relation. The sums in Eqs. 13 and 16 unfortunately are numerically rather unstable for large values of \( N \). They also do not provide analytical expressions in the limiting cases discussed in section IV.

The procedure leading to Eq. 13 can easily be extended to the calculation of expectation values of products of different occupation numbers. Replacing \( n_i \) by \( n_i n_j \) in Eq. 12 with \( i \neq j \) one obtains

\[ \langle n_i n_j \rangle_N = \frac{Z_{N-2}}{Z_N} e^{-\beta (\epsilon_i + \epsilon_j)} (1 - n_i) (1 - n_j) \]

The large \( N \) limit can be treated as following Eq. 13. With the additional assumption \( \langle n_i n_j \rangle_N \approx \langle n_i \rangle_N \langle n_j \rangle_N \) one obtains using Eq. 13 after elementary algebra

\[ \langle n_i n_j \rangle_N \approx [e^{\beta (\epsilon_i + \mu)} + 1] (e^{\beta (\epsilon_j - \mu)} + 1)^{-1}. \]
i.e. the simplest version of Wick’s theorem \( \langle n_i n_j \rangle = \langle n_i \rangle \langle n_j \rangle \) approximately holds for large \( N \) also in the canonical ensemble. For arbitrary values of \( N \) one again can proceed recursively. With the starting value \( \langle n_i n_j \rangle_2 = e^{-\beta (e_i + e_j)}/Z_2 \) one can show by induction

\[
\langle n_i n_j \rangle_N = \frac{1}{Z_N} \sum_{k=2}^{N} (-1)^k Z_{N-k} \sum_{l=1}^{k-1} e^{-\beta |k_i + (k-l)j|}. \tag{19}
\]

This equation also readily follows from Eq. (5b) of reference 3. Expectation values of higher products of occupation number operators are discussed with a new approach in the next section.

### III. WICK’S THEOREM AND WEAKER FORMS OF IT

#### A. General remarks

In this section we address Wick’s theorem and weaker forms of it in a more general setting and consider expectation values of multiple products of creation and annihilation operators. A general \( m \)-particle operator can be written as a linear combination of such a multiple product of \( m \) creation and \( m \) annihilation operators \( \hat{A} \).

\[
\hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} = c_1^{\dagger} c_{k_1} c_2^{\dagger} c_{k_2} \ldots c_m^{\dagger} c_{k_m} c_{l_1} c_{l_2} \ldots c_{l_m}. \tag{20}
\]

For the case of fermions treated here all \( k_i \) and all \( l_j \) have to be different in order to obtain a non-zero expression. The two-particle interaction \( V \) between fermions is an important \( m = 2 \) example. If it is treated in the Hartree-Fock approximation its expectation value in a system of noninteracting fermions occurs. This is one motivation for the following. In a higher order perturbative treatment of a two-particle interaction expectation values of products of operators \( \hat{A}^{(2)} \) occur which can be reordered into operators of the type in Eq. (20). In the following we want to evaluate the expectation value

\[
\langle \hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} \rangle = \text{Tr}(\hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} \rho) \tag{21}
\]

with \( \rho \) being the statistical operator for the canonical or the grand canonical ensemble. Performing the trace in both cases using the occupation number states \( |n_i\rangle_N \) it is obvious that the \( \{l_j\} \) in Eq. (20) have to be a permutation of the \( \{k_i\} \) in order to obtain a nonzero expectation value. This implies

\[
\langle \hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} \rangle = \text{det}(\delta^{(m)})\langle n_{i_1} n_{l_2} \ldots n_{i_m} \rangle \tag{22}
\]

where \( \delta^{(m)} \) is the \( m \times m \) matrix with matrix elements \( \delta^{(m)}_{i j} = \delta_{i j}. \) This result holds for the canonical and the grand canonical ensemble. For \( m = 1 \) this equation reads

\[
\langle c_k^{\dagger} c_l \rangle = \delta_{kl}\langle n_l \rangle. \tag{23}
\]

#### B. The grand canonical ensemble

As mentioned in section II the factorization of \( \rho^{(0)}_{gc} \) (see Eq. (2)) immediately implies

\[
\langle \hat{P}^{(m)} \rangle_{gc} \equiv \langle n_{i_1} \ldots n_{i_m} \rangle_{gc} = \langle n_{i_1} \rangle_{gc} \ldots \langle n_{i_m-1} \rangle_{gc} \langle n_{i_m} \rangle_{gc}. \tag{23}
\]

Introducing the matrix \( \langle c_i^{\dagger} c_j \rangle^{(m)} \) with matrix elements \( \langle c_i^{\dagger} c_j \rangle^{(m)} = \langle c_{i_1}^{\dagger} c_{j_1} \rangle_{gc} \) the expectation value of \( \hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} \) can be written in the two forms

\[
\langle \hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} \rangle_{gc} = \text{det}(\delta^{(m)}) \prod_{i=1}^m \langle n_{i} \rangle_{gc} \tag{24}
\]

Due the multilinearity of the determinant the second form also holds for arbitrary operators \( c_a = \sum_i (\alpha_i) c_i \) in the definition of \( A \). This a a general form of Wick’s theorem for fermions.

For the attempt to express \( \langle \hat{A}_{k_1 k_2 \ldots k_m l_1 l_2 \ldots l_m} \rangle \) in terms of the mean occupation numbers \( \langle n_i \rangle \) also for the canonical ensemble it is useful to present an alternative way to calculate expectation values of the type \( \langle \hat{A}_{c_i} \rangle_{gc} \), where \( \hat{A} \) is an arbitrary product of \( m \) creation and \( m - 1 \) annihilation operators. The essential steps in Gaudin’s method \( 4, 5 \) to determine such expectation values for fermions or bosons are to use Heisenberg type operators

\[
e\beta \hat{H}_0 c_i e^{-\beta \hat{H}_0} = e^{-\beta \epsilon_i} \tag{25}
\]

and the cyclic invariance of the trace. This leads to

\[
\text{Tr}_F \hat{A} c_i e^{-\beta \hat{H}_0} = \text{Tr}_F \hat{A} e^{-\beta \hat{H}_0} c_i e^{-\beta \hat{H}_0} = e^{-\beta \epsilon_i} \text{Tr}_F \hat{A} c_i e^{-\beta \hat{H}_0}. \tag{26}
\]

Now one can use \( c_i \hat{A} = \mp \hat{A} c_i + [c_i, \hat{A}]_\pm \) where the upper (lower) sign is for fermions (bosons). Multiplication with \( e^{\beta \epsilon_i}/Z_F \) yields

\[
\langle c_i^{\dagger} c_i \rangle = \langle c_i^{\dagger} c_i \rangle_{gc} = \langle \hat{A} c_i \rangle_{gc} = \langle [c_i, \hat{A}]_\pm \rangle_{gc}. \tag{27}
\]

For \( \hat{A} = c_j^{\dagger} \) one obtains the expected result

\[
\langle c_j^{\dagger} c_i \rangle_{gc} = \delta_{ij} \frac{\prod_{i=1}^m (\langle n_{i} \rangle_{gc})}{\delta_{ij}} \tag{28}
\]

For the case where \( \hat{A} \) is a product of \( m \) creation and \( m - 1 \) annihilation operators we return to the fermionic case with \( i \rightarrow l_m \) and \( \hat{A} = \hat{P}^{(m-1)} c_{i_m}^{\dagger} \) addressed in Eq. (23). As all \( l_i \) in \( \hat{P}^{(m)} \) differ, \( c_{i_m} \) commutes with \( \hat{P}^{(m-1)} \) i.e. \( [c_{i_m}, \hat{P}^{(m-1)} c_{i_m}^{\dagger}]_\pm = \hat{P}^{(m-1)} \) leading to

\[
\langle n_{i_1} \ldots n_{i_m} \rangle_{gc} = \langle n_{i_1} \ldots n_{i_{m-1}} \rangle_{gc} \langle n_{i_m} \rangle_{gc} \tag{29}
\]

Iteration leads to the complete factorization. Despite the fact that the direct derivation of Eq. (23) using the factorization of \( \rho^{(0)}_{gc} \) is much simpler, Gaudin’s method was shown, as an extension of it can be used also for the case of the canonical ensemble.
C. The canonical ensemble

As Eq. (22) also holds in the canonical ensemble one has again only to address expectation values of products of occupation number operators. In reference 3 a general expression for the expectation value of $m$-particle operators in the position and spin representation was presented. Their Eq. (2) leads for the expectation value of a product of $m$ different occupation number operators to

$$ \langle n_{l_1}...n_{l_m} \rangle_c = \sum_{k=m}^{N} (-1)^{k-m} Z_{N-k} s_{l_1l_2...l_m}^{(k)} $$

(30)

with

$$ s_{l_1l_2...l_m}^{(k)} = \sum_{j_1=1}^{k} \sum_{j_2=1}^{k} ... \sum_{j_m=1}^{k} e^{-\beta \sum_{i=1}^{m} j_i \epsilon_i} \delta_{j_1+j_2+...+j_m,k} \cdot $$

(31)

This generalizes the expressions for $m = 1$ and $m = 2$ presented in section II. For the case of bosons the factor $(-1)^{k-m}$ is missing. We return to this expression in appendix A.

In the following we propose a new approach to the calculation of $\langle n_{l_1}...n_{l_m} \rangle_c$ which provides analytical expressions in the limiting cases for the models discussed in section IV.

In the canonical ensemble the cyclic move of $c_i$ in the trace in Eq. (29) is not allowed as $c_{l_m} | N \rangle$ leaves the Hilbert space with fixed $N$. We therefore have to proceed differently here. We treat expectation values of the type $\langle A c_j^\dagger c_i \rangle$, where $j \neq i$ and $A$ is an arbitrary product of $m-1$ creation and $m-1$ annihilation operators. The cyclic move of $c_j^\dagger c_i$ in the trace in Eq. (29) is possible in the grand canonical as well as the canonical ensemble. Therefore no index for the expectation values is used in the following. The relation

$$ e^{\beta H_0} c_j^\dagger c_i e^{-\beta H_0} = e^{\beta (\epsilon_j - \epsilon_i)} c_j^\dagger c_i $$

(32)

holds without and with the tilde on $H_0$. In order to obtain an equation for $\langle A c_j^\dagger c_i \rangle$ we here use $c_j^\dagger c_i A = A c_j^\dagger c_i + [c_j^\dagger c_i, A]$, with the commutator for fermions as well as bosons after the cyclic move. This leads to

$$ \langle e^{\beta (\epsilon_i - \epsilon_j)} - 1 \rangle \langle A c_j^\dagger c_i \rangle = \langle [c_j^\dagger c_i, A] \rangle. $$

(33)

In order to solve this equation for $\langle A c_j^\dagger c_i \rangle$ the one-particle energies of the states $j$ and $i$ have to differ. We later discuss this condition in more detail and assume $\epsilon_i \neq \epsilon_j$ in the following. The choice $A = c_j^\dagger c_i$ leads to the simplest nontrivial relation. This gives a formula for $\langle c_i^\dagger c_j^\dagger c_i c_j \rangle = \langle n_i (1 - n_j) \rangle$. With $[c_j^\dagger c_i, c_j^\dagger c_j] = n_j - n_i$ Eq. (33) leads to

$$ \langle c_i^\dagger c_j^\dagger c_i c_j \rangle = \frac{\langle n_j \rangle - \langle n_i \rangle}{e^{\beta (\epsilon_i - \epsilon_j)} - 1}, $$

(34)

valid for both ensembles and fermions as well as bosons. A detailed discussion of this result in a slightly modified form will be presented later.

In the following we focus on $\langle P^{(m)} \rangle$ defined in Eq. (28). Only if the spectrum of one-particle energies $\epsilon_i$ is non-degenerate a complete treatment is possible as all quantum numbers $l_i$ in the product $P^{(m)}$ differ. This is e.g. the case for one-dimensional spinless fermions in an external potential, like a box potential or a harmonic well treated as an example in the next section.

Using the anticommutation rule we rewrite the last two occupation number operators in $P^{(m)}$ in the spirit of the simple example just discussed

$$ m_{l_{m-1}} n_m = n_{l_{m-1}} c_{l_{m-1}}^\dagger c_{l_m}^\dagger c_{l_m-1}^\dagger. $$

(35)

With

$$ \bar{A} = P^{(m-2)} c_{l_m-1}^\dagger c_{l_m} $$

(36)

the product of the occupation number operators is given by

$$ P^{(m)} = P^{(m-1)} - \bar{A} c_{l_m-1}^\dagger c_{l_m} $$

(37)

The commutator in Eq. (33) is readily evaluated as $c_{l_m-1}^\dagger c_{l_m} - \bar{A} c_{l_m} c_{l_m-1}^\dagger$ commutes with $P^{(m-2)}$. With $[c_{l_m}^\dagger c_{l_m-1}^\dagger c_{l_m}, c_{l_m-1}^\dagger c_{l_m}] = n_l - n_{l-1}$ used earlier one obtains

$$ \langle [c_{l_m}^\dagger c_{l_m-1}^\dagger, \bar{A}] \rangle = \langle P^{(m-1)} (n_{l_m} - n_{l_m-1}) \rangle. $$

(38)

From Eqs. (37) and (33) one obtains in the non-degenerate case assumed in the following

$$ \langle P^{(m)} \rangle = \frac{\langle P^{(m-2)} (n_{l_{m-1}}) \rangle e^{\beta \epsilon_{l_{m-1}}} - \langle P^{(m-2)} (n_{l_{m}}) \rangle e^{\beta \epsilon_{l_{m}}} \rangle}{e^{\beta \epsilon_{l_{m-1}}} - e^{\beta \epsilon_{l_{m}}} \rangle}. $$

(39)

This holds for the canonical as well as the grand canonical averages. For the case of the canonical ensemble this relation could have been found earlier by using Eqs. (38) and (31) (see appendix A).

For $m = 2$ this equation reads

$$ \langle n_{l_1} n_{l_2} \rangle = \frac{\langle n_{l_1} e^{\beta \epsilon_{l_1}} - \langle n_{l_2} e^{\beta \epsilon_{l_2}} \rangle}{e^{\beta \epsilon_{l_1}} - e^{\beta \epsilon_{l_2}}} \rangle. $$

(40)

This is a slightly different version of Eq. (43).

As a test for the grand canonical ensemble one can put in the Fermi functions for the $\langle n_{l_i} \rangle$ and readily see the factorization which holds in contrast to the canonical ensemble. The deviations from the factorization in this case will be quantitatively studied for simple models in the next section.

With the result for $m = 2$ the calculation of $\langle P^{(3)} \rangle$ using Eq. (39) suggests the following general result

$$ \langle n_{l_1}...n_{l_m} \rangle = \sum_{i=1}^{m} \langle n_{l_i} \rangle \prod_{j \neq i} e^{\beta \epsilon_{l_i}} e^{\beta \epsilon_{l_j}} \rangle. $$

(41)
It is obviously fulfilled for \( m = 2 \). If this is inserted on the right hand side of Eq. (39) for the expectation values of \( m - 1 \) occupation number operators, simple algebra presented in Appendix B completes the inductive proof of Eq. (41). Together with Eq. (22) this shows that one can express the expectation value of an arbitrary \( m \)-particle operator in terms of the expectation values \( \langle n_i \rangle_c \) also within the canonical ensemble. Obviously this new result is more complicated than Wick’s theorem Eq. (23) for the grand canonical average. The complete factorization in this case easily follows from Eq. (41). This is also shown in Appendix B.

From the fact that the use of the Fermi functions in Eq. (41) leads to the factorization of the expectation value one expects that the deviations from Wick’s theorem in the canonical ensemble are large for quantum numbers \( l_i \) where the \( \langle n_i \rangle_c \) differ strongly from \( \langle n_i \rangle_{gc} \). To test this quantitatively we calculate the “Wick ratio”

\[
r_W(l_1, l_2)(T, N) \equiv \frac{\langle n_{l_1} n_{l_2} \rangle_c}{\langle n_{l_1} \rangle_c \langle n_{l_2} \rangle_c}
\]

as well as the correspondingly defined Wick ratio for higher products of occupation number operators for special models. The deviation from Wick’s theorem is quantified by how much \( r_W \) differs from one.

### IV. APPLICATIONS

In this section we present quantitative results for the deviation from Wick’s theorem in the canonical ensemble for two rather different models.

Fermions in one dimension in a harmonic potential are an example of a system with an equidistant one-particle spectrum. Such a system can be realized in ultracold gases [9]. In the non-interacting case exact results for the thermodynamic properties and the mean occupation numbers can be obtained with a recursive method [10]. Here we use these results for the mean occupation numbers in Eqs. (40) and (41) to calculate expectation values of products of occupation number operators for arbitrarily large numbers \( N \) of fermions. This model also plays an important role in the context of the Tomonaga-Luttinger model [11].

In order to address the problem of Eqs. (40) and (41) with degeneracies of the one-particle energies a simple “semiconductor model” is studied with zero width of the valence and conduction bands. The particle number \( N \) is chosen to be equal to the number of valence band states. For this simple model a direct combinatorial method can be used to calculate the canonical mean occupation numbers. It avoids the numerical problems when using Eq. (13) and easily allows to understand how the grand canonical results arises in the large \( N \) limit.

#### A. Fermions in a one-dimensional harmonic trap

We consider \( N \) noninteracting spinless fermions in a system with nondegenerate equidistant one-particle energies \( \epsilon_i \)

\[
\epsilon_i = i \Delta , \quad i = 1, 2, 3, ..., \infty . \tag{43}
\]

By performing the sum over \( n_1 \) in Eq. (4) only, as a first step, a recursive approach leads to an explicit analytical expression for \( Z_N \) [10]. This canonical partition function has the form as for a system of \( N \) uncoupled harmonic oscillators with frequencies \( \omega_m = m\Delta/h, \ m = 1, ..., N \). Proceeding similarly for the mean occupation numbers one obtains the recursion relation [10]

\[
\langle n_i \rangle_N = e^{-\beta \Delta}\langle n_{i-1} \rangle_N + (1 - e^{-\beta \Delta})\langle n_{i-1} \rangle_{N-1}. \tag{44}
\]

Together with the “Schmidt relation” Eq. (13) one can obtain a recursion relation between the mean occupation numbers with the same total particle number only

\[
\langle n_{i+1} \rangle_N = 1 - e^{-\beta \Delta} - (e^{-\beta(N-i)} - e^{-\beta \Delta})\langle n_i \rangle_N . \tag{45}
\]

Using it with \( \langle n_1 \rangle_N = 1 - e^{-\beta \Delta} \) as the starting point, provides an “upward” way to calculate the \( \langle n_i \rangle_N \). Alternatively one can use Eq. (45) to express \( \langle n_i \rangle_N \) in terms of \( \langle n_{i+1} \rangle_N \) and start the downward iteration for \( m + 1 \gg N \) with \( \langle n_{m+1} \rangle_N = 0 \). Together this provides an efficient numerically stable procedure to calculate the mean occupation numbers. In the general case one has to compare \( k_BT \) with two energy scales, \( \Delta \) and \( N \Delta \). In the scaling limit \( N \to \infty \) with fixed \( \beta \Delta \) the recursion relation Eq. (45) for \( \bar{n}_t \equiv \langle n_{N+i} \rangle_N \) simplifies to

\[
\bar{n}_{i+1} = 1 - q^{-i} \bar{n}_i , \quad \bar{n}_i = q^i(1 - \bar{n}_{i+1}) , \tag{46}
\]

whith \( q = e^{-\beta \Delta} \). For 1d fermions with a linear dispersion this scaling limit corresponds to the addition of an infinite “Dirac sea” [12]. Due to the symmetry relation [10]

\[
\bar{n}_{-i} = 1 - \bar{n}_{i+1} \tag{47}
\]

only the upward or the downward recursion has to be used. As long as \( k_BT \ll N \Delta \) holds, Eq. (46) provides an excellent approximation for very large but finite \( N \). Only how \( k_BT \) compares to \( \Delta \) matters in this limit. For \( (N \Delta \gg k_BT \gg \Delta \) the \( \bar{n}_i \) approach the grand canonical Fermi function \( f_l = 1/(e^{\beta(-l/2)\Delta} + 1) \), while for \( k_BT \ll \Delta \) there are appreciable deviations [10].

After this summary of previous results we address the Wick ratio \( r_W \) for this model. With the definition \( \bar{n}_l \equiv \langle \bar{n}_{N+i} \rangle_N \) Eq. (45) reads

\[
\langle n_{N+i}n_{N+i} \rangle = \frac{\bar{n}_{i+1} - q^i \bar{n}_i}{1 - q^i} \tag{48}
\]

For arbitrary values of \( i \) and \( l \) the expectation value \( \langle n_{N+i}n_{N+i} \rangle \) follows from the numerical values for the
mean occupation numbers. As in the scaling limit $N \to \infty$ various analytical results can be obtained we focus on this limit where Eq. (46) can be used to obtain the mean occupation numbers.

In Fig. 1 we present results for the Wick ratio $r_{W}^{i,i,i} = \langle (n_{N+i}n_{N+i})/\bar{n}_{i}\rangle$ for $q = 0.75$ as a function of $l \neq 0$ for different values of $i$. The asymptotic values for large positive and negative values of $l$ are discussed in the text.

For $i \gg 1$ and $j = 1,2,3$ the expectation values $\bar{n}_{i+j}$ are again using Eq. (46) to a sufficient approximation given by $q^{i+j}$. This yields $\langle P_{i}^{(3)} \rangle_{c} \approx q^{i}q^{i+1}q^{i+2}q^{3}$, i.e. 

$$\langle n_{N+i,N+i+1,N+i+2} \rangle_{c} \approx \bar{n}_{i}\bar{n}_{i+1}\bar{n}_{i+2} q^{3}.$$  

For large $l$ the Wick ratio $r_{W}^{i,i+1,i+2}$ is therefore given by $q^{i}$ in agreement with the numerical results in Fig. 2 for $q = 0.5$ and 0.75. For $q = 0.9$ one has to go larger values of $i$ to see the asymptotic behaviour.

Realistic values of $q$ differ for the two applications of this model mentioned earlier. For fermions in a 1d harmonic trap the value of the temperature and $\Delta$ can be independently experimentally tuned, i.e. $q$ can be chosen quite arbitrarily. For free fermions with a linearized dispersion $\Delta \sim 1/L$ holds for box of length $L$ and the limit $L \to \infty$ leads to $q \to 1$, implying a Wick ratio of one as in the grand canonical ensemble.

**B. Zero bandwidth semiconductor model**

A simple model with $M$ degenerate valence band states and $M$ degenerate conduction band states is considered

$$H = \sum_{i=1}^{M} \epsilon_{v_{i}}c_{v_{i}}^\dagger c_{v_{i}} + (\epsilon_{v} + \Delta)c_{v}^\dagger c_{v} = \epsilon_{v}N_{v} + (\epsilon_{v} + \Delta)N_{c}.$$  

(54)

In the following we put $\epsilon_{v} = 0$. Despite the fact that the general case $N \neq M$ is as easily treated as the special case $N = M$, we only present results for the latter in the following. In this case the $N$-fermion ground state is given by the filled valence band. The excited states have $m$ holes in the valence band and $m$ particles in the conduction band. The number of ways to chose $m$ holes in the $N$ valence band states is given by $\binom{N}{m}$. The same result is obtained for the number of ways to put the $m$


particles in the conduction band. Therefore the canonical partition function is given by

$$Z_N = \sum_{m=0}^{N} \left( \frac{N}{m} \right)^2 e^{-m\beta\Delta}. \quad (55)$$

In order to obtain the mean occupation numbers \(\langle n_{c,i}\rangle_c\) for \(\alpha = v, c\) it is sufficient to calculate \(\langle N_{c}\rangle_c\) as \(\langle n_{c,i}\rangle_c\) does not depend on \(i\) and \(\langle N_{v}\rangle_c + \langle N_{c}\rangle_c = N\) holds. Introducing the probability distribution \(p_N(m)\) for the number of electrons in the conduction band the mean occupation of the conduction band is given by

$$\langle N_{c}\rangle_c = \sum_{m=0}^{N} mp_N(m); \quad p_N(m) = \frac{1}{Z_N} \left( \frac{N}{m} \right)^2 e^{-m\beta\Delta}. \quad (56)$$

For not too small values of \(q = e^{-\beta\Delta}\) the probability distribution \(p_N(m)\) for large \(N\) resembles a Gaussian distribution as shown in Fig. 3 for \(N = 50\). For \(k_BT/\Delta = 0.5\) also the grand canonical result is shown for comparison (filled squares). While its average value is close to the canonical result its width is significantly larger. This is discussed quantitatively later.

In the grand canonical ensemble the chemical potential lies in the middle of the bands, \(\mu = \Delta/2\), for the case \(N = M\) considered here. This guarantees \(\langle N\rangle_{gc} = N\) for all temperatures

$$f_c \equiv \langle n_{c,i}\rangle_{gc} = \frac{1}{e^{\beta\Delta/2} + 1} = 1 - \langle n_{v,i}\rangle_{gc}. \quad (57)$$

This is in contrast to the general case \(N \neq M\), in which the chemical potential is temperature dependent. Due to the factorization of \(\rho_{gc}^{(0)}\) the conduction band states \(c, i\) are independently empty with probability \(1 - f_c\) and filled with probability \(f_c\). Therefore the grand canonical distribution function is binomial

$$p_{gc}(m) = \sum_{m=0}^{N} \left( \frac{N}{m} \right) f_c^m (1 - f_c)^{N-m}. \quad (58)$$

with average value \(Nf_c\) and mean square deviation \(Nf_c(1 - f_c)\). The transition of a binomial distribution to a Gaussian distribution in the large \(N\)-limit discussed in textbooks on statistical mechanics. Before addressing the width of \(p_N(m)\) the average occupation numbers \(\langle n_{c,i}\rangle_c\) and \(f_c\) are compared.

In Fig. 4 we show results from the numerical evaluation of \(\langle n_{c,i}\rangle_c\) using Eq. (56). For small values of \(N\) the deviations of the canonical from the grand canonical result are rather large. In the high temperature limit the grand canonical result is approached.

In the extreme low temperature limit \(N^2e^{-\beta\Delta} \ll 1\) one approximately has \(\langle n_{c,i}\rangle \approx N e^{-\beta\Delta}\) which deviates strongly from the grand canonical result \(\approx e^{-\beta\Delta/2}\).

In the large \(N\) limit \(\langle N_{c}\rangle \approx \bar{m}\) where \(\bar{m}\) is the position of the maximum of \(p_N(m)\). Using the Stirling formula \(m! \approx \sqrt{2\pi m/(e^m)}\) valid for \(m \gg 1\) the variable \(m\) in \(p_N(m)\) can be treated as continuous and the position \(\bar{m}\) of the maximum of \(p_N(m)\) is easily obtained setting the derivative of \(p_N(m)\) or \(\ln(p_N(m))\) to zero. With \(d \ln m!/dm \approx \ln m\) one obtains

$$\frac{d \ln(p_N(m))}{dm} \approx 2 \left[ -\ln m + \ln(N - m) \right] + \ln q \quad = 2 \ln \left( \frac{N - m}{m} q^{1/2} \right). \quad (59)$$

Putting the argument of the logarithm equal to 1 the position of the maximum follows as \(\bar{m} = N/(q^{-1/2} + 1)\). With \(q = e^{-\beta\Delta}\) and \(\langle n_{c,i}\rangle = \langle N_{c}\rangle/N\) one finally obtains
in the large $N$ limit

$$
\langle n_{i,i} \rangle_c \rightarrow \frac{1}{e^{\beta \Delta/2} + 1} = \langle n_{i,i} \rangle_{gc} .
$$  

(60)

Next we address the expectation values $\langle n_{\alpha,i n_{\beta,j}} \rangle_c$ with $i \neq j$ when $\alpha = \beta$, in the canonical ensemble. As they are independent of $i$ and $j$ there are only three different types: the $\langle n_{\alpha,i n_{\alpha,j}} \rangle_c$ with $\alpha = \nu$ or $c$ and $\langle n_{c,i n_{\nu,j}} \rangle_c$. The value of the latter follows easily from Eq. (40). As shown in the following the $\langle n_{\alpha,i n_{\alpha,j}} \rangle_c$ are determined by $\langle n_{\alpha,i n_{\nu,j}} \rangle_c$ and $\langle n_{c,i} \rangle_c$. This stems from the fact that $\langle N_c N_v \rangle_c$ can be expressed in terms of $\langle N^2 \rangle_c$ and $\langle N \rangle_c$

$$
\langle N_c N_v \rangle_c = \sum_{m=0}^N m(N - m)p_N(m) = N\langle N \rangle_c - \langle N^2 \rangle_c
$$  

(61)

and with $m(N - m) = N(N - m) - (N - m)^2$ the index $c$ on the right hand side can be replaced by $v$. Using $\langle N_c N_v \rangle_c = N^2\langle n_{c,i n_{\nu,j}} \rangle_c$ this implies

$$
\langle N^2 \rangle_c = N^2(\langle n_{\alpha,i} \rangle_c - \langle n_{c,i n_{\nu,j}} \rangle_c) .
$$  

(62)

For $i \neq j$ one has $\langle N^2 \rangle_c = N(N - 1)\langle n_{\alpha,i n_{\alpha,j}} \rangle_c + N\langle n_{c,i} \rangle_c$. This leads to the promised result

$$
\langle n_{\alpha,i n_{\alpha,j}} \rangle_c = \langle n_{\alpha,i} \rangle_c - \frac{N}{N - 1}\langle n_{c,i n_{\nu,j}} \rangle_c .
$$  

(63)

This allows to calculate the $\langle n_{\alpha,i n_{\alpha,j}} \rangle_c$ in terms of $\langle n_{\alpha,i} \rangle_c$ and $\langle n_{c,i n_{\nu,j}} \rangle_c$ by Eq. (63) gives

$$
\langle n_{c,i n_{\nu,j}} \rangle_c = \frac{\langle n_{c,i} \rangle_c - e^{-\beta \Delta}(1 - \langle n_{c,i} \rangle_c)}{1 - e^{-\beta \Delta}} .
$$  

(64)

If $\langle n_{c,i n_{\nu,j}} \rangle_c$ factorizes in the limit $N \to \infty$ Eq. (63) implies the same for the $\langle n_{\alpha,i n_{\alpha,j}} \rangle_c$ for $i \neq j$.

In Fig. 5 we show the Wick ratios $r^w_W$, $r^w_V$ and $r^{cc}_W$ as a function of temperature for $N = 4$ and $N = 20$. The limiting values for $T \to 0$ and $T \to \infty$ can be understood analytically. At $T = 0$ the valence band is completely occupied, i.e. $\langle n_{\nu,i} \rangle_c = 1 = \langle n_{c,i n_{\nu,j}} \rangle_c$. This implies

$$
r^w_W(T = 0, N) = 1 .
$$  

(65)

As at zero temperature the conduction band is empty $\langle n_{c,i} \rangle_c = 0$, $\langle n_{c,i n_{\nu,j}} \rangle_c = 0$ and $\langle n_{c,i n_{\nu,j}} \rangle_c = 0$. For the Wick ratios $r^w_W$ and $r^{cc}_W$ one therefore encounters a “0/0” problem and the limit $T \to 0$ has to be studied. As mentioned earlier, in the extreme low temperature limit $\langle n_{c,i} \rangle_c \equiv N e^{-\beta \Delta} \ll 1$ holds. With Eq. (64) this leads to

$$
r^w_W(T \to 0, N) = 1 - \frac{1}{N} .
$$  

(66)

Alternatively this can be obtained by simple combinatorics. As the state $v, j$ is supposed to be occupied there are $N - 1$ ways to promote a valence electron to the state $c, i$, leading to $\langle n_{c,i n_{\nu,j}} \rangle_c \approx (N - 1)e^{-\beta \Delta}$. With

$$
\langle n_{c,i} \rangle_c(1 - \langle n_{c,i} \rangle_c) \approx \langle n_{c,i} \rangle_c \approx N e^{-\beta \Delta}
$$

this leads to the result in Eq. (66). We finally address the $T \to 0$ limit of $r^{cc}_W$. There are $N(N - 1)/2$ ways to put two electrons into two prescribed conduction band states, leading to $\langle n_{c,i n_{c,j}} \rangle_c \approx N(N - 1)e^{-2\beta \Delta}/2$. With the result for $\langle n_{c,i} \rangle_c$ one obtains

$$
r^{cc}_W(T \to 0, N) = \frac{1}{2} \left( 1 - \frac{1}{N} \right) .
$$  

(67)

In the high temperature limit $T \to \infty$ simply counting numbers of states determines $\langle n_{\alpha,i n_{\beta,j}} \rangle_c$ with $\alpha, i$ differing from $\beta, j$. The number of ways to put two fermions in these two one-particle states and the other $N - 2$ particles into the remaining $2N - 2$ states is given by $\binom{2N - 2}{N - 2}$ and the partition function by the total number of possible states $\binom{2N}{N}$. This leads to

$$
T \to \infty : \quad r_W \to \frac{1 - 1/N}{1 - 1/(2N)}
$$  

(68)

independently of the upper indices. Without the combinatorics just presented, this value of $r_W$ can be obtained from Eq. (68) realizing that the $\langle n_{\alpha,i n_{\beta,j}} \rangle_c$ with $\alpha, i \neq \beta, j$ are all the same in the infinite temperature limit. One can solve this equation for $x = \langle n_{c,i n_{\nu,j}} \rangle_c = \langle n_{\alpha,i n_{\alpha,j}} \rangle_c$ using $\langle n_{\alpha,i} \rangle_c = 1/2$ and obtains the result of Eq. (68).

In Fig. 6 we show the Wick ratio $r^w_W$ as a function of $1/N$ for different values of $k_BT/\Delta$. The results lie between the “curves” determined by Eqs. (60) and (68). For large $N$ the infinite temperature result is reached quickly with increasing temperature.

We now return to the comparison of the widths of $p_N$ and $p_{gc}$ both shown for $k_BT/\Delta = 0.5$ in Fig. 3. The mean square deviation $\sigma^2$ for both cases is given by

$$
\sigma^2 = \langle N^2_c \rangle - \langle N \rangle^2 = N^2(\langle n_{c,i n_{c,j}} \rangle_c - \langle n_{c,i} \rangle^2) + N\langle n_{c,1} \rangle - \langle n_{c,i n_{c,2}} \rangle_c
$$  

(69)
of $\sigma N$ in the grand canonical case is approximately given by $N$ occupation number operators of one-particle states which can be very large at low temperatures if the product involves numerical approaches presented earlier. The deviations can understand of the deviations from Wick’s theorem in the grand canonical ensemble. To arbitrary order of the products the expectation values are expressed in terms of the expectation values are expressed in terms of the second term is

\[ 0.9 \]

and upper boundary curve of the results are discussed in the text.

Using Wick’s theorem for the grand canonical case the first term on the right hand side vanishes, leading to

\[ (\sigma_c^2)_{gc} = N f_c (1 - f_c) \]

as mentioned earlier.

For the canonical ensemble $\sigma_c^2$ can be expressed in terms of $\langle n_{c,i} \rangle_c$ and $r_W^{(c)}$ as

\[
(\sigma_c^2) = N^2 \langle n_{c,1} \rangle_c^2 (r_W^{(c)} - 1) + N \langle n_{c,1} \rangle_c - r_W^{(c)} \langle n_{c,1} \rangle_c^2 \tag{70}
\]

For large $N$ and not too low temperatures $r_W^{(c)} - 1 \approx -1/(2N)$ holds and the first term of $\sigma_c^2$ which vanishes in the grand canonical case is approximately given by $-N \langle n_{c,1} \rangle_c^2 / 2$. To leading order in $N$ the second term is given by $N \langle n_{c,1} \rangle_c (1 - \langle n_{c,1} \rangle_c) \approx N f_c (1 - f_c)$. In the high temperature limit $(\sigma_c^2)_{gc} \approx 2 (\sigma_c^2)_{c}$ holds, i.e. the width of $p_c$ is larger by a factor $\sqrt{2}$ than that of $p_N$ as can be confirmed in Fig. 3.

V. SUMMARY

With an approach similar to Gaudin’s proof of Wick’s theorem for the grand canonical ensemble new results for expectation values of products of occupation numbers of one-particle states with differing one-particle energies were presented in Eqs. (30a) and (31a). They are valid for the grand canonical as well as the canonical ensemble. To arbitrary order of the products the expectation values are expressed in terms of the average occupation numbers. For two different models it was explicitly shown that these relations allow a deeper understanding of the deviations from Wick’s theorem in the canonical ensemble which go beyond the purely numerical approaches presented earlier. The deviations can be very large at low temperatures if the product involves occupation number operators of one-particle states which are unoccupied at zero temperature.

VI. ACKNOWLEDGEMENTS

The author wants to thank V. Meden and W. Zwerger for a critical reading of the manuscript and useful comments.

Appendix A: Alternative derivation of Eq. (40)

Here we show how Eq. (39) for the canonical ensemble could have been found using Eqs. (30a) and (31a).

In Eq. (39) the sums in $s_{1\ldots l_m}^{(k)}$ run from 1 to $k$. As $j_i \geq 1$ for all $i$ it is obvious that the largest value a $j_i$ can take is $k - m + 1$. As the upper limit of the sums one can also take $\infty$, as the Kronecker delta does its job. Therefore in the following upper limits of the sums are suppressed.

If one multiplies $s_{1\ldots l_m}^{(k)}$ by $e^{\beta \epsilon_m}$ this leads after changing the summation index $j_m$ by one to

\[
e^{\beta \epsilon_m} s_{1\ldots l_m}^{(k)} = \sum_{j_1=1}^{k} \sum_{j_2=1}^{k} \ldots \sum_{j_m=0}^{k} e^{-\beta \sum_{i=1}^{m} j_i \epsilon_i} \delta_{j_1 + \ldots + j_m, k-1}
\]

\[
e^{\beta \epsilon_m} s_{1\ldots l_m}^{(k)} = s_{1\ldots l_m-1}^{(k-1)} + s_{1\ldots l_m-1}^{(k-1)} \tag{A1}
\]

In taking the difference with the according expression where one multiplies with $e^{\beta \epsilon_{m-1}}$, the second terms cancel and one obtains

\[
e^{\beta \epsilon_m - e^{\beta \epsilon_{m-1}}} s_{1\ldots l_m}^{(k)} = s_{1\ldots l_m-1}^{(k-1)} - s_{1\ldots l_m-2}^{(k-1)} \tag{A2}
\]

Eq. (A1) reads for $m \to m - 1$

\[
e^{\beta \epsilon_{m-1}} s_{1\ldots l_m-1}^{(k)} = s_{1\ldots l_m-2}^{(k-1)} + s_{1\ldots l_m-2}^{(k-1)} \tag{A3}
\]

If one performs the corresponding multiplication with $e^{\beta \epsilon_m}$ and takes the difference the comparison with Eq. (A2) yields

\[
e^{\beta \epsilon_m - e^{\beta \epsilon_{m-1}}} s_{1\ldots l_m}^{(k)} = e^{\beta \epsilon_{m-1}} s_{1\ldots l_m-1}^{(k)} - e^{\beta \epsilon_{m}} s_{1\ldots l_m-2}^{(k)} \tag{A4}
\]

Inserting this into Eq. (39) leads to

\[
e^{\beta \epsilon_{m-1}} - e^{\beta \epsilon_{m}} \langle n_{1\ldots l_{m-1}} \rangle_c = \langle n_{1\ldots l_{m-1}} \rangle e^{\beta \epsilon_{m-1}} - \langle n_{1\ldots l_{m-2}l_m} \rangle e^{\beta \epsilon_{m}} \tag{A5}
\]

For $\epsilon_{m-1} \neq \epsilon_{m}$ division proves Eq. (39) in a way different from the one presented in section III.

Appendix B: Induction step in the proof of Eq. (31)

In this appendix the inductive step in the proof of Eq. (31) is presented. Using the abbreviation $x_i = e^{\beta \epsilon_i}$ we assume the formula

\[
\langle n_{1\ldots l_{m-1}} \rangle = \sum_{i=1}^{m-1} \langle n_{i} \rangle \prod_{j

j \neq i}^{m-1} x_i / x_j \tag{B1}
\]
we show that formula Eq. (B1) also holds for m

\[
\langle P^{(m)} \rangle = \frac{\langle P^{(m-2)}n_{l_{m-1}} \rangle x_{m-1} - \langle P^{(m-2)}n_{l_m} \rangle x_m}{x_{m-1} - x_m}.
\]

(B2)

we show that formula Eq. (B1) also holds for m. In both \( \langle P^{(m-2)}n_{l_k} \rangle \) with \( k = m - 1 \) and \( k = m \) all occupation number operators \( n_i \) with \( j \leq m - 2 \) occur. In contrast \( n_{l_{m-1}} \) and \( n_{l_m} \) only appear in one of the two expectation values in Eq (B2). A term proportional to \( \langle n_{l_{m-1}} \rangle \) only results from the first expectation value. Its contribution to \( \langle P^{(m)} \rangle \) is given by

\[
\frac{x_{m-1}}{x_{m-1} - x_m} \prod_{j=1}^{m-2} \frac{x_{m-1}}{x_{m-1} - x_j} = \prod_{j(\neq m-1)} x_{m-1} - x_j.
\]

(B3)

The term proportional to \( \langle n_{l_m} \rangle \) results from the second expectation value

\[
\frac{x_m}{x_m - x_{m-1}} \prod_{j=1}^{m-2} \frac{x_m}{x_m - x_j} = \prod_{j(\neq m)} x_m - x_j.
\]

(B4)

For the terms proportional to \( \langle n_{l_i} \rangle \) with \( j \leq m - 2 \) it is sufficient to consider a single example e.g. \( \langle n_{l_1} \rangle \). With \( p_{m-2}^{(1)} = \prod_{j=2}^{m-2} x_1/(x_1 - x_j) \) and using the recursion relation Eq. (B2) the contribution proportional to \( \langle n_{l_1} \rangle \) in \( \langle P^{(m)} \rangle \) is given by

\[
\frac{1}{x_{m-1} - x_m} p_{m-2}^{(1)} \left( \frac{x_1 x_{m-1}}{x_1 - x_{m-1}} - \frac{x_1 x_m}{x_1 - x_m} \right) = \prod_{j=2}^m \frac{x_1}{x_1 - x_j}.
\]

(B5)

This completes the inductive step for the proof of Eq. (41).

The proof that \( \langle P^{(m)} \rangle \) completely factorizes for the grand canonical average is again easier by induction. For \( m = 2 \) one has

\[
\langle n_{l_1} n_{l_2} \rangle_{gc} = \frac{x_1 \langle n_{l_1} \rangle_{gc} - x_2 \langle n_{l_2} \rangle_{gc}}{x_1 - x_2} = \frac{x_1(x_2 + 1) - x_2(x_1 + 1)}{(x_1 - x_2)(x_1 + 1)(x_2 + 1)} = \langle n_{l_1} \rangle_{gc} \langle n_{l_2} \rangle_{gc}
\]

(B6)

Now we assume that \( \langle P^{(m-1)} \rangle_{gc} \) completely factorizes and use Eq. (B2) for the induction step. This assumption implies \( \langle P^{(m-2)}n_{l_k} \rangle_{gc} \) with \( k = m - 1 \) and \( k = m \) factorizes as \( \langle P^{(m-2)}n_{l_k} \rangle_{gc} = \langle P^{(m-2)} \rangle_{gc} \langle n_{l_k} \rangle_{gc} \). This implies with Eq. (B2)

\[
\langle n_{l_1} \ldots n_{l_m} \rangle_{gc} = \langle P^{(m-2)} \rangle_{gc} \frac{x_{m-1} \langle n_{l_{m-1}} \rangle_{gc} - x_{m-1} \langle n_{l_{m-1}} \rangle_{gc}}{x_{m-1} - x_m} = \prod_{i=1}^m \langle n_{l_i} \rangle_{gc}.
\]

(B7)

This proof is certainly more involved than the one in subsection IIIb.

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