# Calculations of canonical averages from the grand canonical ensemble

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Grand canonical and canonical ensembles become equivalent in the thermodynamic limit, but when the system size is finite the results obtained in the two ensembles deviate from each other. In many important cases, the canonical ensemble provides an appropriate physical description but it is often much easier to perform the calculations in the corresponding grand canonical ensemble. We present a method to compute averages in the canonical ensemble based on calculations of the expectation values in the grand canonical ensemble. The number of particles, which is fixed in the canonical ensemble, is not necessarily the same as the average number of particles in the grand canonical ensemble.

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## I. INTRODUCTION

Whenever we need to work with a system of many quantum particles it is much easier to perform the calculation in the grand canonical ensemble than to do the corresponding calculations in the canonical ensemble. For example, the calculation of the grand canonical partition function for an ideal gas of fermions or bosons is trivial, whereas the computation of the canonical partition function for the same system becomes a formidable task even for a small number of particles. Provided that the system is thermodynamically large, the canonical and grand canonical descriptions agree with each other. There are many quantum systems where the canonical description is more appropriate; these include hot nuclei [1], ultrasmall metallic grains [2], Bose and Fermi gases in atomic traps [3,4], and atoms in plasmas [5]. Therefore, it is important to have a practical theoretical and computational method which enables us to extract canonical averages from corresponding grand canonical calculations.

The problem that we would like to solve in this paper is the following. Suppose that we can perform calculations (or measurements) in the grand canonical ensemble which is characterized by temperature $T$ and chemical potential $\mu$. We would like to compute expectation values of an arbitrary quantity $O$ in the canonical ensemble with temperature $T$ and the number of particles $n$ by using only the averages in the grand canonical ensemble. The number of particles $n$, which is fixed in the canonical ensemble, is not necessarily the same as the average number of particles $\langle N\rangle$ in the grand canonical ensemble.

Earlier works on particle number projection in grand canonical ensembles have been performed to treat hot nuclei [1,6–8], and Bose-Einstein condensation [3,4,9] and to formulate a canonical statistical mean field approximation for mesoscopic systems [10]. Our approach is very different. First, we do not rely on projection operators but extract information from the grand canonical averages by inverting the fluctuation matrix. Second, $\langle N\rangle$ does not necessarily equal $n$ although it might.

## II. THEORY

A quantum mechanical system has the Hamiltonian $H$. The Hamiltonian $H$ commutes with the particle number operator $N$,

$$[H,N]=0. \tag{1}$$

Therefore the Hamiltonian and the particle number operator have the same set of eigenvectors:

$$N|n\alpha\rangle = n|n\alpha\rangle, \tag{2}$$

$$H|n\alpha\rangle = E_{n\alpha}|n\alpha\rangle. \tag{3}$$

Let $O$ be an arbitrary operator. The average in the grand canonical ensemble is

$$\langle O\rangle = \frac{1}{Z}\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}\langle n\alpha|O|n\alpha\rangle, \tag{4}$$

with $Z$ being the grand canonical partition function,

$$Z=\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}, \tag{5}$$

and $\beta = 1/kT$. The average in the canonical ensemble is

$$\langle O\rangle_n = \frac{1}{Z_n}\sum_{\alpha} e^{-\beta E_{n\alpha}}\langle n\alpha|O|n\alpha\rangle, \tag{6}$$

with $Z_n$ being the canonical partition function,

$$Z_n = \sum_{\alpha} e^{-\beta E_{n\alpha}}. \tag{7}$$

We can consider $\langle O\rangle_n$ as a function of $n$ and expand it as a power series

$$\langle O\rangle_n = \sum_{k=0}^{\infty} q_k n^k. \tag{8}$$

With this expansion the grand canonical average (4) becomes (Appendix A)

$$\langle O\rangle = \left\langle \sum_{k=0}^{\infty} q_k N^k \right\rangle. \tag{9}$$

Next, we take the canonical expectation value and add or subtract the grand canonical average,

    

$$\langle O\rangle_n = \sum_{k=0}^{\infty} q_k n^k + \langle O\rangle - \left\langle \sum_{k=0}^{\infty} q_k N^k \right\rangle. \quad (10)$$

Then we cancel the $k=0$ terms in both sums, and the canonical expectation value becomes

$$\langle O\rangle_n = \langle O\rangle - \sum_{k=1}^{\infty} q_k(\langle N^k\rangle - n^k). \quad (11)$$

This expression for the canonical average of the operator $O$ involves only grand canonical expectation values. The coefficients $q_k$ are yet to be calculated. To determine them we introduce the operator

$$\bar{O} = O - \sum_{k=1}^{\infty} q_k N^k \quad (12)$$

and compute the expectation value $\langle \bar{O} f(N)\rangle$, where $f(N)$ is an arbitrary function of $N$. We show in Appendix A that this expectation value can be split:

$$\langle \bar{O} f(N)\rangle = \langle \bar{O}\rangle\langle f(N)\rangle. \quad (13)$$

Since $f(N)$ is an arbitrary function of $N$, Eq. (13) is equivalent to the following system of equations:

$$\langle \bar{O}N\rangle = \langle \bar{O}\rangle\langle N\rangle,$$

$$\langle \bar{O}N^2\rangle = \langle \bar{O}\rangle\langle N^2\rangle,$$

$$\vdots$$

$$\langle \bar{O}N^k\rangle = \langle \bar{O}\rangle\langle N^k\rangle,$$

$$\vdots . \quad (14)$$

If we use the explicit form for operator $\bar{O}$ (12), the system of equations (14) becomes

$$\sum_{k=1}^{\infty} q_k A_{km} = \langle ON^m\rangle - \langle O\rangle\langle N^m\rangle, \quad (15)$$

where the matrix $A_{km}$ is built from the fluctuations

$$A_{km} = \langle N^{k+m}\rangle - \langle N^k\rangle\langle N^m\rangle. \quad (16)$$

The system of linear algebraic equations (15) along with the expansion represents the main result of the paper. Similar equations (although for the case $\langle N\rangle = n$) were obtained by the methods of thermofield dynamics in the context of superconducting nuclei at finite temperature [11,12].

It can be readily shown by the direct differentiation of the partition function (5) that

$$A_{km} = \frac{1}{Z^2\beta^{k+m}}\left( Z\frac{\partial^{k+m}Z}{\partial\mu^{k+m}} - \frac{\partial^k Z}{\partial\mu^k}\frac{\partial^m Z}{\partial\mu^m}\right). \quad (17)$$

Now we prove the convergence of the expansion (11). It is possible to demonstrate, based on simple considerations, that the difference between the canonical and grand canonical averages is [13]

$$\langle O\rangle - \langle O\rangle_n \sim \frac{1}{\langle N\rangle}. \quad (18)$$

The calculation in Appendix C shows that for $k>1$

$$q_k \sim 1/\langle N\rangle^k. \quad (19)$$

Suppose that $n=\langle N\rangle$. Then $(\langle N^k\rangle - n^k) \sim \langle N\rangle^{k-1}$ for large $\langle N\rangle$. Therefore, the corrections to the grand canonical average in Eq. (11) become in this case

$$\sum_{k=1}^{\infty} q_k(\langle N^k\rangle - n^k) \simeq \frac{1}{\langle N\rangle}\sum_{k=1}^{\infty} c_k, \quad (20)$$

where $c_k$ are some coefficients. Comparing (18) and (20) we see that $\Sigma_{k=1}^{\infty} c_k$ is finite. This means that the expansion (11) converges when $\langle N\rangle = n$. We would like to note at this point that each term in the sum (11) is $\sim 1/\langle N\rangle$. This means that the method becomes computationally efficient when it is applied to large systems, since one needs to include fewer terms in the expansion to achieve the same accuracy in this case. Let us consider the corrections to the grand canonical average in Eq. (11) for the case $n=\langle N\rangle + j$, where $j$ is some integral number,

$$\langle O\rangle - \langle O\rangle_n = \sum_{k=1}^{\infty} q_k[\langle N^k\rangle - (\langle N\rangle + j)^k]. \quad (21)$$

We assume that $j/\langle N\rangle \ll 1$. If we substitute the expression for $\langle N^k\rangle$ (C17) into (21) and use the binomial expansion up to the first order in $j/\langle N\rangle$ for $(\langle N\rangle + j)^k$, we obtain

$$\langle O\rangle - \langle O\rangle_n = \sum_{k=1}^{\infty} q_k \langle N\rangle^{k-1}\frac{ck(k-1)}{2}\left(1 - \frac{2j}{c(k-1)}\right). \quad (22)$$

The series (22) always converges for $j=0$, as we just demonstrated. To prove the convergence for $j\neq 0$ we split the sum (22) into two parts: the first part is for $0<k\leq K$ and the second part is for $K<k<\infty$, where $K$ is some positive integer. The first part is always finite and $\sim 1/\langle N\rangle$. By choosing $K$, we can always make $\left(1-\frac{2j}{c(k-1)}\right) \simeq 1$ for $k>K$. Therefore, the convergence of the expansion (11) for the $\langle N\rangle = n$ case implies convergence for any finite difference $|\langle N\rangle - n|$ for which $\frac{|\langle N\rangle - n|}{\langle N\rangle} \ll 1$. We note that these arguments may not work when the matrix $A_{nm}$ is singular. For example, in the case of a low-temperature Fermi gas, all matrix elements $A_{nm}$ tend to zero; therefore the canonical and grand canonical descriptions may deviate from each other in the thermodynamic limit due to the persistent existence of few-particle fluctuations in the grand canonical ensemble [14].

## III. EXAMPLE CALCULATIONS

As an example we consider the system of noninteracting quantum particles distributed on $n_{\text{levels}}$ single-particle energy levels with energies $\varepsilon_l$. The logarithm of the grand canonical partition function is

TABLE I. Occupation numbers and total energy for fermions. FD refers to the Fermi-Dirac statistics in the grand canonical ensemble ($\langle N\rangle=4$). The number of particles in the canonical ensemble is 2. $k_{\max}$ is the number of terms included in expansion (11).

| | | | | | $k_{\max}$ | | | |
|---|---|---|---|---|---|---|---|---|
| $l$ | $\varepsilon_l$ | FD | 1 | 2 | 3 | 4 | 6 | Exact |
| 1 | 1.0 | 0.98 | 0.92 | 0.87 | 0.86 | 0.87 | 0.87 | 0.87 |
| 2 | 2.0 | 0.95 | 0.80 | 0.69 | 0.67 | 0.67 | 0.68 | 0.68 |
| 3 | 3.0 | 0.87 | 0.52 | 0.34 | 0.34 | 0.30 | 0.30 | 0.30 |
| 4 | 4.0 | 0.72 | 0.07 | 0.01 | 0.06 | 0.11 | 0.12 | 0.12 |
| 5 | 5.0 | 0.48 | −0.31 | 0.10 | 0.06 | 0.04 | 0.04 | 0.04 |
| Total energy | | 10.77 | 2.82 | 3.77 | 3.78 | 3.79 | 3.79 | 3.79 |

$$\ln Z = \eta \sum_{l=1}^{n_{\text{levels}}} \ln(1 + \eta e^{\beta(\mu-\varepsilon_l)}), \tag{23}$$

where $\eta=+1$ is for fermions and $\eta=-1$ is for bosons. We set $\beta=1$, $\varepsilon_l=l$, and $n_{\text{levels}}=5$ in all our calculations.

First, we extract averages in the canonical ensemble for the smaller system from the grand canonical ensemble for the larger system. We select the chemical potential $\mu$ in such a way that the average number of particles $\langle N\rangle$ in the grand canonical ensemble is 4. We would like to extract information about the canonical ensemble with $n=2$ particles from this grand canonical ensemble. We compute the occupation numbers and then all physical quantities like the total energy can be calculated with the use of these occupation numbers. To start our calculations, we set $O=n_l$, where $n_l$ is the operator of the number of particles on level $l$. Then we solve the system of linear equations (15) to find the coefficients $q_k$ and use these $q_k$'s to calculate the grand canonical occupation numbers by Eq. (11). The matrix elements $A_{nm}$ are computed by Eq. (17) and with the help of the recurrence relation from Appendix B. The matrix element in the right-hand side of Eq. (15) is computed as the following derivative of the grand canonical partition function (23):

$$\langle n_l N^m\rangle = -\frac{1}{Z\beta^{m+1}}\frac{\partial^{m+1}Z}{\partial\varepsilon_l\,\partial\mu^m}. \tag{24}$$

The results of these calculations are shown in Table I (fermions) and Table II (bosons). The fermionic and bosonic systems both show convergence to the exact results as we include more terms in expansion (11). The convergence for bosons is slower than that for fermions. This is due to the fact that the fluctuations of the occupation numbers $\langle\Delta n_l^2\rangle=\langle n_l\rangle-\eta\langle n_l\rangle^2$ tend to be larger for bosons ($\eta=-1$) than for fermions ($\eta=+1$).

The method also works in the opposite direction; therefore we can compute averages in the canonical ensemble for the larger system using grand canonical averages for the smaller system. We select the grand canonical ensemble with $\langle N\rangle=2$ and compute the occupation numbers in the canonical ensemble of $n=4$ particles. Table III shows the results of these calculations for noninteracting fermions. The convergence to the exact values is as good as in the previous case, thereby demonstrating that the method can also be used to extract the canonical ensemble information for the larger system from the grand canonical calculations of the smaller system. Very similar results were obtained for bosons and we do not show them here.

## IV. CONCLUSIONS

We formulated a method to compute averages in the canonical ensemble based on calculations in the grand canonical ensemble. The number of particles $n$, which is fixed in the canonical ensemble, is not necessarily the same as the

TABLE II. Occupation numbers and total energy for bosons. BE refers to the Bose-Einstein statistics in the grand canonical ensemble ($\langle N\rangle=4$). The number of particles in the canonical ensemble is 2. $k_{\max}$ is the number of terms included in expansion (11).

| | | | | | $k_{\max}$ | | | |
|---|---|---|---|---|---|---|---|---|
| $l$ | $\varepsilon_l$ | BE | 1 | 3 | 5 | 7 | 11 | Exact |
| 1 | 1.0 | 3.43 | 1.52 | 1.52 | 1.47 | 1.44 | 1.42 | 1.42 |
| 2 | 2.0 | 0.40 | 0.33 | 0.33 | 0.37 | 0.39 | 0.39 | 0.39 |
| 3 | 3.0 | 0.12 | 0.10 | 0.10 | 0.11 | 0.12 | 0.13 | 0.13 |
| 4 | 4.0 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.05 | 0.05 |
| 5 | 5.0 | 0.01 | 0.01 | 0.01 | 0.01 | 0.02 | 0.02 | 0.02 |
| Total energy | | 4.81 | 2.68 | 2.69 | 2.77 | 2.82 | 2.84 | 2.85 |

TABLE III. Occupation numbers and total energy for fermions. FD refers to the Fermi-Dirac statistics in grand canonical ensemble ($\langle N\rangle=2$). The number of particles in the canonical ensemble is 4. $k_{\max}$ is the number of terms included in expansion (11).

| | | | $k_{\max}$ | | | | | |
|---|---|---|---|---|---|---|---|---|
| $l$ | $\varepsilon_l$ | FD | 1 | 2 | 3 | 4 | 5 | Exact |
| 1 | 1.0 | 0.80 | 1.18 | 0.92 | 0.98 | 0.99 | 0.99 | 0.99 |
| 2 | 2.0 | 0.60 | 1.18 | 1.01 | 0.97 | 0.93 | 0.97 | 0.97 |
| 3 | 3.0 | 0.36 | 0.91 | 1.02 | 0.96 | 0.97 | 0.91 | 0.91 |
| 4 | 4.0 | 0.17 | 0.51 | 0.70 | 0.72 | 0.73 | 0.77 | 0.77 |
| 5 | 5.0 | 0.07 | 0.23 | 0.35 | 0.38 | 0.37 | 0.36 | 0.36 |
| Total energy | | 4.10 | 9.42 | 10.53 | 10.54 | 10.55 | 10.55 | 10.55 |

average number of particles $\langle N\rangle$ in the grand canonical ensemble. Expansion (11) and the system of linear algebraic equations (15) for the coefficients of expansion are the main result of the paper. We performed test calculations for ideal Fermi and Bose gases, compared our calculations with the exact results, and demonstrated the convergence properties of the expansion (11).

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## APPENDIX A: USEFUL IDENTITIES

Proof that if $\langle O\rangle_n=\Sigma_{k=0}^{\infty}q_k n^k$ then $\langle O\rangle=\langle\Sigma_{k=0}^{\infty}q_k N^k\rangle$:

$$\begin{aligned}\langle O\rangle &= \frac{1}{Z}\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}\langle n\alpha|O|n\alpha\rangle \\ &= \frac{1}{Z}\sum_n e^{\beta\mu n}\sum_\alpha e^{-\beta E_{n\alpha}}\langle n\alpha|O|n\alpha\rangle = \frac{1}{Z}\sum_n e^{\beta\mu n}Z_n\langle O\rangle_n \\ &= \frac{1}{Z}\sum_n e^{\beta\mu n}Z_n\sum_{k=0}^{\infty} q_k n^k = \frac{1}{Z}\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}\sum_{k=0}^{\infty} q_k n^k \\ &= \frac{1}{Z}\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}\langle n\alpha|\sum_{k=0}^{\infty} q_k N^k|n\alpha\rangle = \left\langle \sum_{k=0}^{\infty} q_k N^k\right\rangle.\end{aligned}$$

Proof that $\langle\bar{O}f(N)\rangle=\langle\bar{O}\rangle\langle f(N)\rangle$:

$$\begin{aligned}\langle\bar{O}f(N)\rangle &= \frac{1}{Z}\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}\langle n\alpha|\bar{O}f(N)|n\alpha\rangle \\ &= \frac{1}{Z}\sum_{n\alpha} e^{-\beta(E_{n\alpha}-\mu n)}\langle n\alpha|\bar{O}|n\alpha\rangle f(n) \\ &= \frac{1}{Z}\sum_n e^{\beta\mu n}f(n)\sum_\alpha e^{-\beta E_{n\alpha}}\langle n\alpha|\bar{O}|n\alpha\rangle \\ &= \frac{1}{Z}\sum_n e^{\beta\mu n}f(n)\sum_\alpha e^{-\beta E_{n\alpha}}\langle n\alpha|O-\sum_{k=1}^{\infty} q_k N^k|n\alpha\rangle \\ &= \frac{1}{Z}\sum_n e^{\beta\mu n}f(n)Z_n\left(\langle O\rangle_n-\sum_{k=1}^{\infty} q_k n^k\right) \\ &= \frac{1}{Z}\sum_n e^{\beta\mu n}f(n)Z_n q_0 = \langle f(N)\rangle q_0 = \langle f(N)\rangle\langle\bar{O}\rangle.\end{aligned}$$

## APPENDIX B: RECURRENCE RELATION FOR THE CALCULATIONS OF THE DERIVATIVES

We define $\partial^m=\partial^m/(\partial\mu)^m$. Let

$$\Psi=\ln Z, Z_m=\partial^m Z. \tag{B1}$$

Then

$$Z_m=\partial^m(e^\Psi). \tag{B2}$$

Therefore

$$Z_{m+1}=\partial^m\,\partial(e^\Psi)=\partial^m(\Psi' e^\Psi)=\sum_{k=0}^{m}\frac{m!}{k!\,(m-k)!}Z_k\Psi^{(m-k+1)}, \tag{B3}$$

where

$$\Psi^{(k)}=\partial^k\Psi. \tag{B4}$$

Explicitly,

$$\Psi^{(0)}=\Psi=\eta\sum_{l=1}^{n_{\text{levels}}}\ln B_l,\quad B_l=1+\eta\exp[\beta(\mu-\varepsilon_l)]. \tag{B5}$$

$\eta=1$ for fermions and $=-1$ for bosons.

Assume that

$$\Psi^{(k)}=\sum_{l=1}^{n_{\text{levels}}}\sum_{\sigma=0}^{k}a_\sigma^k(B_l)^{-\sigma}. \tag{B6}$$

Since

$$\partial(B_l)^{-\sigma} = -\sigma\beta[(B_l)^{-\sigma} - (B_l)^{-\sigma-1}], \tag{B7}$$

we get then

$$\Psi^{(k+1)} = \partial\Psi^{(k)} = \sum_{l=1}^{n_{\text{levels}}} \sum_{\sigma=0}^{k} -\sigma\beta a_\sigma^k[(B_l)^{-\sigma} - (B_l)^{-\sigma-1}]. \tag{B8}$$

Since, according to (B6),

$$\Psi^{(k+1)} = \sum_{l=1}^{n_{\text{levels}}} \sum_{\sigma=0}^{k+1} a_\sigma^{k+1}(B_l)^{-\sigma}, \tag{B9}$$

we find that

$$a_\sigma^{k+1} = -\beta[\sigma a_\sigma^k - (\sigma-1)a_{\sigma-1}^k]. \tag{B10}$$

Evidently,

$$a_0^1 = \beta, \quad a_1^1 = -\beta. \tag{B11}$$

## APPENDIX C: SCALING WITH THE NUMBER OF PARTICLES

We use notations (B1)–(B5) from Appendix B. In these notations,

$$\langle N^m\rangle \equiv \frac{Z_m}{Z\beta^m}. \tag{C1}$$

Plugging this into Eq. (B3) we get

$$\langle N^{m+1}\rangle = \sum_{k=0}^{m} \frac{m!}{k!\,(m-k)!}\langle N^k\rangle \frac{\Psi^{(m-k+1)}}{\beta^{m-k+1}}. \tag{C2}$$

In the thermodynamic limit, the sum over $l$ in (B5) can be replaced by an integral. Since the corresponding density of states is proportional to the system volume $V$, e.g., in three-dimensional space it becomes ($\mu$ is the mass of the particle)

$$\rho(\varepsilon) = \frac{V}{\sqrt{2}\pi^2}\left(\frac{\sqrt{\mu}}{\hbar}\right)^3 \sqrt{\varepsilon}, \tag{C3}$$

we see that $\Psi^{(m)} \sim V$. Since $\langle N^m\rangle$ must be proportional to $V^m$, the term with $k=m$ in Eq. (C2) gives the leading contribution. Retaining in (C2) the two leading terms, we get

$$\langle N^{m+1}\rangle \approx \langle N^m\rangle\langle N\rangle + m\frac{\Psi^{(2)}}{\beta^2}\langle N^{m-1}\rangle \tag{C4}$$

with

$$\frac{\Psi^{(2)}}{\beta^2} \equiv \langle N^2\rangle - \langle N\rangle^2 \equiv \sum_l (\langle n_l\rangle - \eta\langle n_l\rangle^2). \tag{C5}$$

Here $\langle n_l\rangle$ are the Bose-Einstein or Fermi-Dirac occupation numbers. Since $\langle N\rangle \gg 1$, we assume in Eq. (C4) that

$$\langle N^m\rangle = \langle N\rangle^m + \frac{\Psi^{(2)}}{\beta^2}\alpha_m\langle N\rangle^{m-2} + O(\langle N\rangle^{m-4}). \tag{C6}$$

Inserting (C6) into (C4) and retaining the leading terms, we get

$$\alpha_{m+1} = \alpha_m + m, \quad \alpha_m = m(m-1)/2. \tag{C7}$$

Thus

$$\langle N^m\rangle \approx \langle N\rangle^m + \frac{\Psi^{(2)}}{\beta^2}\frac{m(m-1)}{2}\langle N\rangle^{m-2}. \tag{C8}$$

Now, we consider the terms $\langle n_l N^m\rangle$. Following Eq. (24) we differentiate Eq. (B3) over $\varepsilon_l$, and, retaining only the leading terms in $V$, we get

$$\langle n_l N^{m+1}\rangle = \langle n_l N^m\rangle\langle N\rangle + \langle N^m\rangle(\langle n_l\rangle - \eta\langle n_l\rangle^2). \tag{C9}$$

We shall look for the solution in the form

$$\langle n_l N^{m+1}\rangle = \langle n_l\rangle\langle N\rangle^{m+1} + \gamma_{m+1}\langle N\rangle^m + O(\langle N\rangle^{m-1}). \tag{C10}$$

Inserting this equation into (C9), we obtain $\gamma_{m+1} = \gamma_m + \langle n_l\rangle - \eta\langle n_l\rangle^2$ and

$$\langle n_l N^{m+1}\rangle \approx \langle n_l\rangle\langle N\rangle^{m+1} + (m+1)(\langle n_l\rangle - \eta\langle n_l\rangle^2)\langle N\rangle^m. \tag{C11}$$

Next, we consider the system of linear equations (15). In the thermodynamic limit, we retain only the first terms in Eqs. (C11) and (C8). If we apply a "weak" thermodynamic limit and retain the next-order terms in Eqs. (C11) and (C8), then

$$A_{km} \approx km\frac{\Psi^{(2)}}{\beta^2}\langle N\rangle^{k+m-2}, \tag{C12}$$

$$\langle n_l N\rangle^m - \langle n_l\rangle\langle N\rangle^m \approx m(\langle n_l\rangle - \eta\langle n_l\rangle^2)\langle N\rangle^{m-1}. \tag{C13}$$

Therefore, assuming that $\Psi^{(m)} \sim V \sim \langle N\rangle$, we get

$$q_k A_{km} \sim \langle N\rangle^{m-1}, \tag{C14}$$

$$q_k\langle N\rangle^{k+m-1} \sim \langle N\rangle^{m-1}, \tag{C15}$$

and therefore

$$q_k \sim 1/\langle N\rangle^k. \tag{C16}$$

The same $\langle N\rangle$ dependence can also be obtained if we express the particle number operator $N$ in terms of creation and annihilation operators and apply Wick's theorem [15] to the matrix elements $\langle N^m\rangle$ and $\langle n_l N^m\rangle$.

Using the fact that $\Psi^{(2)} \sim \langle N\rangle$, we transform Eq. (C8) to the form

$$\langle N^m\rangle \approx \langle N\rangle^m + c\frac{m(m-1)}{2}\langle N\rangle^{m-1}. \tag{C17}$$

Here $c$ is some constant that does not depend on $m$ and $\langle N\rangle$.

It has not escaped our notice that Eqs. (C4) and (C9) break down for bosons at critical and lower temperatures, since, due to the Bose condensation, $\Psi^{(m)}$ becomes proportional to $V^m$.

[1] R. Rossignoli and P. Ring, Ann. Phys. (N.Y.) **235**, 350 (1994).
[2] J. von Delft and D. C. Ralph, Phys. Rep. **345**, 61 (2001).
[3] H. D. Politzer, Phys. Rev. A **54**, 5048 (1996).
[4] C. Herzog and M. Olshanii, Phys. Rev. A **55**, 3254 (1997).
[5] F. Gilleron and J.-C. Pain, Phys. Rev. E **69**, 056117 (2004).
[6] R. Tomas Rodriguez, J. L. Egido, and L. M. Robledo, Phys. Rev. C **72**, 064303 (2005).
[7] K. Tanabe and H. Nakada, Phys. Rev. C **71**, 024314 (2005).
[8] H. Nakada and K. Tanabe, Phys. Rev. C **74**, 061301(R) (2006).
[9] I. Fujiwara, D. ter Haar, and H. Wergeland, J. Stat. Phys. **2**, 329 (1970).
[10] S. A. Ponomarenko, M. E. Sherrill, D. P. Kilcrease, and G. Csanak, J. Phys. A **39**, L499 (2006).
[11] D. S. Kosov and A. I. Vdovin, Z. Phys. A **355**, 17 (1996).
[12] D. S. Kosov and A. I. Vdovin, Izv. Ross. Akad. Nauk, Ser. Fiz. **60**, 94 (1996).
[13] D. A. McQuarrie, *Statistical Mechanics* (University Science Books, Sausalito, CA, 2000).
[14] S. P. Bowen, Y. Zhou, and J. D. Mancini, Phys. Rev. B **46**, 1338 (1992).
[15] G. C. Wick, Phys. Rev. **80**, 268 (1950).