Quantum Gases in the Microcanonical Ensemble near the Thermodynamic Limit

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A new method is proposed for a treatment of ideal quantum gases in the microcanonical ensemble near the thermodynamic limit. The method allows rigorous asymptotic calculations of the average number of particles and particle number fluctuations in the microcanonical ensemble. It gives also the finite-volume corrections due to exact energy conservation for the total average number of particles and for higher moments of the particle number distribution in a system approaching the thermodynamic limit. A present consideration confirms our previous findings that the scaled variance for particle number fluctuations in the microcanonical ensemble is different from that in the grand canonical ensemble even in the thermodynamic limit.

I. INTRODUCTION

The statistical hadron gas approach to nucleus-nucleus (A+A) collisions (see e.g. Ref. [1] and recent review [2]) is rather successful in describing the data on particle multiplicities in a wide range of the collision energies. Usually one considers a thermal system created in A+A collision in the grand canonical ensemble (GCE). The canonical ensemble (CE) [3, 4, 5, 6, 7, 8] or even the microcanonical ensemble (MCE) [9] has been used in order to describe the pp, p+p̅ and e+e− collisions when a small number of secondary particles are produced. In all these cases, the statistical systems are far away from the thermodynamic limit, so the statistical ensembles are not equivalent and exact charge conservation or both energy and charge conservation laws have to be taken into account. The CE is relevant also for systems with a large number of produced particles, e.g., a large number of resultant pions or large nucleon number in p+A collisions, but a small (of the order of 1 or smaller) number of carriers of conserved charges, such as strange hadrons K, antibaryons Ò, or charmed hadrons ß. This may happen not only in elementary but also in p+A or even A+A collisions.

The analysis of the fluctuations is a useful tool to study the properties of the system created during high energy particle and nuclear collisions (see, e.g., Refs. [10, 11, 12, 13, 14, 15, 16, 17] and the review papers [18]). In A+A collisions one prefers to use the GCE because it is the most convenient one from the technical point of view and due to the fact that both the CE and MCE are equivalent to the GCE in the thermodynamic limit when the size of the system tends to infinity. However, the thermodynamic equivalence of ensembles means only that the average values of physical quantities calculated in different ensembles are equal to each other in the thermodynamic limit. It was demonstrated for the first time in Ref. [19] that multiplicity fluctuations are different in the CE and GCE even in the thermodynamic limit. These results have been then verified and extended in Refs. [20, 21, 22]. The particle number fluctuations in the MCE have been considered in our paper [23] and they have been shown to be different from the GCE results even in the thermodynamic limit.

In this paper we present a new method for the study of particle number distribution in the microcanonical ensemble. The method is based on the analysis of the asymptotic behaviour of moments of the particle number distribution. In contrast to the previously used microscopic correlator approach [15], the new method is more rigorous, consistent and mathematically justified. It elucidates some subtleties. Along with fluctuations, it allows to calculate the finite-volume corrections to the thermodynamic quantities.

The paper is organized as follows. In Section II we review the method of microscopic correlator and demonstrate its limitations. A detailed description of our new method is given in Section III. We summarize our consideration in Section IV.

II. MICROSCOPIC CORRELATOR

Let consider the quantum system of non-interacting neutral particles. We review here the application of the method of Ref. [15] to the calculation of the particle number fluctuations in the systems with the exact conservation of energy imposed.
The GCE partition function for a single quantum state with momentum \( p \) has the form

\[
z_p = \sum_n \exp \left( -\frac{\epsilon_p}{T} n \right),
\]

where \( T \) is the system temperature, \( \epsilon_p \equiv \sqrt{p^2 + m^2} \) and \( m \) is the particle mass. The sum in Eq. (1) runs over the number of particles \( n = 0, 1 \) for the Fermi statistics and \( n = 0, 1, 2, \ldots \infty \) for the Bose statistics. Summing up the two terms for the Fermi statistics, or the infinite geometric series for the Bose statistics, one gets:

\[
z_p = \left[ 1 - \gamma \exp \left( -\frac{\epsilon_p}{T} \right) \right]^{-\gamma}.
\]

where \( \gamma = +1 \) and \( \gamma = -1 \) for Bose and Fermi statistics, respectively. The GCE average values are calculated as

\[
\langle n^k_p \rangle_{\text{g.c.e.}} = \sum_n n^k w_p(n),
\]

where

\[
w_p(n) = z_p^{-1} \exp \left( -\frac{\epsilon_p}{T} n \right)
\]
is the probability to observe \( n \) particles in the given quantum state. It is easy to see that

\[
\langle n^k_p \rangle_{\text{g.c.e.}} = \frac{(-T)^k}{z_p} \frac{\partial^k z_p}{\partial \epsilon_p^k}.
\]

For \( k = 1 \) we get the familiar Fermi (Bose) distribution

\[
\langle n_p \rangle_{\text{g.c.e.}} = \frac{1}{\exp \left( \frac{\epsilon_p}{T} \right) - \gamma},
\]

and for \( k = 2 \)

\[
\langle n^2_p \rangle_{\text{g.c.e.}} = \frac{\exp \left( \frac{\epsilon_p}{T} \right) + 1}{\exp \left( \frac{\epsilon_p}{T} \right) - \gamma}^2 = \langle n_p \rangle_{\text{g.c.e.}} \left[ 1 + (1 + \gamma) \langle n_p \rangle_{\text{g.c.e.}} \right].
\]

From Eqs. (6-7) it follows:

\[
\langle (\Delta n_p)^2 \rangle_{\text{g.c.e.}} = \langle n^2_p \rangle_{\text{g.c.e.}} - \langle n_p \rangle_{\text{g.c.e.}}^2 = \langle n_p \rangle_{\text{g.c.e.}} \left[ 1 - \gamma \langle n_p \rangle_{\text{g.c.e.}} \right] \equiv v^2_p.
\]

It is easy to see that \( \gamma = 0 \) in Eqs. (6-7) corresponds to the Boltzmann approximation.

Expressions (6) and (8) are microscopic in a sense that they describe the average values and fluctuation of a single mode with momentum \( p \). However, the fluctuations of macroscopic quantities of the system can be determined through the fluctuations of these single modes. To be more precise, we will demonstrate that the fluctuations can be written in terms of the microscopic correlator \( \langle \Delta n_p \Delta n_k \rangle_{\text{g.c.e.}} \). This correlator can be presented as:

\[
\langle \Delta n_p \Delta n_k \rangle_{\text{g.c.e.}} = v^2_p \delta_{pk}.
\]

The variance \( \langle (\Delta N)^2 \rangle \equiv \langle N^2 \rangle - \langle N \rangle^2 \) of the total number of particles, \( N = \sum_p n_p \), equals to:

\[
\langle (\Delta N)^2 \rangle_{\text{g.c.e.}} = \sum_{p,k} \langle n_p n_k \rangle_{\text{g.c.e.}} - \langle n_p \rangle_{\text{g.c.e.}} \langle n_k \rangle_{\text{g.c.e.}} = \sum_{p,k} \langle \Delta n_p \Delta n_k \rangle_{\text{g.c.e.}} = \sum_p v^2_p.
\]

We have assumed above that the quantum \( p \)-levels are non-degenerate. In fact each this level should be further specified by the projection of a particle spin. Thus each \( p \)-level splits into \( g = 2j + 1 \) sub-levels. It will be assumed that the \( p \)-summation includes all sub-levels too. This does not change the above formulation because of statistical independence of these quantum sub-levels. The degeneracy factor enters explicitly when one substitutes, in the thermodynamic limit, the summation over discrete levels by the integration:

\[
\sum_p \ldots \simeq \frac{gV}{2\pi^2} \int_0^\infty p^2 dp \ldots.
\]
The scaled variance $\omega$ in the thermodynamic limit $V \to \infty$ reads:

$$\omega_{g.c.e.} = \frac{(\langle \Delta N^2 \rangle)_{g.c.e.}}{\langle N \rangle_{g.c.e.}} = \frac{\sum_{p,k} (\Delta n_p \Delta n_k)_{g.c.e.}}{\sum_p \langle n_p \rangle_{g.c.e.}} = \frac{\sum_p v_p^2}{\sum_p \langle n_p \rangle_{g.c.e.}} \approx \frac{\int_0^\infty p^2 dp \ v_p^2}{\int_0^\infty p^2 dp \ \langle n_p \rangle_{g.c.e.}}. \quad (12)$$

The Eq. (12) corresponds to the particle number fluctuations in the GCE. From Eq. (12) one finds $\omega_{g.c.e.} = 1$ in the classical Boltzmann limit ($\gamma = 0$). The effects of quantum statistics lead to $\omega_{g.c.e.} > 1$ for the Bose gas ($\gamma = 1$) and $\omega_{g.c.e.} < 1$ for the Fermi gas ($\gamma = -1$). The strongest effect corresponds to $m/T \to 0$,

$$\omega_{g.c.e.}^{\text{Bose}} = \pi^2/6\zeta(3) \approx 1.368, \quad \omega_{g.c.e.}^{\text{Fermi}} = \pi^2/9\zeta(3) \approx 0.912, \quad (13)$$

and it decreases with increasing $m/T$ (see Fig. 1).

The formula for the microscopic correlator is modified if we impose the exact conservation law on our equilibrated system. For this purpose we introduce the equilibrium probability distribution $W(n_p)$ of the occupation numbers $\{n_p\}$. As a first step we assume that each $n_p$ fluctuates independently according to the Gauss distribution law with mean square deviation $v_p^2$:

$$W(n_p) \propto \prod_p \exp \left[ -\frac{(\Delta n_p)^2}{2v_p^2} \right]. \quad (14)$$

To justify this assumption (see Ref. 13) one can consider the sum of $n_p$ in small momentum volume $(\Delta p)^3$ with the center at $p$. At fixed $(\Delta p)^3$ and $V \to \infty$ the average number of particles inside $(\Delta p)^3$ becomes large. Each particle configuration inside $(\Delta p)^3$ consists of $(\Delta p)^3 \cdot V/(2\pi)^3 \gg 1$ statistically independent terms, each with average value $\langle n_p \rangle$ and scaled variance $v_p^2$. From the central limit theorem it then follows that the probability distribution for the fluctuations inside $(\Delta p)^3$ should be Gaussian. In fact, we always convolve $n_p$ with some smooth function of $p$, so instead of writing the Gaussian distribution for the sum of $n_p$ in $(\Delta p)^3$ we can use it directly for $n_p$.

Now we want to impose the exact conservation laws. The conserved quantity $A$ (the energy and/or conserved charge) can be written in the form $A = \sum_p a(p) n_p$. An exact conservation law means the restriction on the set of occupation numbers $\{n_p\}$: only those which satisfy the condition $\Delta A = \sum_p a(p) \Delta n_p = 0$ can be realized. Let us consider exact energy conservation. Then $A \to E$ (i.e. $a(p) \to \epsilon_p$) and the distribution (14) will be modified because of the energy conservation as:

$$W(n_p) \propto \prod_p \exp \left[ -\frac{(\Delta n_p)^2}{2v_p^2} \right] \delta \left( \sum_p \epsilon_p \Delta n_p \right) \propto \int_{-\infty}^{\infty} d\lambda \ \prod_p \exp \left[ -\frac{(\Delta n_p)^2}{2v_p^2} + i\lambda \epsilon_p \Delta n_p \right], \quad (15)$$
where \( \delta (\epsilon_p \Delta n_p) \) is the Dirac’s \( \delta \)–function. It is convenient to generalize distribution \( \{g(x)\} \) using further the integration along imaginary axis in \( \lambda \)-space. After completing squares one gets:

\[
W(n_p, \lambda) \propto \prod_p \exp \left[ -\frac{\left(\Delta n_p - \lambda v^2_p \epsilon_p\right)^2}{2v_p^2} + \lambda^2 \frac{2}{v_p^2} \epsilon_p^2 \right],
\]

and the average values (i.e. the MCE averages) are now calculated as:

\[
\langle \ldots \rangle = \frac{\int_{-\infty}^{\infty} d\lambda \int_{-\infty}^{\infty} \prod_p dn_p \ldots W(n_p, \lambda)}{\int_{-\infty}^{\infty} d\lambda \int_{-\infty}^{\infty} \prod_p dn_p W(n_p, \lambda)}.
\]

Using Eq. (17) one easily deduces

\[
\langle (\Delta n_p v^2_p \epsilon_p)(\Delta n_k - v^2_k \epsilon_k) \rangle = \delta_{pk} v^2_p, \quad \langle \lambda^2 \rangle = -\left(\sum_p v^2_p \epsilon_p^2\right)^{-1}, \quad \langle (\Delta n_p - v^2_p \epsilon_p)\lambda \rangle = 0.
\]

Therefore, one finds the MCE average for the microscopic correlator

\[
\langle \Delta n_p \Delta n_k \rangle_{m.e.e.} = \delta_{pk} - v^2_p \epsilon_p v^2_k \epsilon_k \langle \lambda^2 \rangle + \langle \Delta n_p \lambda \rangle v^2_k \epsilon_k + \langle \Delta n_k \lambda \rangle v^2_p \epsilon_p
\]

\[
= \delta_{pk} + v^2_p \epsilon_p v^2_k \epsilon_k \langle \lambda^2 \rangle = \delta_{pk} v^2_p - \frac{v^2_p \epsilon_p v^2_k \epsilon_k}{\sum_p v^2_p \epsilon_p^2}.
\]

By means of Eq. (18) one obtains:

\[
\omega_{m.e.e.} = \frac{\langle (\Delta N^2) \rangle_{m.e.e.}}{\langle N \rangle_{g.c.e.}} = \frac{\sum_p v^2_p}{\sum_p \langle n_p \rangle_{g.c.e.}} - \frac{\left(\sum_p v^2_p \epsilon_p\right)^2}{\sum_p \langle n_p \rangle_{g.c.e.} \sum_p v^2_p \epsilon_p^2} \\
\approx \int_{0}^{\infty} p^2 dp \langle n_p \rangle_{g.c.e.} - \frac{\left(\int_{0}^{\infty} p^2 dp v^2_p \epsilon_p\right)^2}{\int_{0}^{\infty} p^2 dp \sum_p v^2_p \epsilon_p^2}.
\]

The Eq. (19) demonstrates that the MCE fluctuations in the thermodynamic limit \( V \to \infty \) can be presented in terms of the GCE quantities. The MCE scaled variances \( \omega_{m.e.e.} \) for different statistics are shown as functions of \( m/T \) in Fig. 2.

The microcanonical suppression effect for the particle number fluctuations increases with the particle mass. In the Boltzmann approximation (\( \gamma = 0 \), \( v^2_p = \langle n_p \rangle_{g.c.e.} = \exp(-\epsilon_p/T) \)) the integrals in Eq. (19) can be calculated analytically:

\[
\int_{0}^{\infty} p^2 dp \exp\left(-\frac{\epsilon_p}{T}\right) = T m^2 K_2\left(\frac{m}{T}\right),
\]

\[
\int_{0}^{\infty} p^2 dp \epsilon_p \exp\left(-\frac{\epsilon_p}{T}\right) = \frac{m^4}{8} \left[ K_4\left(\frac{m}{T}\right) - K_0\left(\frac{m}{T}\right) \right],
\]

\[
\int_{0}^{\infty} p^2 dp \epsilon_p \exp\left(-\frac{\epsilon_p}{T}\right) = \frac{m^5}{16} \left[ K_5\left(\frac{m}{T}\right) + K_3\left(\frac{m}{T}\right) - 2 K_1\left(\frac{m}{T}\right) \right].
\]

Making use of the asymptotic behavior of the modified Hankel function \( K_n(x) \) at \( x \to 0 \) \( (K_0(x) \simeq -\ln x \) and \( K_n(x) \simeq \frac{x}{\pi} \Gamma(n) \left(\frac{x}{\pi}\right)^{-n} \) for \( n \geq 1 \) one gets in the massless limit:

\[
\omega_{m.e.e.}(m = 0) = \frac{1}{4},
\]

i.e. for classical massless particles the MCE the scaled variance is quarter as large as the corresponding scaled variance in the GCE. For the case of Bose and Fermi statistic we obtain:

\[
\omega_{m.e.e.}^{Bose}(m = 0) = \frac{\pi^2}{6\xi(3)} - \frac{135\xi(3)}{2\pi^4} \simeq 0.535, \quad \omega_{m.e.e.}^{Fermi}(m = 0) = \frac{\pi^2}{9\xi(3)} - \frac{405\xi(3)}{7\pi^4} \simeq 0.198.
\]
FIG. 2: The scaled variance \( \omega \) for particle number fluctuation in the microcanonical ensemble for different types of statistics. The lower and upper solid lines correspond to the Fermi and Bose ideal gas, respectively. The dashed line is the Boltzmann approximation.

The \( \omega_{\text{m.c.e.}} \) for bosons is always larger than in the Boltzmann limit and for fermions is always smaller, so we acquire the Bose-enhancement and Fermi-suppression of the fluctuations. They exist also in the GCE. However, the effects due to the quantum statistics in the MCE become stronger than those in the GCE (compare Eqs. (23–25) and Eq. (13)).

As it is seen from Fig. 2, the MCE suppression effects for the fluctuations of massive particles increase with particle mass. One finds that with increasing \( m/T \) ratio the scaled variances for the Bose and Fermi systems approach their Boltzmann limit, \( \omega_{\text{m.c.e.}} \), and from the asymptotic behavior, \( K_n(x) \simeq \sqrt{\frac{\pi}{2}} x \exp(-x) \left(1 + \frac{4n^2-1}{8x} \right) \) at \( x \gg 1 \), it follows that \( \omega_{\text{m.c.e.}} \simeq 3/2(m/T)^{-2} \rightarrow 0 \) at \( m/T \rightarrow \infty \).

Comparing Eq. (18) and Eq. (9) one finds the changes of the microscopic correlator due to the exact energy conservation. First, in the MCE the fluctuations of each mode \( p \) is reduced, i.e. the \( \langle (\Delta n_p)^2 \rangle \) calculated from Eq. (18) is smaller that calculated from Eq. (9). Second, the anticorrelations between different modes \( p \neq k \) absent in the GCE appear in the MCE. These changes of the microscopic correlator result in the suppression effect of the MCE scaled variance \( \omega_{\text{m.c.e.}} \) in a comparison to the GCE one \( \omega_{\text{g.c.e.}} \).

The method considered above has several serious limitations:

- The probability distribution for \( \Delta n_p \) was replaced by the Gaussian distribution (14), but in fact, this two distributions are very different. It is enough to mention that the real distribution is a discrete, and the Gaussian one is continuous. Although the arguments given after the equation (14) suggest that this replacement does not influence the final result in the thermodynamic limit, still, it would be nice to have a more rigorous justification of this fact as well as a recipe for the treatment of finite-size corrections in quantum systems.

- The Exact energy conservation influences not only fluctuations, but also the average values \( \langle n_p \rangle \) and \( \langle n_p^2 \rangle \), and this should result in microcanonical corrections to \( \langle N \rangle_{\text{m.c.e.}} \) and \( \langle N^2 \rangle_{\text{m.c.e.}} \) in the case of finite-volume systems. The approach presented in this section does not allow calculating these corrections.

- It would be desirable to convince ourselves that the present approach gives a correct value for \( \omega_{\text{m.c.e.}} \) despite of the fact that it ignores the finite-volume corrections to \( \langle N \rangle_{\text{m.c.e.}} \) and \( \langle N^2 \rangle_{\text{m.c.e.}} \) which are of the same order as fluctuations \( \langle (\Delta N)^2 \rangle_{\text{m.c.e.}} = \langle N^2 \rangle_{\text{m.c.e.}} - \langle N \rangle_{\text{m.c.e.}}^2 \).

The rigorous method described in the next sections resolves the above issues.
III. THE MOMENTS OF THE PARTICLE NUMBER DISTRIBUTIONS IN THE MCE

In this section we consider a consistent and mathematically justified method for MCE treatment of an ideal gas near and in the thermodynamical limit. Our aim is to find the asymptotic behavior of the thermodynamic quantities (the total particle number and its fluctuations) of a microcanonical thermodynamic system at large volume $V$ in terms of the thermodynamic properties of a grand canonical system, which are easier to calculate.

The methods is based on the analysis of the particle number distribution and its moments. For pedagogical purposes, we first apply our approach to the grand canonical system and then use the gained experience for the treatment of a microcanonical system near the thermodynamic limit $V \to \infty$.

The grand canonical partition function of the ideal quantum gas is given by a product of the grand canonical partition functions $z_p$ for each quantum level $p$:

$$Z_{g.c.e.}(T) = \prod_p z_p = \prod_p \sum_{n_p} \exp \left(-\frac{\epsilon_p n_p}{T} \right) = \sum_{\{n_p\}} W_{g.c.e.}(\{n_p\}) ,$$  \hspace{1cm} (26)

where the sum runs over all possible sets of the occupation numbers $\{n_p\}$. The quantity

$$W_{g.c.e.}(\{n_p\}) = \exp \left(-\frac{\sum_p \epsilon_p n_p}{T} \right) = \prod_p z_p w_p(n_p) ,$$ \hspace{1cm} (27)

is proportional to the probability to observe a given set $\{n_p\}$ of the occupation numbers. Here $w_p(n_p)$ is the probability to observe $n_p$ particles at the level $p$.

To get the (unnormalized) probability distribution for the total particle number we multiply the above expression with the $\delta$-function $\delta \left( \sum_p n_p - N \right)$ and sum over all $n_p$:

$$W_{g.c.e.}(N) = \sum_{\{n_p\}} W_{g.c.e.}(\{n_p\}) \delta \left( \sum_p n_p - N \right) .$$ \hspace{1cm} (28)

Now let us consider the Fourier transform of the above probability distribution:

$$\tilde{W}_{g.c.e.}(\nu) = \sum_N \exp (i\nu N) W_{g.c.e.}(N) .$$ \hspace{1cm} (29)

The $\delta$-function disappears due to the summation:

$$\sum_N \exp (i\nu N) \delta \left( \sum_p n_p - N \right) = \exp \left( i\nu \sum_p n_p \right) ,$$ \hspace{1cm} (30)

this makes the expression factorizable

$$\tilde{W}_{g.c.e.}(\nu) = \sum_{\{n_p\}} \exp \left( i\nu \sum_p n_p \right) W_{g.c.e.}(\{n_p\}) = \prod_p z_p \sum_{n_p} \exp (i\nu n_p) w_p(n_p) = \prod_p \tilde{w}_p(\nu) z_p .$$ \hspace{1cm} (31)

Here we have introduced a Fourier transform $\tilde{w}_p(\nu)$ of the single-level probability distribution $w_p(n_p)$:

$$\tilde{w}_p(\nu) = \sum_{n_p} \exp (i\nu n_p) w_p(n_p) .$$ \hspace{1cm} (32)

One can rewrite the equation as

$$\tilde{W}_{g.c.e.}(\nu) = \exp \left( \sum_p \log \tilde{w}_p(\nu) \right) \prod_p z_p .$$ \hspace{1cm} (33)

The summation in the exponential can be replaced by integration, if the system is sufficiently large:

$$\tilde{W}_{g.c.e.}(\nu) = \exp \left[ \frac{gV}{(2\pi)^3} \int d^3p \log \tilde{w}_p(\nu) \right] \prod_p z_p .$$ \hspace{1cm} (34)
Let us expand the logarithm in the integral into a Taylor series:

$$
\log \tilde{w}_p(\nu) = \log \tilde{w}_p(0) + \sum_{j=1}^{\infty} i^j \frac{m_j(p)}{j!} \nu^j,
$$

(35)

where, in particular, (see Appendix)

$$
m_1(p) = \langle n_p \rangle_{g.c.e.},
$$

(36)

$$
m_2(p) = \langle (n_p - \langle n_p \rangle)^2 \rangle_{g.c.e.} \equiv v_p^2.
$$

(37)

If one uses the normalized probability distribution for \( w_p(n) \), then the first term in (35) is zero and the expression (34) takes the form

$$
\tilde{W}_{g.c.e.}(\nu) = \exp \left[ \sum_{j=1}^{\infty} \frac{i^j}{j!} \frac{gV}{(2\pi)^3} \int d^3p m_j(p) \right] \prod_p z_p.
$$

(38)

Now one can calculate the moments of the probability distribution \( W_{g.c.e.}(N) \) using the values of the function \( \tilde{W}_{g.c.e.}(\nu) \) and its derivatives at \( \nu = 0 \) (see Appendix). The value

$$
\tilde{W}_{g.c.e.}(0) = \prod_p z_p
$$

(39)

is used for the normalization. The first derivative is related to the average number of particles:

$$
\langle N \rangle_{g.c.e.} = \frac{1}{i \tilde{W}_{g.c.e.}(0)} \left. \frac{d\tilde{W}_{g.c.e.}(\nu)}{d\nu} \right|_{\nu=0} = \frac{gV}{(2\pi)^3} \int d^3p \langle n_p \rangle_{g.c.e.} \equiv \bar{N}.
$$

(40)

Similarly,

$$
\langle N^2 \rangle_{g.c.e.} = \frac{1}{\tilde{W}_{g.c.e.}(0)} \left. \frac{d^2\tilde{W}_{g.c.e.}(\nu)}{d\nu^2} \right|_{\nu=0} = \bar{N}^2 + \frac{gV}{(2\pi)^3} \int d^3p v_p^2.
$$

(41)

The above results for the GCE are known from the textbooks. The purpose of this consideration is to demonstrate how our method works and to clarify our further step – a treatment of the MCE. The MCE partition function of the ideal quantum gas is given by

$$
Z_{m.c.e.}\{n_p\} = \sum_{\{n_p\}} \delta \left( \sum_p \epsilon_p n_p - E \right),
$$

(42)

where the sum, similarly to Eq. (20), runs over all sets of the occupation numbers \( \{n_p\} \). The probability to observe a given set \( \{n_p\} \) is proportional to

$$
W_{m.c.e.}\{n_p\} = \delta \left( \sum_p \epsilon_p n_p - E \right).
$$

(43)

Nothing changes if we multiply the last expression by \( 1 = \exp(E/T) \exp(-E/T) \):

$$
W_{m.c.e.}\{n_p\} = \exp \left( \frac{E}{T} \right) \exp \left( -\frac{E}{T} \right) \delta \left( \sum_p \epsilon_p n_p - E \right).
$$

(44)

The parameter \( T \) has the meaning of the temperature of a grand canonical system, which will be defined later.

Using the properties of the \( \delta \)-function, one can replace \( E \) in the second exponent by \( \sum_p \epsilon_p n_p \):

$$
W_{m.c.e.}\{n_p\} = \exp \left( \frac{E}{T} \right) \exp \left( -\frac{\sum_p \epsilon_p n_p}{T} \right) \delta \left( \sum_p \epsilon_p n_p - E \right).
$$

(45)
We replace the summation in the exponential by integration

$$\exp \left( - \sum_p \frac{\epsilon_p n_p}{T} \right) = \prod_p \exp \left( - \frac{\epsilon_p n_p}{T} \right) = \prod_p w_p(n_p) z_p ,$$

(46)

where $z_p$ is the grand canonical partition function for the single $p$-level, $w_p(n_p)$ is the probability to observe $n_p$ particles at this level. The grand canonical system is assumed to have the same quantum levels as the microcanonical system under consideration. The $\delta$-function in (45) can be represented as

$$\delta \left( \sum_p \epsilon_p n_p - E \right) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\lambda \exp \left[ i\lambda \left( \sum_p \epsilon_p n_p - E \right) \right] ,
$$

(47)

therefore,

$$W_{m.c.e.}(\{n_p\}) = \frac{1}{2\pi} \exp \left( \frac{E}{T} \right) \int_{-\infty}^{+\infty} d\lambda \exp \left( -i\lambda E \right) \prod_p w_p(n_p) z_p \exp \left( i\lambda n_p \epsilon_p \right)
$$

$$+ C \int_{-\infty}^{+\infty} d\lambda \exp \left( -i\lambda E \right) \prod_p w_p(n_p) \exp \left( i\lambda n_p \epsilon_p \right) ,
$$

(48)

where we have introduced the notation

$$C = \frac{1}{2\pi} \exp \left( \frac{E}{T} \right) \prod_p z_p .
$$

(49)

The constant $C$ is a normalization factor and is irrelevant to the physical quantities we are interested in.

Similarly to Eq. (28), we get the (unnormalized) probability distribution for the total particle number by multiplying the above expression with the $\delta$-function $\delta \left( \sum_p n_p - N \right)$ and summing over all possible sets $\{n_p\}$:

$$W_{m.c.e.}(N) = C \int_{-\infty}^{+\infty} d\lambda \exp \left( -i\lambda E \right) \prod_p w_p(n_p) \exp \left( i\lambda n_p \epsilon_p \right) \delta \left( \sum_p n_p - N \right) .
$$

(50)

We perform a Fourier transformation of $W_{m.c.e.}(N)$:

$$\tilde{W}_{m.c.e.}(\nu) = \sum_N \exp (i\nu N) . W_{m.c.e.}(N)
$$

(51)

The $\delta$-function disappears due to $\delta \left( \sum_p n_p - N \right)$, and the integrand becomes factorizable:

$$\tilde{W}_{m.c.e.}(\nu) = C \int_{-\infty}^{+\infty} d\lambda \exp \left( -i\lambda E \right) \prod_p \sum_{n_p} w_p(n_p) \exp \left[ i\lambda n_p \epsilon_p \right]
$$

$$= C \int_{-\infty}^{+\infty} d\lambda \exp \left( -i\lambda E \right) \prod_p \tilde{w}_p(\nu + \lambda \epsilon_p)
$$

$$= C \int_{-\infty}^{+\infty} d\lambda \exp \left( -i\lambda E \right) \prod_p \tilde{w}_p(\nu + \lambda \epsilon_p) = C \int_{-\infty}^{+\infty} d\lambda \exp \left[ -i\lambda E + \sum_p \log \tilde{w}_p(\nu + \lambda \epsilon_p) \right] .
$$

(52)

We replace the summation in the exponential by integration

$$\tilde{W}_{m.c.e.}(\nu) = C \int_{-\infty}^{+\infty} d\lambda \exp \left[ -i\lambda E + \frac{gV}{(2\pi)^3} \int d^3 p \log \tilde{w}_p(\nu + \lambda \epsilon_p) \right] ,
$$

(53)

and expand the logarithm in the integral into the Taylor series:

$$\log \tilde{w}_p(\nu + \lambda \epsilon_p) = \log \tilde{w}_p(0) + \sum_{j=1}^{\infty} \frac{m_j(p)}{j!} (\nu + \lambda \epsilon_p)^j .
$$

(54)

This yields

$$\tilde{W}_{m.c.e.}(\nu) = C \int_{-\infty}^{+\infty} d\lambda \exp \left[ -i\lambda E + \sum_{j=1}^{\infty} \frac{gV}{j! (2\pi)^3} \int d^3 p m_j(p) (\nu + \lambda \epsilon_p)^j \right] .
$$

(55)
The first term of the sum in the exponential can be rewritten as

$$i \frac{V}{(2\pi)^3} \int d^3p (n_p) \left( \nu + \lambda \epsilon_p \right) = i \left( \nu \bar{N} + \lambda \bar{E} \right),$$

(56)

where $\bar{N}$ is the average total particle number in the grand canonical system, and

$$\bar{E} = \frac{V}{(2\pi)^3} \int d^3p \langle n_p \rangle \left( \nu + \lambda \epsilon_p \right),$$

(57)

is its average total energy. The temperature of the GCE has been arbitrary so far. Now we fix it so that the average energy of the GCE equals the energy of the MCE: $\bar{E} = E$. In this case the term $-i\lambda E$ is annihilated by $i\lambda \bar{E}$. Finally one gets

$$W_{m.c.e.}(\nu) = C \int_{-\infty}^{+\infty} d\lambda \exp \left[ \nu \bar{N} + \sum_{j=2}^{\infty} \frac{i^j}{j!} \frac{V}{(2\pi)^3} \int d^3p m_j(p) (\nu + \lambda \epsilon_p)^j \right].$$

(58)

Let us find the values of the function $W_{m.c.e.}(\nu)$ and its derivatives at $\nu = 0$ as they will be needed to calculate the moments of the probability distribution $W_{m.c.e.}(N)$. From Eq. (58) it follows

$$W_{m.c.e.}(0) = C \int_{-\infty}^{+\infty} d\lambda \exp \left[ \sum_{j=2}^{\infty} \frac{i^j \lambda^j}{j!} \frac{V}{(2\pi)^3} \int d^3p m_j(p) \epsilon_p^j \right].$$

(59)

It is convenient to introduce the notation

$$\sigma^2 = \frac{V}{(2\pi)^3} \int d^3p m_2(p) \epsilon_p^2.$$  

(60)

After replacing the integration variable, $\lambda = x/\sigma$, the integral (59) takes the form

$$W_{m.c.e.}(0) = C \sigma \int_{-\infty}^{+\infty} dx \exp \left( -\frac{x^2}{2} \right) \exp \left[ \sum_{j=3}^{\infty} \frac{i^j \kappa_{jj}}{j!} x^j \right],$$

(61)

where

$$\kappa_{ij} = \frac{1}{\sigma^j} \frac{V}{(2\pi)^3} \int d^3p m_i(p) \epsilon_p^j.$$  

(62)

It is easy to see that

$$\kappa_{ij} \propto V^{1-j/2},$$

(63)

i.e. the coefficients $\kappa_{jj}$, $j \geq 3$ in the second exponent of (61) become small at $V \to \infty$. We expand the second exponential function in Eq. (61) and perform the integration:

$$W_{m.c.e.}(0) = \frac{\sqrt{2\pi C}}{\sigma} \left[ 1 + \left( \frac{1}{8} \kappa_{4,4} - \frac{5}{24} \kappa_{3,3}^3 \right) + O(V^{-2}) \right].$$

(64)

Similarly,

$$\left. \frac{dW_{m.c.e.}(\nu)}{d\nu} \right|_{\nu=0} = -\frac{C}{\sigma} \int_{-\infty}^{+\infty} dx \left( \bar{N} + \sum_{j=2}^{\infty} \frac{i^{j-1} \kappa_{j(j-1)}}{(j-1)!} x^{j-1} \right) \times \exp \left( -\frac{x^2}{2} \right) \exp \left[ \sum_{j=3}^{\infty} \frac{i^j \kappa_{jj}}{j!} x^j \right]$$

$$= \frac{i\bar{N}C\sqrt{2\pi}}{\sigma} \left[ 1 + \left( \frac{\kappa_{2,1} \kappa_{3,3}}{2\bar{N}} - \frac{\kappa_{3,2}}{2\bar{N}} - \frac{5}{24} \kappa_{3,3}^3 + \frac{1}{8} \kappa_{4,4} \right) + O(V^{-2}) \right].$$

(65)
and
\[ \frac{d^2 \tilde{W}_{\text{m.c.e.}}(v)}{dv^2} \bigg|_{v=0} = -\frac{C}{\sigma} \int_{-\infty}^{+\infty} dx \left[ \sum_{j=2}^{\infty} \frac{i^{j-2} \kappa_{j(j-2)} x^j}{(j-2)!} \left( \frac{N_0^2}{\sigma^2} + \sum_{j=2}^{\infty} \frac{i^{j-1} \kappa_{j(j-1)} x^j}{(j-1)!} \right)^2 \right] \]
\times \exp \left( -\frac{x^2}{2} \right) \exp \left[ \sum_{j=3}^{\infty} \frac{i^j \kappa_{jj} x^j}{j!} \right] = -\frac{N_0^2 C \sqrt{2\pi}}{\sigma} \left[ 1 + \left( \frac{\kappa_{20}}{N_0^2} \right)^2 \right.
\left. - \frac{\kappa_{21}^2}{N_0^2} - \frac{\kappa_{32}}{N_0} + \frac{\kappa_{21} \kappa_{33}}{N_0} - \frac{5}{24} \kappa_{33}^2 + \frac{1}{8} \kappa_{44} \right) + O(V^{-2}) \right]. \quad (66)

Now the moments of the probability distribution \( W_{\text{m.c.e.}}(N) \) can be calculated:
\[ \langle N \rangle_{\text{m.c.e.}} = \frac{1}{iW_{\text{m.c.e.}}(0)} \frac{d^2 \tilde{W}_{\text{m.c.e.}}(v)}{dv^2} \bigg|_{v=0} = \frac{N_0}{1 + \frac{1}{2N_0^2} (\kappa_{21} \kappa_{33} - \kappa_{32}) + O(V^{-2})} \quad (67) \]
and
\[ \langle N^2 \rangle_{\text{m.c.e.}} = \frac{1}{W_{\text{m.c.e.}}(0)} \frac{d^2 \tilde{W}_{\text{m.c.e.}}(v)}{dv^2} \bigg|_{v=0} = \frac{N_0^2}{1 + \left( \frac{\kappa_{20} - \kappa_{21}^2}{N_0^2} + \frac{\kappa_{21} \kappa_{33} - \kappa_{32}}{N_0} \right) + O(V^{-2})}. \quad (68) \]

As it should be, \( \langle N \rangle_{\text{m.c.e.}} \) and \( \langle N^2 \rangle_{\text{m.c.e.}} \) approach, respectively, the grand canonical values \( N_0 \) and \( N_0^2 \) in the thermodynamical limit. The leading finite-volume corrections decay as \( 1/V \). Calculation of higher-order corrections is straightforward.

As is seen, the correction terms containing \( \kappa_{21} \kappa_{33} - \kappa_{32} \) contribute both to \( \langle N \rangle_{\text{m.c.e.}} \) and \( \langle N^2 \rangle_{\text{m.c.e.}} \), but cancel each other in the scaling variance,
\[ \omega_{\text{m.c.e.}} = \frac{\langle N^2 \rangle_{\text{m.c.e.}} - \langle N \rangle_{\text{m.c.e.}}^2}{\langle N \rangle_{\text{m.c.e.}}} = \frac{\kappa_{20} - \kappa_{21}^2}{N_0} + O(V^{-1}) = \frac{\int d^3p \, v_p^2 \int d^3p \, v_p^2 c_p^2}{\int d^3p \, v_p^2 c_p^2} - \frac{(\int d^3p \, v_p^2 c_p^2)^2}{\int d^3p \, n_p} + O(V^{-1}), \quad (69) \]
so that the result for fluctuations is indeed the same as in the previous section [14].

**IV. SUMMARY**

We have proposed a new method for a microcanonical treatment of quantum gases near a thermodynamic limit. The method is based on the analysis of moments of the particle number distribution in the microcanonical ensemble. For particle number fluctuations in the thermodynamic limit it leads to the same results as the microscopic correlator method [15]. However, the new method is more mathematically rigorous and consistent, and it elucidates some subtleties. It gives, therefore, a justification of our previous findings [23] that the scaled variance for particle number fluctuations in the microcanonical ensemble is different from that in the grand canonical ensemble even in the thermodynamic limit. Along with fluctuations, the new method allows calculating the finite-volume corrections to the thermodynamic quantities in the microcanonical ensemble. This can not be done within the microscopic correlator calculations. Our approach can be straightforwardly extended to the system of charged particles with exact charge conservation laws taken into account.

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APPENDIX A: FOURIER TRANSFORM OF A PROBABILITY DISTRIBUTION

Let us consider a probability distribution \( W(x) \). The Fourier transform of this distribution is given by:

\[
\tilde{W}(y) = \int dx e^{ixy} W(x) ,
\]

(A1)

or, for a discrete variable \( x \),

\[
\tilde{W}(y) = \sum_x e^{ixy} W(x) .
\]

(A2)

It is easy to check that the derivatives of the function \( \tilde{W}(y) \) are related to the average values of \( x^k \):

\[
\langle x^k \rangle = \frac{1}{W(0)} \left. \left( \frac{1}{i} \frac{d}{dy} \right)^k \tilde{W}(y) \right|_{y=0} .
\]

(A3)

The central moments of the distribution \( W(x) \) can be conveniently calculated using \( \log \tilde{W}(y) \):

\[
m_k = \left. \left( \frac{1}{i} \frac{d}{dy} \right)^k \log \tilde{W}(y) \right|_{y=0},
\]

(A4)

where

\[
m_1 = \langle x \rangle ,
\]

(A5)

\[
m_2 = \langle (x-\langle x \rangle)^2 \rangle ,
\]

(A6)

\[
m_3 = \langle (x-\langle x \rangle)^3 \rangle ,
\]

(A7)

\[
m_4 = \langle (x-\langle x \rangle)^4 \rangle - 3\langle (x-\langle x \rangle)^2 \rangle^2 ,
\]

(A8)

etc.

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