

## Statistical Physics in a Finite Volume with Absolute Conservation Laws

Sen Cheng

Department of Physics and Astronomy and  
National Superconducting Cyclotron Laboratory,  
Michigan State University, East Lansing, Michigan 48824-1321

**Abstract.** Recursion relations are used to exactly calculate the partition function of a canonical ensemble in which all additive charges as well as the total isospin are strictly conserved. The ensemble can consist of particles that obey either classical or quantum statistics. Recursion relations are also employed to compute observables such as multiplicity distributions and isospin fluctuations.

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### 1. Introduction

Results from a canonical ensemble that obeys exact conservation of additive charges and isospin can be useful in a variety of applications. For example, the unexpected isospin imbalances of CENTAURO events [1] could be explained by employing a Gaussian thermal source and restricting the pion emission to isoscalar pairs only. The pion multiplicity distributions become broader as compared to those of independent pion emission, thus resulting in larger fluctuations [2,3]. This finding could be further substantiated by replacing the Gaussian thermal source by a canonical ensemble and the ad-hoc assumption of isoscalar pairs emission by conservation of total isospin and its projection.

Another potential area of application is the modeling of relativistic heavy ion collisions. Here, hydrodynamical models are used to describe the early stages of the collision, when the density is so high that the particles behave collectively as a fluid. As the collision progresses the density falls, the system breaks up, and hydrodynamics is not applicable anymore. Therefore, the break-up and later stages of the collision have to be described by other means such as, for example, microscopic transport models [4]. When switching to a microscopic transport model from a macroscopic hydrodynamical prescription, particles must be formed from the fluid such that momentum and energy as well as isospin and all

other charges are conserved. Currently, most schemes for generating particles are based on the grand canonical ensemble. However, exact conservation within each event and within each computational cell is essential for studies on fluctuations and balance functions [5].

Partition functions for canonical ensembles conserving charges can be written quite easily, but they are very difficult to compute for large systems because the number of partitions that have to be summed over increases rapidly [6]. This difficulty can be overcome by rewriting the partition function as a recursion relation. These recursion relations were applied to ensembles of classical particles in [7] and to Fermi systems in [8].

In this work we add total isospin conservation to the canonical ensemble and derive the appropriate recursion relations. Furthermore, isospin fluctuations in the canonical ensembles, which, for example, are relevant for CENTAURO event studies, are calculated. A Monte Carlo algorithm that employs these recursion relations to generate particles is part of ongoing work and will be presented in the future. As our focus is the development of the computational technique, we show sample calculations for simple systems rather than comparisons to experimental results.

## 2. Recursion Relations with Classical Statistics

### 2.1. Partition Functions

The partition function for a canonical ensemble of  $A$  particles conserving a charge  $Q$ , where  $Q$  could be a vector containing several charges, is defined as

$$Z_{A,Q} = \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle, \quad (1)$$

where  $\alpha$  labels some quantum state with the appropriate quantum numbers,  $\beta$  is the inverse temperature, and  $H$  is the Hamiltonian of the system. Using the single particle partition function

$$\omega_k = \sum_i \exp(-\varepsilon_i^{(k)}/T), \quad (2)$$

which is simply a sum of Boltzmann weights over all available states  $i$ , the partition function can be written in a more tractable form as a sum over partitions subject to particle number and charge conservation

$$Z_{A,Q} = \sum_{\langle \sum v_k a_k = A; \sum v_k q_k = Q \rangle} \prod_{k=1}^N \frac{\omega_k^{v_k}}{v_k!}. \quad (3)$$

$N$  is the number of particle types,  $v_k$  is the number of particles of type  $k$ , and  $q_k$  is the charge of one particle. The particle number  $a_k$  indicates how many times a particle contributes to the main conserved quantity, e.g., in the case of multi-fragmentation,  $a_k$  would be the mass number of the nuclei.

The computational challenge of Eq. (3) is hidden in the number of partitions to be summed over. Assuming  $a_k = 1$  for all  $k$ , the number of partitions is

$$J(A,N) = \frac{(A+1)!}{(A+2-N)!}, \quad (4)$$

which is prohibitive to compute for large  $A$  or  $N$ . However, summing over all partitions can be bypassed when using recursion relations as derived in [7]

$$Z_{A,Q} = \frac{1}{A} \sum_j a_j \omega_j Z_{A-a_j, Q-q_j}. \quad (5)$$

If intermediate values are stored, Eq. (5) requires a linear runtime in both,  $A$  and  $N$ .

To conserve isospin as well, a sum over all possible isospin configurations for a given partition,  $\{\mathbf{v}_k\}$ , and isospin weights  $W(I, M | \{\mathbf{v}_k\})$  have to be included in the partition function

$$\Omega_{A,I,M,Q} = \sum_{\langle \sum \mathbf{v}_k a_k = A; \sum \mathbf{v}_k q_k = Q \rangle} \sum_{\{\mathbf{v}_k\}} W(I, M | \{\mathbf{v}_k\}) \prod_{k=1}^N \frac{\omega_k^{\mathbf{v}_k}}{\mathbf{v}_k!}. \quad (6)$$

This partition function can be converted to a recursion relation by inserting  $\frac{1}{A} \sum_{j=1}^N a_j \mathbf{v}_j = 1$

$$\Omega_{A,I,M,Q} = \frac{1}{A} \sum_{j=1}^N a_j \omega_j \sum_{\langle \sum \mathbf{v}_k a_k = A; \sum \mathbf{v}_k q_k = Q \rangle} \sum_{\{\mathbf{v}_k\}} W(I, M | \{\mathbf{v}_k\}) \frac{\omega_j^{\mathbf{v}_j-1}}{(\mathbf{v}_j-1)!} \prod_{k \neq j} \frac{\omega_k^{\mathbf{v}_k}}{\mathbf{v}_k!}. \quad (7)$$

The summation indices can be switched

$$\mathbf{v}'_k = \begin{cases} \mathbf{v}_k & , k \neq j \\ \mathbf{v}_k - 1 & , k = j \end{cases} \quad (8)$$

if the sum over isospin configurations is split:

$$\sum_{\{\mathbf{v}_k\}} W(I, M | \{\mathbf{v}_k\}) = \sum_{l'=|M-m_j|}^{I_j+I} \langle I_j m_j; l', M - m_j | IM \rangle^2 \sum_{\{\mathbf{v}'_k\}} W(l', M | \{\mathbf{v}'_k\}). \quad (9)$$

Finally, the recursion relation with conserved total isospin turns out to be

$$\Omega_{A,I,M,Q} = \frac{1}{A} \sum_j a_j \omega_j \sum_{l'=|M-m_j|}^{I+I_j} \langle I_j m_j; l', M - m_j | IM \rangle^2 \Omega_{A-a_j, l', M-m_j, Q-q_j}. \quad (10)$$

## 2.2. Multiplicity Distributions

We derive a recursion relation for the multiplicity distribution of a set  $B$  of particle types. The probability of observing  $n$  particles of a type contained in the set  $B$  can be expressed in terms of factorial moments [7]

$$P_{B,A,I,M}(n) = \sum_{l \geq n} F_{B,A,I,M}(l) \frac{(-1)^{l-n}}{(l-n)! n!}, \quad (11)$$

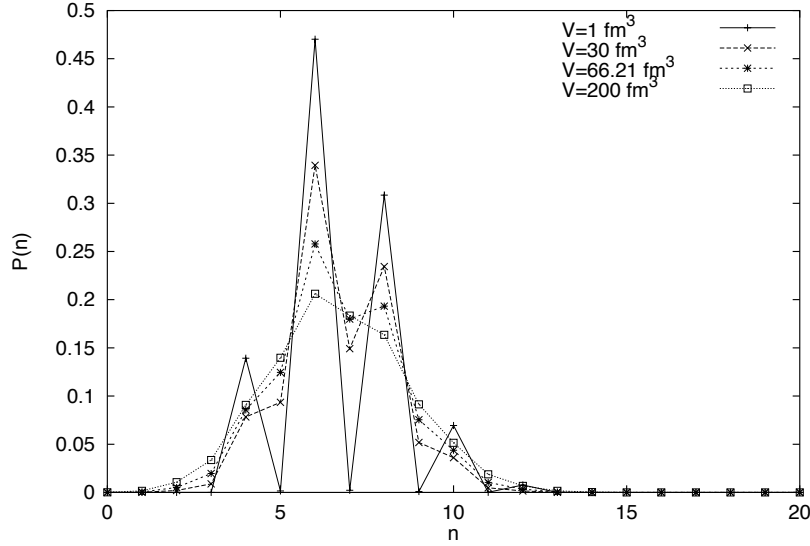
for which recursion relations can be found more easily. Following the procedure in the previous subsection the recursion relation for the factorial moment is found to be

$$F_{B,A,I,M}(n) = \sum_{k \in B} \omega_k \sum_{l'} \langle I_k m_k; l', M - m_k | IM \rangle^2 \frac{\Omega_{A-a_k, l', M-m_k}}{\Omega_{A,I,M}} F_{B,A-a_k, l', M-m_k}(n-1), \quad (12)$$

which leads to the recursion relation for the multiplicity distribution

$$P_{B,A,I,M}(n) = \frac{1}{n} \sum_{k \in B} \omega_k \sum_{I'} \langle I_k m_k; I', M - m_k | IM \rangle^2 \frac{\Omega_{A-a_k, I', M-m_k}}{\Omega_{A, I, M}} P_{B, A-a_k, I', M-m_k}(n-1). \quad (13)$$

To test Eq. (13) we implemented a program that included the pseudo-scalar and vector mesons as well as their decays. Figure 1 shows the multiplicity distribution for neutral pions: the system was constrained to be in an isospin singlet at a temperature of 170 MeV and had to produce a total of 20 pions. For this and all following sample calculations we



**Fig. 1.** Multiplicity distribution of neutral pions for several volumes. The calculation includes all pseudo-scalar and vector mesons and their weak decays. The system was constrained to an isospin singlet at a temperature of 170 MeV. The total number of pions was a fixed  $A = 20$ .

need to make an assumption about the energy states that are available to the particles and that have to be summed over in the single particle partition function of Eq. (2). We required that the linear momentum  $k$  in one dimension satisfy the condition

$$kR = \pi \left( n + \frac{1}{2} \right), \quad (14)$$

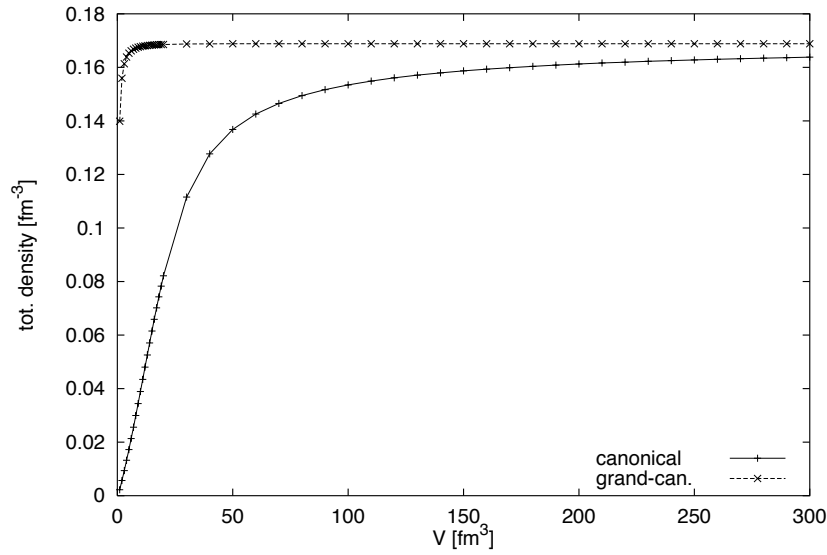
where  $n = 0, 1, 2, \dots$  and  $R$  is the size of the system. The half integers on the RHS, instead of the more usual integers, were inspired by the MIT bag model and lead to a reduction of zero-point surface energy effects. This becomes important for systems that are confined to a small volume. By assuming that our model systems are confined to a cube of volume  $V$ ,

we obtain the energy states

$$\epsilon_{n,m,l} = \sqrt{\frac{\pi^2}{R^2} [(n + 1/2)^2 + (m + 1/2)^2 + (l + 1/2)^2] + M^2}, \quad (15)$$

where  $n, m, l = 0, 1, 2, \dots, M$  is the mass of the particle, and  $R = V^{1/3}$ .

The even-odd asymmetry in Fig. 1 for small volumes that vanishes for larger volumes can be understood in the following way. At small volumes and low temperatures the system minimizes the number, not the mass, of particles produced; it prefers to produce heavy particles that decay into multiple pions rather than producing pions or kaons. These heavy particles ( $\omega$ ,  $\eta$ ,  $\eta'$ ) decay into an odd number of pions (and also into an odd number of neutral pions). Because the number of heavy particles has to be even to make 20 pions, as we imposed, the number of neutral pions is strongly favored to be even. At higher volumes or temperatures low mass particles dominate and the even-odd asymmetry vanishes.



**Fig. 2.** Total number density of a system of only pions in an isosinglet at a temperature of 170 MeV. Shown are calculations for a grand-canonical and a canonical ensemble with classical statistics.

The factorial moment from Eq. (12) corresponds to the density, when  $n = 1$ . For a system of pions in an isosinglet, particle production is significantly suppressed at low volume, but converges towards the grand-canonical result at large volumes (Fig. 2).

### 3. Recursion Relations with Quantum Statistics

For a canonical ensemble of quantum particles with charge conservation the recursion relation for the partition function was given in [8]:

$$Z_{A,Q} = \frac{1}{A} \sum_k \sum_{n=1}^{\infty} C_n^{(k)} Z_{A-n, Q-q_k}, \quad (16)$$

where  $C_n^{(k)} = (\pm 1)^{n-1} \sum_i \exp(-n\varepsilon_i^{(k)}/T)$ . To derive a partition function  $\Omega_{A,I,M,Q}$  that conserves total isospin as well, we first observe that, if the Hamiltonian of the system is independent of  $M$ , then so is the partition function. Then the partition function conserving total isospin can be related to one that conserves only the projection  $Z_{A,M,Q} = \sum_{I \geq M} \Omega_{A,I,M,Q}$ . Therefore

$$\Omega_{A,I,M,Q} = Z_{A,M,Q} - Z_{A,M+1,Q}. \quad (17)$$

To calculate densities the 2-point function is needed

$$\langle a_i^\dagger a_j \rangle = \frac{\delta_{ij}}{Z_A} \sum_n (\pm 1)^{n-1} \exp(-n\varepsilon_i/T) Z_{A-n}, \quad (18)$$

which, however, can only be used when conserving additive quantities, but not isospin. The 4-point function serves to calculate higher moments

$$\langle a_i^\dagger a_j^\dagger a_k a_l \rangle = \frac{1}{Z_A} (\delta_{il} \delta_{jk} \pm \delta_{ik} \delta_{jl}) \sum_{n_i, n_j} (\pm 1)^{n_i + n_j} \exp(-n_i \varepsilon_i/T - n_j \varepsilon_j/T) Z_{A-n_i-n_j}. \quad (19)$$

### 4. Isospin Fluctuations

For classical particles the isospin fluctuation

$$\sigma = \sum_{I=0} \langle I | (n_+ + n_- - 2n_0)^2 | I \rangle, \quad (20)$$

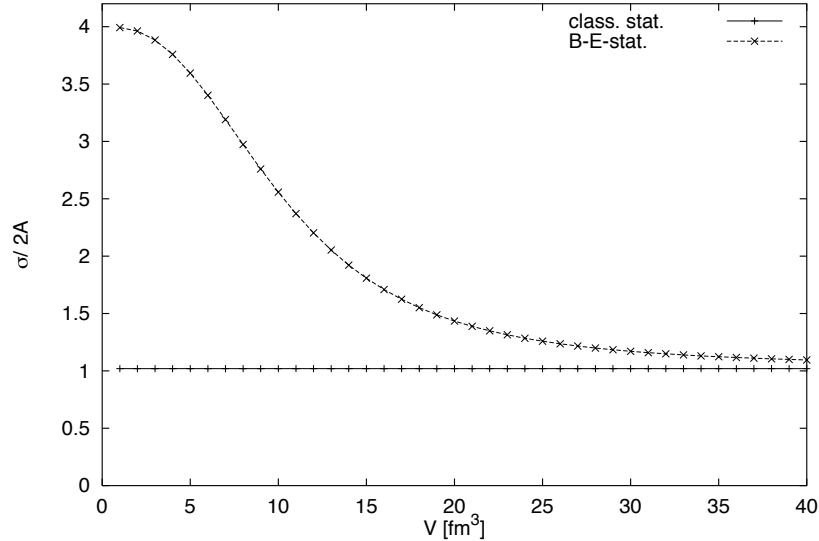
where  $n_+, n_-, n_0$  are the densities of the respective pions, can be readily computed with the recursion relations derived above. However, for quantum particles we cannot compute the density, let alone the higher moments, when conserving total isospin. Therefore, we need to rewrite Eq. (20) in terms of isospin projection states.

The operator in Eq. (20), itself a product of spherical tensor components, can be written as a decomposition into other spherical tensor components  $A_{JM}$

$$(n_+ + n_- - 2n_0)^2 = 6T_{20}T_{20} = 6 \sum_{J,M} \langle 20; 20 | JM \rangle A_{JM}. \quad (21)$$

By the Wigner-Eckart theorem only  $A_{00}$  contributes when contracted between isosinglet states,  $\sigma = 6 \sum_{I=0} \langle I | A_{00} | I \rangle$ , which, after some algebra, becomes

$$\sigma = \frac{6}{5} \left( \sum_{M=0} - \sum_{M=1} \right) \left\langle M \left| \frac{3}{2}n_+ + \frac{3}{2}n_- + n_0 + \frac{1}{6}(n_+ + n_- - 2n_0)^2 \right| M \right\rangle. \quad (22)$$



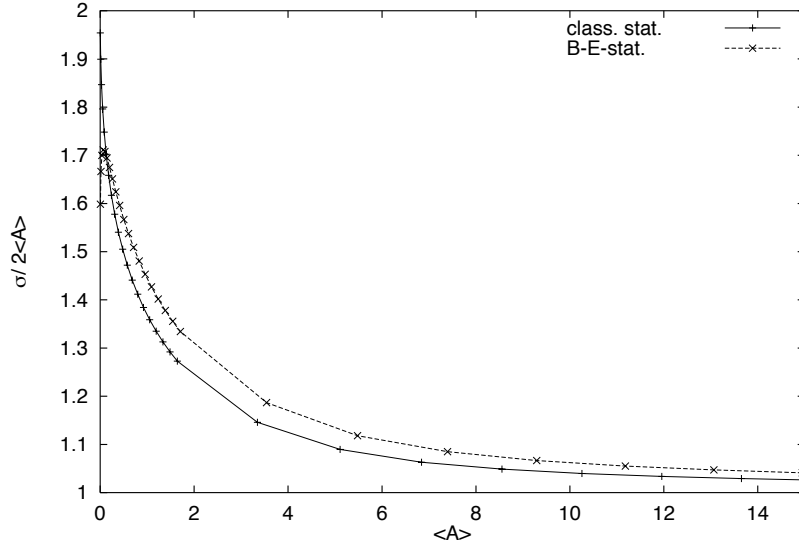
**Fig. 3.** Isospin fluctuations as a function of volume for a system of pions at a temperature of 170 MeV with a fixed number of pions,  $A = 20$ . Shown are calculations with classical and Bose-Einstein statistics. The isospin fluctuations are divided by  $2A$ , the expected isospin fluctuation for a gas of independent pions.

In Figs. 3 and 4 we compare classical to Bose-Einstein statistics in calculations of isospin fluctuations for a system of pions at  $T = 170$  MeV. The fluctuations are divided by  $2A$ , the expected fluctuation for an independent pion gas, to highlight the difference. When the system is fixed to contain 20 pions (Fig. 3), the isospin fluctuation for classical particles does not depend on the volume, as the relative composition of the classical pion gas does not. Bose-Einstein particles, however, prefer to be all in the same state, when the volume becomes small, thus enhancing the isospin fluctuations. When the number of pions is not fixed, the isospin fluctuations converge towards the value for an independent pion gas as the system increases in size (Fig. 4).

## 5. Conclusions

Recursion relations have been derived for a canonical ensemble in which all additive charges as well as the total isospin are strictly conserved. In the case of classical statistics we derived recursion relations for the partition function and multiplicity distribution. For quantum statistics we obtained a recursion relation for the partition function and density. Work is under way to derive the recursion relation for the multiplicity distribution in the latter case.

These recursion relations can be applied to an arbitrary number of particle types and conserved additive charges. They can be computed correctly within the numerical precision



**Fig. 4.** Isospin fluctuations as a function average pion number for a system of pions at a temperature of 170 MeV. Shown are calculations with classical and Bose-Einstein statistics. The isospin fluctuations are divided by  $2\langle A \rangle$ , the expected isospin fluctuation for a gas of independent pions.

of the computer in a reasonable runtime as our sample calculations show. We can now move forward and apply this technique to physical problems and in Monte Carlo algorithms that generate particles with exact conservation of additive charges and isospin. We also derived a method to quickly calculate isospin fluctuations, which makes use of the recursion relations we obtained.

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