Steady state of isolated systems versus microcanonical ensemble

M. Gazdzicki,1,2 M. I. Gorenstein,3,4 A. Fronczak,5
P. Fronczak,5 and M. Mackowiak-Pawlowska5

1Geothe-University Frankfurt am Main, Germany
2Jan Kochanowski University, Kielce, Poland
3Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine
4Frankfurt Institute for Advanced Studies, Frankfurt, Germany
5Faculty of Physics, Warsaw University of Technology,
Koszykowa 75, PL-00-662 Warsaw, Poland

Abstract

A simple dynamical model of particle creation and annihilation in an isolated assembly of particles with conserved energy and fixed volume, the Cell Model, is formulated. With increasing time particle number distribution, obtained by averaging over many systems, approaches a time-independent, steady state distribution. Dependence of the steady state distribution on creation and annihilation conditional reaction probabilities is studied. The results obtained for the steady state are compared with predictions of statistical mechanics within the microcanonical ensemble. In general, the predictions of both models are different. Special conditions needed for their agreement are derived and discussed. The differences between the steady state and microcanonical ensemble show that distinction should be introduced between two classes of models of particle production in high energy collisions. Namely, the statistical models postulating particle creation according to microcanonical ensemble, and the dynamical models assuming particle production via successive, local, creation and annihilation reactions.
I. INTRODUCTION

In modelling an assembly of many particles, one usually refers to a probabilistic approach for calculating system macroscopic properties. Isolated systems of interacting particles are expected to evolve from an arbitrary starting conditions to a steady state, i.e. the state whose macroscopic properties are independent of time. It is popular to believe that the steady state (SS) properties can be calculated within statistical mechanics. Indeed, numerous experimental results on properties of many-particle steady states are in agreement with statistical mechanics. However, the success of statistical mechanics remains unexplained, especially from the point of view of its dynamical foundations [1].

The basic ensemble of microstates in statistical mechanics is the one formulated for isolated systems [2], the so-called microcanonical ensemble (MCE). Other statistical ensembles, like canonical and grand canonical ensembles, can be straightforwardly derived from the MCE. The MCE is defined by all conserved quantities of the system, its volume $V$ and possible microstates. Here it is assumed that energy $E$ is the only conserved quantity. Thus, there are only two independent thermodynamic variables, $E$ and $V$.

The key postulate of statistical mechanics is that all MCE microstates have equal probabilities to appear. Properties of the MCE, like particle number distribution, are easy to calculate for an ideal gas of particles in which the total energy is equal to the sum of single particle energies. Obviously the energy conservation introduces a correlation between particles.

In contrast to statistical mechanics, dynamical models do not postulate probabilities of the microstates. Instead, these probabilities depend on properties of elastic and inelastic reactions between particles. The reactions lead to a time walk of a dynamical system from microstate to microstate starting from an assumed microstate at $t = 0$. Considering a large number of systems with $E$ and $V$ at a given time $t$ one gets an ensemble of microstates. In general, the microstate probability distribution depends on time and a starting microstate distribution. Let us assume that the probability distribution for $t \to \infty$ approaches a distribution which is independent of a starting distribution of microstates. This asymptotic distribution will be called the SS distribution, and the corresponding ensemble of microstates
will be referred to as the SS ensemble. In general, the SS depends on reactions between particles. They determine probabilities of transitions between the microstates. Of course, the MCE lacks such a dependence. Thus, one may expect that the SS ensemble and MCE are different.

In this paper, we introduce a simple approach for modelling an assembly of identical particles which are subject to creation and annihilation reactions, the Cell Model (CM). Correlations due to quantum statistics are not considered. The CM satisfies the energy conservation and allows to calculate the particle number distribution. Special conditions needed to reach the agreement between the SS and MCE predictions are established and discussed.

Isolated systems discussed in this paper do not actually occur in experiments or in nature. Probably the closest to isolated systems are multi-particle systems created in high energy collisions between particles or nuclei. They show many features which can be described within statistical mechanics \[3-5\], in particular microcanonical ensemble surprisingly well describes basic features of experimental data \[6-8\]. The question whether one can distinguish between particles being "born" according to the MCE or resulting from a time-lasting local creation and annihilation reactions motivated this work.

The paper is organized as follows. Section II introduces the Cell Model. In Sec. III the MCE corresponding to the Cell Model is formulated. The model presented here is a Markov chain on a countable microstate space that follows a random walk. This allows to calculate a time-dependence of particle number distribution using a Monte Carlo technique as presented in Sec. IV. Moreover analytical results for the steady state are obtained in Sec. V. Section VI presents a comparison between the results for the SS and MCE. The conditions needed for the agreement between the SS and MCE are derived and discussed. Closing remarks presented in Sec. VII end the paper.

To assure a minimum confusion in subsequent sections, we henceforth summarize here employed terminology:

(i) The label system refers to an assembly of particles with energy \(E\) and volume \(V\).

Number of particles \(N\) in the system changes in time \(t\) due to reaction between particles.
(ii) **Microstate** is a specific microscopic configuration of particles in the system at time $t$.

(iii) **State** refers to an ensemble of microstates.

(iv) **Steady state** labels an ensemble of microstates to which systems approach for $t \rightarrow \infty$.

(v) **Ergodicity** refers to a model property that any microstate has zero probability to never recur.

(vi) **Particle number distribution**, $P(N,t)$, is a probability distribution of $N$ calculated for many systems at time $t$. Mean particle number is given by $\langle N \rangle(t) \equiv \sum_N N P(N,t)$.

II. **CELL MODEL: BASIC ASSUMPTIONS**

The CM is introduced to study properties of isolated systems in the SS and compare the results with the corresponding MCE findings. In this paper, the comparison is limited to particle-number distribution. The number of particles in the system changes in time due to creation and annihilation reactions (inelastic reactions) which take place in $V$ space cells$^1$, $v = 1, \ldots, V$. Then, a new distribution of particles in cells is drawn from all possible microstates with a given particle number. This mimics the effect of elastic reactions. The formation time of a new microstate is assumed to be $\Delta t = 1$. Thus, in the model, time is discrete, $t = 0, 1, 2, \ldots$.

It is assumed that reactions are taking place independently in cells, and energy is conserved in each reaction separately. This local energy conservation leads, of course, to the energy conservation in the whole system. For simplicity, only two values of single particle energy are allowed: $\varepsilon = 1$ and 2. The microstates in the CM are thus defined by the set of ”occupation numbers” $(n_{1,1}, n_{2,1}; \ldots; n_{1,V}, n_{2,V})$, where $n_{\varepsilon,v}$ gives the number of particles having energy $\varepsilon$ in the $v$-th cell. All possible combinations of these sets should satisfy the

---

$^1$ The number of cells in the CM plays the role of volume in statistical mechanics.
energy conservation,

\[
\sum_{v=1}^{V} n_{1,v} + \sum_{v=1}^{V} 2n_{2,v} \equiv N_1 + 2N_2 = E .
\]  

(1)

III. CELL MODEL: MICROCANONICAL ENSEMBLE

In this section the MCE which corresponds to the CM is formulated and the MCE particle number distribution is derived. For given \( E \) and \( N = N_1 + N_2 \), one gets

\[
N_1 = \sum_{v=1}^{V} n_{1,v} = 2N - E , \quad \text{and} \quad N_2 = \sum_{v=1}^{V} n_{2,v} = E - N .
\]  

(2)

Consequently, the number of microstates is equal to

\[
W_{mce}(N; E, V) = W(N_1; E, V)W(N_2; E, V) = \binom{N_1 + V - 1}{N_1} \binom{N_2 + V - 1}{N_2} ,
\]  

(3)

i.e., for each arrangement of \( N_1 \) indistinguishable particles of energy \( \epsilon = 1 \) in \( V \) cells, one can have any arrangement of \( N_2 \) indistinguishable particles of energy \( \epsilon = 2 \) in \( V \) cells. The expressions for \( W(N_\epsilon; E, V) \) correspond to the well known result [9] for the number of different arrangements of \( N_\epsilon \) unlabeled balls (particles) among \( V \) labeled boxes (cells). The assumption of indistinguishable (unlabeled) particles implies that any permutation of particles, either in a cell or between different cells, does not produce a new microstate.

The total number of microstates for all possible pairs \((N_1, N_2)\), \( W_{mce}(E, V) \), is given by:

\[
W_{mce}(E, V) = \sum_{N=\lceil E^2 \rceil}^{E} W_{mce}(N; E, V) ,
\]  

(4)

where \( \lceil E^2 \rceil = \frac{E}{2} \) for even \( E \), and \( \lceil E^2 \rceil = \frac{E+1}{2} \) for odd \( E \).

The MCE assumes that all microstates with energy \( E \) (Eq. (1)) appear with equal probability. This allows to calculate the MCE particle number distribution as:

\[
P_{mce}(N; E, V) = \frac{W_{mce}(N; E, V)}{W_{mce}(E, V)} .
\]  

(5)
Examples of $P_{mce}(N; E, V)$ are shown in the following sections.

IV. CELL MODEL: MONTE CARLO APPROACH

In this section, the time evolution of a system is considered using a discrete-time Monte Carlo approach. It starts at $t = 0$ from an arbitrary microstate and then, in the consecutive time steps $t \geq 0$, it runs as follows:

(i) The initial numbers of particles with energy $\varepsilon = 1$ and 2, which are correspondingly equal to $N_1^I(t)$ and $N_2^I(t)$ (where $N_1^I(t) + 2N_2^I(t) = E$), are used to randomly draw an initial microstate $(n_{1,1}, n_{2,1}; \ldots; n_{1,V}, n_{2,V})$ with $\sum_{v=1}^{V} n_{1,v} = N_1^I$ and $\sum_{v=1}^{V} n_{2,v} = N_2^I$. This "random drawing" mimics the effect of elastic reactions.

(ii) Then creation and annihilation reactions take place. The reactions change the initial microstate $(n_{1,1}, n_{2,1}; \ldots; n_{1,V}, n_{2,V})$, into a final one, $(n_{1,1}^F, n_{2,1}^F; \ldots; n_{1,V}^F, n_{2,V}^F)$, with particle numbers $N_1^F(t) = \sum_{v=1}^{V} n_{1,v}^F$ and $N_2^F(t) = \sum_{v=1}^{V} n_{2,v}^F$.

(iii) The multiplicities $N_1^F(t)$ and $N_2^F(t)$ are then used to draw (elastic reactions) an initial microstate at $t + 1$ with $N_\varepsilon^I(t + 1) = N_\varepsilon^F(t)$.

(iv) Then the above sequence of executing elastic and inelastic reactions repeats in the next time step.

The assumed local energy conservation, that is met in each cell, implies the following relation between the initial and final cell multiplicities:

$$n_{1,v}^I(t) + 2n_{2,v}^I(t) = n_{1,v}^F(t) + 2n_{2,v}^F(t) ,$$

and the global energy conservation can be expressed as

$$N_1^F(t) + 2N_2^F(t) = E = \text{const} .$$
Correspondingly, the total number of particles at time \( t \) is equal to

\[
N(t) = N_F^1(t) + N_F^2(t).
\] (8)

Here, we consider a version of the CM in which the following creation and annihilation reactions \( (n_{I,1}^1, v_{1,1}) \rightarrow (n_{F,1}^1, n_{F,1}^2, v_{1,1}) \) take place:

(i) Annihilation \( (3, 0) \rightarrow (1, 1) \) with probability \( A_3 \),

(ii) Annihilation \( (2, 1) \rightarrow (0, 2) \) with probability \( A_4 \),

(iii) Creation \( (1, 1) \rightarrow (3, 0) \) with probability \( C_3 \),

(iv) Creation \( (0, 2) \rightarrow (2, 1) \) with probability \( C_4 \).

Indices 3 and 4 indicate the cell energy. The probabilities \( A \) and \( C \) are conditional probabilities of a reaction given an initial cell multiplicity. They are assumed to be independent of time and range from zero to one.

Then, for any values of \( E, V \) and conditional reaction probabilities, the time evolution of the system can be calculated using Monte Carlo simulations. Note that the implementation of the classical indistinguishable particles in dynamical simulations is not a straightforward task. Thus, we provided a practical algorithm for this problem (see Appendix A).

By construction, the particle number \( N \) at time \( t \) is a random variable. Thus, when following the time evolution of many systems starting from the same microstate a non-trivial particle number distribution \( P(N, t) \) is obtained\(^2\). This is illustrated in Fig. 1(a), which shows time dependence of the multiplicity distribution for \( E = 100, V = 20 \) and the initial multiplicity distribution \( P(N, 0) = \delta_{N,50} \). In Fig. 1(b), the time evolution of \( P(N, t) \) for the same system parameters but completely different initial microstate distribution, i.e. \( P(N, 0) = \text{const} \), is shown to converge to the same SS distribution like in the former case, i.e.

\[
\lim_{t \to \infty} P(N, t) = P_{ss}(N; E, V).
\] (9)

\(^2\) Note, that since \( N_F^1(t) = N_{I,1}^1(t + 1) \) and \( N_F^2(t) = N_{I,2}^2(t + 1) \), it follows that for a system approaching a SS one has \( P(N^F) = P(N^I) \).
FIG. 1: Examples of time evolution of $P(N,t)$ for CM with $E = 100$ and $V = 20$. (a) $P(N,0) = \delta_{N,50}$, (b) $P(N,0) = \text{const}$.

The above observation arises from the fact that the CM is an ergodic Markov chain, and as such, regardless of the initial conditions, it is always characterized by a unique stationary distribution (see Appendix B).

Figure 2 presents a comparison between $P_{\text{mce}}(N;E,V)$ (5) and $P_{\text{ss}}(N;E,V)$ (9) for different settings of the model parameters. The agreement between the SS and MCE distributions is observed only in some special cases, e.g., for equal conditional reaction probabilities: $A_3 = A_4 = C_3 = C_4$. In the case of arbitrarily-set conditional reaction probabilities, $P_{\text{mce}}(N;E,V)$ and $P_{\text{ss}}(N;E,V)$ usually differ significantly.

V. CELL MODEL: ANALYTICAL APPROACH

In this section an analytical expression for the particle number distribution in the steady state is derived within the discrete-time master equation (MEq) approach (see, e.g., Ref. [10]). It is assumed that for a system in the steady state a probability of having more than one inelastic reaction at a given time step can be neglected. This leads to the follow-
FIG. 2: The SS particle number distribution as compared to the MCE one. Gray histograms show numerical Monte Carlo simulation results for the CM with $V = 10$ and $E = 100$. Lines represent the MCE results \cite{5}. Conditional reaction probabilities used are the following: (a) $A_3 = A_4 = C_3 = C_4 = 1$, (b) $A_3 = A_4 = C_4 = 1$, $C_3 = \frac{1}{2}$.

The master equation for the time dependence of particle number probability distribution, $P(N,t)$:

\[ \Delta P(N,t) = A_3 \left( \frac{(N_1-1)+V-2}{V-2} \right) \left( \frac{(N_2-1)+V-2}{V-1} \right) P(N+1,t) \]
\[ + A_4 \left( \frac{(N_1+2)+V-1}{V-1} \right) \left( \frac{(N_2+1)+V-1}{V-1} \right) P(N+1,t) \]
\[ + C_3 \left( \frac{(N_1-3)+V-2}{V-2} \right) \left( \frac{(N_2+V-2)}{V-1} \right) P(N-1,t) \]
\[ + C_4 \left( \frac{(N_1-2)+V-2}{V-1} \right) \left( \frac{(N_2+V-1)}{V-1} \right) P(N-1,t) \]
\[ - A_3 \left( \frac{(N_1+V-1)}{V-1} \right) \left( \frac{N_2+V-1)}{V-1} \right) P(N,t) \]
\[ - A_4 \left( \frac{(N_1-2)+V-2}{V-1} \right) \left( \frac{(N_2-1)+V-2}{V-1} \right) P(N,t) \]
\[ - C_3 \left( \frac{(N_1+V-1)}{V-1} \right) \left( \frac{N_2+V-1)}{V-1} \right) P(N,t) \]
\[ - C_4 \left( \frac{(N_1+2)+V-2}{V-1} \right) \left( \frac{(N_2-2)+V-2}{V-1} \right) P(N,t) \]

(10)
where $\Delta P(N, t) = P(N, t + 1) - P(N, t)$.

The first term in the right-hand side of Eq. (10) states that systems with $N$ particles ($N_1$ with energy 1 and $N_2$ with energy 2) are created by reducing by one particle multiplicity in systems with $N+1$ particles, as a result of the reaction: $(3, 0) \rightarrow (1, 1)$. For this reaction, initial numbers of particles with energy 1 and 2 are equal to $N_1 + 2$ and $N_2 - 1$, respectively. Probability of this reaction is the product $w_1 w_2 w_3$ of probabilities of three independent events, namely:

(i) $w_1 = P(N+1, t)$ to have $N+1$ particles ($N_1 + 2$ of energy 1 and $N_2 - 1$ of energy 2);

(ii) there are exactly 3 particles of energy 1 and no particles of energy 2 in a given cell:

$$w_2 = \frac{\binom{N_1-1}{V-2}}{V-2} \frac{\binom{N_2-1}{V-2}}{V-2} \frac{\binom{N_1+2}{V-1}}{V-1} \frac{\binom{N_2-1}{V-1}}{V-1} \quad (11)$$

(iii) $w_3 = A_3$ that the reaction $(3, 0) \rightarrow (1, 1)$ occurs.

The other terms in the right-hand side of the MEq (10) are derived in a similar way. Constructing these terms, one needs to remember that the energy conservation requires $N+1 = (N_1 + 2) + (N_2 - 1)$, and $N-1 = (N_1 - 2) + (N_2 + 1)$.

For fixed values of $E$ and $V$, the SS solution of the MEq (10) can be obtained from the condition

$$\Delta P(N, t) = 0 \quad (12)$$

using recursive relations with the initial condition $P(E - 1) = 0$ (details are provided in Appendix C). The solution reads:

$$P_{ss}(N; E, V) = \frac{W_{ss}(N; E, V)}{W_{ss}(E, V)} \quad (13)$$
FIG. 3: The SS particle-number distributions for $E = 80$, $V = 20$, and four sets of conditional reaction probabilities: (I) $A_3 = 0.2$, $A_4 = 0.3$, $C_3 = 0.4$, $C_4 = 0.6$, which satisfy Eq. (20) for $r = 2$, (II) $A_3 = A_4 = C_3 = C_4 = 1$, which satisfy Eq. (5), (III) $A_3 = 0.6$, $A_4 = 0.1$, $C_3 = 0.3$, $C_4 = 0.3$, and (IV) $A_3 = 0.4$, $A_4 = 0.6$, $C_3 = 0.2$, $C_4 = 0.3$, which satisfy Eq. (20) for $r = 0.5$. (a) Comparison of the Monte Carlo (gray histograms) and MEq results (lines). (b) Numerical confirmation of Eq. (26). Points stand for results of Monte Carlo simulations, lines represent SS solutions of the MEq.

where, for even values of $E$,

\[ W_{ss}(N; E, V) = \binom{N_1 + V - 1}{V - 1} \binom{N_2 + V - 1}{V - 1} T(N; E, V), \]

\[ T(N; E, V) = \prod_{k=E/2}^{N-E} \frac{(2k-E)(E-k+V-3) C_3 + (E-k-1)(2k-E+V-2) C_4}{(2k-E)(E-k+V-3) A_3 + (E-k-1)(2k-E+V-2) A_4}, \]

\[ W_{ss}(E, V) = \sum_{N=E/2}^{E} W_{ss}(N; E, V). \]

where, from the definition of the empty product, $T(E/2; E, V) = 1$. Let us note, that in the pathological case of $C_3 = C_4 = 0$ one has $T(N; E, V) = \delta_{N,E}$. In this case one gets $P_{ss}(N; E, V) = \delta_{N,E}$. It can be also shown that the second pathological case, $A_3 = A_4 = 0$, boils down to $P_{ss}(N; E, V) = \delta_{N,E}$. To show this, one has to reformulate the solution of the MEq by solving it with the initial condition $P(E + 1) = 0$ (cf. Appendix C). For all possible choices of $E$ and $V$, and the conditional reaction probabilities $A_3$, $A_4$, $C_3$, $C_4$, the analytical expression (13) for the SS multiplicity distributions agrees with numerical Monte
This observation, though evident in itself, allows to see quite non-obvious feature of comparison, the SS result for $\langle N \rangle$ is also shown (solid line).

When dividing the numerator and denominator of each factor in the product $T(N; E, V)$ by an arbitrary constant parameter $\alpha$, the resulting SS distribution does not change. This observation, though evident in itself, allows to see quite non-obvious feature of $P_{ss}(N; E, V)$. Namely, putting, for example, $\alpha = C_3$ one finds that, for fixed $E$ and $V$, $P_{ss}(N; E, V)$ only depends on three independent parameters - the ratios of the conditional reaction probabilities: $C_4/C_3$, $A_3/C_3$, and $A_4/C_3$, correspondingly.

Additionally, assuming that $\alpha \geq 1$ one can study the effect of rescaled conditional reaction probabilities (i.e. $A_3/\alpha$, $A_4/\alpha$, $C_3/\alpha$, $C_4/\alpha$), on the CM convergence towards the stationary state. This is illustrated in Fig. 4 where the time dependence of the mean particle number is plotted for different values of $\alpha$ and with other model parameters fixed. The results are calculated using the Monte Carlo approach. In the figure, the mean particle number for the SS calculated using the MEq approach is also plotted for a comparison. As expected Monte Carlo results approach the MEq one with increasing time and the convergence is slower for larger values of $\alpha$. 

FIG. 4: Mean particle number, $\langle N \rangle$ as a function of the time $t$ calculated for systems with $E = 100$, $V = 20$, $A_3 = A_4 = C_3 = C_4 = 1$, and for $\alpha = 1$ (circles), $\alpha = 2$ (dots), and $\alpha = 4$ (crosses). The convergence curves were obtained within Monte Carlo simulations averaged over 1000 runs. For comparison, the SS result for $\langle N \rangle$ is also shown (solid line).
VI. STEADY STATE VERSUS MICROCANONICAL ENSEMBLE

In this section, the particle number distributions calculated for the SS are compared with the corresponding MCE distributions, and the limits of MCE applicability in dynamical systems are discussed. Firstly, we discuss conditions needed for the agreement between the steady state and MCE. Secondly, these conditions are somewhat relaxed, resulting in the grand micro canonical ensemble. Thirdly, the most general case of the SS distribution is considered, that does not correspond to any known distribution of statistical mechanics. Finally, an extreme case of only one type of reactions (creation or annihilation) changing particle number is discussed.

(i) One notes that the SS distribution (13) differs from the MCE one (5) by the factor \( T(N; E, V) \), which comprises a dependence on the conditional reaction probabilities. Thus the SS distribution coincides with the MCE one provided that \( T(N; E, V) = 1 \). This is the case for the special selection of the conditional reaction probabilities, namely,

\[
A_3 = C_3, \quad A_4 = C_4 .
\]  

(17)

Then the number of independent parameters of the SS distribution is reduced from three to one, which corresponds to the ratio \( C_3/C_4 = A_3/A_4 \). Thus for any allowed value of this ratio, and for all values of \( E \) and \( V \), the SS predictions agree with the MCE ones.

The condition (17) for the equivalence of the SS and MCE was derived within the specific version of the CM discussed in this paper as an example. Below a more general considerations are presented which are valid for any version of the Cell Model which is the ergodic Markov chain model (see Appendix B). One considers two microstates, \( X = (n_{1,1}^X, n_{2,1}^X; \ldots; n_{1,V}^X, n_{2,V}^X) \) and \( Y = (n_{1,1}^Y, n_{2,1}^Y; \ldots; n_{1,V}^Y, n_{2,V}^Y) \), which can be transformed to each other with conditional probabilities \( B(X \rightarrow Y|X) \) and \( B(Y \rightarrow X|Y) \), respectively. The conditional probability \( B(X \rightarrow Y|X) \) is a probability of the transition \( X \rightarrow Y \) given the microstate \( X \). Thus the transition probability is equal
to $P(X \rightarrow Y) = B(X \rightarrow Y | X)P(X)$ (respectively, $P(Y \rightarrow X) = B(Y \rightarrow X | Y)P(Y)$), where $P(X)$ is the probability of a microstate $X$.

Let us assume that the conditional probabilities of forward and backward transitions are equal for all pairs of microstates, $B(X \rightarrow Y | X) = B(Y \rightarrow X | Y)$. Then one first postulates that the starting (at $t = 0$) distribution of microstates in a large ensemble of systems is equal to the MCE one, i.e., all microstates have the same probability to appear, $P(X) = P(Y)$. Consequently, after the first time step ($t = 1$) all microstates have the same probability to appear, as by the assumption, the numbers of forward and backward transitions are equal. This is, of course, also the case after each subsequent time step. One concludes that the microstate distribution is time independent and, thus, the corresponding SS is equivalent to the MCE. But within the ergodic Markov models (see Appendix B), the SS is independent of a starting distribution (see Appendix B). Therefore, one shows that equal conditional transition probabilities for $X \rightarrow Y$ and $Y \rightarrow X$ transitions result in a steady state which is equal to the MCE. Moreover the transition probabilities for forward and backward transitions are equal: $P(X \rightarrow Y) = P(Y \rightarrow X)$. This corresponds to the so-called detailed balance in the system.

(ii) Let us relax the condition (17) by introducing a parameter, $r$, defined as:

$$C_3 = rA_3, \quad C_4 = rA_4.$$  \hspace{1cm} (18)

Then, for fixed $E$ and $V$, the number of independent parameters in $P_{ss}(N; E, V)$ increases from one to two and the factor $T(N; E, V)$ in Eq. (15) reads

$$T(N; E, V) = r^{N - \frac{E}{k}}.$$  \hspace{1cm} (19)

For $r = 1$ one gets $T(N; E, V) = 1$ and recovers the previously discussed result (17), which coincides with MCE. For $r \neq 1$ the SS particle-number distribution (13) can be
written in the form:

\[ P_{ss}(N; E, V) = W_{mce}(N; E, V) \frac{\exp(-\mu N)}{Z_{gmce}(E, V, \mu)} \equiv P_{gmce}(N; E, V, \mu) , \]

where \( \mu \equiv -\ln(r) \) resembles a dimensionless chemical potential, and \( Z_{gmce}(E, V, \mu) \) is a normalization factor. \( Z_{gmce}(E, V, \mu) \) stands for the partition function of the grand microcanonical ensemble (GMCE). In this ensemble energy is conserved, whereas particles can be exchanged with a particle bath. An example distribution of the form (20) is presented in Fig. 3.

One can show that the condition (18) follows from the assumption of the balance of transitions between states with \( N \) and \( N + 1 \) particles. Note, that the \( N \) and \( N + 1 \) states, in general, include many different microstates. Thus the balance condition discussed here (the coarse balance) is different than the detailed balance condition discussed previously. As an example let us consider the creation reaction \((1, 1) \rightarrow (3, 0)\) and the corresponding annihilation reaction. The other transitions lead to the same conclusions. The coarse balance condition for these reactions reads:

\[ P_{ss}(N; E, V)\omega_{N\rightarrow N+1} = P_{ss}(N+1; E, V)\omega_{N+1\rightarrow N} , \]

where \( P(N) \) is given by Eq. (13) while the transition probabilities \( \omega_{N\rightarrow N+1} \) and \( \omega_{N+1\rightarrow N} \) can be read from the MEq (14):

\[ \omega_{N\rightarrow N+1} = C_3 \frac{(N_1+V-3)}{(V-2)} \frac{(N_2+V-3)}{(V-2)} \]

\[ \omega_{N+1\rightarrow N} = A_3 \frac{(N_1+V+1)}{(V-1)} \frac{(N_2+V-2)}{(V-2)} . \]

After a short algebra one gets

\[ \frac{C_3}{A_3} = \frac{T(N+1; E, V)}{T(N; E, V)} , \]
which can be written as

$$\frac{C_3}{A_3} = \frac{fC_3 + gC_4}{fA_3 + gA_4},$$

(25)

where $f \equiv f(N; E, V)$ and $g \equiv g(N; E, V)$. Finally by cross-multiplying one gets

$$\frac{C_3}{A_3} = \frac{C_4}{A_4} \equiv r.$$

(26)

(iii) Now, let us consider the most general case of unconstrained conditional reaction probabilities. As already mentioned, in this case the SS multiplicity distribution depends on three (arbitrary chosen) ratios of the conditional reaction probabilities (e.g., $C_4/C_3$, $A_3/C_3$, and $A_4/C_3$) and as a rule the steady state is different from MCE and GMCE and the detailed balance is not fulfilled. Examples of $P_{ss}(N; E, V)$ are presented in Figs. 2 and 3.

(iv) One can also consider an extreme case with only annihilation reactions taking place, i.e., $A_3 > 0$, $A_4 > 0$ and $C_3 = C_4 = 0$. Then all systems approach microstates with a minimum number of particles, $N_{\min} = \lceil \frac{E}{2} \rceil$, allowed by the energy conservation, i.e. $P_{ss}(\lceil \frac{E}{2} \rceil; E, V) = 1$ and $\forall_{N \neq \lceil \frac{E}{2} \rceil} P_{ss}(N; E, V) = 0$. Similarly for the model with only creation reactions taking place, the systems approach microstates with the maximum number of particles, $N_{\max} = E$, i.e. $P_{ss}(E; E, V) = 1$ and $\forall_{N \neq E} P_{ss}(N; E, V) = 0$. The $P_{ss}(N; E, V)$ distributions for the two extreme settings of the conditional reaction probabilities are different and different than the corresponding MCE distribution. But the detailed balance is fulfilled in the SS. Namely, there are no inelastic reactions and probabilities of forward and backward elastic reactions is, by definition, equal. Thus, one concludes that the detailed balance alone does not guarantee the agreement between the SS and MCE. It should be mentioned, however, that the extreme settings of the conditional reaction probabilities, the Cell Model does not correspond to the ergodic Markov chain. The ergodicity is one of the basic properties of statistical mechanics.

Let us note that the presented results are consistent with the maximum entropy formulation of statistical mechanics [11]. This formulation boils down to maximization of the
entropy

\[ S \equiv - \sum_i p_i \ln p_i , \]  

(27)

under given constrains, where \( p_i \) are the microstate probabilities, and \( i \) runs from 1 to the total number of microstates \( W_{mc}(E,V) \). Then, imposing the constrain of \( \sum_i p_i = 1 \), one can derive MCE with particle-number distributions given by Eq. (5). Imposing additional constrain - the average number of particles, one finds grand microcanonical ensemble with \( P_{ss}(N;E,V) \) given by Eq. (20) with non-zero chemical potential \( \mu \). Finally, for the conditional reaction probabilities that do not fulfill Eq. (18), the resulting ensemble has a general form that cannot be related to any known ensemble of statistical mechanics.

VII. CLOSING REMARKS

One expects that a steady state of isolated systems depends on features of reactions between particles. The micro canonical ensemble describes isolated systems within statistical mechanics and it is independent of reactions between particles. Thus the steady state and MCE are expected to be different. In view of this, the success of statistical mechanics is difficult to understand.

In an attempt to answer this puzzle a simple model of particle annihilation and creation, the Cell Model, was developed in this paper. The model predicts a particle-number distribution. Its time evolution to a steady state was calculated using the Monte Carlo numerical simulations, whereas an analytical expression for the steady state distribution was obtained using the master equation approach.

Within the model the steady state distribution depends on the system volume and energy as well as on three parameters related to annihilation and creation reactions. For almost all sets of randomly selected reaction parameters the steady state is different than the micro canonical ensemble. This agrees with the naive expectations. Moreover it seems to be supported by Monte Carlo calculations performed within the relativistic quantum molecular dynamics (RQMD) [12]. The RQMD steady state disagrees with the corresponding MCE.
Differences between the steady state and microcanonical ensemble suggest that it is necessary to distinguish between models assuming creation of the whole phase space at once according to the MCE, and models in which particles appear and disappear via creation and annihilation reactions which takes place locally (e.g., in cells of the Cell Model) and drive the system to a steady state. An instantaneous creation of the whole microstate is assumed in several models of particle production in high energy collisions \cite{13,15}. Note, that these models imply a non-local particle production. Particles created in the whole system volume at once have to "communicate" instantaneously in order to "adjust" their energies such to satisfy the global energy conservation.

The reaction parameters of the Cell Model can be adjusted to grant the agreement between the steady state and MCE. This takes place when the annihilation and creation conditional reaction probabilities are equal. This requirements also leads to the detailed balance in the steady state, but the detailed balance does not imply the agreement between the steady state and MCE.

For the conditional creation probabilities proportional to the annihilation ones with the same proportionality factor for different reactions, one gets the particle number distribution in the steady state which disagrees with the MCE one. The distribution is equal to the distribution for the grand micro canonical ensemble with the dimensionless chemical potential equal to logarithm of the proportionality factor. Thus this case imitates an agreement of the steady state with the predictions of statistical mechanics. The condition of proportionality of the conditional creation and annihilation probabilities is derived from the assumption of the balance of transitions between particle number states, the coarse balance.

Based on the results presented in this paper one may speculate that the success of statistical mechanics in modelling various phenomena in nature, in particular particle creation in high energy collisions \cite{3,4} may be related to the following scenarios:

(i) Nature prefers interactions which have the same conditional probabilities of forward and backward reactions,

(ii) Statistical mechanics with different possible ensembles is flexible enough to describe steady states with different constrains than an ensemble which fits them,
(iii) Nature creates systems according to microcanonical ensemble.

Note that the results presented here refer to isolated systems, which do not actually occur in experiments or in nature. Probably the closest to isolated systems are multiparticle systems created in high energy collisions between particles or nuclei. Many features of particle production in these processes resemble predictions of statistical mechanics. Thus we hope that this work may, in particular, shed light on particle production mechanism in high energy collisions.

Acknowledgments

We would like to thank D.V. Anchishkin, St. Mrowczynski, Yu. Shtanov and Marysia Prior for fruitful discussions, comments and corrections. The work of by the Program of Fundamental Research of the Department of Physics and Astronomy of NAS (M.I.G), the National Science Centre of Poland under grants no. 2015/18/E/ST2/00560 (A.F.), no. 2016/21/D/ST2/01983 (M.M.P.) as well as by the German Research Foundation under grant GA1480/2-2 (M.G.).

Appendix A: Listing of the algorithm used in numerical simulations of CM

Here we provide listing of the algorithm for simulating CM model. The CM function contains the main loop that iterates over a specified number of time steps of the simulation. At each iteration the algorithm performs two operations. First, it generates two sequences of cell multiplicities for particles $N_1$ and $N_2$ (lines 35-36 in the Algorithm 1). It can be done with the help of the auxiliary function RANDOMCOMPOSITION which computes a random composition of $N$ elements into $V$ groups. In the second part of the main loop (lines 37-54) the appropriate reactions take place. Here, one can easily extend the number of possible reactions to adapt the algorithm for the calculation of other models.
Algorithm 1 Algorithm for CM model

Input: Energy $E$, number of cells $V$, transition rates $A_3, A_4, C_3, C_4$, number of simulation steps totalsteps

Output: Number of particles in each step $M$

1. function RandomComposition($N, V$) \hfill \textsuperscript{16} adapted from
2. Let $n = \{n_i \mid i = 1, 2, ..., V\}$ be a sequence of occupation numbers
3. Let $a = \{a_i \mid i = 1, 2, ..., V\}$
4. $c_1 \leftarrow V - 1$
5. $c_2 \leftarrow N + V - 1$
6. $i \leftarrow 0$
7. while True do
8. \hspace{1em} $i \leftarrow i + 1$
9. \hspace{1em} if $c_2 \cdot \text{random} \leq c_1$ then
10. \hspace{2em} $c_1 \leftarrow c_1 - 1$
11. \hspace{2em} $a_{c_1} \leftarrow i$
12. \hspace{1em} if $c_1 \leq 0$ then
13. \hspace{2em} \hspace{1em} break
14. \hspace{1em} end if
15. \hspace{1em} end if
16. $c_2 \leftarrow c_2 - 1$
17. end while
18. $n_1 \leftarrow a_1 - 1$
19. for each $j : 2 \leq j \leq V - 1$ do
20. \hspace{1em} $n_j \leftarrow a_j - a_{j-1} - 1$
21. end for
22. $n_V \leftarrow N + V - 1 - a_{V-1}$
23. return $n$
24. end function

function CM($E, V, A_3, A_4, C_3, C_4$, totalsteps)

25. Let $n = \{n_i \mid i = 1, 2, ..., V\}$ be a sequence of cell multiplicities for $N_1$ particles
26. Let $m = \{m_i \mid i = 1, 2, ..., V\}$ be a sequence of cell multiplicities for $N_2$ particles
27. Let $M = \{M_i \mid i = 1, 2, ..., \text{totalsteps}\}$ be a sequence of particle multiplicities in consecutive steps of simulation
28. $step \leftarrow 0$
29. $N_1 \leftarrow E$
30. $N_2 \leftarrow 0$
31. while $step \leq \text{totalsteps}$ do
32. \hspace{1em} $step \leftarrow step + 1$
33. \hspace{1em} $n \leftarrow \text{RandomComposition}(N_1, V)$
34. \hspace{1em} $m \leftarrow \text{RandomComposition}(N_2, V)$
35. for each $v : 1 \leq v \leq V$ do
36. \hspace{2em} if ($n_v = 3$) $\wedge$ ($m_v = 0$) $\wedge$ (random $< C_3$) then
37. \hspace{3em} $N_1 \leftarrow N_1 - 2$
38. \hspace{3em} $N_2 \leftarrow N_2 + 1$
39. \hspace{2em} end if
40. \hspace{2em} if ($n_v = 2$) $\wedge$ ($m_v = 1$) $\wedge$ (random $< C_4$) then
41. \hspace{3em} $N_1 \leftarrow N_1 - 2$
42. \hspace{3em} $N_2 \leftarrow N_2 + 1$
43. \hspace{2em} end if
44. \hspace{2em} if ($n_v = 1$) $\wedge$ ($m_v = 1$) $\wedge$ (random $< A_3$) then
45. \hspace{3em} $N_1 \leftarrow N_1 + 2$
46. \hspace{3em} $N_2 \leftarrow N_2 - 1$
47. \hspace{2em} end if
48. \hspace{2em} if ($n_v = 0$) $\wedge$ ($m_v = 2$) $\wedge$ (random $< A_4$) then
49. \hspace{3em} $N_1 \leftarrow N_1 + 2$
50. \hspace{3em} $N_2 \leftarrow N_2 - 1$
51. \hspace{2em} end if
52. end for
53. $M_{step} \leftarrow N_1 + N_2$
54. end while
55. return $M$
56. end function
Appendix B: Monte Carlo Cell model as Markov Chain

Here, we show that CM always converges to a unique stationary distribution \( P_{st}(N; E, V) \).

For a given energy\(^3\) \( E \), CM is a finite-state Markov chain with states described by the macroscopic quantity \( N \in \{ \frac{E}{2}, \ldots, E \} \). Let \( \mathcal{M} \) be the transition probability matrix. Elements \( \mathcal{M}_{ij} \) of this matrix denote the probability that CM is in the state \( j \) at time \( t + 1 \), given that it was observed in the state \( i \) at time \( t \). Then, one can associate with \( \mathcal{M} \) a digraph \( \mathcal{G} \) in which each node corresponds to a state of \( \mathcal{M} \), and \( \mathcal{G} \) contains edge \((i, j)\) if and only if \( \mathcal{M}_{ij} > 0 \) \[^{17}\]. In Fig. 5 we show a spanning subgraph of \( \mathcal{G} \) that is further used to prove convergence in distribution of \( N \).

In general, to show that any Markov chain converges to a unique stationary distribution one has to show that it is ergodic. In order for the Markov chain to be ergodic, it must satisfy three properties: i) the chain must be irreducible, ii) positive recurrent and iii) aperiodic.

i) Since a Markov chain over \( \mathcal{G} \) is irreducible iff \( \mathcal{G} \) is strongly connected (i.e. there is a path between any pair of nodes \( i, j \) in \( \mathcal{G} \)), then it is easy to see from Fig. 5 that CM is indeed irreducible.

ii) CM is recurrent because every irreducible Markov chain with a finite space of states is always recurrent.

iii) A sufficient test for an irreducible Markov chain to be aperiodic is that its associated digraph \( \mathcal{G} \) contains at least one self-loop (i.e., \( \mathcal{M}_{ii} > 0 \) for some state \( i \)). This is certainly true for CM (see Fig. 5), where it is always possible that no reaction in the

\[^{3}\text{In what follows, without loss of generality, we assume that } E \text{ is even.}\]
system occurs in a single time step (i.e. the number of particles does not change).

Appendix C: Derivation of \( P_{ss}(N; E, V) \) from MEq

To solve the master equation (10), one inserts \( N_1 = 2N - E \) and \( N_2 = E - N \) into this equation. In the stationary regime, when the left side of this equation is equal to 0, its SS solution - \( P_{ss}(N; E, V) \) (here for simplicity denoted as \( P(N) \)) - can be found for even values of \( E \) via a recursive scheme starting with the initial condition \( P(\frac{E}{2} - 1) = 0 \). In particular, the first three probabilities can be expressed by the probability \( P(\frac{E}{2}) \) as follows:

\[
P \left( \frac{1 + E}{2} \right) = P \left( \frac{E}{2} \right) \frac{E V (V + 1)}{2(2V + E - 2)} P \left( \frac{E}{2} \right) T \left( \frac{1 + E}{2} \right),
\]
\[
P \left( \frac{2 + E}{2} \right) = P \left( \frac{E}{2} \right) \frac{E (E - 2)V (V + 1)(V + 2)(V + 3)}{24(2V + E - 2)(2V + E - 4)} T \left( 2 + \frac{E}{2} \right),
\]
\[
P \left( \frac{3 + E}{2} \right) = P \left( \frac{E}{2} \right) \frac{E (E - 2)(E - 4)V (V + 1)(V + 2)(V + 3)(V + 4)(V + 5)}{720(2V + E - 2)(2V + E - 4)(2V + E - 6)} T \left( 3 + \frac{E}{2} \right),
\]

where

\[
T \left( \frac{1 + E}{2} \right) = \frac{C_4}{A_4},
\]
\[
T \left( \frac{2 + E}{2} \right) = T \left( \frac{1 + E}{2} \right) \frac{2(2V + E - 8)C_3 + (E - 4)V C_4}{2(2V + E - 8)A_3 + (E - 4)V A_4},
\]
\[
T \left( \frac{3 + E}{2} \right) = T \left( \frac{1 + E}{2} \right) T \left( \frac{2 + E}{2} \right) \frac{4(2V + E - 10)C_3 + (E - 6)(V + 2)C_4}{4(2V + E - 10)A_3 + (E - 6)(V + 2)A_4},
\]

and, in general,

\[
P \left( \frac{k + E}{2} \right) = P \left( \frac{E}{2} \right) \frac{(V)_{2k} (\frac{E}{2} + V - k)}{(2k)! (\frac{E}{2} + 1 - k)} T \left( k + \frac{E}{2} \right),
\]

where the Pochhammer symbol \((a)_b = a(a+1)...(a+b-1)\) refers to a rising factorial starting at \(a\). By noting that for integer \(a\) and \(b\)

\[
(a)_b = \frac{(a + b - 1)!}{(a - 1)!} = \binom{a + b - 1}{a - 1} b!,
\]

22
one obtains:

\[ P\left(k + \frac{E}{2}\right) = P\left(\frac{E}{2}\right) \frac{\left(\frac{E}{V-1}\right)^{2k+E-1}}{\left(\frac{E}{V-1}\right)^{2k}} \frac{T\left(k + \frac{E}{2}\right)}{T\left(k + \frac{E}{2}\right)} . \]

Finally, substituting \( N = k + \frac{E}{2} \) into the last equation, one gets the solution of MEq, cf. Eqs. (13) and (14):

\[ P(N) = P\left(\frac{E}{2}\right) \frac{\left(\frac{E-N}{V-1}\right)^{2N-E-1}}{\left(\frac{E}{V-1}\right)^{2N}} T(N) , \]

where \( T(N) \equiv T(N; E, V) \) is given by Eq. (15) and the term \( P\left(\frac{E}{2}\right) \) can be calculated from the normalization condition:

\[ \sum_{N=E}^{2E} P(N) = 1 . \]

The steady state distribution \( P_{ss}(N; E, V) \) for odd values of \( E \) can be found in a similar way, by performing a recursion with the initial condition \( P\left(\frac{E-1}{2}\right) = 0. \)

[1] R. Jancel, *Foundations of Classical and Quantum Statistical Mechanics* (Pergamon, London, 1964); I.E. Farquhar, Ergodic Theory in Statistical Mechanics, (Interscience, New York, 1964); P.L. Krapivsky, S. Redner, E. Ben-Naim *A Kinetic View of Statistical Physics* (Cambridge University Press, New York, 2010)

[2] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Oxford: Pergamon) 1975;

[3] F. Becattini, U.W. Heinz, Z. Phys. C 76, 269 (1997) Erratum: [Z. Phys. C 76, 578 (1997)]

[4] F. Becattini et al., Phys. Rev. C 69, 024905 (2004).

[5] A. Andronic, P. Braun-Munzinger, J. Stachel, Nucl. Phys. A 772, 167 (2006).

[6] F. Becattini, Z. Phys. C 69, 485 (1996).

[7] L. Ferroni and F. Becattini, Eur. Phys. J. C 71, 1824 (2011) doi:10.1140/epjc/s10052-011-1824-x [arXiv:1109.5185 [hep-ph]].

[8] V. V. Begun, M. Gazdzicki, M. I. Gorenstein, M. Hauer, V. P. Konchakovski and B. Lungwitz, Phys. Rev. C 76, 024902 (2007) doi:10.1103/PhysRevC.76.024902 [nucl-th/0611075].
[9] W. Feller, An Introduction to Probability Theory and its Applications, Vol. 1 (John Wiley & Sons Inc.) 1957.

[10] N. G. van Kampen, Stochastic Processes in Physics and Chemistry (North-Holland, Amsterdam) 2004.

[11] E. T. Jaynes, Phys. Rev. 106, 620 (1957).

[12] M. Belkacem et al., Phys. Rev. C 58, 1727 (1998).

[13] R. Hagedorn, Nuovo Cim. Suppl. 3, 147 (1965).

[14] M. Gazdzicki, M. I. Gorenstein, Acta Phys. Pol. B 30, 2705 (1999).

[15] P. Castorina, D. Kharzeev, H. Satz, Eur. Phys. J. C 52, 187 (2007).

[16] A. Nijenhuis, H.S. Wilf, Combinatorial Algorithms for Computers and Calculators (Academic Press) 1978.

[17] D.R. Shier, K.T. Wallenius, Applied Mathematical Modeling: A Multidisciplinary Approach, Chap. 13, CRC Press (1999)