Equivalence of ensembles in creation-annihilation nonequilibrium models

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We consider a class of stochastic models on a lattice in which particles are created and annihilated with given rates. The class include very distinct models such as the contact process and the stochastic Ising model. We show how to set up stochastic models with the dynamics that conserve the number of particles that are equivalent, in the thermodynamic limit, to the creation-annihilation models. We also obtain a formula that allows the calculation of the rates with respect to the ensemble of constant particle number.

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I. INTRODUCTION

The use of distinct ensembles in equilibrium statistical mechanics was introduced by Gibbs and consists of a powerful tool in the study of the thermodynamical properties of statistical models. There is a standard procedure for passing from one ensemble to another [1–3]. The main feature of the transformation is that a quantity that is held fixed in one ensemble becomes a fluctuating variable in the other. For instance, in the canonical ensemble the number of particles is constant, whereas in the grand-canonical ensemble it fluctuates. The descriptions of systems by distinct ensembles become equivalent in the thermodynamic limit.

The procedure introduced by Gibbs is appropriate for equilibrium systems, that is, systems described by the Gibbs probability distribution, but cannot be used in nonequilibrium systems. Here we are concerned with the construction of distinct ensembles for nonequilibrium systems of particles described by the probabilistic dynamic rules whose time evolution is governed by a master equation. We show the equivalence between two types of stationary state ensembles: the constant rate ensemble, in which particles are created and annihilated with fixed given rates, and the constant particle number ensemble, defined by the dynamic rules in which the number of particles is kept constant.

The possibility of using distinct ensembles in nonequilibrium models was advanced by Ziff and Brosilov [4] in their study of a irreversible surface-reaction system. More recently, Tomé and de Oliveira [5] introduced the conserved contact process, a version of the ordinary contact process with strictly conserved particle number. In this process, particles jump around over the sites of a regular lattice, falling down only on empty sites that have at least one neighboring site occupied. The conserved contact process displays properties that, in the thermodynamic limit, are identical to those of the ordinary contact process, including universal as well as nonuniversal quantities, and was identified as the contact process in an ensemble of constant particle number. This was indeed confirmed by the numerical simulations in one dimension [5] and more than one dimension [6]. Hilhorst and Wijland [7] provided a proof of the equivalence between the two stationary state ensembles.

We consider here a class of stochastic models on a lattice in which particles are created and annihilated with given rates. The creation and annihiliation can be a simple process, such as a spontaneous process, or more complex, such as a catalylic process. We show that these models, which we call constant rate models, are equivalent, in the thermodynamic limit, to the models defined by the dynamic rules that conserve the number of particles (or magnetization in the case of the stochastic Ising model), which we call constant particle number models. Examples of constant rate models include the ordinary contact process and similar models [8–12], and the Glauber model [13] and any other one-spin flip stochastic dynamics of the Ising model [10,14–18]. Examples of constant particle number models include the conservative contact process [5], and the Kawasaki stochastic dynamics [19] and similar dynamics in which two up-down spins exchange places [20]. An equivalence between the constant rate ensemble and the constant particle number ensemble is shown here by using a method similar to that used by Hilhorst and Wijland [7].

The application of the present method in the case of the lattice-gas (the Ising) model, in particular, allows us to obtain formulas that connect the chemical potential (the magnetic field) to certain averages with respect to the ensemble of conserved particle number (magnetization). Some of these formulas for the chemical potential have been obtained previously by a distinct method [21,22].

II. TRANSITION RATES

Let us denote by η_i the occupation variable attached to site i, of a lattice, with $\eta_i=0$ or 1 according to whether site i is empty or occupied. The vector $\eta=(\eta_1,\eta_2,\ldots,\eta_N)$ will represent the collection of occupation variables in a lattice with N sites. We consider stochastic models composed by two subprocesses: creation of a single particle $(0\to1)$, with transition rate $k_c w_i^c(\eta)$, and annihilation of a single particle $(1\to0)$, with transition rate $k_a w_i^a(\eta)$. The constants k_c and k_a are, respectively, the strengths of the creation and annihilation rates and

$$w_i^c(\eta)=(1-\eta_i)c_i(\eta), \tag{1}$$

$$w_i^a(\eta)=\eta_i a_i(\eta), \tag{2}$$

where $c_i(\eta)$ and $a_i(\eta)$ do not depend on η_i. Since these two subprocesses are mutually exclusive, the one-site transition rate $w_i(\eta)$ from state η_i to state $1-\eta_i$ can be written as the sum

$$w_i(\eta)=k_c w_i^c(\eta)+k_a w_i^a(\eta). \tag{3}$$

Actually, any one-site process can be understood as a creation-annihilation process, as the one-site transition rate can always be written in the form (3).

The numerical simulation of the creation-annihilation process just defined can be performed as follows. At each time step a site of the lattice is chosen at random. If it is empty, then a particle is created with probability proportional to $k_c c_i(\eta)$. If it is occupied, then the particle is annihilated with probability proportional to $k_a a_i(\eta)$.

The stochastic process associated to an ensemble of constant particle number is a two-site process whose transition rate $w_{ij}(\eta)$ from state (η_i,η_j) to state $(1-\eta_i,1-\eta_j)$ is given by

$$w_{ij}(\eta)=w_i^a(\eta)w_j^c(\eta), \tag{4}$$

or

$$w_{ij}(\eta)=(1-\eta_i)\eta_j a_i(\eta)c_j(\eta). \tag{5}$$

The numerical simulation of the constant particle number model can be performed as follows. At each time step a randomly chosen particle jumps from its place to an empty site chosen randomly. The jumping probability is proportional to the product $a_i(\eta)c_j(\eta)$, where i is the departing site and j is the arriving site. In this manner, both the processes of creation and annihilation of particles of the constant rate model are replaced by just a jumping process in the constant particle number model.

III. CONSTANT RATE ENSEMBLE

The time evolution of the probability distribution $P(\eta,t)$ is governed by the master equation

$$\frac{d}{dt}P(\eta,t)=\sum_i \{w_i(\eta^i)P(\eta^i,t)-w_i(\eta)P(\eta,t)\}, \tag{6}$$

where η^i is the vector $\eta^i=(\eta_1,\eta_2,\ldots,1-\eta_i,\ldots,\eta_N)$ and $w_i(\eta)$ is the one-site creation-annihilation transition rate given by Eq. (3).

An equivalent description of the system is made through the time evolution of the correlation functions. Let us define the state function $f_A(\eta)$ by

$$f_A(\eta)=\prod_{i\in A}\eta_i, \tag{7}$$

where the product is over the sites belonging to a given set A. From the master equation it is straightforward to show that

$$\frac{d}{dt}\langle f_A\rangle=\sum_{i\in A}\langle\{f_A(\eta^i)-f_A(\eta)\}w_i(\eta)\rangle, \tag{8}$$

where

$$\langle f(\eta)\rangle=\sum_\eta f(\eta)P(\eta,t) \tag{9}$$

denotes the average of any state function $f(\eta)$. The set of equations for all correlations is equivalent to the master equation. This description is appropriate for taking the thermodynamic limit, since the summation on the right-hand side of Eq. (8) involves a finite number of terms even for an infinite system.

Substituting the transition rate (3) into (8) one obtains the time evolution of the correlation in the form

$$\frac{d}{dt}\langle f_A\rangle=k_c\sum_{i\in A}\langle\{f_A(\eta^i)-f_A(\eta)\}w_i^c(\eta)\rangle+k_a\sum_{i\in A}\langle\{f_A(\eta^i)-f_A(\eta)\}w_i^a(\eta)\rangle. \tag{10}$$

Now we use the obvious relation $\eta_i(1-\eta_i)=0$ to show that

$$f_A(\eta)w_i^c(\eta)=0 \quad \text{if} \quad i\in A, \tag{11}$$

$$f_A(\eta^i)w_i^a(\eta)=0 \quad \text{if} \quad i\in A, \tag{12}$$

so that

$$\frac{d}{dt}\langle f_A\rangle=k_c\sum_{i\in A}\langle f_A(\eta^i)w_i^c(\eta)\rangle-k_a\sum_{i\in A}\langle f_A(\eta)w_i^a(\eta)\rangle. \tag{13}$$

In particular,

$$\frac{d}{dt}\langle\eta_i\rangle=k_c\langle w_i^c(\eta)\rangle-k_a\langle w_i^a(\eta)\rangle, \tag{14}$$

so that, in the stationary state, one has

$$k_c\langle w_i^c(\eta)\rangle=k_a\langle w_i^a(\eta)\rangle. \tag{15}$$

IV. CONSTANT PARTICLE NUMBER ENSEMBLE

The two-site process is governed by the following master equation:

$$\frac{d}{dt}P(\eta,t)=\frac{1}{N}\sum_{ij}\{w_{ij}(\eta^{ij})P(\eta^{ij},t)-w_{ij}(\eta)P(\eta,t)\}, \tag{16}$$

where η^{ij} is the vector $\eta^{ij}=(\eta_1,\ldots,1-\eta_i,\ldots,1-\eta_j,\ldots,\eta_N)$, and N is the total number of sites in the lattice. The transition rate $w_{ij}(\eta)$ is given by Eq. (4) and the model strictly conserves the number of particles.

An equivalent description in terms of the correlations can also be made here. The time evolution of the correlation $\langle f_A\rangle$ is given by

$$\frac{d}{dt}\langle f_A\rangle_c=\frac{1}{N}\sum_{ij}\langle\{f_A(\eta^{ij})-f_A(\eta)\}w_{ij}(\eta)\rangle_c, \tag{17}$$

where the notation $\langle\cdots\rangle_c$ stands for the average with respect to the conservative dynamics.

Taking into account that

$$f_A(\eta^{ij})=f_A(\eta^j) \quad \text{if} \quad i\notin A, j\in A, \tag{18}$$

$$f_A(\eta^{ij})=f_A(\eta^i) \quad \text{if} \quad i\in A, j\notin A, \tag{19}$$

$$f_A(\eta^{ij})=f_A(\eta) \quad \text{if} \quad i\notin A, j\notin A, \tag{20}$$

we may write the time evolution of $\langle f_A\rangle_c$ as

$$\frac{d}{dt}\langle f_A\rangle_c=\frac{1}{N}\sum_{i\in A}\sum_{j\in A}\langle\{f_A(\eta^{ij})-f_A(\eta)\}w_i^a(\eta)w_j^c(\eta)\rangle_c + \frac{1}{N}\sum_{i\in A}\sum_{j\notin A}\langle\{f_A(\eta^{i})-f_A(\eta)\}w_i^a(\eta)w_j^c(\eta)\rangle_c + \frac{1}{N}\sum_{i\notin A}\sum_{j\in A}\langle\{f_A(\eta^{j})-f_A(\eta)\}w_i^a(\eta)w_j^c(\eta)\rangle_c . \tag{21}$$

Using the obvious relation $\eta_i(1-\eta_i)=0$ we may write the following identities:

$$f_A(\eta^{ij})w_i^a(\eta)=0 \quad \text{if} \quad i\in A, \tag{22}$$

$$f_A(\eta^{i})w_i^a(\eta)=0 \quad \text{if} \quad i\in A, \tag{23}$$

$$f_A(\eta)w_j^c(\eta)=0 \quad \text{if} \quad j\in A, \tag{24}$$

which allows us to write

$$\frac{d}{dt}\langle f_A\rangle_c=-\frac{1}{N}\sum_{i\in A}\sum_{j\notin A}\langle f_A(\eta)w_i^a(\eta)w_j^c(\eta)\rangle_c + \frac{1}{N}\sum_{i\notin A}\sum_{j\in A}\langle f_A(\eta^{j})w_i^a(\eta)w_j^c(\eta)\rangle_c . \tag{25}$$

V. EQUIVALENCE OF ENSEMBLES

In this section we show the equivalence between the constant rate ensemble and the constant particle number ensemble. Let us define the quantities

$$\kappa_a(\eta)=\frac{1}{N_B}\sum_{i\notin A}w_i^a(\eta), \tag{26}$$

$$\kappa_c(\eta)=\frac{1}{N_B}\sum_{j\notin A}w_j^c(\eta), \tag{27}$$

where N_B is the number of sites not belonging to A. This permits us to write

$$\frac{d}{dt}\langle f_A\rangle_c=-\frac{N_B}{N}\sum_{i\in A}\langle f_A(\eta)w_i^a(\eta)\kappa^c(\eta)\rangle_c + \frac{N_B}{N}\sum_{j\in A}\langle f_A(\eta^{j})w_j^c(\eta)\kappa_a(\eta)\rangle_c . \tag{28}$$

We may now take the thermodynamic limit $N\to\infty$, which implies $N_B/N\to 1$ since the set A remains finite. Assuming the law of large number to be valid, the quantities κ_a and κ_c approach the averages $\langle w_i^a(\eta)\rangle_c$ and $\langle w_i^c(\eta)\rangle_c$, respectively, in the limit $N_B\to\infty$. This amounts to replace κ_a by $\langle w_i^a\rangle_c$ and κ_c by $\langle w_i^c\rangle_c$ in Eq. (28). Therefore, in the thermodynamic limit we obtain

$$\frac{d}{dt}\langle f_A\rangle_c=-\langle w_i^c(\eta)\rangle_c\sum_{i\in A}\langle f_A(\eta)w_i^a(\eta)\rangle_c + \langle w_i^a(\eta)\rangle_c\sum_{j\in A}\langle f_A(\eta^{j})w_j^c(\eta)\rangle_c , \tag{29}$$

which is equivalent to Eq. (13) as long as

$$k_c/k_a=\langle w_i^a(\eta)\rangle_c/\langle w_i^c(\eta)\rangle_c . \tag{30}$$

This formula allows us to calculate the rates with respect to the ensemble of constant particle number. Equation (30) establishes the equivalence between the ensembles in the stationary regime. For the time-dependent regime, however, Eq. (30) might not always hold. For instance, if the initial state is such that the averages of κ_a and κ_c are not constants, Eq. (30) cannot be satisfied [7].

VI. CONTACT PROCESS

In the ordinary contact process [10,12], the creation of particles is a catalytic process, whereas the annihilation is spontaneous. It is a constant rate model defined by the one-site transition rate

$$w_i(\eta)=(1-\eta_i)\frac{1}{z}\sum_{\delta}\eta_{i+\delta}+\alpha\eta_i , \tag{31}$$

where the summation in δ is over the z nearest neighbor sites, from which we may write

$$k_c=1, \quad w_i^c(\eta)=(1-\eta_i)\frac{1}{z}\sum_{\delta}\eta_{i+\delta}, \tag{32}$$

$$k_a=\alpha, \quad w_i^a(\eta)=\eta_i , \tag{33}$$

where α is the strength of the annihilation process. The conserved contact process [5] is defined by the jump transition rate given by Eqs. (4), (32), and (33), and defines a constant particle number model. According to Eq. (30) we have [5]

$$\alpha=(1/\rho)\langle w_i^c(\eta)\rangle_c , \tag{34}$$

where $\rho=\langle\eta_i\rangle_c$ is the density of particle. This formula allows us to calculate the rate α with respect to the ensemble of constant particle number.

VII. LATTICE-GAS MODEL

It is possible to set up a dynamics of the lattice-gas model in terms of a creation-annihilation process. The lattice-gas model, which is equivalent to the Ising model, is defined by the equilibrium Gibbs probability

$$P(\eta)=(1/Z)\,e^{-\beta\phi(\eta)}, \tag{35}$$

where

$$\phi(\eta)=\sum_{i<j}\varepsilon_{ij}\eta_i\eta_j-\mu\sum_i\eta_i , \tag{36}$$

with ε_{ij} being the interaction between the particles at sites i and j and μ being the chemical potential.

There are several stochastic processes that describe the dynamics of the lattice-gas model. All of them are set up by the use of detailed balance. For the models with one-site transition rates, the detailed balance reads

$$w_i(\eta^i)P(\eta^i)=w_i(\eta)P(\eta), \tag{37}$$

or, taking into account Eqs. (35) and (36),

$$w_i(\eta)/w_i(\eta^i)=\exp\{(1-2\eta_i)[-\beta\phi_i(\eta)+\beta\mu]\}, \tag{38}$$

where

$$\phi_i(\eta)=\sum_j \varepsilon_{ij}\eta_j . \tag{39}$$

Any one-site transition rate $w_i(\eta)$ that satisfies the detailed balance (38) defines a process associated to the constant rate ensemble. Writing $w_i(\eta)$ in the form given by Eq. (3) we obtain from Eq. (4) the transition rate $w_{ij}(\eta)$ associated to the constant particle number ensemble. It is worth mentioning that $w_{ij}(\eta)$ so obtained also satisfies the detailed balance.

The condition (38) does not suffice to define uniquely a transition rate and we are free to define specific one-site transition rates for the Ising model. For instance, we may define

$$w_i(\eta)=k\exp\{-\eta_i[-\beta\phi_i(\eta)+\beta\mu]\}, \tag{40}$$

where k is a constant. The transition rate (40) can be written as a sum of a creation rate and an annihilation rate. Comparing it with the form (3) we may write

$$k_c=k, \quad w_i^c(\eta)=(1-\eta_i), \tag{41}$$

$$k_a=ke^{-\beta\mu}, \quad w_i^a(\eta)=\eta_i e^{\beta\phi_i(\eta)}. \tag{42}$$

The transition rate corresponding to the constant particle number model is obtained by substituting w_i^c and w_i^a in Eq. (4). Using Eq. (30) we write down a formula for obtaining the chemical potential

$$e^{\beta\mu}=[1/(1-\rho)]\langle \eta_i e^{\beta\phi_i(\eta)}\rangle_c , \tag{43}$$

where $\rho=\langle \eta_i\rangle_c$ is the density of particles. This formula has been obtained previously by a distinct procedure in which a particle is removed from the system [21,22].

We may also define another transition rate that satisfies Eq. (38) such as

$$w_i(\eta)=k\exp\{(1-\eta_i)[-\beta\phi_i(\eta)+\beta\mu]\}, \tag{44}$$

where k is a constant. Using the same reasoning as before we arrive at the following formula:

$$e^{-\beta\mu}=(1/\rho)\langle (1-\eta_i)e^{-\beta\phi_i(\eta)}\rangle_c , \tag{45}$$

which is another formula that allows us to get the chemical potential with respect to an ensemble of constant particle number and has been obtained previously by a distinct procedure in which a particle is added to the system [21,22].

VIII. CONCLUSION

We have studied a class of creation-annihilation stochastic models on a lattice and have shown how to set up equivalent stochastic models with the dynamics that conserve the number of particles. The constructed constant particle number models are shown to be equivalent, in the thermodynamic limit, to the constant rate models. We have also obtained formulas that allow us to calculate the rates with respect to the ensemble of constant particle number. These formulas were applied to the conserved contact process and to the stochastic lattice gas model for which we obtained expressions for the calculation of the chemical potential with respect to the canonical ensemble.

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