# Conciliating synchronicity with spatial discretization, exclusion, interactions, and detailed balance

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The construction of a discrete stochastic system of interacting particles that evolves through a fully synchronous evolution rule while satisfying detailed balance is a highly demanding task. As a consequence, the presence of nontrivial interaction fields can make synchronicity and thermodynamic equilibrium look as two conflicting counterparts. We show that, with the proper prescriptions, the process of migration of particles in a lattice of mutually exclusive nodes can be simulated with a fully synchronous algorithm, which we call parallel Kawasaki dynamics (PKD), that incorporates site exclusion, local interactions, and detailed balance without the need of system partitioning schemes. We show that the underlying pseudo-Hamiltonian (which is *derived* from the PKD dynamics instead of being assumed *a priori* as usual in a sequential Monte Carlo scheme) is temperature dependent and causes the resulting equilibrium properties to differ substantially from the conventional hopping model when the system is near critical conditions.

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With their multifarious applications and simple implementation, lattice gases represent a branch of computational modeling where a physical system, parametrized in a state space of highly reduced complexity (at least in comparison with off-lattice molecular systems) and equipped with opportune evolutionary laws, can return an approximate but indeed reasonable meso- or macroscale representation of a great variety of chemical and physical phenomena [1–8]. Remarkable attention is still devoted to the Ising model [9] and all the variations on it. Among them, the (sequential) Kawasaki dynamics, where spin exchanges replace the Ising spin flips to mimic the displacement of a particle from a lattice node to another [10], is one of the most widely known. However, a synchronous formulation satisfying detailed balance (DB) does exist for the Ising model [11], but it does not for the Kawasaki dynamics. This is because, whereas imposing DB in a sequential Monte Carlo (MC) lattice gas is a relatively simple matter, even in the presence of highly nontrivial interaction fields [12–14], it might turn out to be much more tricky for a synchronous evolution mechanism. The most evident symptom of the conflict among full synchronicity, mutual exclusion, interactions, and thermodynamic equilibrium is that, at least to our knowledge, up to now there is no lattice model that can be considered as the parallel counterpart of the Kawasaki dynamics, i.e., there is no particle-conserving cellular automata (CA) rule satisfying all these requirements at the same time. Even if we do not consider explicit particle-particle interaction fields, very few fully synchronous discrete systems exist which satisfy DB or at least the semi-DB property—in these models the mutual exclusion, if present [15], is the only form of interaction and it holds on the *channels* that connect neighboring nodes rather than on the nodes themselves, causing the node occupation state to range between zero and the number of channels per node and therefore not to satisfy a total exclusion principle [16,17]. On the other hand, partitioning strategies exist that allow restraints and conservation laws to be implemented just like in sequential MC algorithms [18,19] and are perfectly suitable in many physical problems. Nevertheless, although near critical conditions the lack of DB does not prevent certain classes of nonequilibrium CA rules from possessing an underlying Hamiltonian at large scales [20], and although the nonequilibrium nature of a model does not prevent it from properly reproducing real physical phenomena, nor from being amenable to thorough analysis and classification [21], the formulation of a proper synchronous evolution rule for the Kawasaki dynamics satisfying DB at the microscopic level and obeying some known lattice Hamiltonian (or pseudo-Hamiltonian) without space decomposition nor demons [22] is still of remarkable interest.

Starting from a recently proposed equilibrium CA of mutually exclusive nodes [23] we introduce a fully synchronous interacting model for the Kawasaki dynamics of particles traveling in a lattice under the DB restraint. Our model, which we call parallel Kawasaki dynamics (PKD), is synchronous in its very nature rather than being a parallelization scheme for the sequential Kawasaki dynamics (SKD). In this work we derive the underlying pseudo-Hamiltonian and show how the equilibrium properties it produces differ from those obtained in SKD.

Let us consider a system made of a lattice $\mathcal{L}$ of $L$ nodes arbitrarily arranged (each denoted by $r$) and $N$ indistinguishable particles (each occupying one of the lattice nodes). An exclusion principle holds on the nodes so every node occupancy, denoted $n(r)$, can have value 0 or 1, respectively, if the node is empty or occupied by one particle. As a consequence, the lattice density, $\rho = N/L$, satisfies $0 \leqslant \rho \leqslant 1$. We indicate as $\boldsymbol{\eta} = \cup_r n(r)$ any of the possible occupancy configurations [satisfying $\sum_r n(r) = N$]. The system evolves in discrete time steps $t = 0, \tau, 2\tau, \ldots$ of arbitrary duration $\tau$. During each step, every node, say, $r$, can either retain or try to release its guest particle to one of the $\nu_r$ nodes connected to it if it is occupied, otherwise it can remain empty or receive a particle from one of the connected $\nu_r$ nodes. If we define the quantity $\nu_m = \sup_{r\in\mathcal{L}} \nu_r$ as the highest node connectivity in the lattice, the *neighborhood* of $r$, indicated as $\mathcal{I}_r$, then can be defined as $\mathcal{I}_r := \{r' \in \mathcal{L} | p(r \to r') > 0 \wedge r \neq r'\}$, where $p(r \to r')$ is the probability of a *lone* particle to jump into node $r'$ given that it is currently located at node $r$. In analogy with Ref. [23],

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we have $p(r \to r') = \exp\{\beta n(r)[\varepsilon(r) - \psi(r,r')]\}/\nu_m$ (with $r \neq r'$), where $\beta = (k_B T)^{-1}$, where $k_B$ is the Boltzmann constant and $T$ is the temperature, $\varepsilon(r) \leqslant 0$ is the adsorption energy at the node $r$, and the term $\psi(r,r') = \psi(r',r) \geqslant 0$ is the energy barrier between the nodes $r$ and $r'$. The probability of the host node itself to be chosen as the destination node reads, consequently, $p(r \to r) = 1 - \sum_{r' \in \mathcal{I}_r} p(r \to r')$. In order to coexist with synchronicity, we require the jump probability at each time step to depend only on the current configuration. This implies that we need to discard any conventional Monte Carlo scheme based on trial moves and acceptance-rejection criteria. Furthermore, mutual interactions among occupied nodes must be defined accordingly. Our choice is that the configuration in the neighborhood of an occupied node changes its probability of releasing its guest particle from $p(r \to r')$ into $\widetilde{p}(r \to r'|\boldsymbol{\eta}_r)$, called *pointing probability* and defined as the probability of a particle in $r$ to attempt a jump into $r'$ (or, in order to introduce a terminology that we will use throughout the rest of the paper, to *point towards* $r'$), given that the current local configuration is $\boldsymbol{\eta}_r$,

$$\widetilde{p}(r \to r'|\boldsymbol{\eta}_r) = \frac{p(r \to r')}{Z(r,\boldsymbol{\eta}_r)}[\overline{n}(r') + n(r')\phi(r,r')], \qquad (1)$$

where $\boldsymbol{\eta}_r = \cup_{r' \in \mathcal{I}_r} n(r')$ is the configuration of the occupancies in the neighborhood of node $r$, $\overline{n}(\cdot)$ is a shorthand notation for $1 - n(\cdot)$ and $\phi(r,r')$, satisfying $\phi(r,r) = 1$ and $\phi(r,r') = \phi(r',r) \geqslant 0$, is a dimensionless interaction parameter that modifies the tendency of the particle in $r$ to point towards the node $r'$ if that node is occupied. If it is, a repulsive, noninteracting, or attractive effect is produced respectively through $0 \leqslant \phi(r,r') < 1$, $\phi(r,r') = 1$, and $\phi(r,r') > 1$ [e.g., $\phi$ could be formulated as $\exp(-\beta\varepsilon_\phi)$, where $\varepsilon_\phi \in \mathbb{R}$ is an interaction energy]. In Eq. (1), $\widetilde{p}$ is normalized by

$$Z(r,\boldsymbol{\eta}_r) = \sum_{r' \in \mathcal{I}_r^0} p(r \to r')[\overline{n}(r') + n(r')\phi(r,r')], \qquad (2)$$

where $\mathcal{I}_r^0 := r \cup \mathcal{I}_r$ is the extended neighborhood of node $r$ (i.e., the neighborhood $\mathcal{I}_r$ *plus* the node $r$ itself). $Z(r,\boldsymbol{\eta}_r)$ turns out to be a key quantity since its negative logarithm represents the interacting part of the lattice Hamiltonian on the node $r$ when the configuration is $\boldsymbol{\eta}$.

Given this apparatus, we implement a synchronous evolution rule allowing particle migration while preventing any conflicts to arise by means of the following three prescriptions [23]: (i) Empty sites can be pointed to and reached by a particle in a neighboring site, whereas occupied sites can be pointed to but cannot be reached; (ii) if two or more particles point to the same site, no one of them will be allowed to reach it; and (iii) if one or more particles are pointing to a site occupied by another particle, that particle must stay at rest.

At each time step, say $t$, at every occupied node (independently of the other nodes), say $r$, whose neighborhood occupancies are configured as $\boldsymbol{\eta}_r$, we select a target node by associating to the site $r$ itself and to each neighbor $r' \in \mathcal{I}_r$ the random Boolean $\xi^t(r \to r')$, having value 1 with probability $\widetilde{p}(r \to r'|\boldsymbol{\eta}_r)$ and 0 otherwise. The matrix $\boldsymbol{\xi}^t$ is called the *matrix of directions* at time $t$. Obviously we impose $\sum_{r' \in \mathcal{I}_r^0} \xi^t(r \to r') = 1$, so every particle can choose only one target node at a time. Once $\boldsymbol{\xi}^t$ is determined, we move the particles according to a discrete evolution equation of the form

$$\boldsymbol{\eta}^{t+\tau} = \widehat{\omega}_{\boldsymbol{\xi}^t} \circ \boldsymbol{\eta}^t, \qquad (3)$$

where $t$ is the time and $\widehat{\omega}_{\boldsymbol{\xi}^t}$ is an evolution operator that transforms the input configuration, $\boldsymbol{\eta}^t$, into the output configuration, $\boldsymbol{\eta}^{t+\tau}$, according to the matrix of directions $\boldsymbol{\xi}^t$ and the prescriptions (i)–(iii). A detailed mathematical formulation of prescriptions (i)–(iii) can be found in our previous work [24]. However, although the evolution rule is the same as in Ref. [24], since the probability distribution governing the matrix of directions of the PKD, Eqs. (1) and (2), differs markedly and is much more general than the noninteracting counterpart, the PKD model shown in this work turns out to be able to behave very differently from the model studied in our seminal paper.

The most important aspect of PKD is that the pointing probability $\widetilde{p}(r \to r'|\boldsymbol{\eta}_r)$, Eq. (1), and the evolution rule, Eq. (3), couple perfectly in a CA dynamics that satisfies the DB requirement, i.e., $[P(\boldsymbol{\eta}^i)/P(\boldsymbol{\eta}^o)][\Omega(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o)/\Omega(\boldsymbol{\eta}^o \to \boldsymbol{\eta}^i)] = 1$, where $P(\boldsymbol{\eta})$ is the equilibrium probability of the system to be configured as $\boldsymbol{\eta}$, and $\Omega(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o)$ is the transition probability from $\boldsymbol{\eta}^i$ (input) to $\boldsymbol{\eta}^o$ (output), given by

$$\Omega(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o) = \sum_{\boldsymbol{\xi}} \delta[\boldsymbol{\eta}^o - \widehat{\omega}_{\boldsymbol{\xi}} \circ \boldsymbol{\eta}^i] \times \prod_{r \in \mathcal{L}} \sum_{r' \in \mathcal{I}_r^0} \xi(r \to r')\widetilde{p}\big(r \to r'|\boldsymbol{\eta}_r^i\big), \qquad (4)$$

where $\delta[\cdot]$ is the Krœnecker $\delta$ function, taking the value 1 if $\widehat{\omega}_{\boldsymbol{\xi}} \circ \boldsymbol{\eta}^i = \boldsymbol{\eta}^o$ and zero otherwise. Once one becomes familiar with the PKD evolution criteria, realizing that DB holds is straightforward. Here we discuss the DB relation in PKD and we derive the equilibrium distribution by using very intuitive arguments. The reader interested in a more in-depth study of this subject can find it in the Supplemental Material [25]. Together with prescriptions (i)–(iii), which solve any kind of competition in the collective migration process, the fact that every particle interacts only with the nodes it can point to [this can be seen from Eq. (1)] allows us to factorize the right-hand side of Eq. (4) into two contributions, respectively, from the *moving* and from the *resting* particles, i.e., $\Omega(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o) = \Omega_{\mathrm{mov}}(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o)\Omega_{\mathrm{rest}}(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o)$. By realizing that (1) every time a particle jumps from $r$ to $r'$ it is necessarily verified that the pointed node ($r'$) was free before the jump and that no other particles were pointing to it nor to $r$ and that (2) all the possible combinations of particle directions that cause one or many of them to stay at rest during the forward transformation $\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o$ also cause them to rest during the backward process $\boldsymbol{\eta}^o \to \boldsymbol{\eta}^i$ and vice versa, we can write

$$\frac{\Omega_\alpha(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o)}{\Omega_\alpha(\boldsymbol{\eta}^o \to \boldsymbol{\eta}^i)} = \prod_{r \in \mathcal{L}} \left[\frac{e^{\beta\varepsilon(r)}}{Z\big(r,\boldsymbol{\eta}_r^i\big)}\right]^{\Delta_\alpha^{io}(r)} \left[\frac{e^{\beta\varepsilon(r)}}{Z\big(r,\boldsymbol{\eta}_r^o\big)}\right]^{-\Delta_\alpha^{oi}(r)} \qquad (5)$$

with $\alpha = \mathrm{mov,rest}$ and $\Delta_{\mathrm{mov}}^{io}(r) = n^i(r)\overline{n}^o(r)$, $\Delta_{\mathrm{mov}}^{oi}(r) = n^o(r)\overline{n}^i(r)$, and $\Delta_{\mathrm{rest}}^{io}(r) = \Delta_{\mathrm{rest}}^{oi}(r) = n^i(r)n^o(r)$. If we use Eq. (5) to compute the transition probability ratio $\Omega(\boldsymbol{\eta}^i \to \boldsymbol{\eta}^o)/\Omega(\boldsymbol{\eta}^o \to \boldsymbol{\eta}^i)$ and we put that ratio in the detailed balance relation, we find that the equilibrium distribution of

configurations is given by

$$P(\boldsymbol{\eta}) \propto \prod_{r\in\mathcal{L}} [e^{-\beta\varepsilon(r)} Z(r,\boldsymbol{\eta}_r)]^{n(r)}. \tag{6}$$

As it happens in the case of full synchronization of the Ising model [26], the distribution function $P(\boldsymbol{\eta})$ of the PKD is non-Gibbsian and is characterized by a *pseudo*-Hamiltonian which, if we formally cast the right-hand side of the relation (6) into the form $e^{-\beta\mathcal{H}_\beta(\boldsymbol{\eta})}$, can be written as $\mathcal{H}_\beta(\boldsymbol{\eta}) = \mathcal{H}^{(0)}(\boldsymbol{\eta}) + \mathcal{H}^{\rm pp}_\beta(\boldsymbol{\eta})$, where $\mathcal{H}^{(0)}(\boldsymbol{\eta}) = \sum_r n(r)\varepsilon(r)$ is the interaction energy of the guest particles with the host lattice and the particle-particle interactions (besides mutual exclusion) are defined as

$$\mathcal{H}^{\rm pp}_\beta(\boldsymbol{\eta}) = -\sum_{r\in\mathcal{L}} \frac{n(r)}{\beta} \ln\left\{1 - \frac{1}{\nu_m}\sum_{r'\in\mathcal{I}_r} n(r') \times e^{\beta[\varepsilon(r)-\psi(r,r')]}[1-\phi(r,r')]\right\}. \tag{7}$$

The first peculiarity we notice in Eq. (7) is that the temperature dependence of $\mathcal{H}^{\rm pp}_\beta$ cannot be eliminated. Analogously to the pseudo-Hamiltonian of Little's model, this causes conventional thermodynamic relations involving partial derivatives with respect to the temperature to be no longer applicable [27]. Second, since the interaction between a particle in $r$ and a particle in the neighbor site $r'$ depends on the configuration of both the neighborhoods of $r$ and $r'$, the nature of PKD interactions is multibody rather than pairwise. The equilibrium properties arising from performing a PKD algorithm over a lattice do not differ qualitatively from the ones shown by a lattice obeying standard Kawasaki dynamics, except for the critical behavior in the case of repulsive interactions. For simplicity, let us assume $\mathcal{L}$ to be one-dimensional with periodic boundary conditions ($\nu = \nu_{\rm m} = 2$), $\phi$ and $\varepsilon$ to be space independent, and $\psi = 0$ everywhere in the system. Since the pseudo-Hamiltonian, Eq. (7), in this case reads $\mathcal{H}_\beta(r) = n(r)\{\varepsilon - \beta^{-1}\ln[1 - \frac{1}{2}e^{\beta\varepsilon}(1-\phi)N_r]\}$, where $N_r$ is the number of occupied first neighbors of site $r$, we achieve the situation of strongest repulsion for $\phi = 0$ and $\varepsilon = 0$ that causes $\mathcal{H}_\beta(r)$ to go to $+\infty$ when the number of occupied neighbors of $r$ is $N_r = 2$. This means that the two allowed saturation configurations show *pairs* of neighboring occupied nodes separated by one empty node, i.e., $\cdots$ ■■□■■□■■□ $\cdots$, giving a critical occupancy of $N_m = 2Q\{\frac{L}{3}\} + Q\{[L - 3Q\{\frac{L}{3}\}]/2\}$, where $Q\{A/B\}$ denotes the quotient between the two integers $A$ and $B$. Therefore, for $\phi = 0$ and $\varepsilon = 0$ a critical loading $\rho_c := \lim_{L\to\infty} \frac{N_m}{L} = \frac{2}{3}$ exists at which an infinite chemical potential is required to add a new particle in the system. This behavior is a consequence of the form that the grand partition function, $\Xi = \sum_N \lambda^N Q_N$ (where $Q_N$ is the canonical Partition function, $\lambda = e^{\beta\mu}$, and $\mu$ is the chemical potential), assumes near critical conditions. One can easily show that, starting from the expression for $\mathcal{H}_\beta(r)$ for the one-dimensional lattice,

$$\lim_{\varepsilon\to 0^-} \Xi = \sum_N \lambda^N \phi^{1-\Theta(N_m-N)} \sum_k c_{k,N}\phi^k,$$

where $\Theta(q)$ is the discrete Heaviside step function (taking the value 0 if $q < 0$ and 1 otherwise) and the $c_{k,N} > 0$ for $N = 0,\ldots,L \vee k = 0,\ldots,N$ and $c_{k,N} = 0$ otherwise. This is due to the fact that, when $N > N_m$, every possible configuration contains at least one local arrangement in which the two first-neighboring sites around a particle are both occupied. For such a situation the contribution from site $r$, i.e., $e^{-\beta\mathcal{H}_\beta(r)}$, reads $e^{\beta\varepsilon}[1 - e^{\beta\varepsilon}(1-\phi)]$, which becomes $\phi$ in the limit $\varepsilon \to 0^-$. For $0 \leqslant \phi \ll 1$, the weight of the configurations with $N > N_m$ decreases until it becomes null when $\phi = 0$. On the other hand, as $\varepsilon$ becomes slightly less than zero (as well as for $\phi$ slightly greater than zero), $\mathcal{H}_\beta$ and $\mu$ turn out to be always finite, causing the isotherm to show a finite step around $\rho_c$. Once the value of chemical potential at the top of the step is reached, the system has enough energy to host more particles until there is complete saturation of the lattice. The effect on the chemical potential step caused by the departure of $\varepsilon$ from zero to more negative values is shown in Fig. 1(a), where isotherms for a one-dimensional lattice are obtained from simulations in the canonical ensemble using the sublattice method [24] in all cases except $\varepsilon < 10^3 \wedge \rho > \rho_c$, where the grand-canonical ensemble was adopted instead (with sequential insertion or deletion but parallel displacement moves) due to the drastic dynamical slowdown which causes the sublattice method to be less accurate. As we can see, the more $\varepsilon$ departs from zero, the more the $\mu$ step decreases until it disappears completely. The effect of increasingly positive $\phi$ is qualitatively the same. Analogous behavior is shown for a square lattice ($\nu = 4$), Fig. 1(b), but with the slightly higher critical loading of

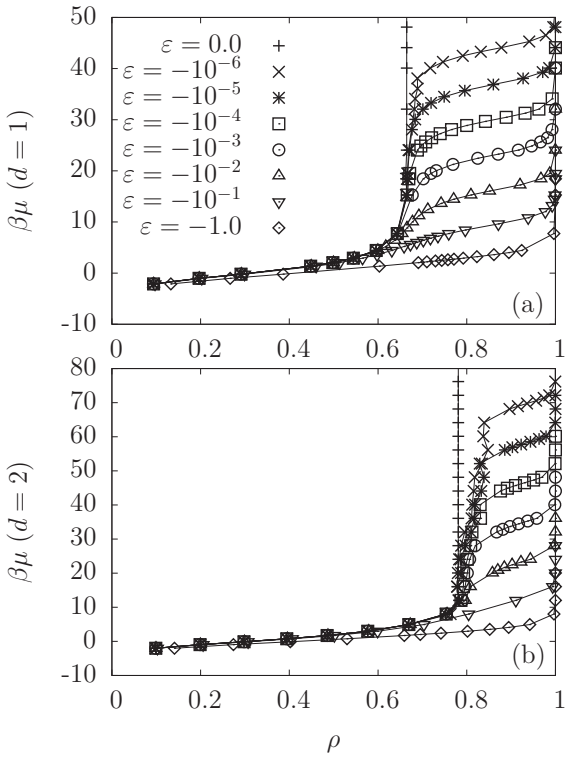


FIG. 1. Adsorption isotherms (chemical potential, $\mu$, in units of kJ mol$^{-1}$, vs site density, $\rho$, dimensionless) for the one-dimensional PKD lattice with $\phi = 0$ for several values of adsorption energy $\varepsilon$. The temperature is fixed at 300 K. The size of the systems is $L = 8192$ for $d = 1$ and $L = 128^2$ for $d = 2$. For each point in the figure, simulation data were obtained by up to 20 simulations, each one made of $10^7$ steps (after equilibration). Error bars are smaller than the size of the points.

$\rho_c \sim 0.78$, due to the fact that in critical conditions the saturation configurations are those in which every particle is surrounded by one empty neighbor and three occupied ones.

We remark on some major differences with respect to the SKD with infinite lateral repulsion. First, in SKD the critical loading in the one-dimensional system is $\rho_c^{\text{seq}} = 1/2$, corresponding to the two configurations where filled and empty sites are alternating in the one-dimensional lattice, because the interaction energy is infinite for a particle having one as well as two occupied neighboring sites [28]. Second, in SKD an infinitely large lateral repulsion causes $\mu \to \infty$ for $\rho \to \rho_c^{\text{seq}}$ for $\varepsilon = 0$ as well as for $\varepsilon < 0$.

In conclusion, although the resulting non-Gibbsian character of the equilibrium distribution of configurations (whose critical behavior differs substantially from the sequential Kawasaki counterpart) seems to limit its applicability to isothermal systems far from critical conditions, the PKD evolution rule represents a further, meaningful step toward the formulation of general parallel evolution algorithms where full synchronicity does not conflict with strict detailed balance.

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