Metastability on the steady states in a Fermi-like model of counterflowing particles

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In this work we propose a two-dimensional extension of a previously defined one-dimensional version of a model of counterflowing particles, which considers an adapted Fermi-Dirac distribution to describe the transition probabilities. In this modified and extended version of the model, we consider that only particles of different species interact and they hop through the cells of a two-dimensional rectangular lattice with probabilities taking into account diffusive and scattering aspects. We show that for a sufficiently low level of randomness (α ≥ 10), the system can relax to a mobile self-organized steady state of counterflow (lane formation) or to an immobile state (clog) depending sensitively on the initial conditions if the system has an average density near the crossover value (ρc). We also show that for certain suitable mixing of the species, we peculiarly have 3 different situations: (i) The immobile,(ii) Mobile organized by lanes, and (iii) Mobile without lane formation for the same density value. All of our results were obtained by performing Monte Carlo simulations.

Countering streams of particles [1-3] can lead to interesting patterns such for example charged colloids [4]. Exactly as pedestrian organize their motion to make that system flow, particles without a “natural intelligence”, self-propelled or simply oriented by a field, sometimes can organize their motion by lanes. However, exclusion effects seems to bring clogging/jamming phenomena [5, 6], although the formation of condensates is not mandatorily observed only in counterflowing systems [7].

Recently, we have developed a model with exclusion based on Fermi-Dirac distribution [6] from an extension of a simple model without exclusion previously defined in [2]. The easiness and coverage of this extended model is related to the manipulation of a single parameter that can model systems going from hard body systems with exclusion up to systems completely random and without exclusion effects. We have previously shown that such systems have an interesting transition from a clogging phase to a mobile phase that we have described with many order parameters such as mobility, Gini coefficient, over different situations [7].

The extension of this Fermi model for the counterflowing streams of particles in two dimensions has not yet studied and it deserves our attention. In this paper we propose a two-dimensional version of the Fermi-model to describe the counterflowing streams of particles on a lattice. We show that the system can present metastable events between a clogging and a lane phase, which to the best of our knowledge was never observed in similar systems of particles. Thus in this paper, we qualitatively and quantitatively explore this phenomena in details.

Our paper is organized as follows: we present one of the possible formulations (the more appropriate in our conception) of the modeling in two dimensions. We show that a renormalization is required for d = 2, but that naturally recovers d = 1 previously studied by us in our first contributions about this topic. After, by concluding the paper, we present our results and a few conclusions and summaries are presented.

We start defining our scenario: a rectangular system of $V = L_x L_y$ cells with periodic boundary conditions (toroidal lattice) where $N$ particles of two species, namely $A$ and $B$, can move. Each cell has a maximum occupation level denoted by $\sigma_{\text{max}}$. Our particles are able to hop only to its neighboring cells where particles of the species $A$ tend to move to the +x direction (along the toroid) whilst particles of the species $B$ tend to move to the −x direction, exactly as the effect of an electric field longitudinally applied, considering that particles of species $A$ are oppositely charged to the particles of species $B$. In our model, particles only interact with particles of the opposite type. Thus a particle of species $A$ that occupies the cell $(x, y) = (i\epsilon, j\epsilon)$ hops to its neighboring cell $(x, y) = (i\epsilon + \epsilon, j\epsilon)$ at the instant $t = \tau l$ according to a Fermi-like distribution of probability given by

$$P_{i,j}^{(l)} \rightarrow (i+1,j) = \frac{1}{Z^{(l)}} \frac{1}{1 + \epsilon^\alpha (B_{i,j}^{(l)} - \sigma_{\text{max}})}, \quad (1)$$

where $B_{i,j}^{(l)}$ is the number of particles of the species $B$ in the cell, $\alpha$ is the parameter that control the randomness of the dynamics, $\epsilon$ is the step-length (linear dimension of the cells) and $\tau$ is the time spend to perform the transition. Here $Z^{(l)}$ is a normalization factor to be defined later.

We define the probability of the particles to move along the $y$-direction as a product of two factors: scattering and diffusion. The scattering factor is defined as the complement of the chances of a particle to move in the direction of the toroid, i.e., the complement of the Eq. [1] In a similar way, the diffusion factor consist on the chances of a particle to enter the neighboring cell in the $y$-direction, which depends on the level of occupation of the target cell.

By this logic, we describe the chances of the particle $A$ to move to a cell in the transversal direction of the toroid
as
\[
p_{(i,j)\rightarrow(i,j\pm1)}^{(l)} = \frac{e^\alpha(B_{i,j}^{(l)}-\sigma_{\text{max}})^2(1 + e^\alpha(B_{i,j}^{(l)}+\sigma_{\text{max}})-1)}{Z^{(l)}(1 + e^\alpha(B_{i,j}^{(l)}+\sigma_{\text{max}})}
\]

(2)
taking into consideration the diffusive and scattering factor in its composition. Here the normalization factor is defined as: \[Z^{(l)} = \sum_{(i',j')} p_{(i',j')\rightarrow(i,j')}^{(l)},\]
where \((i',j')\) denotes that sum is taken over the nearest neighboring cells to which the movement is allowed. However, to keep the similarities with the original model, the particles also have to have the chances of remaining in its cells. So we also define the probability of a particle \(A\) to stay in its cell as the complement of the sum of all probabilities of movement. But that part is tricky, because we must take into account that \(0 \leq Z^{(l)} \leq 2\) and thus we have to make use of a necessary simple algorithm in our MC simulations to overcome the two following possible situations:

- \(Z^{(l)} \leq 1\): in this scenario we have \(p_{(i,j)\rightarrow(i,j)}^{(l)} = 1 - Z^{(l)}\) and the equations 1 and 2 are not normalized by the factor \(Z^{(l)}\);
- \(Z^{(l)} > 1\): in this case the particle will certainly move and the equations 1 and 2 are normalized by the factor \(Z^{(l)}\).

By symmetry, a particle of the species \(B\) in the cell \((x, y) = (i, j)\) hops to its neighboring cell \((x, y) = (i \pm \epsilon, j \pm \epsilon)\) at the instant \(t = \tau l\) with probability:
\[p_{(i,j)\rightarrow(i-1,j)}^{(l)} = \frac{1}{Z^{(l)}}(1 + e^\alpha(A_{i-1,j}-\sigma_{\text{max}})-1)\]
and similarly:
\[p_{(i,j)\rightarrow(i,j\pm1)}^{(l)} = \frac{1}{Z^{(l)}}(1 + e^\alpha(A_{i,j\pm1}-\sigma_{\text{max}})-1(1 + e^\alpha(A_{i-1,j}-\sigma_{\text{max}})).\]

The main parameter of the adapted Fermi-like distribution in our model is \(\alpha\) once it controls the randomness of the dynamics that can range from a purely random scenario to a deterministic case where the relation between the cell’s occupation and the limitation factor (\(\sigma_{\text{max}}\)) is paramount. In the context of counter-flowing particle dynamics, \(\alpha\) can be associated with the magnitude of an external field applied to oppositely charged particles.

We can understand the influence of \(\alpha\) on the dynamics by focusing on the two extreme situations: (i) \(\alpha \to 0\) and (ii) \(\alpha \to \infty\). In the case (i) \(\alpha \to 0\) the dynamics is completely random with particles \(A(B)\) moving cell by cell with probability 1/2 towards the \(+x\) or \(-x\) direction if the particle is from the \(A(B)\) species and with 1/4 to the \(\pm y\) direction. It is easy to notice that there is no chance of particles to stay in its cells. On the other hand, in the contrasting situation (ii) \(\alpha \to \infty\) however, the system behaves with deterministic dynamics such as the lattice gases and the set of possible configurations of occupation of the surrounding cells will define with certainty the movement of all particles except for the particular case in which the target cell happen to have \(\sigma = \sigma_{\text{max}}\). In that case, a local random decision is made as a result of \(\rho = 1/2\) or 1/4 depending on the direction of the occupied cell, although we do not expect it to substantially alter the bulk behavior of the system. Moreover, it is important to mention that we have a notorious computational advantage in using this model, since we are not obliged in checking by brutal force if cells satisfies the occupation limit \(\sigma_{\text{max}}\) such as systems with nearest neighbor exclusion [9][10].

To describe the state of the dynamics we define the mobility, denoted as \(M(t) = \frac{1}{N} \sum_i \xi_i(t)\), where \(\xi_i(t)\) is a binary parameter that assumes the value 1 when a particle moves in the \(x\)-direction and assumes the value 0 otherwise. The mobility stands as a current of particles or simply the fraction of the particles that perform a step along its species’s drift direction. When jamming/clog occurs the mobility drops to zero. While an opposite scenario occurs like particle’s self-organization in lane formation, the mobility will tend to one as a result of the optimal flow. To capture the lane-organized state we define the order parameter in the \(x\)-direction, or simply “x-order parameter”, denoted as \(\Phi_x = \frac{1}{N} \sum_{k=1}^{Lx} |A_k - B_k|\), where \(A_k = \sum_{j=1}^{Lx} A_{j,k}\) and \(B_k = \sum_{j=1}^{Lx} B_{j,k}\) are the marginal sum over the \(j\) variable (cells along the \(y\)-direction) of the number of particles of each species. By the definition of \(\Phi_x\) we see that it will tend to one when the system is in a lane-organized state along the toroid which represents an optimal state of flow due to the lack of particles moving in the opposite direction.

The mobility parameter is only possible to be calculated when performing MC simulations, differently from \(\Phi_x\) that depends only on the spacial concentration of particles and can also be measured when one integrates the recurrence relations that emerge from a mean field approximation of the Eqs. 1 and 2 for the species \(A\) as well as it can be done for the species \(B\), similarly to what was made in Ref. 11.

We implemented standard MC simulations where the MC step consists of choosing \(N\) particles at random of the \(N\) possible particles and sequentially updating its position before moving to the next MC step. In all of our results we use \(N_A = N_B = N/2\) and a number of runs following the relation \(N_{\text{run}} = 100000/N + 10000\) unless told otherwise.

A detailed study of the influence of \(\alpha\) and \(\sigma_{\text{max}}\) were explored in our previous contributions in one dimensional systems [6], [7], and in this current paper, we concentrate our study in a situation where the clogging is expected (\(\alpha\) large and \(\sigma_{\text{max}} = 1\)) and therefore the most important situation to be explored.

Our first result is to analyze the time evolution of mobility and \(\Phi_x\) for considerably low stochastic level \(\alpha = 20\) [11] and for three different values of densities: \(\rho = 0.5\), \(\rho = 1.0\) and \(\rho = 1.5\). At this regime we expect the system of dimensions \(L_x = 256\) and \(L_y = 64\),
to present a high mobility scenario for low density whilst for high density case we expect the system to jam. The Figs. 1 and 2 shows the expected behavior for the two present extreme cases of density (plot (a) and (c)) as we can see $M(t)$ and $\Phi_x(t)$ for each of the ten runs rapidly reaching the steady state. The case of intermediate density, i.e., $\rho = 1.0$, surprisingly shows a metastable steady state as we can see by the plot (c) in the Figs. 1 and 2. The present case reveals that for a certain specific density, the steady state of each run depends sensibly on the initial conditions as we can observe by the splitting of the mobility and the $x$-order parameter. We can also observe in the plot (c) of Figs. 1 and 2 that it is a bimodal situation, since there is no intermediate steady state of mobility other than the fully mobile self-organized state or the jammed state.

To better understand this metastability phenomena, we studied the system’s dependence on the density $\rho = N/V$. By knowing that the dynamics relax to a bimodal steady state of extremely different outcomes, where for each run the mobility and $\Phi_x$ do not change after a sufficient time, we implemented the same criteria to stop the time evolution as used in the previous work based on the slope of the time dependent curve to consider when the system has reached the steady state. The considered criteria consists on making a linear fitting on $M(t)$ and $\Phi_x(t)$ averaged over consecutive large number of time intervals $\Delta t$ and so comparing the slope of the fitted curve to an error value $\eta$. In this work, we used $\Delta t = 1000$

Figure 1. Time evolution of mobility for ten different runs (different seeds) of a system with dimensions of $L_x = 256$ and $L_y = 64$ and with $\alpha = 20$. The dynamics relaxes to a state of optimal flow when $\rho = 0.5$ (a) and relax to an immobile state when $\rho = 1.5$ (c). For $\rho = 1.0$ (b), the system presents a metastable steady state where either the mobile or the immobile phase can arise depending sensibly on the initial conditions.

and $\eta = 10^{-7}$ as it was shown in Ref. [6] to be a good choice. Now focusing on the study of the density’s influence on the metastability behavior, we simulated a total of $N_{run} = 10^5/N + 10^4$ different runs to calculate the probability of lane formation (the number of times that the system reaches the lane pattern at steady state divided by $N_{run}$), which is denoted as $p_{lanc}$, similarly the probability of clog formation, denoted as $p_{clog}$, and the probability of any outcome other than the two previous cases, denoted as $p_{else} = 1 - p_{clog} - p_{lanc}$.

The Fig. 3 shows us the probabilities the system have of reaching each one of the three possible steady states as a function of $\rho$ for a system of width $L_y = 2$ (purposefully quite narrow) and different values of length $L_x = 2^5$ (black), $L_x = 2^6$ (red), $L_x = 2^7$ (green), and $L_x = 2^8$ (blue). We can observe that the system shows the expected lane formation state for small densities regardless of the size of the system. When the system has sufficiently large density ($\rho \geq 0.5$ for $L_x = 2^5$ for example) clogging starts to emerge as stationary state and the bimodal meta-stable scenario arises. With larger density values, $p_{clog}$ keeps increasing whilst $p_{lanc}$ decreases until both curves crosses each other over and the most probable scenario for the dynamics shifts.

The inset plot of Fig. 3 shows us that the standard deviation of the $p$ has its maximum value at the crossover density where $p_{lanc} = p_{clog} = 1/2$ and thus we define the crossover density $\rho_c \equiv p_{lanc} = p_{clog} = 1/2$. As the Fig. 3 suggests, the lengthier the system is, the more the crossover density appears to decrease asymptotically and at the same time the range of density at which the metastability phenomena occurs becomes smaller with
Crossover density is therefore simulated in the case studied until this point of equal concentrations \( \rho = \rho_c \). Here we performed simulations to obtain a plot of \( \rho \) against the level of occupation \( \rho_c \). We plotted the standard deviation of the probabilities having their maximum value \( \rho_c \) decreasing with larger system.

Let us continue with our finite size scaling study, but now one changes the width of a long system. We show in the Fig. 3 the probabilities of the stationary state uniquely. In order to conclude, it is important to comment some points about \( \alpha \). We used a sufficiently large value of \( \alpha \) during all our manuscript. But this was not duly justified. Here we performed simulations to obtain a plot of \( \rho \) against the level of occupation \( \rho_c \). We noticed that the crossover density asymptomatically increases from \( \rho_c \approx 0.5 \) up to a maximum \( \rho_c \approx 1.2 \) for systems with \( L_y \geq 2 \).

For all the curves we begun by simulating a scenario of one species \( (c_A = 0) \), which means \( p_{\text{lane}} = 1 \) and obviously it represents a fake state of lane formation for the fact that there is not induced self-organization when only one species is considered.

Fig. 5(a) shows an expected behavior for the dynamics because the level of occupation \( (\rho) \) of the system assures the lane formation despite the growth of the concentration of the species \( A \). However, the case of \( \rho = \rho_c \) (Fig. 5(b)) shows that \( p_{\text{lane}} \) gradually decreases as \( c_A \) grows. Finally in Fig. 5(c) which corresponds \( \rho > \rho_c \), we observe the arise of a new possibility: a transitional scenario where the system do not self-organize itself and neither relax to a jammed state. In that case, the overall density \( \rho \) is above the crossover level so the growth of \( c_A \) around \( c_A \approx 0.2 \) makes the particles \( A \) stand as impurities for the movement of \( B \) but are not sufficient to make system immobile. In this case we can have self organized systems and also unorganized motion patterns, which makes us believe that the term “chaotic” is the best suited to describe it since the system can lose its ordering pattern. When the mixing of species tend to the same relative concentration of \( \alpha \) which makes us believe that the term “chaotic” is the best suited to describe it since the system can lose its ordering pattern. When the mixing of species tend to the same

Figure 3. The probabilities of lane formation (filled circles), jamming (empty circles) and relaxation to any other state in between (lines) for a system with width of \( L_y = 2 \) for \( L_x = 2^5 \) (black), \( L_x = 2^6 \) (red), \( L_y = 2^3 \) (green) and \( L_x = 2^8 \) (blue). We are able to see that the crossover density asymptomatically decreases as the length of the system increases. The inset plot shows the standard deviation of the probabilities having their maximum value \( \rho_c \) decreasing with larger systems.

Figure 4. The probabilities of lane formation (filled circles), jamming (empty circles) and relaxation to any other state (lines) for a system with length \( L_x = 128 \). We plotted the results for different widths: \( L_y = 2 \) (black), \( L_y = 2^3 \) (red), \( L_y = 2^3 \) (green), and \( L_y = 2^4 \) (blue). We notice that the crossover density increases from \( \rho_c \approx 0.5 \) up to a maximum \( \rho_c \approx 1.2 \) for systems with \( L_y \geq 2 \).
part of this manuscript, and using $\rho = 0.5 < \rho_c$ (plot (a)), $\rho = \rho_c = 1.2$ (plot (b)), and $\rho = 3.0 > \rho_c$ (plot (c)) in Fig. 6.

The result suggests that only for $\rho = \rho_c$, and $\alpha > 10$ we can observe the metastability, but for small values of $\alpha$, the system is moderately mobile which is expected since

that the interaction between opposite species is weak.

By concluding, in this paper we extend for two dimensions the Fermi-like model for the counterflowing streams of particles. We show that for a suitable density of particles the system under balance/symmetry between the species: $c_A = c_B$, the system is metastable since it evolves to only two possible steady states: one characterized for an immobile regime (clogged) and another mobile self-organized regime represented by a pattern of lanes of particles. Our results also suggest that an imbalance/asymmetry between the species: $c_A \neq c_B$, can generate in addition to these two patterns, an alternative situation characterized by a random mobile state since the dominance of one of species, makes the system to macroscopically behave as a single flux.

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[11] For $\alpha = 20$ the system is essentially deterministic, which is exactly our purpose since only in this regime the metastable states can occur. For this reason, we concentrate a discussion about $\alpha$ in the final of this paper presenting a plot to justify this initial choice of our study.