Negative differential mobility in interacting particle systems

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(Received 7 December 2017; revised manuscript received 29 March 2018; published 29 May 2018)

Driven particles in the presence of crowded environment, obstacles, or kinetic constraints often exhibit negative differential mobility (NDM) due to their decreased dynamical activity. Based on the empirical studies of conserved lattice gas model, two species exclusion model and other interacting particle systems we propose a new mechanism for complex many-particle systems where slowing down of certain *non-driven* degrees of freedom by the external field can give rise to NDM. To prove that the slowing down of the non-driven degrees is indeed the underlying cause, we consider several driven diffusive systems including two species exclusion models, misanthrope process, and show from the exact steady state results that NDM indeed appears when some non-driven modes are slowed down deliberately. For clarity, we also provide a simple pedagogical example of two interacting random walkers on a ring which conforms to the proposed scenario.

DOI: 10.1103/PhysRevE.97.052137

Systems in thermal equilibrium react to small external drive by generating a current which is proportional to the drive and the equilibrium fluctuation of the current [1]. The current flows along the direction of the drive, and the mobility, i.e., the ratio of the average particle current to the external force, remains necessarily positive [2,3]. There is no such restriction in nonequilibrium and both absolute mobility and differential mobility can become negative. Absolute negative mobility (ANM) or conductance refers to the situation when the current flows in the direction opposite to the drive [4–9]. Negative differential mobility (NDM) results when the current decreases with increasing drive [10,11]. It has been observed in various electronic systems [12–15], and in context of particle [10,16,17] and thermal transport [18–20]. In particular, the occurrence of NDM of driven tracer particles in the presence of static obstacles [21–25] or in steady laminar flow [26] or crowded medium [27,28] have been studied extensively in recent years. In context of many-particle systems, NDM has also been observed in the presence of kinetic constraints [29] or obstacles [25,30–32].

Much effort has been made recently to understand the mechanism of NDM in driven systems. What appears crucial for the emergence of NDM is the 'trapping' of the *driven* particles [21,24], characterized by a decrease in the so-called 'traffic' or dynamical activity with increasing bias [33,34]; the obstacles or the crowded environment typically slow down the particle movement, in turn reducing the 'traffic' or dynamical activity which results in NDM. However, the picture can be more complicated in multi-component driven diffusive systems where, in general, the current constitutes contributions from many degrees of freedom (different particle types or modes). In fact, recently it has been shown that a driven tracer in an exclusion process, where the current has two distinct components, can exhibit ANM even around equilibrium [35]. In general, in interacting driven systems, each degree of freedom or mode could experience the external field differently; in particular, the field might affect the time-scales of modes which are not directly biased, and in turn influence the behavior of the current.

In this article we propose a new mechanism: *'slowing down' of non-driven modes in driven interacting particle systems can lead to negative differential mobility.* This proposition is motivated from empirical studies of NDM in several lattice models of which we present two specific examples here, namely an M-chain conserved lattice gas system and a two-species exclusion model. We demonstrate that occurrence of NDM in these systems is associated with a decrease of time-symmetric current or traffic of non-driven modes; the traffic is 'slowed down' due to inter-particle interactions. To prove that the slowing down is indeed the cause, and not the effect, of NDM, we introduce and study several exactly solvable models where some non-driven modes are slowed down deliberately by making a suitable choice of jump rates. We demonstrate that NDM occurs as a direct consequence of the slowing down; without it the NDM disappears.

Our first example is the conserved lattice gas model (CLG) on a $L \times M$ periodic lattice [36] where the site variable $\tau_{ij} = 1,0$ with $i = 1,2\dots L$ and $j = 1,2\dots M$ represents the presence or absence of a particle at the site (i,j); $\rho = \frac{1}{LM}\sum_{ij}\tau_{ij}$ denotes the density. The particles in this M-chain model can move if and only if they have exactly one vacant neighboring site; in absence of any external drive, each jump occurs with unit rate. Now we apply a local field ε along the x-direction that changes the jump rates to the right (left) neighbor to p (q) respecting the local detailed balance condition [37] $\varepsilon = \ln\frac{p}{q}$ with $k_BT = 1$. The particle hopping in y-directions remains unaffected. We work in the phase $\rho > \frac{1}{2}$ where the system is ergodic [36]. Using Monte Carlo simulations we measure the average current $j_{x,y} = (\langle n_r^{x,y}\rangle - \langle n_l^{x,y}\rangle)/L$, where $\langle n_r^{x,y}\rangle$ $(\langle n_l^{x,y}\rangle)$ are the steady state average of the number of right (left) jumps in unit time. This system shows a negative differential mobility for large drive ε, as can be seen from the non-monotonic behavior of j_x shown in Fig. 1(a). The current in y-direction j_y remains zero, however, the time-scale

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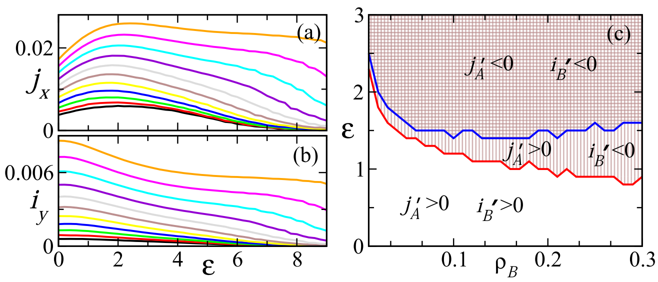

FIG. 1. (a) Current j_x and (b) traffic i_y in the M-chain CLG as functions of ε for different density ρ in the range $0.55 \leqslant \rho \leqslant 0.65$. (c) Phase diagram of the two species exclusion dynamics (1) in ρ_B-ε plane: NDM ($j'_A < 0$) occurs in a region where the traffic of B particles slows down (i.e, $i'_B < 0$). Here, $\rho_A = 0.1$, $\alpha = 0.01$, and $w = 0.1$.

of y-jumps are affected due to the hard-core interaction which is clearly visible from the average 'traffic' or time-symmetric current $i_y \equiv (\langle n_r^y\rangle + \langle n_l^y\rangle)/L$, plotted in Fig. 1(b). In fact, it turns out that dependence of i_y on ε is similar to that of j_x for large ε. This observation indicates the presence of a strong correlation between the current j_x along the driven direction x and the traffic i_y in the transverse (or non-driven) direction.

The next example is a one-dimensional exclusion model with two different particle species, A and B—each species can be considered as a separate current carrying mode. The particles interact via hardcore repulsion; $\tau_i = 0, A, B$ denotes the site occupancy on a periodic lattice of size L. The A particles are driven by a biasing field $\varepsilon = \ln \frac{p}{q}$, they exchange with Bs with rate α, and the dynamics of B particles is taken independent of ε,

$$A0 \underset{q}{\overset{p}{\rightleftharpoons}} 0A, \quad AB \underset{\alpha}{\overset{\alpha}{\rightleftharpoons}} BA, \quad \tau B0 \underset{w}{\overset{u_\tau}{\rightleftharpoons}} \tau 0B. \tag{1}$$

Here, $u_\tau = w + (1-w)\delta_{\tau,0}$, with τ being the occupancy of the left neighbor of the B particle, and does not depend on the biasing field ε that drives As. Note that the B particles experience a constant bias quantified by w, but they are still *non-driven* with respect to ε. We measure the current $j_A = (\langle n_r^A\rangle - \langle n_l^A\rangle)/L$ of A particles and the average 'traffic' $i_B = (\langle n_r^B\rangle + \langle n_l^B\rangle)/L$ of the B particles for different values of the parameters. Figure 1(c) shows the phase diagram in ρ_B-ε plane for fixed values of w,α and $\rho_A = 0.1$, where the presence of NDM and decreasing traffic are marked as shaded regions. Clearly, the presence of NDM is always associated with the decreased traffic of the non-driven modes.

In interacting systems, it is not uncommon that an external driving field affects some non-driven modes [38–40]. The examples presented above are special in a way that the effect is to increase the time-scale, i.e., slow down the traffic of the non-driven modes; occurrence of NDM appears to be correlated with the same. However, whether NDM is the effect of this slowing down or rather it is the cause, is not clear at this stage. To show that the slowing down of non-driven degrees can indeed 'cause' NDM, in the following we introduce and investigate a set of models and show explicitly from exact steady state results that any deliberate slowing down of non-driven modes by external bias can result in NDM.

Two random walkers: As a simple prototypical example of two interacting current-carrying modes we consider two distinguishable particles, denoted by A and B, on a periodic lattice interacting via hardcore exclusion (A and B cannot occupy the same site), following a dynamics:

$$A0 \underset{q}{\overset{p}{\rightleftharpoons}} 0A, \quad B0 \underset{\psi}{\overset{\psi}{\rightleftharpoons}} 0B. \tag{2}$$

In this two random walkers (TRW) model the external field ε affects the particles differently: A is biased to move towards right as $\varepsilon = \ln(p/q) > 0$, whereas B performs an unbiased random walk with jump rate ψ. Clearly, they are the cartoon representations of the driven and non-driven modes of realistic interacting systems. Traffic of the B particle is proportional to the jump rate ψ and we intend to prove below that NDM occurs in this system when ψ is decreasing function of ε, and it disappears when $\psi \equiv \psi(\varepsilon)$ is constant or increasing.

We use the so-called 'matrix product ansatz' [41] to express the steady state weight $P(C)$ for any configuration C in a matrix product form: $P(C) = \mathrm{Tr}[\prod_{i=1}^L X_i]$, where the matrix $X_i = \hat{A}\delta_{\tau_i,A} + \hat{B}\delta_{\tau_i,B} + \hat{E}\delta_{\tau_i,0}$ represents occupancy τ_i of the site i. The matrices $\hat{A}, \hat{B}, \hat{E}$ must obey the following algebra to satisfy the Master equation in the steady state:

$$\hat{A}^2 = 0 = \hat{B}^2, p\hat{A}\hat{E} - q\hat{E}\hat{A} = \omega\hat{A}, \hat{B}\hat{E} - \hat{E}\hat{B} = \frac{\omega}{\psi}\hat{B}, \tag{3}$$

where ω is an auxiliary scalar. We find a 2×2 matrix representation of the algebra (3) with a choice $\omega = \psi\frac{p-q}{\psi+q}$,

$$\hat{A} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \hat{B} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \hat{E} = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix}, \tag{4}$$

where $\gamma = \frac{p+\psi}{q+\psi}$. The partition function of the system of size L is then $Z_L = \sum_C P(C) = \frac{\gamma^{L-1}-1}{\gamma-1}$. The average stationary current of A particle is

$$j_A = p\langle A0\rangle - q\langle 0A\rangle = \omega\frac{Z_{L-1}}{Z_L} \simeq \frac{(p-q)\psi}{(p+\psi)}, \tag{5}$$

where we have taken the thermodynamic limit $L \to \infty$ in the last step. Due to the presence of the interaction, the B particle also exhibits a stationary current which depends on ε; in fact, $j_B = j_A$ (as expected in the absence of particle exchange) and the total particle current $j = j_A + j_B = 2\frac{(p-q)\psi}{(p+\psi)}$. The response of the current j to a small increase in ε is quantified by the differential mobility $j'(\varepsilon)$, where the prime denotes derivative with respect to ε. Equilibrium corresponds to $\varepsilon = 0$, i.e., $p = q$ (remember that $q = e^{-\varepsilon}p$) and in this case, the mobility, as expected, is positive irrespective of the functional form of ψ. On the other hand, in the large driving limit $\varepsilon \to \infty$, assuming p and p' remain finite, we have

$$j'(\infty) = -\lim_{\varepsilon\to\infty}\frac{p^2\psi^2}{(p+\psi)^2}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\frac{1}{p}+\frac{1}{\psi}\right). \tag{6}$$

This sets a criterion for NDM in the TRW model: if asymptotically the increasing rate of ψ^{-1} is larger than the decreasing rate of p^{-1}, then there will be a finite bias $\varepsilon^* > 0$ above which the response is negative. Since the inverse rates measure the diffusion time scales, and the particles here interact via strong repulsive interaction (here hardcore), this criterion is in tune with the proposition given in Ref. [27]. In particular, for the cases $q = 1/(1+e^\varepsilon)$ (i.e., $p = 1-q$) or $q = e^{-\varepsilon}$ ($p = 1$), any choice of $\psi(\varepsilon)$ for which $\psi'(\infty) < 0$ would

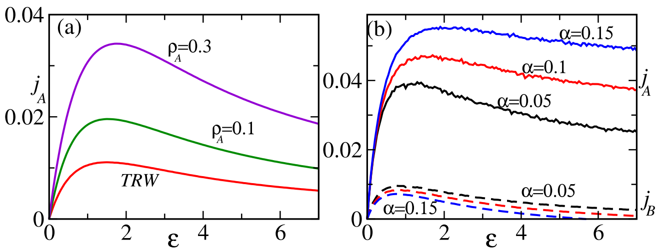

FIG. 2. NDM in two-species exclusion model. (a) j_A obtained from exact steady state results for $\alpha = 0$ are shown for $\rho_B = \rho_A = 0.1, 0.3$; the threshold values are $\varepsilon^* = 1.53, 1.76$, respectively. For the TRW model we plot $j_A/200$ for better visibility. (b) For $\alpha > 0$, j_A (solid lines) and j_B (dashed lines) are obtained from simulations with $L = 1000, \rho_A = 0.1, \rho_B = 0.3$, and different $\alpha = 0.05, 0.1$, and 0.15.

exhibit NDM. Current $j_A = j/2$ as a function of ε for $q = e^{-\varepsilon}, \psi(\varepsilon) = 1/(1+\varepsilon)$ is shown in Fig. 2(a); NDM occurs here for $\varepsilon > \varepsilon^* = 1.505$.

The TRW model, being a toy model of two current carrying modes, lacks some important features of realistic driven systems. In the following we study several more complex driven interacting systems and show that a similar mechanism indeed induces NDM.

Two-species exclusion process: Our next example is a generalized version of dynamics (2) with an added particle exchange dynamics

$$A0 \underset{q}{\overset{p}{\rightleftharpoons}} 0A, \quad B0 \underset{\psi}{\overset{\psi}{\rightleftharpoons}} 0B, \quad AB \underset{\alpha}{\overset{\alpha}{\rightleftharpoons}} BA. \tag{7}$$

Unlike the TRW model, now we have macroscopic numbers of A and B particles with conserved densities ρ_A and ρ_B, respectively.

First let us consider the case $\alpha = 0$. In absence of particle exchange the number of As (Bs) trapped between to consecutive Bs (As) are conserved and thus the configuration space is not ergodic. We choose to work in a sector with exactly one $A(B)$ particle between any two consecutive Bs(As); the configurations are now $C \equiv \{A0^{n_1}B0^{n_2}A0^{n_3}B0^{n_4}\ldots B0^{n_{2N}}\}$, each having exactly N number of As and Bs, and $\sum_i n_i = L - 2N$ number of vacancies. The steady state weights of this particular equal density ($\rho_A = \frac{N}{L} = \rho_B$) sector, can be obtained exactly using the matrix product ansatz, by representing $A, B, 0$ as matrices $\hat{A}, \hat{B}, \hat{E}$, respectively. The required matrix algebra in this case turns out to be the same as Eq. (3) indicating Eq. (4) as a possible representation. However, unlike the TRW model, here we need to deal with finite densities $\rho_{A,B}$. The grand canonical partition function is now $Z_L = \mathrm{Tr}[(z\hat{A} + \hat{B} + \hat{E})^L]$, where z is the fugacity associated with only A particles. In the thermodynamic limit, $Z_L = \lambda_+(z)^L$, where $\lambda_\pm(z) = \frac{1}{2}(1 + \gamma \pm \sqrt{(1-\gamma)^2 + 4z})$ are the eigenvalues of $(z\hat{A} + \hat{B} + \hat{E})$ and $\gamma = (p+\psi)/(q+\psi)$. This leads to $\rho_A = z\frac{\mathrm{d}}{\mathrm{d}z}\ln\lambda_+(z) = z/(\lambda_+^2 - \lambda_+\lambda_-)$. The steady state current of A particles is now

$$j_A = z(p\langle A0\rangle - q\langle 0A\rangle) = \frac{z(p - q\gamma)}{\lambda_+^2(\lambda_+ - \lambda_-)}. \tag{8}$$

Explicit calculation shows that the current of B particles $j_B = \psi(\langle B0\rangle - \langle 0B\rangle)$ is the same as j_A (as expected for $\alpha = 0$), thus $j = 2j_A$. The differential response $\frac{\mathrm{d}j}{\mathrm{d}\varepsilon}$ becomes negative as the field ε is increased beyond some threshold ε^*, which depends on the densities $\rho_A = \rho_B$ as shown in Fig. 2(a) for $p = 1, q = e^{-\varepsilon}$, and $\psi(\varepsilon) = 1/(1+\varepsilon)$.

For $\alpha > 0$, we do not have an exact solution, however, Monte Carlo simulations confirm that the model still exhibits NDM in a fairly large range of particle densities. Figure 2(b) shows j_A and j_B versus ε for different values of α for $\rho_A = 0.1, \rho_B = 0.3$.

Asymmetric misanthrope process. We also investigate systems without hardcore exclusion, namely an asymmetric misanthrope process (AMP) [42] on a one-dimensional lattice where each site i can hold any number of particles $n_i \geqslant 0$. The particles can hop to their right or left nearest neighbors with a rate that depends on the occupation of both departure and arrival sites,

$$\{n_i, n_{i+1}\} \underset{u_l(n_{i+1}+1, n_i-1)}{\overset{u_r(n_i, n_{i+1})}{\rightleftharpoons}} \{n_i - 1, n_{i+1} + 1\}; \tag{9}$$

the functional form of the rate functions $u_{r,l}(.)$, for right and left hops are different. This dynamics conserves density $\rho = \sum_i n_i/L$. The asymmetric rate functions correspond to driving fields $E_{mn} = \ln\frac{u_r(m,n)}{u_l(n+1,m-1)}$ acting on bonds with local configurations (m,n). Clearly, if $E_{mn} = 0\ \forall m,n$, we have $u_r(m,n) = u_l(n+1, m-1)$ and the system is in equilibrium satisfying the detailed balance condition with all configurations being equally likely.

We now choose a set of specific rate functions:

$$u_r(m,n) = \begin{cases} \psi & n = 0 \\ 1 & n > 0 \end{cases}; \quad u_l(m,n) = \begin{cases} \psi & m = 1 \\ e^{-\varepsilon} & m > 1, n = 0, \\ \frac{1}{2} & m > 1, n > 0 \end{cases}$$

$$\text{implying,} \quad E_{mn} = [\ln 2 + (\varepsilon - \ln 2)\delta_{m,1}](1 - \delta_{n,0}). \tag{10}$$

Here, the hopping of isolated particles to *vacant* neighbors is not biased, as both the rightward hop and corresponding reverse hop occur with the same rate ψ; we consider them as non-driven modes. Jumps to occupied neighbors are however biased by an external field which depends on the occupation of the departure site: ε when the departure site has only one particle or otherwise a constant field $\ln 2$.

To explore the possibility of NDM in this system we did a Monte Carlo simulation with $\psi(\varepsilon) = 1/(1+\varepsilon)$. Figure 3(a)

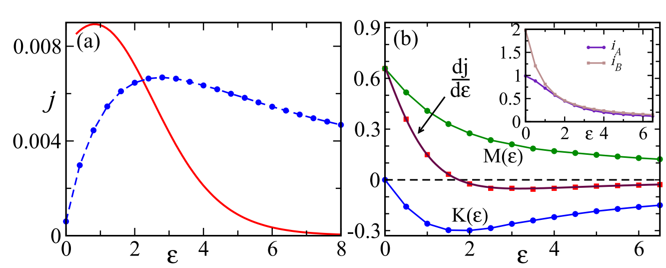

FIG. 3. (a) Current j versus ε for AMP dynamics (10) for density $\rho = 0.15$. Circle: $\psi = 1/(1+\varepsilon)$ (simulations), solid line: exact results for ψ given by Eq. (11). (b) Entropic and frenetic components of the linear response in the TRW model $K(\varepsilon)$ and $M(\varepsilon)$ measured from simulations ($L = 100$). The inset shows the traffic i_A, i_B.

shows the particle current j versus ε (symbols) which depicts a non-monotonic behavior; once again we see that slowing down a non-driven mode results in NDM. This behavior of current can be understood more rigorously from the exact steady state weights of AMP, which has a factorized form $P(\{n_i\}) \sim \prod_i f(n_i)$ when the rate functions satisfy certain conditions [42]. In the present case, these conditions require

$$\psi(\varepsilon) = \frac{2 - e^{\varepsilon} + 2\delta(1 - e^{-\varepsilon})}{3e^{\varepsilon} - 4} \tag{11}$$

with $\delta = \frac{1}{4}(e^{\varepsilon} - 2 + \sqrt{4 + 12e^{\varepsilon} + e^{2\varepsilon}})$, when $f(n) = \delta^{n-1} \forall n > 0$ and $f(0) = 1$. Note that $\psi(\varepsilon)$ in Eq. (11) is a decreasing function for all ε, but the model is well defined only in the regime $\varepsilon > \ln \frac{4}{3}$, where $\psi > 0$. The grand canonical partition function is $Z_L = F(z)^L$ with $F(z) = \sum_n f(n) z^n = 1 + \frac{z}{1 - \delta z}$, where fugacity z controls the particle density through $\rho(z) = zF'(z)/F(z) = z[(1 - \delta z)(1 + z - \delta z)]^{-1}$. Finally, the current is

$$j = \frac{1}{2F(z)^2}[(F(z) + 2\psi - 2e^{-\varepsilon} - 1)(F(z) - 1 - z) + 2z(1 - \psi)(F(z) - 1)]. \tag{12}$$

Figure 3(a) shows j as a function of ε for density $\rho = 0.15$; NDM is observed for $\varepsilon \gtrsim 0.9$.

Nonequilibrium response relation: Away from equilibrium, the linear response of current J can be expressed as a sum of two nonequilibrium correlations [33],

$$\frac{d}{d\varepsilon}\langle J \rangle = \frac{1}{2}\langle S'(\omega); J \rangle - \langle D'(\omega); J \rangle, \tag{13}$$

where $S(\omega)$ and $D(\omega)$ are the entropy (anti-symmetric under time reversal) and 'frenesy' (symmetric) associated with a trajectory ω during time interval $[0,t]$ [33]; primes denote derivatives with respect to ε and $\langle f; g \rangle \equiv \langle fg \rangle - \langle f \rangle \langle g \rangle$. For a single driven tracer, $S' = J$ and the entropic term is simply the variance of the current while the frenetic one depends on the details of the specific dynamics. A large frenetic contribution which may occur, for example, in the presence of traps or obstacles, can make the overall response negative [21,24]. To understand how the entropic and frenetic components of mobility compete in systems where the escape rate (or the time-symmetric traffic) of the driven particle or mode is fixed whereas a *non-driven mode* is slowed down, let us consider the example of TRW model with $p + q = 1$. Since the driving is associated with the A particle only, we have $S' = J_A$, where J_A is the time-integrated current of the A particle during the time $[0,t]$. The change in dynamical activity is now

$$D'(\omega) = \frac{(p - q)}{2} I_A - \frac{\psi'}{\psi} I_B - (p' + \psi')t_{AB} - (q' + \psi')t_{BA},$$

where $t_{AB}(t_{BA})$ refers to the total time during which B sits immediately to the right (left) of A. For the stationary current $j = \lim_{t\to\infty}\langle J \rangle / t$, the entropic component is then given by $M(\varepsilon) = \lim_{t\to\infty}\langle J_A; J \rangle / 2t$ and the frenetic component $K(\varepsilon) = -\lim_{t\to\infty}\langle D'(\omega); J \rangle / t$.

Figure 3(b) shows plots of $M(\varepsilon)$ and $K(\varepsilon)$ obtained from simulations. Similar to the single particle case, $M(\varepsilon)$ remains positive for all $\varepsilon > 0$, whereas $K(\varepsilon)$ becomes negative resulting in NDM above a threshold field. The inset shows the average time-symmetric traffic $i_{A,B}$, both decrease as the driving is increased; the unbiased B particle, being slowed down by the field ε, in turn slows down the A particle.[1]

Conclusion. In this article, we address the question of negative differential mobility (NDM) in interacting driven diffusive systems. Usually NDM occurs when the driven particles are slowed down (increased time-scale of motion) by the external field. Here, we propose an alternate mechanism and show that NDM can occur in interacting multi-component systems when the drive slows down some other, non-driven, degree of freedom. This proposition is motivated from the empirical study of NDM in several systems including conserved lattice gas models [36] and a two-species exclusion model introduced here. To prove that the slowing down of a non-driven degree can indeed lead to NDM we study several exactly solvable models, the simplest one being a pedagogical example of two distinguishable random walkers on a periodic lattice interacting via exclusion, only one of which is driven by an external field. NDM appears there only when the non-driven particle is deliberately slowed down by the external field. Other, more complex, exactly solvable examples of the two-species exclusion process and asymmetric misanthrope process are also studied where the same mechanism leads to NDM for large driving. In these models explicit dependence of jump rates on the driving field might appear simplistic, or even unrealistic, but the main purpose of introducing them is to illustrate and validate the proposition put forward in this article. We believe this mechanism provides a new direction to the occurrence of NDM in interacting particle systems, in contrast to the existing ones—jamming, kinetic constraints, or trapping of driven modes.

Acknowledgments. U.B. would like to acknowledge the support from the Indo-French Centre for the promotion of advanced research (IFCPAR) under Project No. 5604-2.

[1]Note that in absence of any interaction between A and B, i_A would be a constant since $p + q = 1$.

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