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Monte Carlo simulations of interacting particle mixtures in ratchet potentials

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Abstract
There are different models of devices for achieving a separation of mixtures of particles by using the ratchet effect. On the other hand, it has been proposed that one could also control the separation by means of appropriate interactions. Through Monte Carlo simulations, we show that inclusion of simple interactions leads to a decrease of the ratchet effect and therefore also a separation of the mixtures.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The ratchet effect is the appearance of a directional flow in systems composed by particles lying on a substrate that provides a spatially periodic and asymmetric potential in the non-equilibrium regime. Since these currents depend (in magnitude and direction) on the characteristics of the potential and can vary with the kind of particles, several devices have been proposed for achieving segregation of particles. The proposed models are mostly based on one-dimensional (1D) systems [1–3, 6, 7], neglecting any interaction among the particles, and those who take into account the interactions do not consider the hard core (HC) effect [4, 5]. This is because its inclusion made it quite difficult to solve the coupled Langevin equations for the time evolution or the Fokker–Planck equation in the mean field approximation.

The study of 1D systems (which do not exist in nature) has been justified considering its application to systems characterized as 'quasi-1D' without a clear meaning. In the absence of any interaction, this would mean that the ratchet potential depends only on a coordinate, and the other dimension is not relevant. However, with the inclusion of interactions (or the HC), it is difficult to imagine a realistic interaction which depends only on that coordinate. Therefore, 1D systems are not appropriate when interaction effects are considered in transport phenomena. In particular, in 1D systems the inclusion of the simplest realistic interaction (the HC) completely prevents segregation; meanwhile, in the quasi-dimensional systems as described above, this does not occur. Thus, in order to elucidate the effect of the HC and interactions on the transport and segregation of particles, we use Monte Carlo techniques in two-dimensional (2D) systems. These types of techniques have also been used to study the diffusion in highly confined hard disc fluid mixtures [8].

2. The system

We consider a cell of length L with n_a particles in the ratchet potential $V_\alpha(x)$, and n_b particles were not affected by any potential (neutral particles).

$$V_\alpha(x) = \begin{cases} \dfrac{U_o}{2}\left(\cos\left[\dfrac{\pi}{\alpha}\left(\dfrac{(\alpha+1)x}{L}\right)\right]\right), & 0 \leqslant \dfrac{x}{L} \leqslant \dfrac{\alpha}{(\alpha+1)}, \\ \dfrac{U_o}{2}\left(\cos\left[\pi\left((\alpha+1)\dfrac{x}{L}-\alpha\right)\right]\right), & \dfrac{\alpha}{(\alpha+1)} \leqslant \dfrac{x}{L} \leqslant 1. \end{cases} \tag{1}$$

For $\alpha > 1$ the minima of the wells of the ratchet are displaced to the right, while if $\alpha < 1$, the minima are displaced to the left. Figure 1 displays the potential equation (1) for $\alpha = 1/3$.

The temperature fluctuates between the two values T_l (low) and T_h (high), with periodic boundary conditions in the

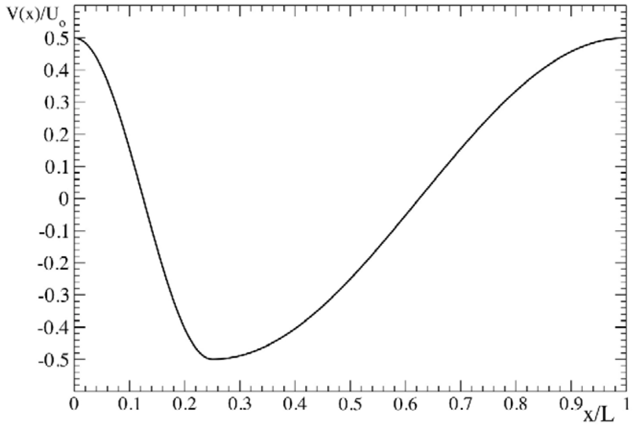

Figure 1. Ratchet potential with $\alpha = 1/3$.

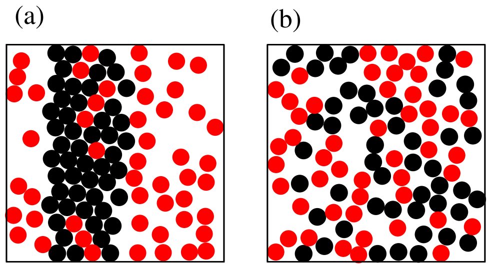

Figure 2. Typical configuration of the system with only HC as interaction ($r_{hc} = 0.04$). Black (red) discs correspond to *a* non-neutral (*b* neutral) particles. (a) T_l and (b) T_h.

x-direction. For 2D systems the boundary condition in the y-direction is hard wall. In our calculations we take as the unit of energy the depth of the ratchet potential (U_o) and the unit of length, the length of the cell (L).

We include the interactions $v_{i,j}$ (as a step function) given by equation (2) among the particles besides the HC and v_s takes different values if the particles are identical or not. r_{min} stands for the hard core radius (r_{hc}) or 0 if this is neglected:

$$v_{i,j} = \begin{cases} v_s & \text{for } r_{min} \leqslant r_{i,j} \leqslant r_{max}, \\ 0 & \text{for } r_{max} \leqslant r_{i,j} \end{cases} \tag{2}$$

with

$$r = \begin{cases} \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} & \text{for 2D}, \\ |x_i - x_j| & \text{for 1D}. \end{cases} \tag{3}$$

Rejected Monte Carlo simulations for 1D and 2D systems were performed in order to analyze the displacement of particles. Each time a particle leaves the cell to the right (left), it is re-injected to the left (right) and moves forward (backward) one cell. After N_p passes, we calculate the histogram of the cell displacement, the fraction of particles moving forward (backward) n cells ($f(n)$), for each type of particles. The temperature flips from high to low each $N_f \ll N_p$ pass.

The system behavior under different bath temperatures is displayed in figure 2. The figure shows the typical 2D system configurations at two temperatures without interaction ($v_s = 0$ for all particles). The values were $n_a = 50$, $n_b = 50$,

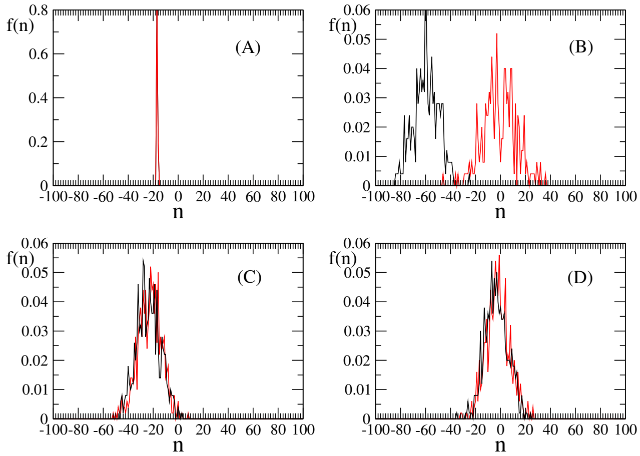

Figure 3. The fraction of particles $f(n)$ versus n number of cells for 1D systems. The black (red) line corresponds to *a* non-neutral (*b* neutral) particles: (A) with HC, (B) without interaction, (C) without HC but attractive interaction among identical particles and repulsive in the other case and (D) without HC but repulsive interaction among identical particles and attractive in the others.

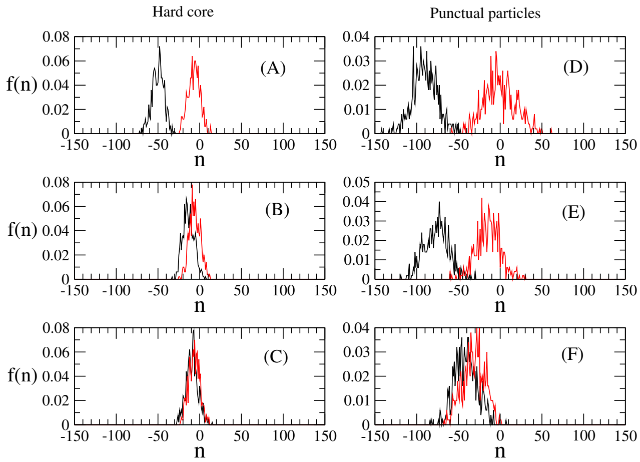

Figure 4. The fraction of particles $f(n)$ versus n number of cells for 2D systems. Black (red) corresponds to *a* non-neutral (*b* neutral) particles: (A) with HC, (B) with HC and attractive interaction among identical particles and repulsive for the others, (C) with HC and repulsive interaction among identical particles and attractive in the other case, (D) without interaction, (E) the same as (C) but without HC and (F) the same as (D) but without HC.

$N_p = 9 \times 10^6$, $N_f = 10^4$, $L = 1$, $U_0 = 1$, $v_s = 0$, $T_l = 0.01$ and $T_h = 6$, $\alpha = 1/3$, $r_{hc} = 0.04$ (for the 2D system). When the additional interactions equation (2) is included, $|v_s| = 0.15$ and $r_{max} = 0.12$.

In figure 3, panel (A) corresponds to the 1D system with HC, where there is observed no particle separation, and the histograms are identical although they present a left drag. In figure 3(B) (without HC), diffusion is observed only for neutral particles, while for the others a left drift is found besides diffusion. The histograms shown in figure 3(C) refer to attractive interaction among identical particles and repulsive interaction in the other case, both show a left drift without any segregation. In figure 3(D) the interaction is repulsive among the identical particles and attractive in the others. It is observed that the ratchet effect does not appear.

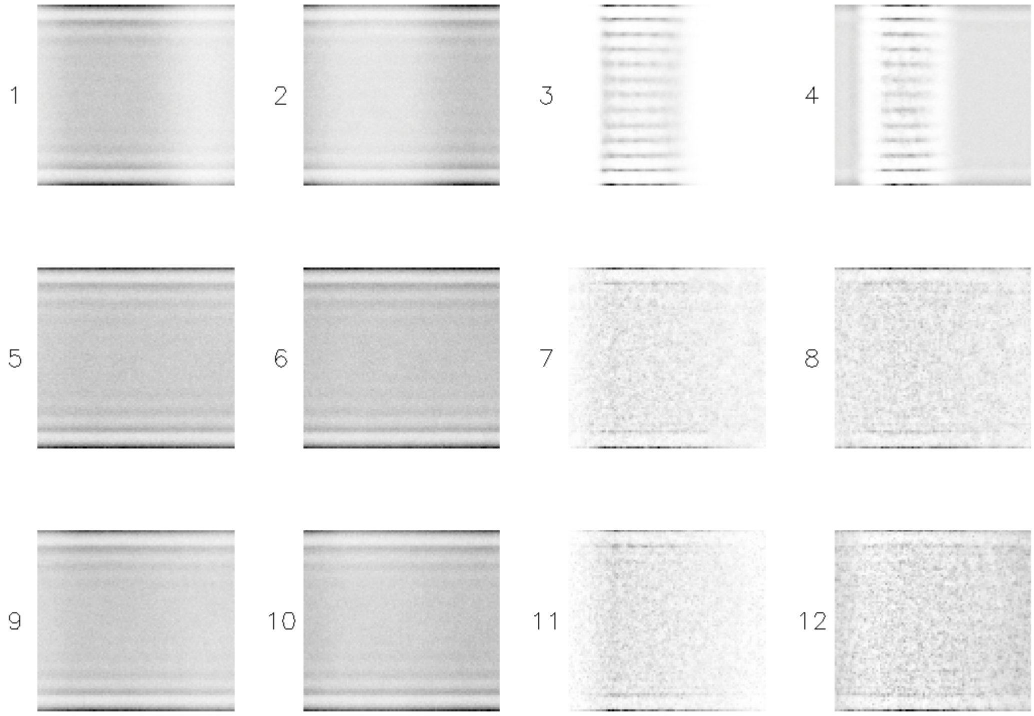

Figure 5. The density of particles. The first row corresponds to HC interaction. The second row corresponds to HC and repulsive interaction between identical particles and attractive interaction among different particles. The third row corresponds to HC and attractive interaction between identical particles and repulsive interaction among others. The first (third) column corresponds to a particles at T_h (T_l). The second (fourth) column corresponds to b particles (neutral) at T_h (T_l).

As expected, the inclusion of HC eliminates any possibility of segregation of particles in the 1D system (see figure 3(A)). Even when HC is not considered, if there is repulsion between particles of different types, there is an effective HC at T_l (see figure 3(C)). In some 1D models without HC [4, 5], opposite displacements for different kinds of particles are obtained by controlling the interaction. In our case this behavior was not obtained. This is due to the repulsive interaction works as an effective HC at low temperatures, so there is always a drag effect.

For 2D systems, taking into account the HC effect as the only interaction present, the neutral particles are dragging to the left (see figure 4(A)). In figure 4(B) is displayed the effect of attraction among identical particles and repulsion in different particles, and in figure 4(C) the interaction is repulsive among identical particles and attractive in the different particles. In both cases the ratchet effect diminishes, although the drag remains from neutral particles to the left. In figures 4(D)–(F) the interactions are the same as above but without HC.

The inclusion of HC has significant effects as can be seen by comparing figures 4(A) and (D). This interaction in all cases decreases the possibility of segregation and diffusion (compare figures 4(B) and (E) or figures 4(C) and (F)). By adding the interactions equation (2) to the system with HC, it can be seen that the segregation diminishes considerably (figure 4(B)) or disappears completely (figure 4(C)).

Figure 5 shows the particle density for the cases discussed above (2D and HC). Panels 1–4 have only HC interaction between particles, panels 5–8 have repulsive interaction between identical particles and attractive interaction among different ones, and panels 9–12 have attractive interaction between identical particles and repulsive among others. Panels 1, 2, 5, 6, 9 and 10 correspond to T_h and the remaining panels to T_l, while panels 1, 5, 3, 7, 9 and 11 correspond to the a particles and the remaining to b particles (neutral). The asymmetry is evident for the case without interaction. By including interactions, the densities become similar (the asymmetry disappears) and because of that, the ratchet effect decreases.

3. Summary and conclusions

The effect of HC eliminates the possibility of segregation in 1D systems. Even if HC is not considered, when repulsive interactions between particles of different type are included there is an effective HC at T_l. On the other hand, always neglecting the HC, if the interaction between identical particles is repulsive and attractive among different particles, the configurations for T_l are messy and the ratchet effect is lost. In the 2D system the inclusion of HC has a significant effect to diminish both diffusion and particle segregation. The effect of other interactions considered here decreases even further the achievement of segregation.

Acknowledgments

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References

[1] Marchesoni F and Savel'ev S 2009 *Phys. Rev.* E **80** 011120
[2] Savel'ev S, Marchesoni F, Hängui P and Nori F 2004 *Europhys. Lett.* **67** 179–185

[3] Savel'ev S, Marchesoni F, Hänggi P and Nori F 2004 *Phys. Rev.* E **70** 066109
[4] Savel'ev S, Marchesoni F and Nori F 2003 *Phys. Rev. Lett.* **91** 010601
[5] Savel'ev S, Marchesoni F and Nori F 2004 *Phys. Rev. Lett.* **92** 160602
[6] Carusela M F, Fendrik A J and Romanelli L 2010 *Int. J. Bifurcation Chaos* **20** 263–9
[7] Borromeo M and Marchesoni F 2005 *Acta Phys. Pol.* B **36** 1421–9
[8] Ball C D, MacWilliam N D, Percus J K and Bowles R K 2009 *J. Chem. Phys.* **130** 054504