Driven diffusive systems with a moving obstacle: a variation on the Brazil nuts problem

LETTER TO THE EDITOR

Driven diffusive systems with a moving obstacle: a variation on the Brazil nuts problem

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Abstract. We present some surprising results of computer simulations on the driven diffusive motion of a 'polymer' in a 'sea of monomers'. The particles move on a lattice subject to a driving field that biases jump rates in a direction perpendicular to the polymer which occupies L sites (monomers occupy one site). This produces a stochastic asymmetric simple exclusion dynamics of the polymer-monomer lattice system. Simulations on a two-dimensional square lattice exhibit unexpected behaviour of the polymer velocity as a function of its length: the velocity $V(L)$ first decreases and then *increases*. This may have relevance for the size segregation of particulate matter which results from the relative motion of different size particles induced by shaking (the Brazil nuts phenomenon). The location of the minimum of $V(L)$ depends on the nature of the driving fields and on the density.

When you shake a can of mixed nuts, the Brazil nuts rise to the top. This phenomenon is the canonical example of size segregation of particulate matter produced by shaking. In general, size segregation as a result of vibratory motion is an important dynamical process common to many industrial systems. Powder separation by the vibration of a non-uniform mixture [1] is just one example: the larger particles move relative to the smaller ones, yielding a system segregated primarily on the basis of size.

Rosato, Strandburg, Prinz and Swendsen (RSPS) [1, 2] conducted a series of computer simulations on mixtures exhibiting such a segregation. Specifically, they studied a two-dimensional system of large and small disks of equal mass. The disks are subject to a gravitational force in the vertical direction and interact with each other and with the walls of their 'container' through a hard-core potential. They simulated the shaking process by quickly (instantaneously) lowering the 'container' by some prescribed amplitude. The disks, which now have space to move, manoeuver themselves according to Monte Carlo metropolis dynamics under the influence of gravity. After all of the disks have settled, they consider one cycle complete and repeat the process. Their simulations gave results consistent with experiments; after many shakes, the larger disks lie on top of the smaller ones in a non-equilibrium stationary state.

RSPS explained the phenomenon as follows: in the shaking process particles are subjected to stochastic forces which make them move both vertically and horizontally, as long as there are voids large enough to receive them. Large particles which require large voids will then be blocked by smaller disks jumping in front of them. This prevents the large particle from falling as rapidly as the smaller ones, and it therefore moves up relative to the container.

Motivated by their work, we investigated the behaviour of a simple lattice gas system which should exhibit a similar size-dependent relative motion. Namely, we studied the relative steady state velocities of different sized particles in a driven diffusive system on a periodic lattice. The relative velocity between the large and small particles, $u(L) = V(L) - V(1)$, is in the direction opposite to the 'gravitational field' due to the 'blocking' of the larger by the smaller ones which can jump 'diffusively' in front of it.

We measured the velocity of a single large particle, a polymer, as a function of its length, L, expecting to see it decrease monotonically. We were, therefore, surprised to discover that after an initial decrease, the velocity actually reached a minimum at some critical length and then increased. This critical length depended on the driving field and monomer density. That is, the segregation rates (between the large particle and the smaller ones far from it) first increased, and then decreased.

The *equilibrium* properties of multicomponent lattice gases and polymers in solution have been extensively studied for many years. For the *non-equilibrium* properties this is not so, the effort having been directed almost exclusively at simple lattice gases [3, 4, 5]. The presence of the large particle whose motion is not Markovian complicates the analysis and make exact results difficult to obtain. We therefore turned to computer simulations. We present the results of these simultations and offer a heuristic explanation of what we believe to be occurring.

We chose the simplest model exhibiting the dynamical behaviour of a two-component mixture: a two-dimensional square lattice, Z^2, with two types of particles—monomers and (rigid) polymers. A monomer, as the name implies, occupies one site, and a polymer more than one. The particles interact by exclusion; no more than one particle per site is permitted. A monomer at site x waits an exponential time with parameter one and then selects a direction α, $\alpha =$ north, south, east or west, with probability b_α. If the neighbouring site y in the direction α is unoccupied at that time, the particle jumps to that site; otherwise it does not move.

For a system containing only monomers the product measure is stationary for the dynamics [5]. That is, if one places monomers at each site x independently with probability ρ, then this distribution is stationary with respect to the dynamics. Consequently, there is no structure to the density profile as seen from a tagged monomer.

Placing a polymer into the system complicates matters. We assumed, in order not to introduce more difficulties, that the polymer is rigidly aligned in the horizontal (east-west) direction. That is, all of the sites occupied by it lie in the same row. The polymer moves according to a dynamics similar to that of the monomers: we choose one site on the polymer, say the most eastern, to control its dynamics. The polymer waits an exponential time with mean one and then selects a direction α with probability b_α and attempts to jump in that direction. Every site which the polymer would occupy after the move must be empty to permit a move. For a polymer to move to the east or the west, then only the site next to that end must be unoccupied. If, on the other hand, it tries to move north or south, L sites must be empty for the move to be made. Note that the size of the polymer does not affect the exponential waiting time.

When the driving field $E = 0$, that is, all b'_α are equal, we have a Kawasaki (particle conserving) dynamics at infinite temperature. The stationary state of the system as seen from the polymer is still a product measure at some specified uniform monomer density ρ. Our interest then is in the stationary states of this system when there is a constant field in the $-y$-direction: this means that $b_{\text{south}} > b_{\text{north}}$. To find the behaviour of the system we carried out computer simulations.

We performed the simulations on two-dimensional square lattices containing N^2 sites with periodic boundary conditions in both directions. First we place the tracer particle of length L, $L = 1, 2, \ldots$, on the empty lattice. We then randomly occupy some of the remaining sites with $\rho(N^2 - L)$ monomers so that the probability of finding a monomer on a non-tracer site is exactly known.

The random number generator selects a lattice site. If unoccupied, it chooses another. Once an occupied site is reached, the particle at that location attempts a move to a neighbouring site as dictated by the jump rates. With probability $b_\perp = b_{\text{east}} = b_{\text{west}}$ the particle attempts to move eastward or westward. It attempts south with probability $b_\parallel = b_{\text{south}}$ and north with probability $1 - b_\parallel - 2b_\perp = b_{\text{north}}$. This simulates a continuous time process. For most (though not all) of our work, we imagine an infinite driving field that prevents moves north, that is, $b_\parallel + 2b_\perp = 1$.

After the decision is made (by the random number generator) in what direction to move, the occupancy of the target site is checked. If empty, the move is successful, and the process repeats. For the polymer to move north or south all of the adjacent L sites in the chosen direction must be empty. The jump rates guarantee that the only conserved quantity is particle number.

Finite size effects and finite run times were our two overriding concerns. To estimate these, we simulated pure monomer systems with different jump rates and particle densities and measured the average velocity of a tracer monomer. For a pure monomer system we know exactly the average velocity of a tracer monomer, $V(1) = b(1 - \rho)$, where $b = b_{\text{south}} - b_{\text{north}}$. This stems from the previously mentioned fact that a tracer monomer will see a uniform distribution at density ρ, so the probability that the site adjacent to the monomer is empty is $1 - \rho$. We compared the simulations to the exact theoretical value and for runs of 40 000 Monte Carlo steps per site (MCS) found that the simulated monomer velocities were typically within one per cent of their exact values.

In order to estimate the finite size effects for polymers we checked the velocity dependence of two different length polymers on a series of six lattices of increasing size. In figure 1 we plot the velocity of an $L = 3$ and an $L = 6$ polymer as a function of lattice size. For these plots the density of monomers is 0.5 and the jump rates are $b_\perp = 0.25$ and $b_\parallel = 0.5$. We let the system evolve for 10 000 MCS so that it reaches a stationary state. Over the next 40 000 MCS interval we determine the tracer velocity. We define this quantity as $\Delta X / \Delta t$ where ΔX is the net displacement in the field direction and Δt measured in MCS is the time over which the displacement occurred. These velocities are determined from three independent runs, each of 40 000 MCS. It appears that the velocities approach an asymptotic value as the lattice size increases. The surprising thing here is that for large lattices $V(6) > V(3)$ in spite of the hard-core exclusion dynamics which requires more sites to be empty for longer polymers to move. We provide a heuristic explanation of this phenomenon later in this letter.

In figure 2 we show the normalised velocity, $V(L)/V(1)$, of the polymer as a function of its length for three different driving fields. The jump rates are as above. For these simulations we used a 64×64 lattice. The system evolved to a stationary state for 10 000 MCS, and we determined velocities over the following 40 000 MCS interval. We find as before that beyond a certain length which depends on the field that the velocity actually starts to increase.

We have simulated the dynamics for various monomer densities and driving fields and find that the minimum is controlled by the ratio of field bias to perpendicular
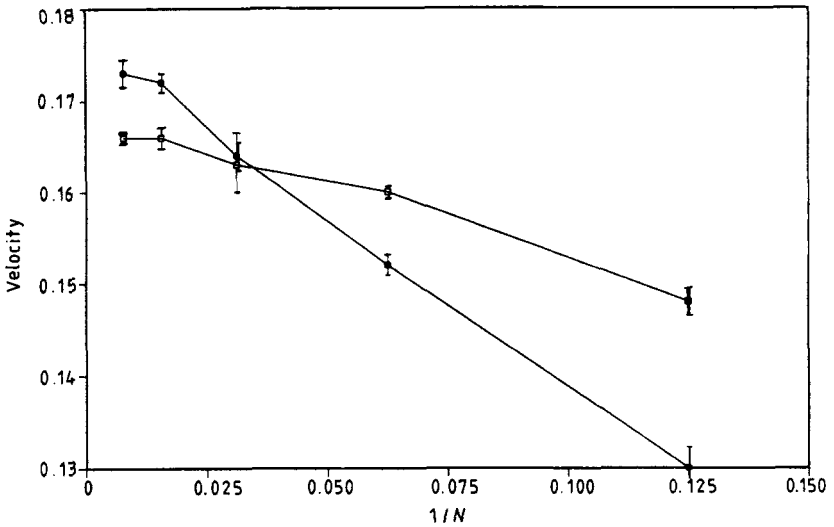
Figure 1. Tracer velocity as a function of inverse lattice size. Squares represent a tracer with $L = 3$ and filled circles, $L = 6$. The monomer density and velocity are both 0.5.
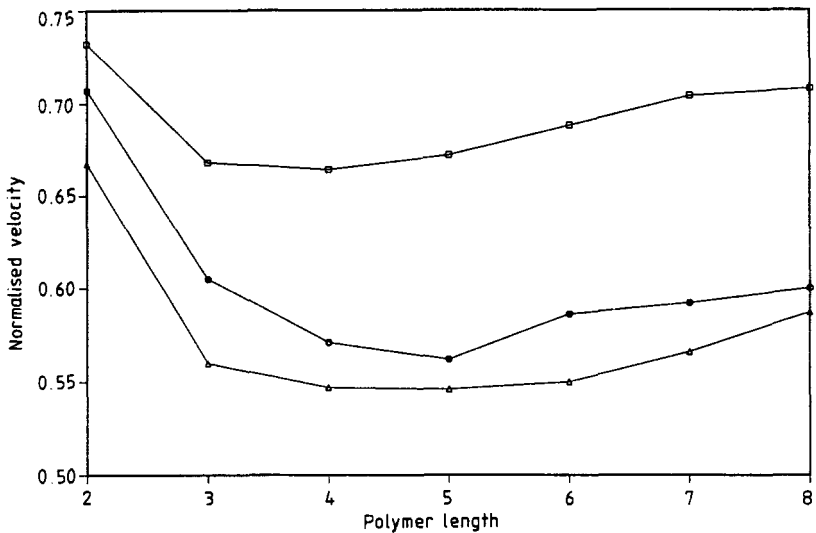

Figure 2. Normalised velocity $V(L)/V(1)$ as a function of length for infinite driving field. Squares represent $\rho = 0.5$, $b_\perp = 0.25$ and $b_\parallel = 0.5$. Filled circles represent $\rho = 0.5$, $b_\perp = 0.25$ and $b_\parallel = 0.4$. Triangles, $\rho = 0.5$, $b_\perp = 0.35$, and $b_{/\text{parallel}} = 0.3$. The lattice is 64×64.

jump rates. A smaller ratio shifts the minimum to longer polymers and, given some fixed parameters, we see no minima for the lengths simulated. Strong finite size effects prohibit us from studying longer polymers on a 64×64 lattice.

One might be tempted, as a first approximation, to say that the velocity is given by $V(L) = b(1 - \rho)^L$. This assumes a uniform density profile and ignores correlations between monomers. Such an approximation fails badly.

To explain the anomalous behaviour of the velocity $V(L)$, we proceed in two steps: we argue first that the blocking is primarily at the edges of a long polymer and second

that the presence of the polymer produces a density profile in which the density at the edges actually decreases as L increases.

To simplify matters, consider the case where the polymer has length $L \gg 1$, and there is no motion northward. Since even one occupied site below the polymer will block the polymer motion, the field will create a low-density region below and a high-density region above the polymer. Particles from the sides diffuse into this region and are carried 'down-wind'. The longer the polymer, the farther downward and sideways will extend the depletion region, and the faster monomers will move when in this region. In fact, the field will most likely carry the monomers away before they can move under the centre region of the polymer far inward from the edges. Most of the sites directly under the polymer are never occupied. It is only near the edges that blocking occurs. Now, the larger this depletion region in the horizontal direction, the fewer particles there are to come in from the sides to block the polymer, and so its velocity increases. This effect is enhanced by the motion of the polymer itself. As the polymer travels through this low-density area it creates a fan-shaped low-density region which now extends *above* the polymer. This is due entirely to the motion of the polymer. For a fixed polymer there is a special symmetry in the monomer–hole dynamics which prevents this wing from forming.

The density profiles, as seen from the polymer, bear out this picture qualitatively. There is a depletion region below the polymer which sweeps above it in a wing-like shape. Immediately above the polymer there is a region where the density is higher than the initial monomer density. This is illustrated in figure 3.
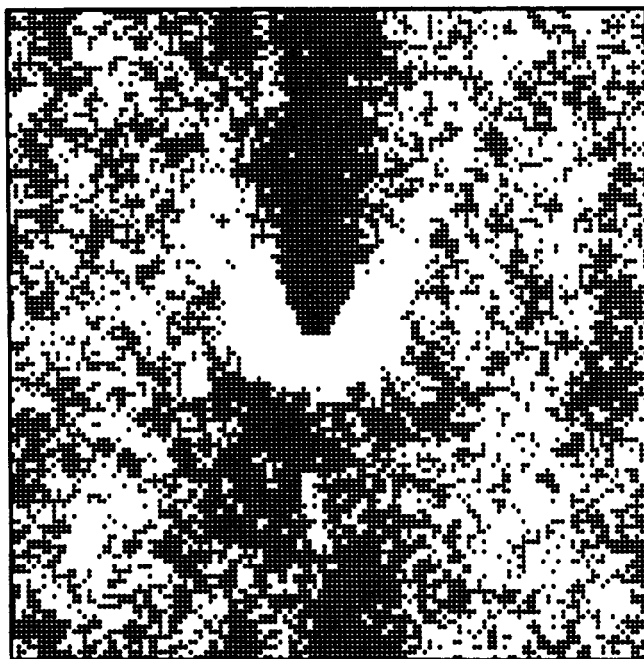

Figure 3. We show the high-density regions of monomers as viewed from the moving frame of the polymer. High-density sites ($\rho > 0.5$) appear as black squares with size proportional to density. Sites with low density appear white. Note the wing or fan effect. The lattice is 128×128, $b_\perp = 0.25$, $b_\parallel = 0.5$.

To carry out a quantitative analysis seems difficult. There is obviously a delicate balance between two competing effects: (1) longer polymers require more sites to be unoccupied to move, and (2) longer polymers deplete a larger region. The net results, as the simulations show, depend on the density of monomers and details of the jump rates.

We explain the change in the curves when the driving field is reduced or the perpendicular jump rates are enhanced by noting that under these conditions monomers can penetrate farther inward under the polymer before the field carries them away. With such rates, more sites under the polymer can be affected and it is not until longer polymers are used that other factors can negate this effect. As noted previously when the field is decreased, the minimum is shifted to longer polymers.

As further evidence for our interpretation we have (at the suggestion of H van Beijeren) carried out simulations in which there was no exclusion between the monomers—the polymer, however, was still blocked by the monomers. The velocity $V(L)$ now decreased monotonically with L. This indicates that the increase in the motion of the monomers with lowered density is an important ingredient in creating the wing effect.

This wing effect, however, does not appear to be necessary for the anomalous behaviour. We have performed simulations where the polymer is fixed at the origin, and the monomers act as before. What we record is the number of times that all of the sites immediately below the polymer are empty. A plot of percentage of time empty against polymer length bears a striking resemblance in form to the velocity curves for the moving polymer; see figure 4. For this case we can rigorously prove, and computer simulations support, that the average density at the sites along the polymer axis is equal to the initial uniform density (no wing effect). We find this by constructing an equivalent dynamics which exploits the precisely opposite behaviour of monomers and holes under the action of the field. We see a surprising behaviour in spite of the fact that there is no longer a wing effect. The motion, in the mobile polymer case,
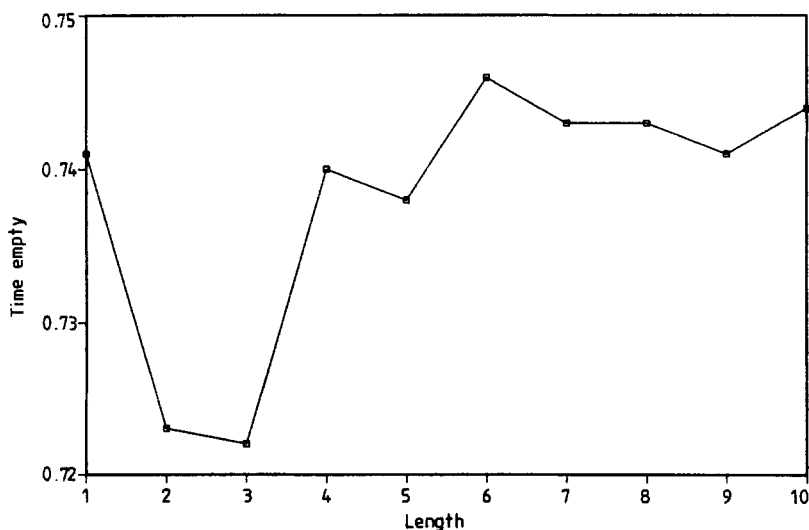

Figure 4. Percentage of time which all of the sites immediately below the polymer is empty as a function of length. The density is 0.5, $b_\perp = 0.25$ and $b_\parallel = 0.5$. The lattice is 128×128 and the data was recorded over 90 000 MCS.

then, creates the wing-like feature which serves to enhance an already existing anomalous behaviour.

We summarise our argument as follows: the action of the field is to transform the blocking from a bulk effect to an edge or boundary effect. This, coupled with the reduced density at the boundaries due to the entire length of the polymer, is responsible for the results we find in computer simulations. Assuming our heuristics are correct, a natural question is: what is the asymptotic velocity as a function of length? Does it approach a constant value, or does it decrease again?

In an effort to better understand the phenomena discussed here, we are currently studying diffusive flow with a drift past a fixed obstacle†. This sounds like a textbook problem but is apparently not in the literature. We are also still hoping to obtain some rigorous results concerning the stationary state as viewed from a tagged polymer.

What implications does this anomalous behaviour have on the model of RSPS? There are certainly important differences between their model and ours. In particular their system does not permit the establishment of a stationary state, since after each shake the system settles to rest. This stationary state relative to the tracer particle may be the essential feature which allows for the surprising behaviour. It seems, however, possible that such behaviour might be observed at greater amplitudes of shaking and larger ratio of disk radii. That is, larger disks might rise at a slower rate.

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† Work in progress with J Keller.