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October 15, 2018

Dear PRE Editors,

We would like to submit the paper "On The Diffusion of Sticky Particles in 1-D" for consideration in PRE. In it we create a new paradigm for modelling complex flow, combining the simplest particle-based model for flow with the simplest particle-based model for attraction, the Symmetric Exclusion Process and the Ising model. A remarkable discovery is that this "Sticky Particle Model" has a nonequilibrium transition between two types of flow, something not generally believed impossible in 1D without long-range interactions or an external field. As with the SEP and Ising models, the simple nature of the model makes it representative of a wide range of flow problems. We also demonstrate well-defined limiting behaviour of the density and flow. Simple explanations of these observations escape us, but should open up the field to follow-up test and developments of overarching theories on nonequilibrium thermodynamics such as maximum entropy, maximum entropy production of maximum flow.

After introducing the model, we analyse it in depth with three different techniques: Monte Carlo simulation, Transition rate matrices, and mean field theory.

The paper has some history. We originally submitted to PRL where the referees felt we hadn't proved our case. We are confident in our results, but the refereeing at PRL made it clear that attempting to cram both simulation and mean field theory into a letter format could not be done in a clear manner.

Since the PRL submission, we developed the transition matrix approach which provides yet more evidence and explanation of the model. We are confident that this, and extended numerical evidence of the transition such as the fluctuation peak in 7 would convince the referees. For this reason, we choose to submit our more thorough exposition to PRX. The editors there have read it, and they say that the paper's audience is probably not general enough to publish it there, and have recommended that we forward it on the PRE.

Below we make a point-by-point response to the previous PRL referees. PRX also asked about the division of materials between paper and SM: We note the recurrent theme in both reviews that the paper needed to be more comprehensive in presenting the data. This, along with the new semi-analytic results from the Transition Matrix approach, justifies the expansion of the paper.

It seems that our "historical" MFT-first presentation of the work, overemphasized the importance of MFT. Consequently, we have restructured the paper to start with our new Transition matrix analysis, followed by the simulations and finally the MFT. For ease of comparison, results from all three methods are presented in some figures.

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Second Report of Referee A – LQ16123/Hellier

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The authors have not remedied the problems in the original version of the manuscript: the manuscript does not contain simulation results to support the mean-field picture, which is based on a number of approximations.

We are well aware of the deficiencies of MFT, which breaks down at the transition. We present more simulation results here to explain what happens when MFT fails, not to "support" the MFT picture.

Since mean-field theory is known to overestimate phase transitions in one-dimensional models (e.g. the 1D Ising model), there are reasons to be concerned about the correctness of the manuscript. Note that in principle it should not be difficult to provide such simulation results (see the second point below for more detail).

Previously we did not include enough about the simulations convince referee A. By switching from PRL to regular paper format, we have included far more comprehensive details of the simulation and evidence for the transition: the slope changes in Fig 3 and 4, the different flow character in Fig 5, and the peak in density fluctuations in Fig 7.

In its present form, I do not think the manuscript solves an outstanding problem or significantly advances a certain field. The authors think they do, because, as they state in their reply, they believe that equation (1) is "a significant achievement" and "the difficulty of doing it is probably why this apparently-obvious model has not been previously published." I disagree with these statements: equation (1) is based on simple mean-field arguments and similar equations have been derived before in the literature (see the third point below for more detail).

Below you can find arguments to substantiate my critique:

1) The authors state that "the referees have looked primarily at the more trivial aspects of the work".

In my original report I have expressed concerns about the validity of the main result, which is based on mean-field arguments. Since the main result of the present work uses certain assumptions (mean-field theory), and since no evidence is provided concerning the validity of these assumptions, I do not think my critique is about trivial aspects.

2) The authors state that "Referee A, in particular, has misunderstood the main result."

Analyses of the SPM model itself, not just the mean field theory is the definitive aspect of the work. For very sticky particles, MFT predicts a negative diffusion constant - which breaks the mean field assumption. This is indicated

of a transition in the full system which is more fully described by simulation and TRM.

This refers to the fact that in my original report I have stated "that the main result seems to be an artifact of the approximative nature of mean-field theory". I think this remains a valid criticism, which has not been remedied in the revised manuscript. The manuscript presents no evidence for the existence of a nonequilibrium phase transition in the simulation results of the model.

I am not stating that such a nonequilibrium phase transition does not exist, but rather that the authors do not provide the required evidence to claim this transition exist.

In the original report, the referee said that the nonequilibrium phase transition seemed to be an artifact of MFT. We accept this criticism of the original PRL, but the additional simulation data in this extended version provides the required evidence

For example, figure 1 of the revised manuscript shows a clear discrepancy between simulations and mean field theory: mean-field theory describes a phase transition from a phase with nonzero flux to a phase with zero flux, whereas in simulations there is a smooth crossover from a regime where the flux is proportional to "lambda" to a regime where the flux is proportional to λ^4. From the presented data one can thus not conclude that the nonequilibrium phase transition predicted by mean-field theory exists in the actual model.

This is exactly correct. The MFT predicts zero-flux and the breakdown of the mean field approximation. MFT indicates that there is a transition, but MFT cannot describe the nature of the region in which MFT is inapplicable. The simulation shows a different type of transition. There is still flow in the low lambda region (fig 5), at least until the flow is so slow that it becomes impractical and only our newly added semi-analytic TRM approach can correctly describe the behaviour (Fig 4).

How can the authors show the existence of a phase transition? They could present curves for different system sizes and use finite size scaling to show that simulation results converge to mean-field theory. Such an analysis is not presented in the manuscript.

We have now done this. Figs 6 and 7 show that the system-size dependence of flow and fluctuations converges very quickly at low lambda. From Fig 3&4 it is evident that convergence is even faster at higher lambda, as would be expected. This rapid convergence makes it impossible to do finite-size scaling to characterize the transition. However, as we mention above, there is conclusive evidence for a transition from simulation and TRM results as shown Figs 3,4 5 and 7. It is also evident in these figures that the low lambda behaviour is different from the MFT.

3) The authors state that "the analytic derivation of the mean-field solution (eq. 1, derived in the SM) is a significant achievement" and "the difficulty of doing it is probably why this apparently obvious model has not been previously published."

This statement is incorrect because equation (1) is a mean-field equation for the occupation probabilities. Mean-field equations are relatively easy to derive: this is confirmed by the authors' derivation presented in the SM, which is very simple. Note also that similar mean-field derivations have been presented in other papers on lattice gases: see for example section 2.2 of the review paper "RA Blythe, MR Evans, Journal of Physics A: Mathematical 2007" and section

4 of the review paper "Cecile Appert-Rolland, Maximilian Ebbinghaus, Ludger Santen, Phys. Reports, 2015".

Perhaps it was inappropriate to speculate as to why work hasn't been done before. The "similar" work of our Edinburgh colleagues Blythe and Evans has over 500 citations, so although the MFT is not the main result here, we are comfortable describing it as significant.

4) The authors state: "The model is defined in terms of rates, and because we did not notice it at first, we feel that detailed balance is not trivial and worth proving (see Referee B point 1). Most well-known jamming models defined by rates, e.g. ASEP, do not have detailed balance. It is sometimes tacitly assumed that this lack of detailed balance is necessary for non-trivial flow behavior. An important aspect of this work is to demonstrate that obtaining non-trivial flow *can* be achieved in a model with detailed balance."

This statement is incorrect, since the model is a specific example of a class of reversible lattice gases studied before in the literature. See the book "Large Scale Dynamics of Interacting Particles, H. Spohn" for an overview of this research, and see also the paper "H Spohn, Long range correlations for stochastic lattice gases in a non-equilibrium steady state, Journal of Physics A: Mathematical and General, 1983", for more details. It is a well known fact that such lattice gases on a ring satisfy detailed balance.

This is a minor point about a comment in the response rather than the paper. We said that "Most well-known jamming models defined by rates, e.g. ASEP, do not have detailed balance.". We didn't claim that all of them do, and the referee correctly points out a class of models which do have detailed balance and jamming behaviour (for 3 or more dimensions).

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This is my second report on the manuscript "On The Diffusion of Sticky Particles in 1-D", by JDM Hellier and GJ Ackland. The revised version is an improvement over the original manuscript but my opinion on its meeting of the specific criteria for acceptance in the Physical Review Letters remains unaltered. Honestly, I believe that this paper belongs in a more specialised journal such as the Physical Review E. In addition, I think that the paper should benefit from being merged with the supplemental material, since some of the results are much better understood after reading it.

We respectfully disagree with the referee here. However, we accept the point that the results are better understood when merged with the SM. It echoes the criticism of lack of convincing proof from Ref A. Now that we also have the Transition Rate Matrix results to consider, the switch to PRX becomes even more essential

Finally, a rather technical point on the detailed balance proof in the supplemental material (but the authors say that the proof of detailed balance is important for them, so I would like to clarify this). What the authors are saying is that the "equilibrium" distribution of their model is

(equations not transcribed from pdf)

in the Ising Hamiltonian, as I said in my first report. So, the model the authors are proposing is a particular case of a 1d Ising system, with both external field and nearest neighbour interaction, with Kawasaki dynamics. The thing is that, with the authors motivation as a "sticky" particle-hole system, the

intensity of the external field and the nearest-neighbour coupling are linked, the latter being one-half of the former, and this yields non- intuitive behaviour (the reported phase transition). I think this should be clearly stated in the long paper I encourage the authors to write.

The referee maps our model in the equilibrium case to a spin Ising model with a field. We stated the equivalence in the original manuscript, but the extra space allows us to discuss this mapping explicitly in section IIB. The referee's derivation is correct, but overlooks that the SPM is defined by its dynamics, not the Hamiltonian. This is not a trivial distinction because, under (particle hopping) Kawasaki dynamics, the density is conserved ($\sum \sigma_i$ constant). The "field" term cannot affect the system and its link to the coupling cannot cause the non-intuitive behaviour. Had we been considering spin-flips and Glauber dynamics the situation would have been as the referee describes.