PRL 106, 079602 (2011)

PHYSICAL REVIEW LETTERS

provided by Open Access LM 18 FEBRUARY 2011

Hinsch, Reese, and Frey Reply: We have carefully reviewed our simulation algorithm and found that the original implementation featured a bias on the passive part that favored moves to the right by a small fraction of order N^{-1} . Repeating the simulations with the corrected algorithm, we have now obtained density profiles in good agreement with the simulations by Jiang *et al.* [1]. In particular, our revised simulations also indicate that the mean field phase diagram, calculated by our analytical approach [2], seems to be exact.

Neither our corrected algorithm nor the simulations of Jiang *et al.* [1] were designed to simulate the actual dynamics of the system, but are sequential updating algorithms. Therefore, we decided to scrutinize these results upon comparing them with simulations based on the Gillespie algorithm, which gives an exact solution for the stochastic dynamics; see, e.g., Ref. [3]. As shown in Fig. 1(a), the obtained density profiles are in good qualitative agreement, but show slight quantitative deviations.

We have conducted simulations with different established random number generators and have not found any dependence of our results on the used sequence of random numbers. We would like to point out, however, that deviations between the results obtained from a Gillespie and an updating algorithm for large systems are most likely due to insufficient sampling in the updating algorithms. In order to obtain valid averages, the time window for sampling configurations has to be much larger than the typical correlation time T. The latter is estimated as the mean passage time of a particle through the active part, $T \sim N$. As is well known, the expected error in the simulations should then scale with the inverse square root of the number of statistically independent configurations. In an updating algorithm this implies that the number of moves required for sampling should scale as N^3 [see Fig. 1(b)]. This scaling is a peculiarity of the considered lattice gas, as the diffusion rate scales with system size by construction. This leads to the supplemental power of N in addition to the usual N^2 scaling for a diffusion process. We think that in update algorithms this large number of relaxation steps is important to note in the particular case of large system sizes.

In conclusion, we attribute the deviation from mean field theory claimed in the original Letter [2] to a faulty simulation algorithm.



FIG. 1 (color online). (a) Density profiles on the active part of the lattice with N = 500 and $n_p = 0.38$ for various diffusion strengths d. Data were acquired using our revised updating algorithm (thick lines) and a Gillespie algorithm (thin lines), of which we ran 100 simulations, each recording 100 independent configurations of the particle density on the lattice. To assure independence of consecutive configurations, we chose a sampling time T = N and equilibrated the system for a time $\sim 2N$. (b) Number of updates as a function of system size in the Gillespie algorithm. After an equilibration of the system $(n_p =$ 0.38 and d = 0.65) for a time 5N, the number of updates performed in the Gillespie algorithm were counted over a time interval 15N, and from that the average number of updates in the sampling time T = N were determined. This shows that in an update algorithm the number of updates has to grow like N^3 for the observation time to be larger than the correlation time.

We thank R. Jiang and collaborators for their attentive and careful revision of our original work.

Hauke Hinsch, Louis Reese, and Erwin Frey Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS) Department of Physics Ludwig-Maximilians-Universität München Theresienstrasse 37, D-80333 München, Germany

Received 11 November 2010; published 18 February 2011 DOI: 10.1103/PhysRevLett.106.079602 PACS numbers: 64.60.Ht, 05.40.-a, 05.60.-k, 05.70.Ln

- [1] R. Jiang *et al.*, previous Comment, Phys. Rev. Lett. **106**, 079601 (2011).
- [2] H. Hinsch and E. Frey, Phys. Rev. Lett. 97, 095701 (2006).
- [3] D.T. Gillespie, J. Comput. Phys. 22, 403 (1976); J. Phys. Chem. 81, 2340 (1977).