LETTER TO THE EDITOR

Nonequilibrium reweighting on the driven diffusive lattice gas

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Abstract
The nonequilibrium reweighting technique, which was recently developed by
the present authors, is used for the study of nonequilibrium steady states. The
renewed formulation of nonequilibrium reweighting enables us to use the
very efficient multi-spin coding. We apply the nonequilibrium reweighting
technique to the driven diffusive lattice gas model. Combining with the
dynamical finite-size scaling theory, we estimate the critical temperature T_c and
the dynamical exponent z. We also argue that this technique has an interesting
feature that enables explicit calculation of derivatives of thermodynamic
quantities without resorting to numerical differences.

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Most phenomena occurring in nature are in nonequilibrium states. Nonequilibrium systems,
such as epidemics [1], vehicular traffic [2], biological networks [3] and catalysis [4] have
attracted a lot of attention. Monte Carlo simulation has become a standard tool in scientific
computing, and advanced simulation methods, such as cluster algorithms [5, 6] and generalized
ensemble methods [7–10] have been developed. However, many advanced Monte Carlo
methods are not applicable to nonequilibrium systems. Efficient Monte Carlo algorithms for
nonequilibrium simulation are much needed.

Quite recently, the present authors [11] have developed a reweighting method for
nonequilibrium systems based on sequential importance sampling (SIS) [12, 13]. With
nonequilibrium reweighting, only simulation at a single temperature is required to obtain
information for a range of temperatures. The nonequilibrium reweighting method differs
conceptually from conventional Monte Carlo methods. In many Monte Carlo methods, a
sequence of micro-states is sampled by using the Boltzmann distribution. One can interpret this
as sampling over a 'path' generated by the associated Monte Carlo updates. Thermodynamic
quantities are then averaged over this path. In nonequilibrium reweighting, many paths are
first sampled with a trial distribution that is not necessarily equal to the Boltzmann distribution.
Then thermodynamic quantities are calculated based on the relative probability between the
trial distribution and the Boltzmann distribution. The relative probability is called 'weights' in
literature, which we shall use hereafter. The advantage of this is that one could sample many

paths at one temperature and then calculate required thermodynamic quantities for a range of temperatures.

Moreover, Saracco and Albano [14, 15] have proposed an effective analysis of nonequilibrium phase transitions, in the study of the driven diffusive lattice gas model [16], using a dynamical finite-size scaling theory. The behaviour of nonequilibrium phase transitions can be extracted from short-time dynamics [17–19]. If we combine the advantages of dynamical finite-size scaling and nonequilibrium reweighting, we can achieve an effective way of simulation for nonequilibrium systems.

In this letter, we apply the nonequilibrium reweighting method [11] to the study of nonequilibrium steady states [20, 21]. We illustrate our method on the driven diffusive lattice gas model [16]. We reformulate the nonequilibrium reweighting method and implement very efficient multi-spin coding [22, 23]. We also make modifications to the dynamical finite-size scaling relation, which was originally proposed by Saracco and Albano [14, 15], so that the advantages of reweighting and dynamical finite-size scaling can be combined.

Let us start by explaining the driven diffusive lattice gas model proposed by Katz, Lebowitz and Spohn (KLS) [16]. This system is one of the most well-known nonequilibrium models exhibiting a nonequilibrium steady state. It was first proposed as a model for super-ionic conductors, and attained its popularity due to its complex collective behaviour. It is constructed as a $L_x \times L_y$ square lattice with *half-filled* lattice sites having periodic boundary conditions. Its Hamiltonian is given by

$$\mathcal{H} = -4 \sum_{\langle ij, i'j' \rangle} n_{ij} n_{i'j'}, \tag{1}$$

where the summation is over nearest lattice sites. The variable $n_{ij} = 1$ when the site is filled and $n_{ij} = 0$ otherwise. Attempts for each particle to jump to an empty nearest-neighbour site are given by the Metropolis rate [24],

$$T_{\beta, E}(\sigma'|\sigma) = \min[1, \exp(-\beta(\Delta\mathcal{H} - \epsilon E))], \tag{2}$$

where σ and σ' are the system configurations before and after the jump, $\Delta\mathcal{H}$ represents the change in energy due to the jump, E is a constant driving force, $\epsilon = -1, 0$ or 1 depending on whether the jump is against, orthogonal or along the direction of the drive, and $\beta = 1/T$ is the inverse temperature of the thermal bath. The L_y direction is taken as the direction of the drive. The KLS model exhibits an order–disorder second-order phase transition. In the ordered phase, strips of high- and low-density domains are formed along the direction of the drive. In the final steady state, the particles are condensed into a single strip parallel to the direction of the drive [25]. Hence the order parameter can be defined as the density profile along the direction of the drive [14], and moments of the order parameters are given by

$$\rho^k = \frac{1}{(L_x/2)} \sum_{j=1}^{L_x} \left| \frac{1}{L_y} \sum_{i=1}^{L_y} n_{ij} - \frac{1}{2} \right|^k, \tag{3}$$

where $n_{ij} = 0$ or 1 as defined in equation (1), and $k = 1, 2, 4$ represents the first, second and fourth moments of the order parameter, respectively.

We briefly review the nonequilibrium reweighting based on SIS, and show the implementation on the KLS model. Define a path $\vec{x}_t$, a sequence of points in phase space σ_i which were visited during the course of simulation, as

$$\vec{x}_t = (\sigma_1, \sigma_2, \ldots, \sigma_t). \tag{4}$$

This path can be sampled by using the Monte Carlo method at an inverse temperature β and a constant drive E. The objective is to calculate the appropriate weights for computing the thermal average of a quantity Q at another inverse temperature β' and another drive E',

$$\langle Q(t)\rangle_{\beta',E'} = \sum_{j=1}^{n} w_t^j Q(\vec{x}_t^j) \Big/ \sum_{j=1}^{n} w_t^j, \tag{5}$$

where the sum is over all sampled paths indexed by j and w_t^j are the weights. The number of paths is denoted by n. To calculate the weights, the following steps are implemented,

(1) Suppose $\vec{x}_t^j = \left(\sigma_1^j, \ldots, \sigma_t^j\right)$ up to time t is sampled from a simulation at the inverse temperature β and drive E.

(2) To go from t, choose a pair of neighbouring lattice sites at random. If one of the two sites is empty, move the particle to the empty site with the rate, $T_{\beta,E}(\sigma'^j|\sigma_t^j)$, which is the Kawasaki spin exchange process. σ'^j denotes the system configuration after the move.

(3) An incremental weight δw^j has different values according to two possible outcomes,

   (a) If the move is accepted; $\sigma_{t+1}^j = \sigma'^j$ and $\delta w^j = T_{\beta',E'}(\sigma'^j|\sigma_t^j)\big/T_{\beta,E}(\sigma'^j|\sigma_t^j)$.

   (b) If the move is rejected; $\sigma_{t+1}^j = \sigma_t^j$ and $\delta w^j = \left[1 - T_{\beta',E'}(\sigma'^j|\sigma_t^j)\right]\big/\left[1 - T_{\beta,E}(\sigma'^j|\sigma_t^j)\right]$.

The weights at $t+1$ are given by this incremental weight through the relation $w_{t+1}^j = \delta w^j \times w_t^j$ with $w_1^j = 1$.

For each path $j \in \{1, \ldots, n\}$, these steps are repeated until some predetermined maximum Monte Carlo time is reached.

We make a comment on the technical detail of calculating the weights. For the case of infinite drive ($E = \infty$), possible values of incremental weights δw_i are,

$$\begin{aligned}
\delta w_0 &= 1, \\
\delta w_1 &= \exp(-12(\beta' - \beta)), \\
\delta w_2 &= \exp(-8(\beta' - \beta)), \\
\delta w_3 &= \exp(-4(\beta' - \beta)) \\
\delta w_4 &= (1 - \exp(-12\beta'))/(1 - \exp(-12\beta)), \\
\delta w_5 &= (1 - \exp(-8\beta'))/(1 - \exp(-8\beta)), \\
\delta w_6 &= (1 - \exp(-4\beta'))/(1 - \exp(-4\beta)).
\end{aligned} \tag{6}$$

The weights can then be written as a product of incremental weights,

$$w_t^j = (\delta w_1)^{h_1^j(t)}(\delta w_2)^{h_2^j(t)} \cdots (\delta w_6)^{h_6^j(t)}, \tag{7}$$

where $h_1^j(t) \cdots h_6^j(t)$ are the number of hits on the incremental weights $\delta w_1 \cdots \delta w_6$ during the course of simulation from time 1 to t. Note that δw_0 is irrelevant in equation (7). Generalization of this counting method to the case of finite E is trivial. Since the calculation of weights has been reduced to accumulating a histogram, the multi-spin coding technique [22] can be implemented not only for the spin update process but also for the calculation of the histogram of incremental weights. For system configuration updates, we follow the multi-spin coding technique similar to the case of the Kawasaki spin exchange model [23]. Once the histogram $h_1^j(t) \cdots h_6^j(t)$ is obtained, using equation (7) allows us to reweight to a large number of temperatures (drives) with negligible extra computational effort. A large increase in efficiency has been obtained by a new formulation of the nonequilibrium reweighting. The details of the multi-spin coding for the nonequilibrium reweighting will be given elsewhere.

For the dynamical finite-size scaling, we use the following equation,

$$\rho^k = b^{-\frac{k\beta}{\nu_\parallel}} \rho^{*(k)} \left(b^{-z}\tau, b^{\frac{1}{\nu_\parallel}}\epsilon, b^{-1}L_y, b^{-\frac{\nu_\perp}{\nu_\parallel}}L_x, b^{x_0}\rho_0 \right), \tag{8}$$

where k is the kth moment of the order parameter, $\rho^{*(k)}$ is the scaling function for the kth moment, b is the spatial rescaling factor, $\epsilon = (T - T_c)/T_c$, β is the critical exponent for the order parameter (it should not be confused with the inverse temperature), $\nu_\parallel$ and $\nu_\perp$ are the critical exponents for the correlation length parallel and orthogonal to the drive, respectively. z is the dynamical exponent and τ is Monte Carlo steps per site. In addition to the original scaling form of Saracco and Albano [14, 15], our scaling form has a term $b^{x_0}\rho_0$ to reflect the initial system configuration [18, 19]. x_0 is an independent exponent and $\rho_0 \ll 1$ is the order parameter of the initial configuration. This term was also suggested in a comment to Albano and Saracco's paper [15]. Simulations have to be started with a chosen value of ρ_0 for all samples. We prepare our initial configuration with $\rho_0 = 0$ by inserting $L_y/2$ particles for each column in the lattice and then shuffling each column independently. Letting $b = \tau^{1/z}$, we have

$$\rho^k = \tau^{-\frac{k\beta}{\nu_\parallel z}} \rho^{*(k)} \left(\tau^{\frac{1}{\nu_\parallel z}}\epsilon, \tau^{-\frac{1}{z}}L_y, \tau^{-\frac{\nu_\perp}{\nu_\parallel z}}L_x, \tau^{\frac{x_0}{z}}\rho_0 \right). \tag{9}$$

In the limit of $L_x \to \infty$ at the critical temperature ($\epsilon = 0$) with $\rho_0 = 0$, the ratio-of-moments reduces to a scaling function with a single argument,

$$\frac{\langle \rho^4 \rangle}{\langle \rho^2 \rangle^2} = g(\tau^{-1/z}L_y) \qquad \text{with} \quad \rho_0 = 0, \epsilon = 0, L_x \to \infty. \tag{10}$$

By plotting the ratio-of-moments versus τL_y^{-z} at T_c and $\rho_0 = 0$, neglecting corrections to scaling, the curves for different system sizes L_y will collapse into a single curve. A measure of goodness-of-fit can be defined for the 'curve-collapse' as

$$\eta = \frac{1}{x_{\max} - x_{\min}} \int_{x_{\min}}^{x_{\max}} \left| g_{L_{y1}}(x) - g_{L_{y2}}(x) \right| \mathrm{d}x, \tag{11}$$

where $g_{L_{y1}}(x) = g(\tau L_{y1}^{-z})$ and $g_{L_{y2}}(x) = g(\tau L_{y2}^{-z})$. Our task is to choose T_c and z which minimize η. In using relation (10), we should check that the system size L_x orthogonal to the drive is large enough. At this point, we should mention that other authors [26, 27] have studied the KLS model using finite-size scaling at nonequilibrium steady states. While we focus on dynamical behaviour, other finite-size scaling methods were developed for analysis at steady states.

We now show the results of the Monte Carlo simulation for the KLS model. We first illustrate the reweighting for the order parameter, and then show how reweighting can be combined with dynamical finite-size scaling (equation (10)) to calculate the critical temperature and dynamical exponent. Figure 1 shows how data over a range of temperatures can be extracted from simulations at a single temperature. The temporal evolution of the order parameter ρ for the infinite drive ($E = \infty$) was investigated for 64×32 lattice. Simulations were performed at $T = 3.160$, and data were reweighted to nearby temperatures, $T = 3.150, 3.155, 3.165, 3.170$ (from top to bottom). Averages were taken over 4.096×10^6 samples. We made independent calculations directly at $T = 3.150$, for example, to check the effectiveness of the reweighting. The deviation of the data between the reweighted ones from $T = 3.160$ and the direct ones at $T = 3.150$ is found to be the same within statistical errors.

We also made simulations for the finite drive ($E \approx 0.5$). We illustrate the reweighting over both E and T. We performed two simulations at $(T, E) = (2.765, 0.515)$ and $(2.780, 0.500)$ for 32×32 lattice. The combination of the order parameters is made by using $\bar{\rho} = \left(\sum_{k=1}^2 \rho_k / \Delta_k^2 \right) / \left(\sum_{k=1}^2 1 / \Delta_k^2 \right)$, where $\rho_{1,2}$ and $\Delta_{1,2}$ are the order parameter and error
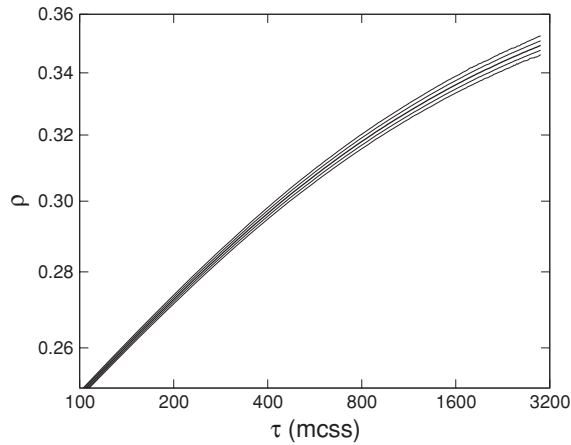
Figure 1. Plot of order parameter with infinite drive for 64×32 lattice with actual simulation performed at $T = 3.160$ shown with a bold line. From top to bottom values of T are 3.150, 3.155, 3.160, 3.165, 3.170. Averages were taken over 4.096×10^6 samples.
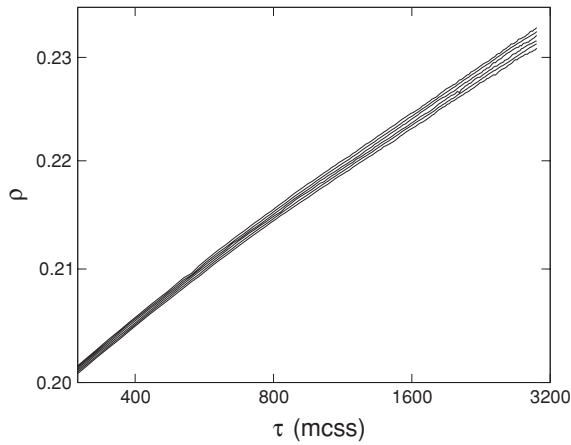

Figure 2. Plot of order parameter with finite drive for 32×32 lattice with actual simulation performed at $(T, E) = (2.765, 0.515)$ and $(T, E) = (2.780, 0.500)$. Reweighted data are combined using a weighted mean. From top to bottom values of T and E are $(T, E) = (2.760, 0.520)$, $(2.765, 0.515)$, $(2.770, 0.510)$, $(2.775, 0.505)$, $(2.780, 0.500)$, $(2.785, 0.495)$. Averages were taken over 2.048×10^6 samples for each simulation.

estimates from the first and second simulations, respectively. Figure 2 shows the temporal evolution of the order parameter for several temperatures and drives. Data were reweighted to several values at $(T, E) = (2.760, 0.520)$, $(2.770, 0.510)$, $(2.775, 0.505)$, $(2.785, 0.495)$. Averages were taken over 2.048×10^6 samples for each simulation. Generally, we found that reweighting is effective when the distributions $P_{\beta, E}(\vec{x}_t^j)$ and $P_{\beta', E'}(\vec{x}_t^j)$ have sufficient overlaps. Error bars and fluctuations of weights [13] can also be used as quantitative measures on the effective range of reweighting.

To determine T_c, we use the dynamical finite-size scaling of the ratio-of-moments (equation (10)). Here we concentrate on the infinite drive ($E = \infty$). We simulated 64×64 and 64×128 lattices, and calculated the ratio of the moments, $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$. Before going into the
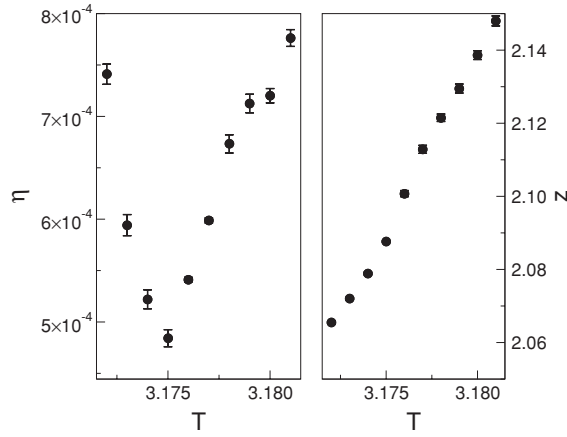
Figure 3. Plots showing the goodness-of-fit η and corresponding values of dynamical exponent z for various temperatures. Data are generated by fitting ratio-of-moments for $L_y = 64$ and $L_y = 128$ between the range $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2 = 1.2$ and 1.405. T_c is estimated from the temperature with the best fit ($T_c = 3.175 \pm 0.002$). Error bars were generated by fitting several ranges of ratio-of-moments.
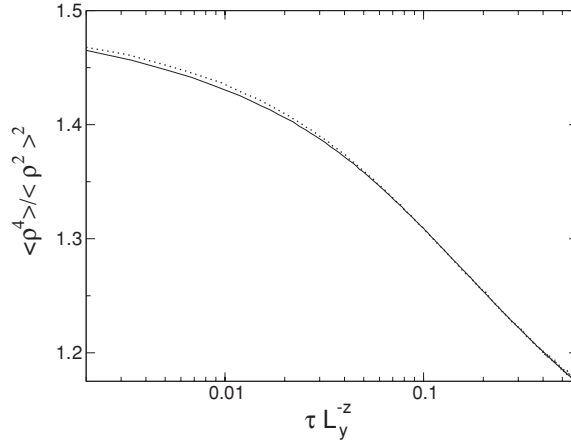

Figure 4. Scaling plot of $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$ versus τL_y^{-z} for $z = 2.09$, $L_y = 64$ (solid line) and $L_y = 128$ (dotted line) at $T = 3.175$. Initial system configurations were prepared with $\rho_0 = 0$.

discussion of the fitting, we make a comment on the system size L_x whether we can consider as $L_x \to \infty$. We performed simulations for both $L_x = 64$ and $L_x = 128$, and confirmed that the ratio of moments for $64 \times L_y$ and $128 \times L_y$ coincided with each other to within statistical fluctuations. Thus, we may regard that $L_x = 64$ is large enough. Since $\nu_\parallel > \nu_\perp$ for the KLS model, the correlation length orthogonal to the drive, $\xi_\perp$, develops slowly; hence, $L_x = 64$ is large enough to use the scaling relation (10). Now we show the fitting procedure. Fitting was performed for several temperatures near T_c, which were reweighted from the data obtained at a single temperature, and for each temperature we adjusted the value of z such that the goodness-of-fit η, equation (11), becomes minimum. Figure 3 shows η for several temperatures and the values of z used to calculate η. The best fit occurs at $T_c = 3.175 \pm 0.002$; the error bar on T_c is estimated by including all neighbouring temperatures where the mean values of η are within two standard deviations of η at $T = 3.175$. The value of z within

$T = 3.175 \pm 0.002$ is $z = 2.09 \pm 0.01$, and we use this value as our estimate of the dynamical exponent. Figure 4 shows the scaling plot of $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$ as a function of τL_y^{-z} for 64×64 (solid line) and 64×128 (dotted line) lattice sizes at $T = 3.175$ and $z = 2.09$. The curves are almost indistinguishable at this scale although some corrections to scaling can be observed below $\tau L_y^{-z} = 0.02$. To study the corrections to scaling, the goodness-of-fit for ratio-of-moments for smaller sizes, that is, 64×32 and 64×64 lattices, was also calculated using a similar procedure. The best fit occurs at $T = 3.155 \pm 0.005$ with $z = 2.23 \pm 0.03$. The estimate for T_c increases with the system size, whereas that for z decreases. Our estimates of T_c and z are compatible with the recent estimates for the infinite lattice, $T_c = 3.1980 \pm 0.0002$ [27], $T_c = 3.200 \pm 0.010$ [15], $z = 2.016 \pm 0.040$ [15]. A more systematic analysis of the corrections to scaling to get a precise estimate of T_c and several critical exponents for infinite lattice will be left to a separate publication. Before closing we show the actual procedure of the reweighting for each system size. For 64×32 lattice, 4.096×10^6 samples were used for the simulation at $T = 3.16$. For 64×64 lattice, 8.19×10^5 samples were used for each simulation at $T = 3.174$ and 3.180. Results were then reweighted to other temperatures and combined using a weighted mean, $\bar{r} = \left(\sum_{k=1}^2 r_k / \Delta_k^2 \right) / \left(\sum_{k=1}^2 1 / \Delta_k^2 \right)$. Here $r_{1,2}$ and $\Delta_{1,2}$ are the ratio-of-moments and error estimates from the first and second simulations, respectively. For 64×128 lattice size, 1.64×10^5 samples were used for each simulation at $T = 3.174, 3.177$ and 3.180, and reweighted results were combined using the same procedure.

To summarize, we have studied the use of nonequilibrium reweighting based on SIS for the nonequilibrium steady states. We have reformulated the nonequilibrium reweighting method, which is convenient for the multi-spin coding. As a result, a large increase in efficiency has been achieved for the performance of simulations. We have applied the nonequilibrium reweighting to the driven diffusive lattice gas model (the KLS model). Combining with the dynamical finite-size scaling theory, we have estimated T_c and the dynamical exponent z.

Finally, we make a remark on possible applications. The nonequilibrium reweighting method is very general and has some very interesting properties. For example, the fluctuation–dissipation theorem does not hold for nonequilibrium systems and derivatives of thermodynamic quantities had been estimated using finite differences [28]. With reweighting, derivatives can be calculated directly by differentiating the weights explicitly, that is,

$$\frac{\mathrm{d} \langle Q(t) \rangle_{\beta'}}{\mathrm{d} \beta'} = \frac{\sum_{j=1}^n Q(\vec{x}_t^j) \frac{\mathrm{d} w_t^j}{\mathrm{d} \beta'}}{\sum_{j=1}^n w_t^j} - \langle Q(t) \rangle_{\beta'} \frac{\sum_{j=1}^n \frac{\mathrm{d} w_t^j}{\mathrm{d} \beta'}}{\sum_{j=1}^n w_t^j}. \tag{12}$$

Here, $\mathrm{d} w_t^j / \mathrm{d} \beta'$ can be obtained by differentiating equation (7) with respect to β'. We believe that the nonequilibrium reweighting method will have applications in several directions.

Acknowledgments

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