Nonequilibrium Reweighting on the Driven Diffusive Lattice Gas

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The nonequilibrium reweighting technique, which was recently developed by the present authors, is used for the study of the nonequilibrium steady states. The renewed formulation of the nonequilibrium reweighting enables us to use the very efficient multi-spin coding. We apply the nonequilibrium reweighting 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 epidemic [1], vehicular traffic [2], biological network [3], and catalysis [4], have captured 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, 8, 9], have been developed. However, many advanced Monte Carlo methods are not applicable to nonequilibrium systems. Efficient Monte Carlo algorithms for nonequilibrium simulation are highly demanded.

Quite recently, the present authors [11] have developed a reweighting method for nonequilibrium systems based on the 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 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 behavior of nonequilibrium phase transitions can be extracted from short time dynamics [17, 18, 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 paper, we apply the nonequilibrium reweighting method [11] to the study of the 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 with 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 behavior. 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

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

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 neighbor site are given by the Metropolis rate [24],

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

where $\sigma$ and $\sigma'$ 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 $e^4$, and moments of the order parameters are given by

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

(3)

where $n_{ij} = 0$ or 1 as defined in Eq. $\textbf{1}$, 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 of the KLS model. Define a path $x_t$, a sequence of points in phase space $\sigma_i$ which were visited during the course of simulation, as

$$
x_t = (\sigma_1, \sigma_2, \cdots, \sigma_t).
$$

(4)

This path can be sampled using the Monte Carlo method at an inverse temperature $\beta$ 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 $\beta'$ and another drive $E'$,

$$
\langle Q(t) \rangle_{\beta', E'} = \frac{\sum_{j=1}^n w_j^t Q(x_t^j)}{\sum_{j=1}^n w_j^t},
$$

(5)

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

1. Suppose $x_t^j = (\sigma_1^j, \cdots, \sigma_t^j)$ up to time $t$ is sampled from a simulation at the inverse temperature $\beta$ and drive $E$.

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

3. An incremental weight $\delta w^j$ has different values according to two possible outcomes,

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

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

The weights at $t + 1$ is given by this incremental weight through the relation $w_{t+1}^j = \delta w^j \times w_t^j$ with $w_0^j = 1$.

For each path $j \in \{1, \cdots, n\}$, 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 case of infinite drive ($E = \infty$), possible values of incremental weights $\delta w_i$ are,

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

(6)

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

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

(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 $\delta w_0$ is irrelevant in Eq. $\textbf{7}$. 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 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 Eq. $\textbf{7}$ allows us to reweight to a large number of temperatures (drives) with negligible extra computational efforts. A large increase of 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,

$$
\rho^k = b^{\frac{k}{\nu_\perp}} \rho^{\epsilon(k)}(b^{-ze_\perp}, b^{-ve_x}, b^{-1} L_y, b^{-v_y} L_x, b^{-c_0} \rho_0),
$$

(8)

where $k$ is the $k$th moment of the order parameter, $\rho^{\epsilon(k)}$ is the scaling function for the $k$th moment, $b$ is the spatial rescaling factor, $\epsilon = (T - T_c)/T_c$, $\beta$ 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 $\tau$ is Monte Carlo steps per site. In addition to the original scaling form of Saracco and Albano [14] [15] [16], our scaling form has a term $b^{c_0} \rho_0$ to reflect the initial system configuration [15] [16]. $x_0$ is an independent exponent and $\rho_0 \ll 1$ is the order parameter of the initial configuration. Simulations have to be started with a chosen value of $\rho_0$ 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 $b = \tau^{1/2}$, we have

$$
\rho^k = \tau^{-\frac{k}{\nu_\parallel}} \rho^{\epsilon(k)}(\tau^{-\frac{e_\perp}{v_x}} L_y, \tau^{-\frac{e_\perp}{v_y}} L_x, \tau^{\frac{c_0}{c_0}} \rho_0).
$$

(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,

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

By plotting the ratio-of-moments versus $\tau L_y^{-z}$ 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

$$\eta = \frac{1}{x_{\text{max}} - x_{\text{min}}} \int_{x_{\text{min}}}^{x_{\text{max}}} \left| g_{L_y}(x) - g_{L_y}(x) \right| dx, \quad (11)$$

where $g_{L_y}(x) = g(\tau L_y^{-z})$ and $g_{L_y}(x) = g(\tau L_y^{-z})$. Our task is to choose $T_c$ and $z$ which minimize $\eta$. In using the relation Eq. (11), we should check that the system size $L_x$ orthogonal to the drive is large enough. At this point, we should mention that Leung [26] has studied the KLS model using finite size scaling at nonequilibrium steady states. While we focus on dynamical behaviors, his finite size scaling method was 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 (Eq. (11)) 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 $\rho$ for the infinite drive ($E = \infty$) was investigated for $64 \times 32$ 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 $4.096 \times 10^6$ 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 and the direct ones at $T = 3.150$ are 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 $32 \times 32$ lattice. The reweighting of the order parameter is made by using

$$\bar{\rho} = \frac{\sum k \rho_k / \Delta^2_k}{\sum k \Delta^2_k},$$

where $\rho_{1,2}$ and $\Delta_{1,2}$ are the order parameter and error estimates from the first and second simulations, respectively. Figure 3 shows the temporal evolution of the order parameter for several temperatures and drives. Data was 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 $2.048 \times 10^6$ samples for each simulation. Generally, we found that reweighting is effective when the distributions $P_{\beta, E}(\vec{x}_j^t)$ and $P_{\beta', E}(\vec{x}_j^t)$ have sufficient overlaps. Error bars and fluctuations of weights 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 (Eq. (10)). Here we concentrate on the infinite drive ($E = \infty$). We simulated $64 \times 64$ and $64 \times 128$ lattices, and calculated the ratio of the moments, $\langle \rho^4 \rangle / \langle \rho^2 \rangle^2$. Before going into the 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 $\nu_1 > \nu_\perp$ 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 Eq. (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 $\eta$, Eq. (11), becomes minimum. Figure 4 shows $\eta$ for several temperatures and the values of $z$ used to calculate $\eta$. The best fit occurs at $T_c = 3.175 \pm 0.002$; the error bar on $T_c$ is estimated by including all neighboring temperatures where the mean values of $\eta$ are within two standard deviations of $\eta$ 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 $\tau L_y^{-z}$ for $64 \times 64$ (solid line) and $64 \times 128$ (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, $64 \times 32$ and $64 \times 64$ 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 infinite lattice, $T_c = 3.1980 \pm 0.0002$ [27], $T_c = 3.200 \pm 0.010$ [15], $z = 2.016 \pm 0.040$ [12]. 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 $64 \times 32$ lattice, $4.096 \times 10^6$ samples were used for the simulation at $T = 3.16$. For $64 \times 64$ lattice, $8.19 \times 10^5$ samples were used for each simulation at $T = 3.174$ and $3.180$. Results were then reweighted to other temperatures and combined using weighted mean, $\bar{\tau} = (\sum k \tau_k / \Delta^2_k)/(\sum k \Delta^2_k)$. Here $\tau_{1,2}$ and $\Delta_{1,2}$ are the ratio-of-moments and error estimates from the first and second simulations, respectively. For $64 \times 128$ lattice size, $1.64 \times 10^5$ 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 of 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 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,

$$\frac{d\langle Q(t) \rangle_{\beta'}}{d\beta'} = \frac{\sum_{j=1}^n (\langle \vec{x}_j^t \rangle_{\beta'}) \frac{d\vec{x}_j^t}{d\beta'}}{\sum_{j=1}^n w_t^j} - \langle Q(t) \rangle_{\beta'} \frac{\sum_{j=1}^n d\vec{x}_j^t}{\sum_{j=1}^n w_t^j}. \quad (12)$$
Here, $dw'_1/d\beta'$ can be obtained by differentiating Eq. (7) with respect to $\beta'$. We believe that the nonequilibrium reweighting method would have several directions for applications.

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