Rejection-free cluster Wang-Landau algorithm for Hard Core Lattice Gases

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A. A. A. Jaleel, J. E. Thomas, D. Mandal, Sumedha, R. Rajesh, Phys. Rev. E 104, 045310

Hard-Core Lattice Gases

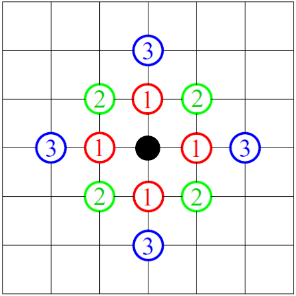


TABLE I. Number density at full packing, $\eta_{\max}$, and the phase at full packing for the different models studied in the paper. d denotes the dimension.

Model	$\eta_{\max}$	Phase at full packing
1-NN($2d$)	1/2	Sublattice
2-NN($2d$)	1/4	Columnar
3-NN($2d$)	1/5	Sublattice
1-NN($3d$)	1/2	Sublattice
2-NN($3d$)	1/4	Sublattice
3-NN($3d$)	1/8	Columnar

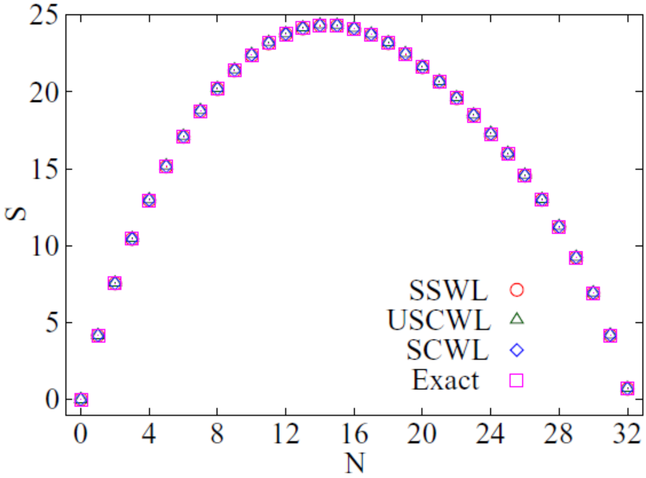
Algorithms

- **Single-Site Wang-Landau Algorithm (SSWL)** - This is based on single site updating. The new configuration is chosen over the older configuration by weight of min $\left[1, \frac{g(N_{old})}{g(N_{new})}\right]$.
- **Unbiased Strip Cluster Wang-Landau Algorithm (USCWL)** - Here we have cluster moves but the new configurations are not weighted by inverse of the density of states. Here also, the new configuration is chosen over the older configuration by weight of min $\left[1, \frac{g(N_{old})}{g(N_{new})}\right]$.
- **Strip Cluster Wang-Landau Algorithm (SCWL)** - We use this algorithm and we have cluster moves and also the new configurations are weighted by inverse of their density of states. Here we don't discard the new configuration by any weight. Hence, rejection free.

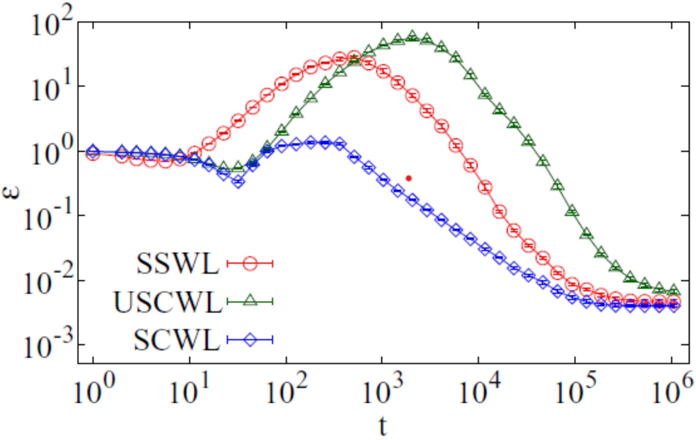
Wang-Landau Protocol

- A configuration of N particles is weighted inversely proportional to $g(N)$, the number of configurations with N particles., $g(N)$ changes continuously during the simulations and is expected to converge to its true value with increasing time.
- We adopt a flat histogram technique where a histogram and entropy is maintained and added by one and given paramter f respectively on the N^{th} bin, where N is the number of particles that are occupied in the configuration that is reached.
- Due to sampling by the inverse of density of states, the histogram will reach a flatness criterion to complete an iteration. We modify $f \to f/2$ and reset the histogram for the next iteration. We repeat the iteration till f becomes less than a set value.

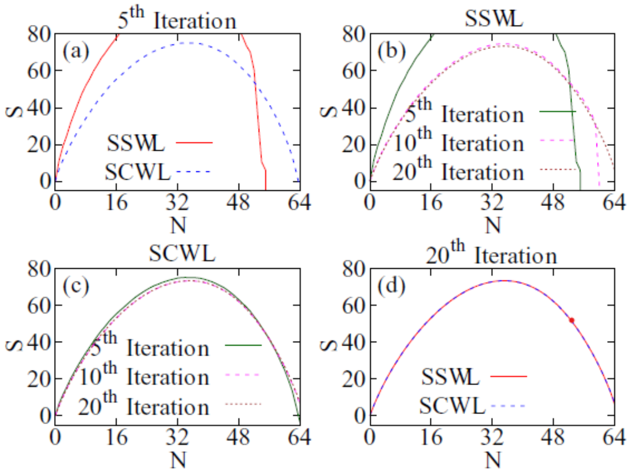
Entropy for 1-NN model.



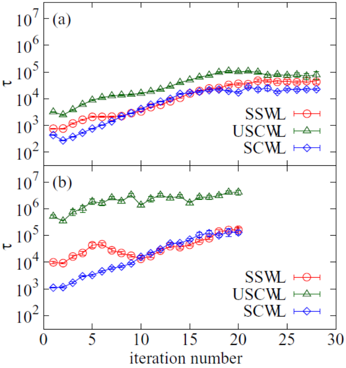
Error for 1-NN model $\left(\frac{1}{N^{max}-1} \sum_{N=1}^{N^{max}} \left| 1 - \frac{S(N)}{S_{ex}(N)} \right| \right)$.



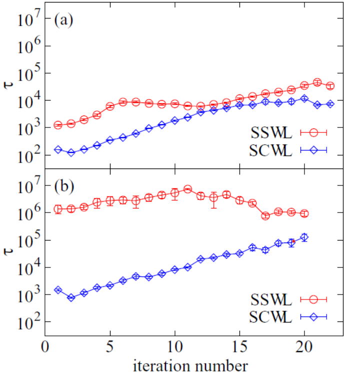
Entropy for 2-NN model with iteration.



Exit times



(a)
(b)
SSWL
USCWL
SCWL
τ
iteration number



(a)
(b)
SSWL
SCWL
τ
iteration number

Applications

Knowing the density of states, we can calculate the average of any observable $O_{k,d}$:

$$\langle O_{k,d} \rangle = \frac{\sum_{N=0}^{N^{max}} O(N) e^{\mu N} g(N)}{\sum_{N=0}^{N^{max}} e^{\mu N} g(N)}$$

We can calculate the compressibility, susceptibility, and pressure defined as

$$\kappa_{k,d} = L^d \left(\langle \rho_{k,d}^2 \rangle - \langle \rho_{k,d} \rangle^2 \right)$$

$$\chi_{k,d} = L^d \left(\langle q_{k,d}^2 \rangle - \langle q_{k,d} \rangle^2 \right)$$

$$P_{k,d}(\mu) = L^{-d} \ln \sum_{n=0}^{N^{max}} e^{\mu N} g(N)$$

and the pressure from the canonical ensemble, $\tilde{P}_{k,d}$:

$$\tilde{P}_{k,d} = \int_0^{\rho} [1-\phi(\rho)] \frac{\partial}{\partial \rho} \left[\frac{\rho}{1-\phi(\rho)} \right] d\rho$$

Near a continuous transition, the finite size scaling of different quantities

$$\kappa_{k,d} \approx L^{\alpha/\nu} f_\kappa((\mu-\mu_c)L^{1/\nu})$$
$$\langle q_{k,d} \rangle \approx L^{-\beta/\nu} f_q((\mu-\mu_c)L^{1/\nu})$$
$$\chi_{k,d} \approx L^{\gamma/\nu} f_\chi((\mu-\mu_c)L^{1/\nu})$$

For numerical analysis, it is useful to define an assosciated quantity, which we will denote by t:

$$t_{k,d} = \frac{\partial \ln \langle q_{k,d} \rangle}{\partial \mu}$$

, and near the transition we have

$$t_{k,d} \approx L^{1/\nu} f_t((\mu-\mu_c)L^{1/\nu})$$

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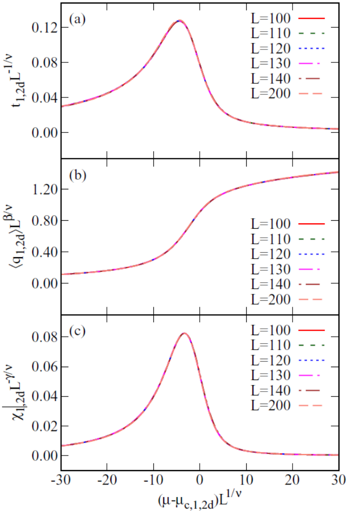
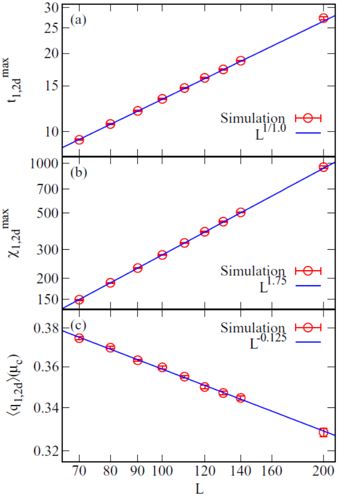
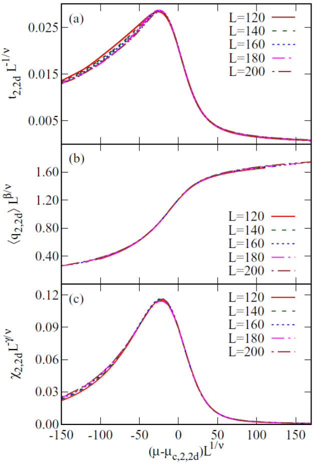
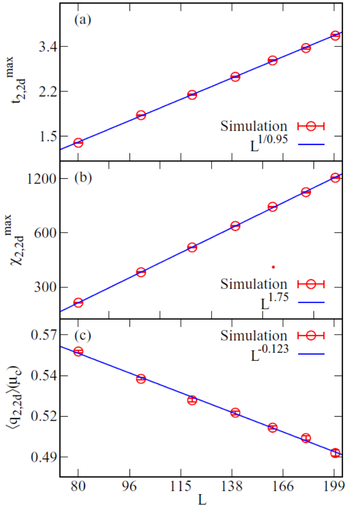
Results (1-NN Model)



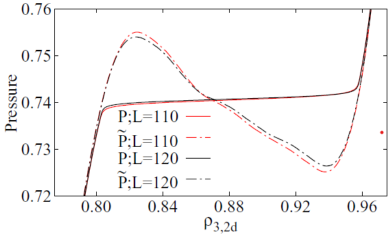


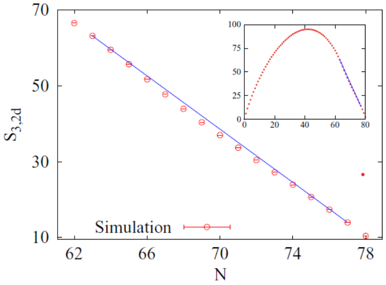
Results (2-NN Model)



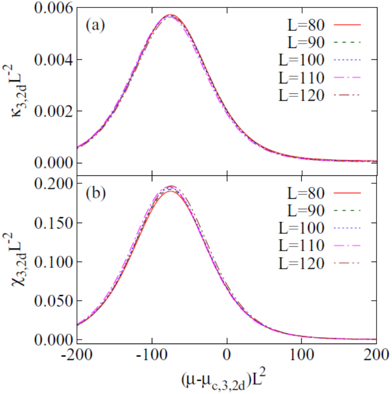


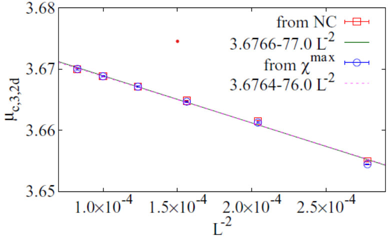
Results (3-NN Model)





Results (3-NN Model)





Thank you