

tionary time series X_1, X_2, \dots, X_T we can define its discrete Fourier transform to be

$$\hat{X}(\omega) := \frac{1}{\sqrt{T}} \sum_{t=1}^T X_t e^{i\omega t} \quad (7)$$

with $\omega = 2\pi m/T$ and $m = 0, 1, \dots, T-1$. It is then straightforward to show [14] that for large T we have

$$\langle |\hat{X}(\omega)|^2 \rangle = f_X(\omega) + O\left(\frac{1}{T}\right). \quad (8)$$

2.1. Autocorrelation times

We now discuss the implications of the general form (1) on two key time scales, the *integrated* autocorrelation time and the *exponential* autocorrelation time.

2.1.1. Integrated Autocorrelation time

From $\rho_X(t)$ the integrated autocorrelation time is defined [15] as

$$\tau_{\text{int},X} := \frac{1}{2} \sum_{t=-\infty}^{\infty} \rho_X(t). \quad (9)$$

If \bar{X} denotes the sample mean of X_1, X_2, \dots, X_T then the variance of \bar{X} satisfies [15]

$$\text{var}(\bar{X}) \sim 2 \tau_{\text{int},X} \frac{\text{var}(X)}{T}, \quad T \rightarrow \infty. \quad (10)$$

It is (10) that accounts for the key role played by the integrated autocorrelation time in the statistical analysis of Markov-chain Monte Carlo time series. If instead of a correlated time series, one considers a sequence of independent random variables, then the variance of the sample mean is simply $\text{var}(X)/T$. It is in this sense that $\tau_{\text{int},X}$ determines how many time steps we need to wait between two “effectively independent” samples.

It can now be seen immediately from (9) that, as noted in the introduction, (1) and (3) imply

$$2\tau_{\text{int},n} = \sum_{t=-\lfloor \tau \rfloor}^{\lfloor \tau \rfloor} \left(1 - \frac{|t|}{\tau}\right), \quad (11)$$

$$= \tau + O(\tau^{-1}) \quad (12)$$

$$= \frac{L}{|v_c|} + O(L^{-1}). \quad (13)$$

Equation (13) provides a very simple exact expression for $\tau_{\text{int},n}$ in terms of the physical parameters of the model. It is quite rare to have such an expression for a non-trivial model.

2.1.2. Exponential Autocorrelation time

Typically, we expect that $\rho_X(t) \sim \exp(-t/\tau_{\text{exp}})$ as $t \rightarrow \infty$, which defines the exponential autocorrelation time τ_{exp} . More precisely [15], one defines the exponential autocorrelation time of observable X to be

$$\tau_{\text{exp},X} := \limsup_{|t| \rightarrow \infty} \frac{-|t|}{\log \rho_X(t)}, \quad (14)$$

and then the exponential autocorrelation time of the system as

$$\tau_{\text{exp}} := \sup_X \tau_{\text{exp},X}, \quad (15)$$

where the supremum is taken over all observables X . The autocorrelation time τ_{exp} measures the decay rate of the slowest mode of the system, and it therefore sets the scale for the number of initial time steps to discard from a simulation, in order to avoid bias from initial non-stationarity. All observables that are not orthogonal to this slowest mode satisfy $\tau_{\text{exp},X} = \tau_{\text{exp}}$.

For the TASEP in continuous time, τ_{exp} was computed analytically in [16, 17] using the exact Bethe Ansatz solution. In particular, it was found that τ_{exp} is $O(1)$ with respect to L in the high and low density phases. We would expect the same behavior to hold generally for the NaSch model.

However, if $\rho_n(t)$ were to have strictly finite support as claimed in (1), then we would have $-|t|/\log \rho_n(t) = 0$ for all $|t| > \tau$, implying that $\tau_{\text{exp},n} \neq \tau_{\text{exp}}$. This would then mean that n is orthogonal to the slowest relaxation mode, which seems implausible. We thus conclude that although (1) provides a very good approximation, $\rho_n(t)$ cannot actually have a strictly finite support.

2.2. Finite-size scaling of $\rho_n(t)$

To obtain a more precise ansatz for $\rho_n(t)$ we therefore fix some $k \in \mathbb{N}$ satisfying $k \leq \lfloor \tau \rfloor$ and set

$$\rho_n(t) = \begin{cases} 1 - |t|/\tau, & |t| \leq k, \\ B e^{-|t|/\tau_{\text{exp}}}, & |t| \geq k+1. \end{cases} \quad (16)$$

Since we know empirically that (1) is a very good approximation, it must be the case that $k/\tau \sim 1$ as $\tau \rightarrow \infty$. Let us then write $\tau = k + \varepsilon$, where the only assumption we make regarding ε is that $\varepsilon/\tau \rightarrow 0$ as $\tau \rightarrow \infty$. Since the continuum limit of $\rho(x\tau)$ should define a continuous function of $x \in \mathbb{R}$ we choose the parameter B by demanding that $1 - |t|/\tau = B e^{-|t|/\tau_{\text{exp}}}$ when $|t| = k$, which yields

$$\rho_n(t) = \begin{cases} 1 - |t|/\tau, & |t| \leq k, \\ \varepsilon e^{-(|t|-k)/\tau_{\text{exp}}/\tau}, & |t| \geq k. \end{cases} \quad (17)$$