1 Worm algorithm for the XY model

The original introduction to the worm algorithm for classical statistical models was given by Prokof'ev and Svistunov in 2001 [1]. However, they do not deeply discuss the XY model but instead the $|\psi|^4$ model, which can recover the XY model in a particular limit. In that sense their discussion is more general; nevertheless here we explain the worm algorithm for the XY model without making it too complicate.

The XY model without magnetic field is defined by the Hamiltonian

$$H = -\sum_{\langle ij\rangle} \vec{s}_i \cdot \vec{s}_j = -\sum_{\langle ij\rangle} \cos(\theta_i - \theta_j), \tag{1}$$

where $\langle ij\rangle$ denotes a sum between the nearest neighbours. The partition function is

$$\begin{aligned} Z &= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \exp\left[\beta \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j)\right] \\ &= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \prod_{\langle ij\rangle} \exp\left[\beta \cos(\theta_i - \theta_j)\right], \end{aligned} \tag{2}$$

where $\beta = 1/T$. If we use the following identity for the exponential

$$\sum_{\nu=-\infty}^{\infty} I_\nu(\beta) \exp(i\nu\theta) = \exp(\beta \cos(\theta)), \tag{3}$$

we rewrite the partition function as

$$Z = \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \prod_{\langle ij\rangle} \left(\sum_{J_{ij}=-\infty}^{\infty} I_{J_{ij}}(\beta) \exp\left[iJ_{ij}(\theta_i - \theta_j)\right] \right) \tag{4}$$

We can express this partition function in a more convenient form if we integrate over the angles. We will explain the idea for the simple case of a 1-dimensional lattice with N sites and periodic boundary, but the final result will be valid for general dimension and can be easily proved. Thus

$$\begin{aligned} Z = &\int_0^{2\pi} \prod_{i=1}^{N} \frac{d\theta_i}{2\pi} \sum_{J_{12}=-\infty}^{\infty} \sum_{J_{23}=-\infty}^{\infty} \cdots \sum_{J_{N1}=-\infty}^{\infty} I_{J_{12}}(\beta) \exp\left[iJ_{12}(\theta_1 - \theta_2)\right] I_{J_{23}}(\beta) \exp\left[iJ_{23}(\theta_2 - \theta_3)\right] \times \\ &\cdots \times I_{J_{N1}}(\beta) \exp\left[iJ_{N1}(\theta_N - \theta_1)\right] \\ = &\sum_{\{J_{ij}\}} I_{J_{12}}(\beta) I_{J_{23}}(\beta) \cdots I_{J_{N1}}(\beta) \int_0^{2\pi} \frac{d\theta_1 d\theta_2 \dots d\theta_N}{(2\pi)^N} \exp\left[i\theta_1 \left(J_{12} - J_{N1}\right)\right] \exp\left[i\theta_2 \left(J_{23} - J_{12}\right)\right] \times \\ &\cdots \times \exp\left[i\theta_N \left(J_{N1} - J_{(N-1)N}\right)\right], \end{aligned} \tag{5}$$

where we define $\sum_{\{J_{ij}\}} \equiv \sum_{J_{12}=-\infty}^{\infty} \sum_{J_{23}=-\infty}^{\infty} \cdots \sum_{J_{N1}=-\infty}^{\infty}$. We can represent the configurations that contribute to the partition function graphically if we interprete J_{ij} as the flux that goes from site i to j[1]. With this in mind, then $J_{ij} = -J_{ji}$ and

$$\begin{aligned}
Z &= \sum_{\{J_{ij}\}} I_{J_{12}}(\beta) I_{J_{23}}(\beta) \cdots I_{J_{N1}}(\beta) \int_0^{2\pi} \frac{d\theta_1 d\theta_2 \dots d\theta_N}{(2\pi)^N} \exp\left[i\theta_1 \left(J_{12} + J_{1N}\right)\right] \exp\left[i\theta_2 \left(J_{23} + J_{21}\right)\right] \times \\
&\cdots \times \exp\left[-i\theta_N \left(J_{N(N-1)} + J_{N1}\right)\right] \\
&= \sum_{\{J_{ij}\}} I_{J_{12}}(\beta) I_{J_{23}}(\beta) \cdots I_{J_{N1}}(\beta) \int_0^{2\pi} \frac{d\theta_1 d\theta_2 \dots d\theta_N}{(2\pi)^N} \exp\left[i\theta_1 \nabla \cdot \mathbf{J}_1\right] \exp\left[i\theta_2 \nabla \cdot \mathbf{J}_2\right] \cdots \exp\left[i\theta_N \nabla \cdot \mathbf{J}_N\right],
\end{aligned} \tag{6}$$

where $\nabla \cdot \mathbf{J}_i \equiv \sum_j J_{ij}$ is the total flux at the site i. Integrating over the angles we see that only when $\nabla \cdot \mathbf{J}_i = 0$, $\forall i = 1, \dots, N$ the configuration contributes to the partition function. Therefore

$$Z = \sum_{\{J_{CP}\}} I_{J_{12}}(\beta) I_{J_{23}}(\beta) \cdots I_{J_{N1}}(\beta). \tag{7}$$

$$\boxed{Z = \sum_{\{J_{CP}\}} \prod_{\langle ij \rangle} I_{J_{ij}}(\beta),} \tag{8}$$

where $\{J_{CP}\}$ stands for "closed path" configuration, which means that the configuration satisfies the condition $\nabla \cdot \mathbf{J}_i = 0$, $\forall i = 1, \dots, N$. As mentioned earlier, eq. (8) is valid for any dimension, the proof is just a generalization of what we have done here. It is usual to refer to eq. (8) as the *flow representation* of Z. The graphical depiction of the configurations that contribute to the partition function is of those ones that at each site the number of bond lines that enter and exit adds up to zero, see for instance fig. 1.

The worm algorithm samples a larger space than the one corresponding to Z. This space is defined by the configurations that contribute to the correlation function

$$G = \int_0^{2\pi} \frac{d\theta_I d\theta_M}{(2\pi)^2} \int_0^{2\pi} \prod_{i \neq I,M} \frac{d\theta_i}{2\pi} \vec{s}_I \cdot \vec{s}_M \prod_{\langle ij \rangle} \exp\left[\beta \cos(\theta_i - \theta_j)\right] \tag{9}$$

$$= \int_0^{2\pi} \frac{d\theta_I d\theta_M}{(2\pi)^2} \int_0^{2\pi} \prod_{i \neq I,M} \frac{d\theta_i}{2\pi} \cos(\theta_I - \theta_M) \prod_{\langle ij \rangle} \exp\left[\beta \cos(\theta_i - \theta_j)\right]. \tag{10}$$

By doing similar steps as with the partition function, it is seen that the correlation function takes the form

$$\boxed{G = \sum_{\{J_{OP}\}} \prod_{\langle ij \rangle} I_{J_{ij}}(\beta),} \tag{11}$$

where $\{J_{OP}\}$ stands for "opened path", which means that the configurations satisfy the condition $\nabla \cdot \mathbf{J}_i = 0$, $\forall i \neq I, M$ and $\nabla \cdot \mathbf{J}_{I,M} = \pm 1$. A graphical example of this kind of configurations is shown in fig. 2.

[1] We can think of J_{ij} as the number of lines that enter and leave the site i in the direction of j. An exiting line adds +1 to the flux, while an entering lines adds -1 (this is just convention).

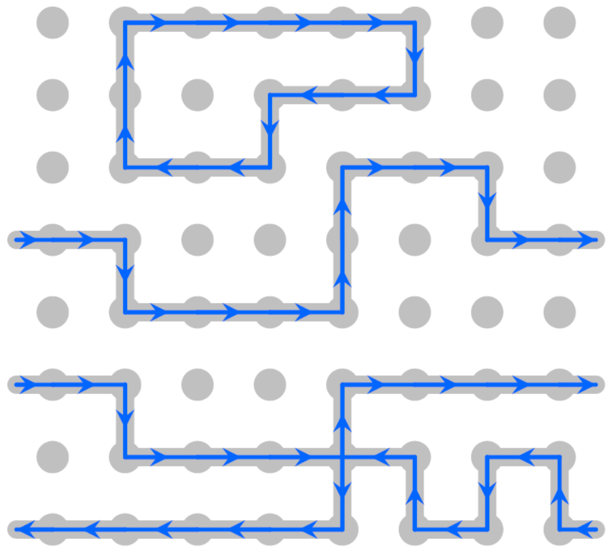

Figure 1: Typical configuration of the partition function. The flux at each site adds up to zero. The figure was taken from ref. [2], where they also comment some ideas of the worm algorithm in the XY model.

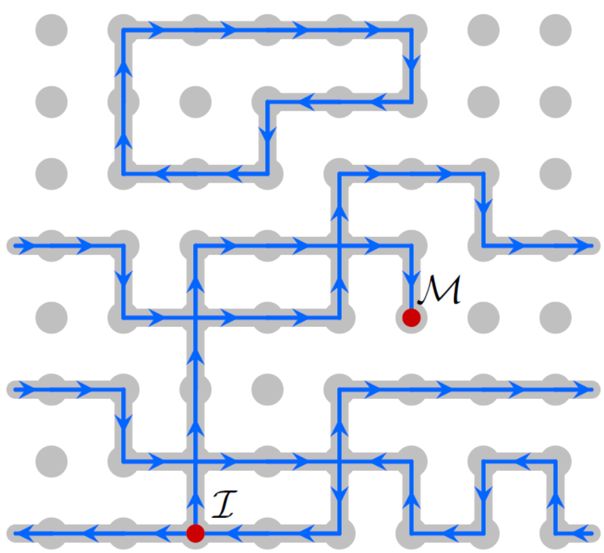

Figure 2: Typical configuration of the correlation function. The flux at each site adds up to zero, except at the sites I and M. The figure was taken from ref. [2].

The idea of the worm algorithm for this model is to sample the $G-$space in such a way that when $I = M$ we recover the $Z-$space. This can be achieved by following these steps:

1. We begin with $I = M$ at some random site on the lattice.
2. We choose one of the neighbors of M, say N, and propose an update of the flux from J_{MN} to $J'_{MN} = J_{MN} + 1$ (note that this also modifies the flux at N).
3. We accept such an update with probability
$$p = \min\left(1, \frac{I_{J'_{MN}}(\beta)}{I_{J_{MN}}(\beta)}\right). \tag{12}$$
If the update is accepted, we move M to N, otherwise we repeat the previous step.
4. We continue repeating steps 2 and 3 until $I = M$. When this happens we choose a random site on the lattice, set $I = M$ there and repeat steps 2 and 3.

After performing these steps several times one can proceed to measure observables. For instance, as it is mentioned in various references [2, 3, 4], the magnetic susceptibility is obtained by measuring the average number of steps that the algorithm takes to go from the G-space to the Z-space. Other usual observables are more tricky to measure. For instance, in order to measure the energy with this algorithm, one has to consider the partition function in the flow representation and find an expression for
$$\langle E\rangle = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} \tag{13}$$
in terms of known quantities with this algorithm, such as the flux variables J_{ij}. To do so we will consider again the simple 1-dimensional case with N sites, one more time everything generalizes easily to d dimensions. Then
$$Z = \sum_{\{J_{CP}\}} I_{J_{12}}(\beta)I_{J_{23}}(\beta)\cdots I_{J_{N1}}(\beta). \tag{14}$$

Computing the derivative we obtain
$$\begin{aligned}\frac{\partial Z}{\partial \beta} &= \sum_{\{J_{CP}\}}\Big(I'_{J_{12}}(\beta)I_{J_{23}}(\beta)\cdots I_{J_{N1}}(\beta) + I_{J_{12}}(\beta)I'_{J_{23}}(\beta)\cdots I_{J_{N1}}(\beta) + \cdots \\ &\quad + I_{J_{12}}(\beta)I_{J_{23}}(\beta)\cdots I'_{J_{N1}}(\beta)\Big) \\ &= \sum_{\{J_{CP}\}}\left(\frac{I'_{J_{12}}(\beta)}{I_{J_{12}}(\beta)} + \frac{I'_{J_{23}}(\beta)}{I_{J_{23}}(\beta)} + \cdots + \frac{I'_{J_{N1}}(\beta)}{I_{J_{N1}}(\beta)}\right) I_{J_{12}}(\beta)I_{J_{23}}(\beta)\cdots I_{J_{N1}}(\beta). \end{aligned} \tag{15}$$

Therefore
$$\boxed{\langle E\rangle = -\left\langle \sum_{\langle ij\rangle} \frac{I'_{J_{ij}}(\beta)}{I_{J_{ij}}(\beta)}\right\rangle,} \tag{16}$$

where the sum runs over nearest neighbors. Equation (16) is valid for general dimension d. One is often interested in determining the specific heat C_V. This is either obtained by numerically differentiating the simulation's outcome of eq. (16) or by computing $\langle E^2 \rangle$ so that one can substitute in the formula

$$C_V = \frac{\partial \langle E \rangle}{\partial \beta} = \beta^2 (\langle E^2 \rangle - \langle E \rangle^2). \tag{17}$$

We will explain how to obtain $\langle E^2 \rangle$ in a similar manner as with $\langle E \rangle$. We start from the usual expression in statistical mechanics

$$Z = \frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} \tag{18}$$

and use equation (15), thus

$$\langle E^2 \rangle = \left\langle \frac{I''_{J_{12}}(\beta)}{I_{J_{12}}(\beta)} + \cdots + \frac{I''_{J_{N1}}(\beta)}{I_{J_{N1}}(\beta)} - \left(\frac{I'_{J_{12}}(\beta)}{I_{J_{12}}(\beta)} \right)^2 - \cdots - \left(\frac{I'_{J_{N1}}(\beta)}{I_{J_{N1}}(\beta)} \right)^2 + \left(\frac{I'_{J_{12}}(\beta)}{I_{J_{12}}(\beta)} + \cdots + \frac{I'_{J_{N1}}(\beta)}{I_{J_{N1}}(\beta)} \right)^2 \right\rangle. \tag{19}$$

Therefore, for general d, we have

$$\boxed{\langle E^2 \rangle = \left\langle \sum_{\langle ij \rangle} \frac{I''_{J_{ij}}(\beta)}{I_{J_{ij}}(\beta)} \right\rangle - \left\langle \sum_{\langle ij \rangle} \left(\frac{I'_{J_{ij}}(\beta)}{I_{J_{ij}}(\beta)} \right)^2 \right\rangle + \left\langle \left(\sum_{\langle ij \rangle} \frac{I'_{J_{ij}}(\beta)}{I_{J_{ij}}(\beta)} \right)^2 \right\rangle. \qquad (20)}$$

This way one can compute C_V with the worm algorithm.

2 Results

In this section we show some low statistics results that were obtained with a simple python implementation of the worm algorithm for the $2d$ XY model. The code can be revised in [5]. All the results correspond to 1 000 measurements with 100 000 thermalization sweeps and 10 decorrelation steps.

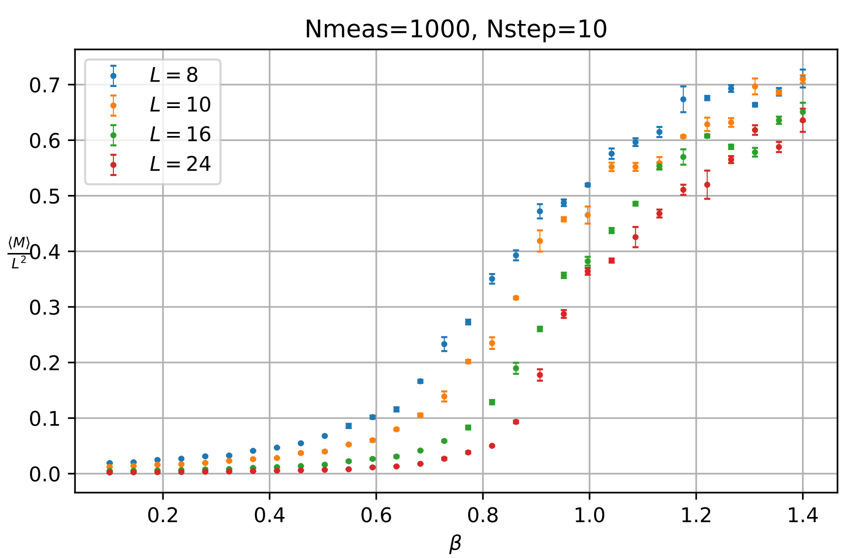

Figure 3: Magnetization density of the $2d$ XY model measured with the worm algorithm for several lattices.

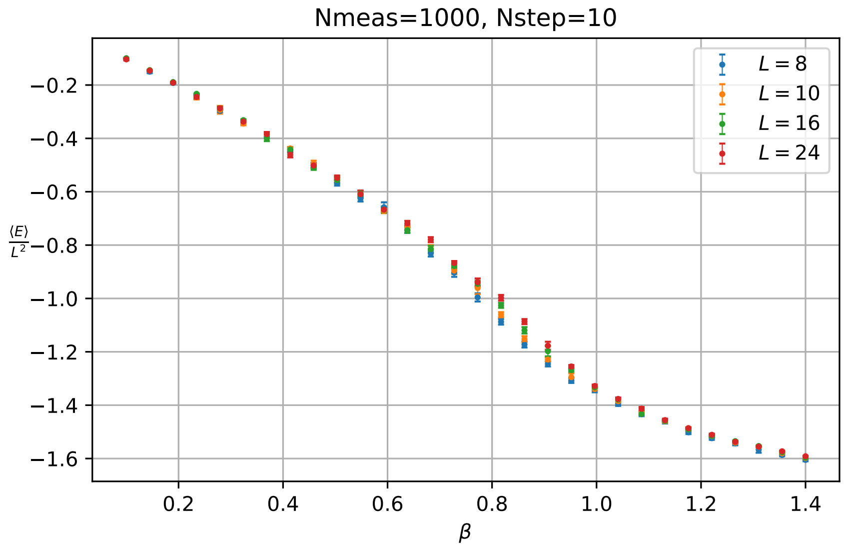

Figure 4: Energy density of the $2d$ XY model measured with the worm algorithm for several lattices.

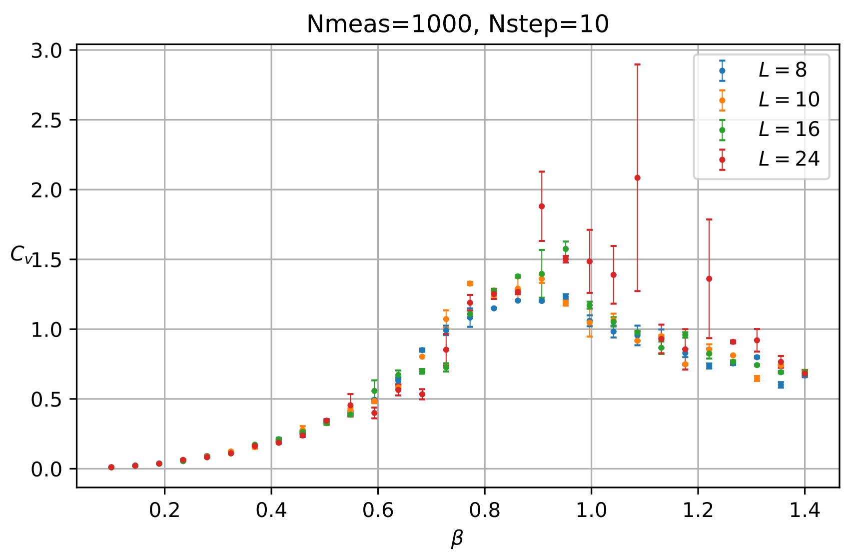

Figure 5: Specific heat of the $2d$ XY model measured with the worm algorithm for several lattices.

References

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[5] https://github.com/Fabian2598/O-2-Model