Fact sheet: Wegner's model for finite systems

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December 1, 2019

1 Wegner's harmonic model - overview

We consider the harmonic model solved by Wegner[3],

$$H = -2Nd + \frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} I(\mathbf{r}-\mathbf{r}')(\phi_{\mathbf{r}} - \phi_{\mathbf{r}'})^2, \tag{1}$$

a low-temperature approximation for the XY model on a d-dimensional lattice of N sites, with the hamiltonian

$$H^{XY} = -\sum_{\mathbf{r},\mathbf{r}'} I(\mathbf{r}-\mathbf{r}')\cos(\phi_{\mathbf{r}} - \phi_{\mathbf{r}'}). \tag{2}$$

In both eqs (1) and (2), the sum is unconstrained, and it counts each edge twice. `Wegner_LMC.py` samples the partition function of eq. (1) using the Metropolis algorithm in arbitrary spatial dimension d on a hypercubic lattice, where $I(\mathbf{r}-\mathbf{r}') = 1$ for nearest neighbors, and $I(\mathbf{r}-\mathbf{r}') = 0$ else. `Wegner_ECMC.py` samples eq. (1) with the event-chain algorithm. In this fact sheet, we obtain the exact partition function, energy and spin correlation functions of this model on a finite lattice with $N = L^D$ sites, slightly extending Wegner. `Wegner_1d_Exact.py` contains a step-by-step implementation of the main analytic formulas of the present fact sheet.

The goal of this fact sheet is double:

- On the one hand, we need the exact formulas for the pair correlation function $g[\mathbf{r} = (L/2, \dots, L/2)]$, which we conjecture to be the slowest variable in Wegner's model, in order to describe the correlation time of LMC and ECMC in this model.
- On the other hand, we derive from this exact solution the direct-sampling algorithm `Wegner_Direct.py` for this model. Exactly solvable models generally give rise to direct-sampling algorithms[2], and Wegner's model is no exception. It is however not clear how to generalize the direct-sampling algorithm from the harmonic model to the XY-model, and it is even more mysterious how to generalize from the analogous harmonic solid[1] to the case of hard disks in the solid phase.

2 Wegner in $1D$, finite N

In one dimension, we consider $L = N$ sites numbered $r = (0, 1, \dots, N-1)$, with Fourier modes $k = (0, 2\pi/N, \dots, (N-1)2\pi/N)$. To simplify notation, we sometimes write $\sum_{k=1}^{N-1}$, when in fact we sum over the Fourier modes $k_1, \dots, k_{N-1}$.

Furthermore, we have

$$I(r) = \begin{cases} 1 & \text{if } r = -1, 1, \text{ with pbc} \\ 0 & \text{else.} \end{cases} \tag{3}$$

Using this choice, we have

$$H = -2N + \sum_{r=0}^{N-1} (\phi_{r+1} - \phi_r)^2 \quad \text{(with pbc: } N \equiv 0\text{).} \tag{4}$$

2.1 Analytical solution

For each choice of $(\phi_0 \dots \phi_{N-1})$ with $\sum_{r=0}^{N-1} \phi_r = 0$, we define Fourier-transformed angles:

$$\hat{\phi}_k = \frac{1}{\sqrt{N}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} \phi_r \tag{5}$$

and express the orginal ϕ_r variables through them as:

$$\phi_r = \frac{1}{\sqrt{N}} \sum_{k=0,2\pi/N,\dots}^{2(N-1)\pi/N} \mathrm{e}^{+ikr} \hat{\phi}_k. \tag{6}$$

`Wegner_1d_Exact` implements this Fourier transform (through a direct summation as in eq. (38), rather than by FFT) and checks that it is consistent, and leads to the expression of the Hamiltonian as

$$H = -2N + \sum_{k=1,N-1} \epsilon_k \hat{\phi}_k \hat{\phi}_{N-k} \tag{7}$$

$$= -2N + 2 \sum_{k=1,N/2-1} \epsilon_k \hat{\phi}_k \hat{\phi}_{-k} + 4\ \hat{\phi}_{N/2}^2 \tag{8}$$

with

$$\epsilon_k = 4 \sin^2 \left(\frac{k}{2} \right). \tag{9}$$

As the Hamiltonian of eq. (1) is real, we have $\hat{\phi}_{N-k} = \hat{\phi}_{-k} = \hat{\phi}_k^*$ (complex conjugate) and $\hat{\phi}_{N/2}$ is real.

The program `Wegner_1d_Exact` illustrates the passage from eq. (4) to eq. (8):

$$H = -2N + \sum_k \sum_{k'} \hat{\phi}_k \hat{\phi}_{k'} \underbrace{\sum_r \left[\mathrm{e}^{ik(r+1)} - \mathrm{e}^{ikr} \right] \left[\mathrm{e}^{ik'(r+1)} - \mathrm{e}^{ik'r} \right]}_{4\sin^2\left(\frac{k}{2}\right)\delta(k'+k,2\pi)}$$

$$= -2N + \sum_{k=1}^{N-1} \epsilon_k \hat{\phi}_k \hat{\phi}_{N-k}, \quad (10)$$

where $\epsilon_k = 4\sin^2(k/2)$.

Next, one introduces the real-valued Fourier components $\hat{\Psi}$ as

$$\hat{\Psi}_k = \frac{1}{\sqrt{2}} \left(\hat{\phi}_k + \hat{\phi}_{-k} \right) \quad \text{for } k = 1, \ldots, N/2-1 \quad (11)$$

$$\hat{\Psi}_{-k} = \frac{1}{i\sqrt{2}} \left(\hat{\phi}_k - \hat{\phi}_{-k} \right) \quad \text{for } k = 1, \ldots, N/2-1 \quad (12)$$

$$\hat{\Psi}_{N/2} = \hat{\phi}_{N/2} \quad (13)$$

with the inverse transform

$$\hat{\phi}_k = \frac{1}{\sqrt{2}} \left(\hat{\Psi}_k + i\hat{\Psi}_{-k} \right) \quad \text{for } k = 1, \ldots, N/2-1 \quad (14)$$

$$\hat{\phi}_{-k} = \frac{1}{\sqrt{2}} \left(\hat{\Psi}_k - i\hat{\Psi}_{-k} \right) \quad \text{for } k = 1, \ldots, N/2-1, \quad (15)$$

and arrives at the representation of the Hamiltonian

$$H = -2N + \sum_{k=1,N/2-1} \epsilon_k \left(\hat{\Psi}_k^2 + \hat{\Psi}_{-k}^2 \right) + 4\ \hat{\phi}_{N/2}^2. \quad (16)$$

Note that we have again a factor of 2 with respect to Wegner, unless we take his eq. (8) to imply a sum over the entire Brillouin zone.

The partition function is given by (maybe some constant prefactors missing)

$$Z = \prod_k \int_{-\infty}^{\infty} d\hat{\Psi}_k \exp\left[-\beta \epsilon_k \hat{\Psi}_k^2 \right]. \quad (17)$$

Let us count degrees of freedom in this system, between the Fourier-transformed version and the real-space version. Indeed, the Fourier modes $1, \ldots, N/2-1$ and $N/2+1, \ldots N-1$ are complex, but they satisfy $\hat{\phi}_k = \hat{\phi}_{N-k}^*$ (this gives $N-2$ degrees of freedom). The Fourier mode $N/2$ is real and gives one degree of freedom, and a total of $N-1$, just as the number of ϕ_r, if we impose that they sum to zero.

The system energy satisfies

$$\langle E \rangle = -2N + \sum_k \epsilon_k \frac{\int_{-\infty}^{\infty} d\hat{\Psi}_k \hat{\Psi}_k^2 \exp\left[-\beta\epsilon_k \hat{\Psi}_k^2 \right]}{\int_{-\infty}^{\infty} d\hat{\Psi}_k \exp\left[-\beta\epsilon_k \hat{\Psi}_k^2 c \right]} = -2N + \sum_k \frac{k_B T}{2}, \quad (18)$$

with $\int_{-\infty}^{\infty} dx \exp\left(-ax^2\right) = \sqrt{\pi}/\sqrt{a}$ and $\int_{-\infty}^{\infty} dx x^2 \exp\left(-ax^2\right) = \sqrt{\pi}/(2a^{3/2})$.

2.2 Spin correlation function

Following Wegner[3], in order to compute the spin-correlation function

$$g(r) = \langle \cos(\phi_0 - \phi_r) \rangle = Re \langle \exp[i(\phi_0 - \phi_r)] \rangle , \tag{19}$$

we note that

$$\begin{aligned} \phi_0 - \phi_r &= \frac{1}{\sqrt{N}} \sum_{k=1}^{N-1} \hat{\phi}_k [1 - \exp(ikr)] \\ &= \frac{1}{\sqrt{N}} \left[\sum_{k=1}^{N/2-1} \hat{\phi}_k \left(1 - \mathrm{e}^{ikr}\right) + \hat{\phi}_{N/2}(1 - \mathrm{e}^{i\pi r}) + \sum_{k=1}^{N/2-1} \hat{\phi}_{-k} \left(1 - \mathrm{e}^{-ikr}\right) \right]. \end{aligned} \tag{20}$$

Writing out the exponentials into sines and cosines, this gives

$$\phi_0 - \phi_r = \sqrt{\frac{2}{N}} \sum_{k=1}^{N/2-1} \left[\hat{\Psi}_k (1 - \cos kr) + \hat{\Psi}_{-k} \sin kr \right] + \frac{1 - (-1)^r}{\sqrt{N}} \hat{\Psi}_{N/2}. \tag{21}$$

These terms are put together as follows for the correlation function (where we integrate over the modes just as in eq. (18)):

$$A : \exp\left\{ - \left[\frac{\sqrt{2}}{\sqrt{N}} (1 - \cos kr) \right]^2 / (4\beta\epsilon_k) \right\} \quad \text{terms with } \hat{\Psi}_k, \tag{22}$$

$$B : \exp\left\{ - \left\{ \frac{\sqrt{2}}{\sqrt{N}} \frac{[1 - (-1)^r]}{\sqrt{2}} \right\}^2 / (16\beta) \right\} \quad \text{term with } \hat{\Psi}_{N/2}, \tag{23}$$

$$C : \exp\left\{ - \left[\frac{\sqrt{2}}{\sqrt{N}} \sin kr) \right]^2 / (4\beta\epsilon_k) \right\} \quad \text{terms with } \hat{\Psi}_{-k}. \tag{24}$$

This yields, in agreement with Wegner's eq. (11), except for the boundary term,

$$g(r) = \exp\left\{ -\frac{2k_B T}{N} \left[\sum_{k=1}^{N/2-1} \frac{\sin^2\left(\frac{kr}{2}\right)}{\epsilon_k} + \frac{1}{32} (1 - (-1)^r)^2 \right] \right\}. \tag{25}$$

To derive eq. (25), one uses

$$\int dx \exp\left(-ax^2\right) = \frac{\sqrt{\pi}}{\sqrt{a}} \tag{26}$$

and

$$\int dx \exp\left(-ax^2 + ibx\right) = \frac{\exp\left(-\frac{b^2}{4a}\right)\sqrt{\pi}}{\sqrt{a}}, \tag{27}$$

so that the ratio of the two integrals equals $\exp\left(-\frac{b^2}{4a}\right)$.

2.3 Direct-sampling algorithm for Wegner's model in one dimension

The direct-sampling algorithm for Wegner's model in one dimension first samples

$$\hat{\Psi}_k = \text{gauss}(\sigma_k = 1/\sqrt{2\beta\epsilon_k}) \tag{28}$$

$$\hat{\Psi}_{-k} = \text{gauss}(\sigma_k = 1/\sqrt{2\beta\epsilon_k}) \tag{29}$$

$$\hat{\phi}_k = \frac{1}{\sqrt{2}}\left(\hat{\Psi}_k + i\hat{\Psi}_{-k}\right) \tag{30}$$

$$\hat{\phi}_{-k} = \frac{1}{\sqrt{2}}\left(\hat{\Psi}_k - i\hat{\Psi}_{-k}\right) \tag{31}$$

$$\hat{\phi}_{N/2} = \text{gauss}(\sigma_k = 1/\sqrt{8\beta}) \tag{32}$$

$$\hat{\phi}_0 = 0 \tag{33}$$

and then performs the inverse Fourier transform of eq. (38). This is implemented in `Wegner_1d_Direct.py` by direct calculation. For large N, fast Fourier methods will be called for.

2.4 Test of the correlations

The Python programs `Wegner_LMC.py`, `Wegner_ECMC.py`, `Wegner_1d_Exact.py`, and `Wegner_1d_Direct.py` cross-check the different ways of computing the correlation functions. Results for $\langle\cos(\phi(0) - \phi(r))\rangle$ are as follows, for $\beta = \sqrt{2}$ and $N = 8$:

r	LMC	ECMC	Exact	Direct
0	1.0	1.0	1.0	1.0
1	0.856557	0.85670	0.85668960	0.8566973
2	0.767048	0.76697	0.76707933	0.7670832
3	0.717807	0.71787	0.71787752	0.7178946
4	0.702133	0.70205	0.70218850	0.7021766

2.5 Asymptotic behavior

Neglecting the oscillating factor in eq. (25), the spin correlation starts at $r = 1$ as

$$g(1) = \exp\left(-\frac{k_B T}{4}\right) = \exp(-r/\xi) \quad \text{with } \xi(r=1) = 4/(k_B T). \tag{34}$$

Using

$$\sum_{i=1}^{N/2-1} \frac{\sin^2\left(\frac{\pi i}{2}\right)}{4\sin^2\left(\frac{\pi i}{N}\right)} \to \frac{N^2}{4\pi^2}\sum_{i=1}^{\infty}\frac{\sin^2\left(\frac{\pi i}{2}\right)}{i^2} = \frac{N^2}{32}, \tag{35}$$

we see that for $r = N/2$, this gives

$$g(N/2) = \exp\left(-\frac{k_B T}{8}\frac{N}{2}\right) = \exp\left(-r/\xi\right) \quad \text{with } \xi(r = N/2) = 8/(k_B T). \quad (36)$$

Fig. 1 shows how the effective correlation length, defined by $g(r) = \exp\left[-r/\xi(r)\right]$, interpolates between 4β (at $r = 1$) and 8β (at $r = N/2$). The latter is enhanced as clockwise and anticlockwise correlations contribute equally across the periodic lattice. The true effective correlation length in the infinite chain equals 4β, as we take the $N \to \infty$ limit before the $r \to \infty$ limit.

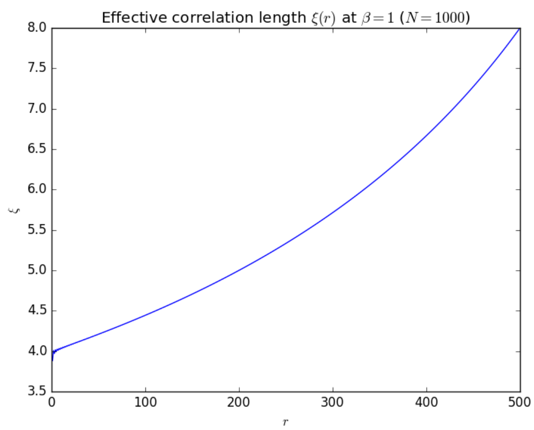

Figure 1: Effective correlation length in the one-dimensional harmonic model with $N = 1000$, $\beta = 1$. The absolute correlation at half-lattice equals $\exp\left(-500/8\right) = 7\times10^{-28}$.

3 Wegner in 2D (and general D), finite N

The higher-dimensional calculation is performed analogously to the one of Section 2, with Fourier-transformed angles $\hat{\phi}_{\mathbf{k}}$ expressed in terms of the real-space angles $\phi_{\mathbf{r}}$:

$$\hat{\phi}_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} \mathrm{e}^{-i\mathbf{kr}} \phi_{\mathbf{r}} \quad (37)$$

and the inverse Fourier transform as:

$$\phi_r = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in B_1} \mathrm{e}^{+i\mathbf{kr}} \hat{\phi}_{\mathbf{k}}. \quad (38)$$

Here, the real-space vectors satisfy $\mathbf{r} = (x, y)$ with $x, y = 0, 1, \ldots, L-1$, whereas the momentum vectors in the first Brillouin zone B_1 satisfy $\mathbf{k} = (k_x, k_y)$ with $k_x, k_y = 0, 2\pi/L...(L-1)2\pi/L$. vectors $\mathbf{r} = (x, y)$, with $x, y = 0, 1, \ldots, L$.

The $N-1$ momentum vectors in the first Brillouin zone are arbitrarily partitioned into the sets B^+, B^-, and B^s (with : $B^+ \cup B^- \cup B^s = B_1$): For any vector $\mathbf{k} \in B^+$, there is a vector $-\mathbf{k} \in B^-$. The vectors with $\mathbf{k} = -\mathbf{k}$ (modulo 2π) make up the symmetric part of the Brillouin zone, B^s. To achieve the partitioning in program `Wegner_2d_Exact.py`, the elements of B_1 are inspected one after the other. If a vector $\mathbf{k}$ satisfies $-\mathbf{k} \neq \mathbf{k}(\mod 2\pi)$, it is added to B^+ and $-\mathbf{k}$ is discarded. Otherwise ($-\mathbf{k} = \mathbf{k}$), it is added to B^s (see `Wegner_2d_Exact`).

3.1 Test of the correlations (2D)

The Python programs `Wegner_LMC.py`, `Wegner_ECMC.py`, `Wegner_2d_Exact.py`, and `Wegner_2d_Direct.py` cross-check the different ways of computing the correlation function $\langle \cos[\phi(0) - \phi(\mathbf{r})] \rangle$. Results are as follows, for $\beta = \sqrt{2}$ and $N = L^2 = 16$:

$\mathbf{r}$	LMC	ECMC	Exact	Direct
(0, 0)	1.0	1.0	1.0	1.0
(1, 0)	0.920335	0.920584	0.920476	0.920448
(2, 0)	0.902103	0.901939	0.902018	0.901984
(3, 0)	0.920455	0.920390	0.920476	0.920550
(0, 1)	0.920412	0.920537	0.920476	0.920405
(1, 1)	0.902135	0.901904	0.902018	0.901788
(2, 1)	0.893888	0.893726	0.893752	0.893438
(3, 1)	0.901951	0.902335	0.902018	0.901848
(0, 2)	0.902025	0.901893	0.902018	0.901683
(1, 2)	0.893785	0.893815	0.893752	0.893466
(2, 2)	0.888785	0.889009	0.888828	0.888513
(3, 2)	0.893733	0.893855	0.893752	0.893334
(0, 3)	0.920403	0.920445	0.920476	0.920476
(1, 3)	0.901776	0.902109	0.902018	0.901854
(2, 3)	0.893715	0.893916	0.893752	0.893614
(3, 3)	0.901903	0.902021	0.902018	0.901873

References

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[3] F. Wegner. Spin-ordering in a planar classical heisenberg model. *Zeitschrift für Physik*, 206(5):465–470, 1967.