Computational Physics (Physics 760) Exercise #5

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Don't forget to make your code available to and useable by your tutor / grader!

5 [20 points] The Ising Model in 2D

Consider the Ising model on a 2 dimensional square lattice with on N sites on a side (N^2 sites in total), and with periodic boundary conditions in both directions. Let the external magnetic field $h = 0$. The model is essentially indistinguishable from before

$$Z[\beta, J] = \sum_{\sigma} e^{-\beta H[J]} \qquad H[J] = -J \sum_{\langle \vec{x}, \vec{y} \rangle} \sigma_{\vec{x}} \sigma_{\vec{y}} \qquad \beta = 1/T \tag{1}$$

with dimensionful parameters (in units where $k_B = 1$). The difference from before is that x and y indicate positions on a 2D torus rather than a 1D ring. To pick a set of dimensionless units we can set $\beta = 1$, so that the only remaining parameter is J (if you prefer, in what follows everywhere you see J think to yourself 'oh yes, βJ').

Onsager showed that this model exhibits a phase transition: At high temperatures (small J) the system is disordered; at low temperatures (large J) the system is strongly correlated and spontaneously magnetizes. The transition happens at the *critical coupling*

$$J_c = \frac{1}{2} \log\left(1 + \sqrt{2}\right) \approx 0.4406867935097715 \cdots \tag{2}$$

We will not explain how he accomplished this achievement; a modern understanding leverages Kramers-Wannier duality. An analytic solution when $h \neq 0$ has yet to be found.

In this exercise we'll study a fixed J. In Exercise 6 we'll study a variety of Js. So you probably want to write your code flexibly to allow good reuse. You may want to save the ensembles you produce to disk.

5.1 [3 pts] Exact Results

The net magnetization $M = \sum_{\vec{x}} \sigma_{\vec{x}}$, and the magnetization per site is $m = \frac{1}{N^2} M$. In 1948 Onsager twice stated at conferences without proof that in the thermodynamic limit

$$\langle |m| \rangle = \begin{cases} 0 & J \leq J_c \qquad \text{(warmer than critical)} \\ \left(1 - \frac{1}{\sinh^4(2J)}\right)^{1/8} & J > J_c \qquad \text{(cooler than critical).} \end{cases} \tag{3}$$

(Don't worry, it was proved by others 3 years later.) We also know the energy per site

$$\epsilon = -J \coth(2J) \left(1 + \frac{2}{\pi}(2\tanh^2(2J) - 1) \times K\left(4\,\text{sech}^2(2J)\tanh^2(2J)\right)\right) \tag{4}$$

where K is the *complete elliptic integral of the first kind*,

$$K(k^2) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2\theta}} \tag{5}$$

but be careful, sometimes that integral is called $K(k)$ without the square; it varies from package to package.

- (2 points) Implement the exactly-known $\langle |m| \rangle$ and ϵ. Don't implement the elliptic K yourself unless you imagine enjoying it. As a way to check your implementation, here is a small table of some selected values

$1/J$	$\langle \lvert m \rvert \rangle$	$\langle \epsilon \rangle$
0.25	1.0000000	-8.000
1	0.9992758	-1.997
2	0.9113194	-0.873
3	0.0000000	-0.272

- (1 point) It is standard to plot as a function of $1/J$ (because $1/(\beta J) \sim T$). Make 2 plots, one for each observable, plotting them against $1/J \in [0.1, 5]$ with fine steps. You should see a sharp, non-smooth feature in $\langle |m| \rangle$ at $1/J_c$, an indicator of the phase transition.

5.2 [6 points] MCMC for the 2D Ising Model

Feel welcome to adapt / expand your 1D code from previous exercises.

- (1 point) Implement a function which, given J and a configuration of spins σ on the 2D square lattice with periodic boundary conditions, computes H.
- (1 point) Implement a function which, given J, a configuration σ, and a location $\vec{x}$, computes

$$\Delta H = H(\sigma \text{ except flip the spin on site } \vec{x}) - H(\sigma) \tag{6}$$

  Make sure this function is *fast*; if it scales with the volume the computations will take a very long time.

- (1 point) Implement the Metropolis-Hastings for sampling from the 2D Ising model, using sweeps of single spin flips.
- (2 points) Generate a *single* ensemble of 10^5 configurations for $J = 0.5$ for each $N = \{4, 8, 12\}$. On 3 separate plots show the Monte Carlo histories of m, $|m|$, and ϵ (measure on each configuration and plot as a function of Monte Carlo time) (you can put the 3 Ns on the same figure). You'll reuse these configurations below.
- (1 point) Remember that as $0.5 = J > J_c \approx 0.44$ we are in the broken phase. How does that related to what you see in the Monte Carlo histories? Keep in mind we proved in class that $\langle m \rangle = 0$ for any finite N. Does that jibe with what you see?

5.3 [3 points] Slow Tunneling Means Long Autocorrelation Times

Recall that the autocorrelation function of a timeseries (for example, a sequence of measurements of a single observable on configurations produced by a Markov chain)

$$C(\Delta t) = \langle (O(t) - \mu)(O(t + \Delta t) - \mu) \rangle = \frac{1}{n - |\Delta t|} \sum_{t_0=0}^{n-|\Delta t|-1} (O(t_0) - \mu)(O(t_0 + \Delta t) - \mu) \tag{7}$$

$$\Gamma(\Delta t) = C(\Delta t)/C(0) \tag{8}$$

can be *Fourier accelerated*, and we can the timeseries' *integrated autocorrelation time* by

$$\tau = \frac{1}{2} + \sum_{\Delta t=1}^{T} \Gamma(T) \tag{9}$$

where the sum can be cut off by T in different ways. Cut the sum off where Γ first crosses 0.

- (2 points) Compute the autocorrelation time τ for m, $|m|$, and ϵ for the two test ensembles above. Do the results comport with the Monte Carlo history figure you made?
- (1 point) Recall that when $h = 0$ we have an extra $\mathbb{Z}_2$ symmetry: σ and $-\sigma$ have the same weight, and this guarantees that $\langle m \rangle = 0$ for any finite N. Write 1 or 2 sentences explaining why the very slow autocorrelation time of m is not important.

5.4 [8 points] The Thermodynamic Limit for One J

You now have an ensemble of 10^5 measurements for $J = 0.5$ for each $N = \{4, 8, 12\}$. For each ensemble use as 'the' autocorrelation time the larger of the autocorrelation times of $|m|$ and ϵ.

- (5 points) Perform a bootstrap analysis estimating the mean and uncertainty for $\langle |m| \rangle$ and $\langle \epsilon \rangle$ for each ensemble. To to ensure you don't under-estimate your uncertainties (by thermalizing and blocking or decimating, for example).
- (2 points) For both observables plot the estimates (with uncertainties as error bars) against $1/N^2$ (so the thermodyanmic limit is at 0). Show the known exact results given above at $1/N^2 = 0$.
- (1 point) Explain what you see in a few sentences.