Exercises for Computational Physics (physics760)
WS 2020 / 21

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Exercise 2 (20 pts. total)

Homework (due Nov.18 at 18:00)

Please note the due date of this homework. Submission of homework *requires* submitting your solutions (e.g. answers to questions, graphs, results in tabular form) in the form of a brief report (please no 100 page submissions!) **AND** a copy of your code that you used to do the simulations. Please address all questions and requirements written below in *italics* and red font in your homework report.

3 Simulating the 2-D Ising model

We now move on to the 2-d Ising model (on a square grid), which as you will find out, exhibits many interesting and non-trivial behavior. The Hamiltonian for this system is the same as the one you encountered in the first homework, but now each site has 4 nearest neighbors. We define the 2-d lattice with $\Lambda = N_x \times N_y$ lattice points and assume periodic boundary conditions in both the x and y directions. Lastly, for simplicity we assume that the coupling J is the same in the x and y directions (i.e. *isotropic coupling*).

1: *Modify your 1D Ising code so that it works in 2 dimensions as described above. Furthermore, implement the Metropolis-Hastings* accept/reject *that was discussed in the lectures (in other words do NOT do a "brute-force" calculation like in the previous homework). Set your code up such that measurements are done after each "sweep" of the lattice, where a "sweep" constitutes looping over all sites on the lattice, and at each site flipping its spin and performing the Metropolis-Hastings* accept/reject *step. In other words, after each "sweep" of the lattice you will have performed Λ accept/reject tests . 10 pts.*

When writing your code, it obviously pays off to keep calculations as efficient as possible. The following questions are meant to guide you in writing efficient routines.

2: *How does the numerical cost of the calculation of the energy (for a given spin configuration) scale with the system size Λ? 1 pt.*

3: *Assuming you've flipped one spin s_i, how does the numerical cost of the calculation of the* change in energy *ΔS scale with the system size Λ? 1 pt.*

Thanks to Onsager and other intelligent people, we know that the 2d Ising model exhibits a thermal phase transition when $h = 0$ at

$$J_c = \frac{1}{2} \log\left(1 + \sqrt{2}\right) \approx 0.440686793509772\ . \tag{1}$$

4: *What is the significance of the critical coupling J_c? 1 pt.*

These same people determined the exact behavior of the magnetization per site and energy per site when $h = 0$ in the thermodynamic limit (see `https://en.wikipedia.org/wiki/Square_lattice_Ising_model`):

$$|m| = \begin{cases} \left(1 - \frac{1}{\sinh^4(2J)}\right)^{1/8} & \forall J > J_c \\ 0 & \forall J \leq J_c \end{cases} \tag{2}$$

$$\epsilon = -J \coth(2J) \left(1 + \frac{2}{\pi}\left(2\tanh^2(2J) - 1\right) K\left(4\mathrm{sech}^2(2J)\tanh^2(2J)\right)\right)\ , \tag{3}$$

where $K(m)$ is the incomplete elliptic integral of the first kind.

5: *Use your algorithm to estimate $\langle m \rangle$ as a function of $h \in [-1, 1]$ for some fixed $J < 1$. Use $N_x = N_y$ for a sample of values between 4 and 20. 2 pts*

6: *Use your algorithm to estimate $\langle \epsilon \rangle$ (average energy per site) as a function of $J \in [.25, 2]$ for $h = 0$. Again use $N_x = N_y$ for various values between 4 and 20. Compare your result to the exact solution in the thermodynamic limit. 2 pts*

7: *Use your algorithm to estimate $\langle |m| \rangle$ (absolute value of the mean magnetization) as a function of $J \in [.25, 1]$* and *$h = 0$. Again use $N_x = N_y$ for various values between 4 and 20. Plot your results as a function of J^{-1} and compare your result to the exact solution in the thermodynamic limit. Explain the physical significance of what you find. What would you see if you instead plotted $\langle m \rangle$ instead of $\langle |m| \rangle$? 3 pts*

8: *(EXTRA CREDIT 4pts). Only do this if interested. You are NOT obligated to do this!*

Estimate the specific heat $C = \Lambda * (\langle \epsilon^2 \rangle - \langle \epsilon \rangle^2)$ holding $h = 0$ fixed and as a function of $J \in [.25, 1]$. Do this for a small number of sizes $N = N_x = N_y$ up to $N \sim 20$ and plot your results **for** *C/J^2 as a function of J^{-1}. What are you seeing?*

If you want, you can compare your result with the exact expression for the specific heat in the thermodynamic limit (with $h = 0$),

$$C = \frac{4J^2}{\pi \tanh^2(2J)} \left(K(\kappa^2) - E(\kappa^2) - \left(1 - \tanh^2(2J)\right)\left[\frac{\pi}{2} + (2\tanh^2(2J) - 1)K(\kappa^2)\right]\right) \tag{4}$$

where $K(m)$ and $E(m)$ are the incomplete elliptic integral of the first and second kind, respectively, and

$$\kappa = \frac{2\sinh(2J)}{\cosh^2(2J)} \tag{5}$$