Exercises for Computational Physics (physics760)
WS 2020 / 21

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Exercise 1 (20 pts. total)

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1 In-class exercises

1.1 Make buddies

If you haven't done so yet, use this opportunity to find a partner to do your homework with. We prefer teams of 2.

1.2 Version control with git

Once you have your team, then please set up a `git` repo. Your tutor might do a hands-on, walk-through presentation about the basic usage of git if there is enough demand by the class. Either way, make sure you:

- Can use of `git` on your own local machine
- Understand and can use the following `git` commands
  - init, status, branch, log, add, commit, show, help, diff
- Commit a change **with an accompanying message of your change** (ie. the heart of version control)
- *Provide access to your tutor!*

2 Homework (due Nov.11 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.

Simulation of the 1-D Ising model

The Ising model is a wonderful sandbox to study critical phenomena with numerical methods. Our main strategy in the coming weeks will be to investigate the Ising model in 2 dimensions, which already shows plenty of interesting behavior. To uncover these features via non-perturbative simulation techniques is our principal goal in this tutorial series.

As a warm up we start with the simpler Ising model in 1 dimension. The analytic solution is known (you might have seen this as an exercise in some solid-state physics lecture), which conveniently allows us to implement, verify and test our code by the exact solution.

2.1 The model

Consider a chain of spins ("1d lattice") with sites labeled by $x \in \{0, \ldots, N-1\}$. To each site x we attach a spin variable $s_x \in \{\pm 1\}$. One specific choice of a spin for each site we call a spin configuration $\mathbf{s} = \{s_x : \forall\, x\}$.

This system of spins is immersed in a heat bath of constant temperature T and in an external magnetic field h. Its dynamics are governed by the Hamiltonian

$$\mathcal{H}(s) = -J \sum_{\langle x,y \rangle} s_x\, s_y - h \sum_x s_x \,. \tag{1}$$

$\langle x, y\rangle$ denotes the nearest-neighbor pair x and y on the chain, J is a real number and we assume periodic boundary conditions. In the heat bath environment the probability for finding the spin system at spin configuration $\mathbf{s} = (s_0, s_1, \ldots, s_{N-1})$ is given by the Boltzmann distribution

$$\mathrm{P}\,(\mathbf{s}) = \exp\left(-\frac{\mathcal{H}(\mathbf{s})}{k_B T}\right) / \sum_{\mathbf{s}'} \exp\left(-\frac{\mathcal{H}(\mathbf{s}')}{k_B T}\right) \equiv \frac{1}{Z} \exp\left(-\frac{\mathcal{H}(\mathbf{s})}{k_B T}\right) \;, \tag{2}$$

where we define

$$Z = \sum_{\mathbf{s}'} \exp\left(-\frac{\mathcal{H}(\mathbf{s}')}{k_B T}\right) \;.$$

as the partition function. The sum in the partition function is over all possible spin field $\mathbf{s} = (s_0, s_1, \ldots, s_{N-1})$ configurations. To simplify notation, let's switch to a system of units such that $k_B = 1$.

In 1d the partition function can be determined analytically as a function of N, J/T, and h/T. We won't derive this result here, but only state it,

$$Z = \lambda_+^N + \lambda_-^N \quad ; \quad \lambda_\pm = \mathrm{e}^{\frac{J}{T}} \left(\cosh(\frac{h}{T}) \pm \sqrt{\sinh(\frac{h}{T})^2 + \mathrm{e}^{-4\frac{J}{T}}} \right) \;. \tag{3}$$

For those who are interested, the derivation can be found here:

https://en.wikipedia.org/wiki/Ising_model

You'll find this expression useful later when comparing your numerical results with exact results.

1: *Discuss the physical meaning of J, in particular the sign of J, and the role it plays in magnets, for example. (3 pts.)*

2: *Clarify what it means to have periodic boundary conditions (nearest neighbors). (1 pt.)*

3: Implement the Ising 1d simulation: determine an estimate for magnetization per spin

$$\langle m \rangle = -\frac{T}{N} \frac{\partial \log Z}{\partial h}\,, \tag{4}$$

and attempt to estimate the error of your estimate.
Since we work with units where $k_B = 1$, what are the relevant dimensionless *ratios in this problem? (1 pt.)*

Use your simulation code to study the dependency of $\langle m \rangle$ on

- *the external field strength h for fixed N*
- *the number of spins N for fixed h*

Compare your numerical results to the exact solution at finite N, as well as to the "infinite volume" (also known as the "thermodynamic limit") solution, i.e. for $N \to \infty$. Provide graphs of your comparisons. Use values of $h \in [-1, 1]$ and N up to $N \sim 20$ (but no larger). Describe your findings on the dependency of $\langle m \rangle$ with N. You can fix $J = 1$ for all simulations. (5 pts.)

Do not forget to submit your (well-written) code with your answers. (10 pts.)