NTNU **Institutt for fysikk**

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Exam in TFY4235 Computational Physics
May 05, 2014
09:00

Allowed help: Alternativ **A**

This problem set consists of 4 pages.

This exam is published on Monday, May 5 at 09:00 hours. You can work on your solution till **Thr. May 08, 2014 at 23:00** ("the deadline"). Before the deadline you should submit your final report in pdf-format via the "its leaning" page of this class. You are prior to this deadline *also* expected[1], to email the final report to me at `Ingve.Simonsen@ntnu.no` with subject TFY4235. [2]

Should you run short on time, you are adviced to spend the time to do properly what you do instead of following a strategy of doing a little bit here-and-there.

Information posted during the exam, like potential misprints, links to papers etc. will be posted on the web-page of the course at `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/#Exam` and/or `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Exam/`. *It is your responsibility to check this information regularly!*

There are no constraints on any aids you may want to use in connection with this exam, including discussing it with anybody. *But, the report and the programs you will have to write yourself. Please attach your programs as appendices to the report. Give as a footnote the names of your collaborators during the exam.* The report may be written in either Norwegian (either variation) or in English.

There are no formal requirements for the format of the report in addition to what was said above. The report should explain what you have been doing, your results, and how you interpret these results. Details should be included to the extent that we as graders can follow your way of reasoning. General background theory that, for instance, can be found i textbooks, is not needed in the report. It is documentation of your work we are interested in!

[1] Useful in the unlikely event that something should go wrong with the its learning submission.

[2] Warning: If your email is too large, the gmail system, to which I also forward my email, may notify you that the message was too large to by delivered to my gmail account. This means that your message was received successfully by the ntnu email system, if you were not informed otherwise.

Remember that if you have written an original and clever code for solving the problem, but are not able to explain it well in the report, it is hard to give you full credit.

I plan to have office hours from 13:00-16:00 on Monday May 05 in case you have questions to the problems. Also the other days of the exam I will be at the department.

Good luck to all of you!

Problem 1.

This problem is devoted to the study of the two dimensional Ising model. We assume a square lattice. Each node i of the lattice has spin S_i taking values -1 or 1, *i.*e. $S_i \in \{-1, 1\}$. The Hamiltonian for the system is

$$H = -J \sum_{\langle i,j \rangle} S_i S_j \tag{1}$$

where $J > 0$ is a positive constant (ferromagnet) and the sum $\langle i, j \rangle$ is over nearest neighbors. This model has a *critical point* at the temperature $T = T_c$. For $T < T_c$, the model is in the ferromagnetic phase for which large domains of similar spins exist. On the other hand, for $T > T_c$ such domains are not present. See course slides for more details.

This problem aims at (1) determining T_c; (2) determining the critical exponent ν (see definitions below). To this end, we will use the heat-bath algorithm (see reference below).

Determination of the critical temperature T_c: A clever method for determining T_c is known as the *gradient-method*; see for instance Physics A **187**, 611 (1992) [1]. The idea underlying the gradient-method is to simulate the Ising model using the heat-bath algorithm on a lattice with a constant temperature gradient over the lattice. By choosing $T > T_c$ on one side of the lattice and $T < T_c$ on the other side, the model will be in the ferromagnetic phase on the side of the lattice where $T < T_c$ and in the paramagnetic phase on the side of the lattice where $T > T_c$. If one has a way of distinguishing the two phases, one may determine the average position of the interface separating these two phases. The temperature associated with this average position is the effective critical temperature T_{eff}. In order to find the true critical temperature T_c, the system size has to be extrapolated to infinity. Given that the quadratic square lattice has dimension $L \times L$, a relevant extrapolation formulae is

$$T_{eff} = T_c + \frac{A}{L^{\nu/(1+\nu)}}. \tag{2}$$

Here ν is the correlation length exponent, and we will determine it below. If T_{eff} is determined for some values of L using the method outlined below, T_c can be determined from Eq. (2) once the exponent ν is known. Assume periodic boundary conditions for the direction orthogonal to the temperature gradient.

Details: In order to determine the interface between the two phases, we use *damage spreading.* Make two identical copies of the $L \times L$ lattice. Along the low temperature edge, *fix* all spins to value $+1$ in one of the copies and to the value -1 in the other. Otherwise let all spins initially be equal. Use the *same* random numbers to update both lattices (so that both lattices would have developed identically had it not been for the difference in spins along the low temperature edge). Compare the two lattices may be done by using the function $\mathrm{xor}(S_i^{(1)}, S_i^{(2)})$ (see also ieor); recall that xor(1,1)=0, xor(1,-1)=1, xor(-1,1)=1, and xor(-1,-1)=0. Measure the distance from the high temperature edge to the first node for which $\mathrm{xor}(S_i^{(1)}, S_i^{(2)}) = 1$. This is the position, x_r, of the interface along row r.

Determine the position of the interface along all rows, and use these results to calculate $\langle x_r \rangle$ and $w = \sqrt{\langle x_r^2 \rangle - \langle x_r \rangle^2}$. These two latter quantities must, furthermore, be averaged over different Monte-Carlo times. From these results calculate the effective temperature, T_{eff}, corresponding to the position $\langle x_r \rangle$, and the temperature standard deviation, ΔT, that is associated with the position standard deviation w.

The correlation length exponent ν is defined as

$$\xi \sim |T - T_c|^{-\nu}\,, \tag{3}$$

where ξ is the correlation length. When the system has a temperature gradient, one has $\xi = w$ and $|T - T_c| = \Delta T$. The relation between w and ΔT is

$$\Delta T = gw, \tag{4}$$

where g is a temperature gradient. If the temperatures of the low- and high-temperature edges are kept fixed as L is changed, it follows that $g \propto 1/L$. By combining Eqs. (3) and (4), one is lead to

$$w \sim (gw)^{-\nu} \sim \left(\frac{w}{L}\right)^{-\nu}. \tag{5}$$

Solving this equation with respect to w results in

$$w \sim L^{\nu/(1+\nu)}. \tag{6}$$

Use Eq. (6) to estimate ν from the "numerical measurements" of w. From your estimate for the exponent ν, obtain the critical temperature T_c by the use of Eq. (2).

References

[1] A. Hansen and D. Stauffer, *The three-dimensional Ising model in a temperature gradient*, Physica A, **189**, 611 (1992).
`http://dx.doi.org/10.1016/0378-4371(92)90064-W`