ETH
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Computational Quantum Physics Exercise 11

FS 12
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Problem 11.1 Wolff algorithm with improved estimators on general lattices

Generalize your implementation of the Wolff algorithm from exercise 9 to work with an arbitrary adjacency list instead of a specific lattice. We will need this in next week's exercise.
Implement improved estimators (Section 7.2.3 of the script) to measure the susceptibility

$$\chi_2 = \sum_n \sigma_0 \sigma_n \tag{1}$$

and the second moment

$$\mu_2 = \sum_n \sigma_0 x_n^2 \sigma_n \,, \tag{2}$$

where x_n is the minimum distance (including periodic boundary conditions) between the two spins. In addition, measure the absolute value of the magnetization

$$|M| = \left| \sum_i \sigma_i \right| . \tag{3}$$

As a test for this week, construct the adjacency list for the three-dimensional cubic lattice. And run simulations for this lattice with coupling $J = 1$ on all bonds at varying temperatures. From your measurements of the above observables compute the connected magnetic susceptibility

$$\langle \chi \rangle = \frac{\beta}{N} \left(N \langle \chi_2 \rangle - \langle |M| \rangle^2 \right) , \tag{4}$$

the inverse temperature being $\beta = 1/k_B T$ as usual. By plotting χ versus βJ you should be able to show that your code gives results consistent with a critical point at $J\beta_c = 0.2216544 \pm 3 \cdot 10^{-7}$ [Talapov, Blöte. J. Phys. A: Math. Gen. **29** 5727 (1996)]. Make sure you show reliable error bars for your data.

Problem 11.2 Improved estimator for χ_4

Next week we will need to measure the connected four-point correlator

$$\langle \chi_{4c} \rangle = \langle \sum_{j,k,l} \sigma_0 \sigma_j \sigma_k \sigma_l \rangle - 3 \langle \sum_j \sigma_0 \sigma_j \rangle^2 = \langle \chi_4 \rangle - 3 \langle \chi_2 \rangle^2 . \tag{5}$$

Show that this can be achieved by measuring the improved estimator [I. Montvay, G. Münster, U. Wolff, Nucl. Phys. B **305**, 143 (1988)]

$$\langle \chi_{4c} \rangle = \frac{1}{N} \langle 3 \sum_{c,c'} N_c^2 N_{c'}^2 - 2 \sum_c N_c^4 \rangle - \frac{3}{N} \langle \sum_c N_c^2 \rangle^2 , \tag{6}$$

where c, c' run over the clusters of a Swendsen-Wang configuration and the expectation values $\langle\rangle$ are to be taken with respect to the different Swendsen-Wang cluster configurations. N_c denotes the size of cluster c.