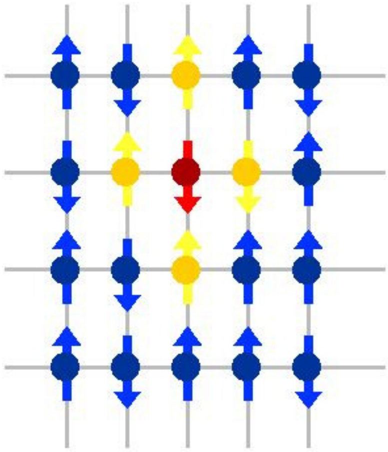
Problem set 2: Metropolis Criterion, Ising Model

1. a. You have generated 100000 configurations of a Lennard-Jones system using (1) simple sampling, (2) importance sampling. How do you calculate the average energy?
   b. Verify that the Metropolis Criterion enforces detailed-balance. (Distinguish between $\Delta E< 0$ und $\Delta E>0$.)
   c. The Glauber algorithm has the following acceptance rule: $W_{ij}=(1-\tanh(\beta(E_j-E_i)/2))$.
   Show that this algorithm enforces detailed balance, too.
   (Hint: $\tanh(x)=(e^x-e^{-x})/(e^x+e^{-x})$.)
   d. Formulate the Metropolis Criterion for a system of hard discs in the canonical ensemble.

2. Consider a d-dimensional system of spins, which can point up ($s_i=+1$) or down ($s_i=-1$). Only nearest neighbors interact („Ising-Model"). We would like to write a Monte Carlo program with which we can determine the statistical properties of such a system.

$$E = -\frac{1}{2}\sum_{i,j=1}^{n} s_i s_j$$



a. How many interactions need to be calculated after a single spin flip in d=1,2,3 dimensions?

b. Write down which steps need to be implemented to simulate the Ising model.

c. Which configurations would you expect at high and at low temperatures. Distinguish between d=1 and d=2,3.

d. If you have access to a computer:
Verify part c for d=2:
(http://bartok.ucsc.edu/peter/java/ising/keep/ising.html) What happens at T=2.629?

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