Phys 535

Lab Session

Question 1 One-dimensional Ising model

Following the outline given in the lecture, program the one-dimensional Ising model

$$E = -\varepsilon \sum_{i=0}^{N-1} s_i (s_{i-1} + s_{i+1})$$

for N spins. Assume periodic boundary conditions, i.e. $s_N = s_0$, $s_{-1} = s_{N-1}$.

- (a) Using N = 20 points, plot energy per spin E/N and magnetization per spin $M/N = \sum s_i/N$ as functions of temperature T.
- (b) Plot the specific heat c_v and the magnetic susceptibility χ as functions of temperature T.
- (c) If you double the number of points, do you get markedly different results?
- (d) What are the options to vectorize the calculation?

Hints:

- Do not forget to discard a number of early values while the system tries to find its equilibrium. The lower the temperature, the longer equilibration will take.
- The IDL function shift(vector, n) takes a vector and performs a cyclic shift of its elements by n.

Question 2 Quantum Monte Carlo

Using the trial wave function

$$\Phi(x) = Axe^{-kx} , \qquad (1)$$

find a Monte Carlo approximation E to the energy E_0 of the ground state for a particle in the potential well

$$U(x) = \begin{cases} \infty , & x < 0 , \\ x , & x \ge 0 . \end{cases}$$

$$(2)$$

- (a) Find E(k) for a set of values of the parameter k, at least $\{0.5, 1, 1.5, 2\}$.
- (b) If you choose a normal distribution for the displacement instead of a uniform one, do the energies change? Can you explain?

Question 3 Simulated annealing

Use *simulated annealing* to find an approximation to the global energy minimum for the one-dimensional Ising model.

Hint: Use your program(s) from Question 1.