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Exercises for Computational Methods in Solid State Theory SS 2014

Exercise Set 5

(Due date: Monday, June 23, 2014)

Exercise 7 (**Exact diagonalization of spin models**) (10 points)

a) Consider the Heisenberg spin dimer with $s = 1/2$.

$$\hat{H} = J\,\vec{S}_1 \cdot \vec{S}_2 \tag{1}$$

Use the basis states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ to find the eigenvalues and eigenvectors of the Hamiltonian analytically. Which is the ground state of the system for $J = 1$?

b) Write a program that evaluates a linear chain of spins with $s = 1/2$ with antiferromagnetic next-neighbour Heisenberg interactions and periodic boundary conditions using full diagonalization of the Hamiltonian.

$$\hat{H} = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j \tag{2}$$

c) Implement the Lanczos algorithm for the Heisenberg chain. Verify your results with the program written in b).

d) Consider the Hamiltonian of the antiferromagnetic next-neighbour Heisenberg chain. Introduce a magnetic field H and set the gyromagnetic ratio to $g = 2$.

$$\hat{H} = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j - g\mu_B H \sum_i S_i^z \tag{3}$$

Plot the average magnetization per lattice site as a function of the applied magnetic field for different lengths of the chain. What do you observe?