Quantum Dynamics: Full diagonalization

Numerical or algebraic solution of the Heisenberg model on a small system

Solve the Heisenberg model on a ring of N sites (i.e. with periodic boundary conditions)

$$\hat{H} \;=\; J \sum_i \hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1} \;-\; h \sum_i \hat{S}_i^z$$

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using a computer. First calculate the complete Hamilton matrix in Fock space, then diagonalize it (see hints below).

Thermodynamics

Calculate the total energy at N=8, βJ=2, h=$J/2$, (result: $E = -2.867\ldots$) as well as the following quantities (plots !):

a) the magnetization per site, $\langle \frac{M}{N} \rangle$ where $M = \sum_i \hat{S}_i^z$, as a function of magnetic field h at βJ=40, N=8. Also vary βJ and N (e.g., use also N=7). Try to explain your results qualitatively.

b) the susceptibility per site $\chi/N = \frac{\beta}{N}(\langle \hat{M}^2 \rangle - \langle \hat{M} \rangle^2)$ at N=8, h=0 as a function of β (it should have a maximum at βJ=$O(1)$); also vary the value of N,

c) and calculate the (approximate) ground state energy *per site* as a function of system size at h=0 and βJ=30 $\approx \infty$.

< O > = (tr O exp(-beta H)) / Z , Z = tr exp(-beta H)

Nonequilibrium Dynamics

Calculate the time evolution for a situation similar to the MPS case. Since the lattice size will be very small, you should choose open boundary conditions and start a single particle close to one edge of the system. Is a linear propagation visible ?

Hints:

With N sites, Fock space has size 2^N and the Hamilton matrix is of size $2^N \times 2^N$. For simplicity, you should calculate the whole matrix (!). Thus, you do not need to make use of the symmetries of $\hat{H}$, nor any conservation laws, nor the fact that the matrix is sparsely populated. Then you should be able to run calculations easily up to about $N = 8$. You can solve the problem numerically (Matlab) or algebraically (Mathematica, Maple). Once you have established the Hamilton matrix, you can then, in these programs, immediately calculate quantities like $\exp(-\beta H)$ (in matlab with the command *expm* – if the matrix is not too terribly large. Leave out factors $\hbar$ and let "J=1". *(continued on next page)*

Strategy for calculating the matrix: You can code the states of Fock space efficiently as whole numbers $I = 0, ..., 2^N - 1$, by interpreting the bit-representation of this number as a spin configuration. Then $I + 1$ can be used as the index of the matrix. Do not calculate each matrix element separately. Instead, first initialize the matrix to zero, then loop over state vectors I and calculate the contributions of each lattice edge $(j, j+1)$ and each lattice site j. It is helpful to encode the lattice structure (which sites are neighbours of each other) separately first.