Numerical many-body methods - Problem Set 1 (Exact Diagonalization)

Due by 18/11/2021

In this exercise we will consider the $J_1 - J_2$ spin-1/2 chain. The Hamiltonian of the system is given by

$$H = J_1 \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_i \vec{S}_i \cdot \vec{S}_{i+2}. \tag{1}$$

We will assume anti-ferromagnetic couplings, i.e. $J_1 > 0, J_2 \geq 0$, and denote the dimensionless ratio $g = J_2/J_1$. For $J_2 = 0$ (i.e. $g = 0$) the problem reduces to the Heisenberg chain we discussed in class. The model with finite J_2 is known to exhibit a phase transition at $g_c \simeq 0.241$. For $g < g_c$ the system is gapless with (antiferromagnetic) spin-spin correlations decaying as a power-law as you will show in this exercise. This is a consequence of the Mermin-Wagner theorem which prevents a 1D system from breaking a continuous symmetry (the spin rotation symmetry in this case) and ordering even at zero temperature (i.e. when the system is in the ground state). At $g = g_c$ the system undergoes a dimerization transition and becomes gapped.

To understand the dimerized phase it is instructive to consider $g = 1/2$. This is known as the Majumdar–Ghosh point and for this ratio the model can be solved exactly (see e.g. the Wikipedia article on "Majumdar–Ghosh model"). In the thermodynamic limit, $N \to \infty$, the ground state is two-fold degenerate and is given as a product state of singlets on every other bond:

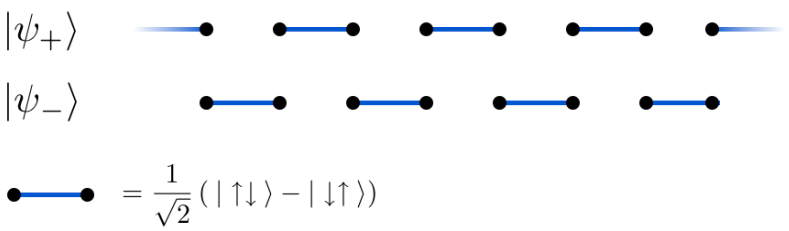

Figure 1: Dimerized ground states at the Majumdar–Ghosh point, i.e. for $J_2/J_1 = 1/2$ (figure taken from Wikipedia). In a finite system the two lowest energy states will be the even and odd superposition of the states depicted in the figure i.e. $|\psi_{1,2}\rangle = \frac{1}{\sqrt{2}}(|\psi_+\rangle \pm |\psi_-\rangle)$ with a splitting exponential in system size.

For g away from 1/2 the correlation length is finite, but the ground state can still be characterized by a finite dimer order parameter (that we will introduce below).

1. Generalize the Lanczos code presented in class to allow for a finite J_2 term. Try to think of different limits in which it is easy to check the ground state energy you obtain (e.g. for $J_1 = 0$ and $J_2 > 0$ the chain decouples into two independent chains with nearest neighbor coupling only).

When answering the questions below consider the following points in the phase diagram: $g = 0, g_c, 1/2$ and another value of g of your choice that lies in the dimerized phase (i.e. $g > g_c$) but away from 1/2.

2. Perform finite-size scaling of the triplet gap (i.e. the energy gap between the ground state in the $S^z = 0$ sector to the lowest state in the $S^z = 1$ sector). Use even system sizes of up to (at least) $N = 22$ sites. To see what this gap converges to in the thermodynamic limit, $N \to \infty$, more clearly plot it as function of $1/N$ (and set the x axis to start at 0). Check that the gap is indeed finite for $g > g_c$. Note that such an excitation in the dimerized phase corresponds to breaking a singlet bond and creating two free spin ups (a.k.a. spinons).

3. Perform finite-size scaling of the singlet gap (i.e. the energy gap to the first excited state in the $S^z = 0$ sector). (Be careful here! Recall that if you see a degenerate state in Lanczos this is due to numerical instabilities.) Check that the gap decays exponentially for $g > g_c$ (this is the gap between the states $|\psi_{1,2}\rangle = \frac{1}{\sqrt{2}}(|\psi_+\rangle \pm |\psi_-\rangle)$ mentioned above). What is the exponent for $g = 1/2$?

4. Calculate the spin-spin correlations in the ground state of the system, i.e. the expectation value of $\langle \vec{S}_1 \cdot \vec{S}_{1+x} \rangle$ as function of x. (Here you can use just the largest system size you considered above.) Note that due to spin-rotation symmetry it is enough to calculate $\langle S^z_1 S^z_{1+x} \rangle$ since $\langle S^z_1 S^z_{1+x} \rangle = \frac{1}{3}\langle \vec{S}_1 \cdot \vec{S}_{1+x} \rangle$. Show that for $g \leq g_c$ these correlations decay as a power law (up to logarithmic corrections that we won't discuss here), while for $g > g_c$ the decay is exponential. Note that this might be hard to observe close to the critical point (since at that point the correlation length diverges), but should be clearly visible for g close to $1/2$. Tips: to see a power law decay use a log-log plot and to see an exponential decay use a semi-log plot. You can change the scale of the axis in Julia (similarly to Python) by `xscale("log")` or `yscale("log")` respectively.

To observe dimerization, bond-bond correlations are typically considered. These are defined as $\langle B_1 B_{1+x} \rangle$, where $B_i = \vec{S}_i \cdot \vec{S}_{i+1}$ (i.e. B_i is the "strength" of the bond between sites i and $i+1$). Here, for simplicity, we will consider $\langle B^z_1 B^z_{1+x} \rangle$ where $B^z_i = S^z_i S^z_{i+1}$. (Note that unlike in the case of spin-spin correlations these are not related to each other in a simple way, but it will be enough to consider the latter correlations to see the ordering.)

5. Calculate $\langle B^z_1 B^z_{1+x} \rangle - \langle B^z_1 \rangle \langle B^z_{1+x} \rangle$ as function of x in the ground state of the system. (Again, use the largest system size you considered above.) What is the behavior of this order parameter for $g \leq g_c$? Show that for $g > g_c$ this order parameter saturates to a finite value (up to the alternating sign). Once again, this might be difficult to see close to g_c but should be clearly visible close to $g = 1/2$.