Università degli studi di Trieste

Dipartimento di Fisica

Advanced Quantum Mechanics

Parity Dependent Quantum Phase Transition in the Ising Chain: Analytical results

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Indice

1 Overview of spin systems

The present work has been made to provide analytical support to the simulations run for the *Advanced Quantum Mechanics* exam held at University of Trieste (a.a. 2022/2023).

1.1 Spin systems

In this section we briefly remind the main features of spin systems. In a spin system, the local Hilbert space is bidimensional: we can choose $\{|\uparrow\rangle, |\downarrow\rangle\}$ as a local basis. The commutation rules satisfied by spin operators are

$$\begin{aligned}\left[\sigma_j^a, \sigma_{j'}^{a'}\right] &= 0 \quad \text{for} \quad j' \neq j \\ \left[\sigma_j^a, \sigma_j^b\right] &= 2i\epsilon^{abc}\sigma_j^c \\ \{\sigma_j^a, \sigma_j^b\} &= 2\delta^{ab}.\end{aligned}$$

Moreover we can define the ladder operators as $\sigma_j^{\pm} = \dfrac{\sigma_j^x \pm i\sigma_j^y}{2}$, satisfying $\{\sigma_j^+, \sigma_j^-\} = 1$. It might appear impossible to describe a spin system through bosons. Given a bosonic operator $\hat{b}$ together with is vacuum state $|0\rangle$ (i.e. $\hat{b}|0\rangle = 0$), in fact, we can construct an infinite dimensional Hilbert space. If we, nevertheless, somehow truncate this space to being composed by two states only, then the spin Hilbert space can be recovered. This truncation - that can be explained through an infinite on-site repulsion for bosons - leads to **hardcore bosons**.

1.2 Mapping to hardcore bosons

Let's now proceed by identifying

$$|0\rangle \leftrightarrow |\uparrow\rangle \quad \text{and} \quad |1\rangle = \hat{b}^\dagger|0\rangle \leftrightarrow |\downarrow\rangle.$$

Consequently, it's straightforward to show that these relations hold:

$$\begin{cases}\sigma_j^+ = b_j \\ \sigma_j^- = b_j^\dagger \\ \sigma_j^z = 1 - 2b_j^\dagger b_j\end{cases} \Rightarrow \begin{cases}\sigma_j^x = b_j^\dagger + b_j \\ \sigma_j^y = i(b_j^\dagger - b_j) \\ \sigma_j^z = 1 - 2b_j^\dagger b_j\end{cases}$$

where we have used the fact that $\sigma^+|\downarrow\rangle = |\uparrow\rangle$, $\sigma^-|\uparrow\rangle = |\downarrow\rangle$. It's crucial to underline that these new operators $b_j^\dagger$ commute on different sites, like spin operators, but they anticommute on the same site. Summing up

$$
\begin{aligned}
[b_i, b_j] &= 0 \quad \text{for} \quad i \neq j \\
\{b_i, b_i^\dagger\} &= 1 \\
b_j|0\rangle &= 0,
\end{aligned}
$$

where we can notice that the hardcore constraint can be easily represented in terms of spinless fermions. Unfortunately, while the mapping from spins to hardcore bosons is valid in each dimension, the one from hardcore bosons to spinless fermions can be done only for $1D$ systems where there's a natural way to define order.

1.3 Jordan-Wigner Transformation

The mapping from hardcore bosons to spinless fermion is made through a highly nonlocal transformation known as Jordan-Wigner transformation. We define

$$b_j = K_j c_j = c_j K_j,$$

where $K_j = e^{i\pi \sum_{l=1}^{j-1} n_l} = \displaystyle\prod_{l=1}^{j-1}(1-2n_l)$ is just a sign and c_j is a fermionic operator satisfying $\{c_i, c_j^\dagger\} = \delta_{ij}$, $\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$. It is easy to show that the b operators satisfy the hardcore boson commutation rules:

$$
\begin{aligned}
b_j^\dagger b_j &= c_j^\dagger K_j^\dagger K_j c_j = c_j^\dagger c_j \\
b_j b_j^\dagger &= K_j c_j c_j^\dagger K_j^\dagger = c_j c_j^\dagger
\end{aligned}
$$

and

$$
\begin{aligned}
b_{j1} b_{j2}^\dagger &= c_{j1} e^{-i\pi \sum_{l=j1}^{j2-1} n_l} c_{j2}^\dagger \\
b_{j2}^\dagger b_{j1} &= c_{j1} e^{-i\pi \sum_{l=j1}^{j2-1} c_{j2}^\dagger}.
\end{aligned}
$$

Other useful and straightforward relations are:

- $b_j^\dagger b_j = c_j^\dagger c_j$
- $b_j^\dagger b_{j+1}^\dagger = c_j^\dagger (1-2n_j) c_{j+1}^\dagger = c_j^\dagger c_{j+1}^\dagger$
- $b_j^\dagger b_{j+1} = c_j^\dagger (1-2n_j) c_{j+1} = c_j^\dagger c_{j+1}$
- $b_j b_{j+1} = c_j (1-2n_j) c_{j+1} = -c_j c_{j+1}$
- $b_j b_{j+1}^\dagger = c_j (1-2n_j) c_{j+1}^\dagger = -c_j c_{j+1}^\dagger$

where it is crucial to use the fact that, for example, $c_j K_j K_{j+1} c_{j+1}$ $= c_j e^{i\pi \sum_{l=1}^{j-1} n_l} e^{i\pi \sum_{l=1}^{j-1} n_l} e^{i\pi n_j} c_{j+1} = -c_j c_{j+1}$ since n_j must be 1 in order to have a nonvanishing action of c_j.

1.4 Summary

It is thus possible to map a one dimensional spin system into a fermionic one using the following chain of mapping.

$$\begin{cases} \sigma_j^+ = b_j \\ \sigma_j^- = b_j^\dagger \\ \sigma_j^z = 1 - 2b_j^\dagger b_j \end{cases} \Rightarrow \begin{cases} \sigma_j^x = b_j + b_j^\dagger \\ \sigma_j^y = i(b_j^\dagger - b_j) \\ \sigma_j^z = 1 - 2b_j^\dagger b_j \end{cases} \Rightarrow \begin{cases} \sigma_j^x = K_j(c_j + c_j^\dagger) \\ \sigma_j^y = iK_j(c_j^\dagger - c_j) \\ \sigma_j^z = 1 - 2n_j \end{cases}$$

We can hence notice that

- $\sigma_j^z = 1 - 2n_j = 1 - 2c_j^\dagger c_j$
- $\sigma_j^x \sigma_{j+1}^x = (c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} + h.c.)$
- $\sigma_j^y \sigma_{j+1}^y = -(c_j^\dagger c_{j+1}^\dagger - c_j^\dagger c_{j+1} + h.c.)$

where for the last two we have used some of the equations of the previous section.

1.5 Boundary Conditions

We can now show that the boundary conditions imposed on a spin system can vary in the corresponding fermionic one according to the parity of the number of fermions. In fact

$$b_L^\dagger b_{L+1} = e^{i\pi \sum_{j=1}^{L-1} n_j} c_L^\dagger c_1 = -e^{i\pi \sum_{j=1}^{L} n_j} c_L^\dagger c_1 = -e^{i\pi N} c_L^\dagger c_1$$

where whe have used the fact that n_L must be 1 in order to have a nonvanishing action of $c_L^\dagger$. Similarly

$$b_L^\dagger b_1^\dagger = e^{i\pi \sum_{j=1}^{L-1} n_j} c_L^\dagger c_1^\dagger = -e^{i\pi N} c_L^\dagger c_1^\dagger.$$

Hence we have PBC if the number of fermions is odd, APBC if the number of fermions is even.

2 The Model

In the following, we are going to consider a quantum Ising chain in a transverse field whose Hamiltonian is given by

$$H = \frac{J}{2} \sum_{j=1}^{N} \left[\sigma_j^x \sigma_{j+1}^x + h\sigma_j^z \right].$$

Using the relations previously derived, we can cast this Hamiltonian into a fermionic one

$$
\begin{aligned}
H &= \frac{J}{2}\sum_{j=1}^{N}\left[(c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} + c_{j+1}c_j + c_{j+1}^\dagger c_j) + h(1-2c_j^\dagger c_j)\right] \\
&= \frac{J}{2}\sum_{j=1}^{N}\left[c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j - 2hc_j^\dagger c_j + c_{j+1}c_j + c_j^\dagger c_{j+1}^\dagger\right] + \frac{JhN}{2},
\end{aligned}
$$

with $c_{N+1} = c_1$ se $N_f = 1 \mod 2$ and $c_{N+1} = -c_1$ se $N_f = 0 \mod 2$, being N_f the parity of the number of fermions. This information can be included in the Hamiltonian by writing it as

$$
H = PH^{(+)}P + LH^{(-)}L
$$

where $P = \dfrac{1+\prod_{j=1}^{N}(1-2c_j^\dagger c_j)}{2}$ is the projector into the even sector of the fermionic Fock space (if there is an even number of fermions $P = 1$, otherwise $P = 0$), $L = 1 - P$ and

$$
\begin{aligned}
H^{(+)} &= \frac{J}{2}\left\{\sum_{j=1}^{N-1}\left[c_j^\dagger c_{j+1} + c_j^\dagger c_{j+1}^\dagger - hc_j^\dagger c_j + \frac{h}{2}\right] - c_N^\dagger c_1 - c_N^\dagger c_1^\dagger\right\} + h.c. \\
H^{(-)} &= \frac{J}{2}\left\{\sum_{j=1}^{N-1}\left[c_j^\dagger c_{j+1} + c_j^\dagger c_{j+1}^\dagger - hc_j^\dagger c_j + \frac{h}{2}\right] + c_N^\dagger c_1 + c_N^\dagger c_1^\dagger\right\} + h.c.
\end{aligned}
$$

It's fundamental to notice that the parity of the number of fermions is not directly related to the parity of the number of sites, but to the total magnetization (the sum over all the sites of the z component of the spin). The Hamiltonian can be diagonalized by Fourier transforming the fermionic fields:

$$
c_j = \frac{e^{i\pi/4}}{\sqrt{N}}\sum_{k\in\Gamma^\pm} e^{ikj}c_k^\pm.
$$

It is useful to stress that the ensembles $\Gamma^\pm$ strongly depend on the boundary conditions. In case of PBC $e^{ikL} = 1 \Rightarrow k = \dfrac{2n\pi}{N}$, whereas in case of APBC $e^{ikL} = -1 \Rightarrow k = \dfrac{\pi(2n+1)}{N}$. Substituting into the Hamiltonian we get

$$
\begin{aligned}
H^{(-)} &= \frac{J}{2}\sum_{j=1}^{N}[\frac{1}{N}\sum_{q,q'} e^{-iqj}e^{iq'j}e^{iq'}c_q^\dagger c_{q'} - \frac{i}{N}\sum_{q,q'} e^{-iqj}e^{-iq'j}e^{-iq'}c_q^\dagger c_{q'}^\dagger + \frac{1}{N}\sum_{q,q'} e^{-iqj}e^{-iq}e^{iq'j}c_q^\dagger c_{q'} \\
&\quad + \frac{i}{N}\sum_{q,q'} e^{iqj}e^{iq}e^{iq'}c_q c_{q'} - \frac{h}{N}\sum_{q,q'} e^{-iq}e^{iq'}c_q^\dagger c_{q'}] + \frac{JhN}{2} \\
&= \frac{J}{2}[\sum_q e^{iq}c_q^\dagger c_q - i\sum_q c_q^\dagger c_{-q}^\dagger e^{iq} + \sum_q e^{-iq}c_q^\dagger c_q + i\sum_q e^{-iq}c_q c_{-q} - h\sum_q c_q^\dagger c_q] + \frac{NhJ}{2} \\
&= \frac{J}{2}\sum_q[(2\cos q - h)c_q^\dagger c_q - ic_q^\dagger c_{-q}^\dagger e^{iq} + ic_q c_{-q}e^{iq}] + \frac{NhJ}{2} \\
&= \frac{J}{2}\sum_{q>0}[(2\cos q - h)c_q^\dagger c_q - \frac{i}{2}[c_q^\dagger c_{-q}^\dagger e^{iq} + c_{-q}^\dagger c_q^\dagger e^{-iq}] + \frac{i}{2}[c_q c_{-q}e^{iq} + c_{-q}c_q e^{-iq}]] \\
&= \frac{J}{2}\sum_{q>0}[(2\cos q - h)c_q^\dagger c_q - \frac{i}{2}[c_q^\dagger c_{-q}^\dagger e^{iq} - c_q^\dagger c_{-q}^\dagger e^{-iq}] + \frac{i}{2}[c_q c_{-q}e^{iq} - c_q c_{-q}e^{-iq}]] \\
&= \frac{J}{2}\sum_{q>0}[(2\cos q - h)c_q^\dagger c_q - \frac{i}{2}[c_q^\dagger c_{-q}^\dagger e^{iq} - c_q^\dagger c_{-q}^\dagger e^{-iq}] + \frac{i}{2}[c_q c_{-q}e^{iq} - c_q c_{-q}e^{-iq}]] \\
&= \frac{J}{2}\sum_{q>0}[(2\cos q - h)c_q^\dagger c_q + \frac{1}{2}\sin q[2c_q^\dagger c_{-q}^\dagger - 2c_q c_{-q}]] \\
&= \frac{J}{2}\sum_{q>0}[(2\cos q - h)c_q^\dagger c_q + \frac{1}{2}\sin q[-2c_{-q}^\dagger c_q^\dagger - 2c_q c_{-q}]].
\end{aligned}
$$

The general form of the Hamiltonian in each sector can thus be written as

$$
H^{(\pm)} = -J\sum_{q\in\Gamma^\pm}\left[(h-\cos q)c_q^\dagger c_q + \frac{1}{2}\sin q\left(c_{-q}^\dagger c_q^\dagger + c_q c_{-q}\right)\right] + \frac{JhN}{2}.
$$

As a last step, we want to define a rotation-like transformation (Bogoliubov transformation) to diagonalize the hamiltonian:

$$
\begin{aligned}
c_q &= \cos\theta_q\ \chi_q + \sin\theta_q\ \chi_{2\pi-q}^\dagger\ (\forall\ q \text{ in } H^{(+)} \text{ or } \forall\ q \neq 0 \text{ in } H^{(-)})) \\
c_{-q}^\dagger &= -\sin\theta_q\ \chi_q + \cos\theta_q\ \chi_{2\pi-q}^\dagger \\
c_0 &= \chi_0 \text{ (only for } H^{(-)}).
\end{aligned}
$$

Let's substitute these transformations into the Hamiltonian, momentarily omitting the constant term:

$$
\begin{aligned}
H^{(+)} = &- J \sum_{q\in\Gamma^+} \Big[(h-\cos q)(\cos\theta_q \chi_q^\dagger + \sin\theta_q \chi_{2\pi-q})(\cos\theta_q\chi_q + \sin\theta_q\chi_{2\pi-q}^\dagger)\Big] + \\
&- \frac{J}{2}\sum_{q\in\Gamma^+} \sin q \Big[(\cos\theta_{-q}\chi_{-q}^\dagger + \sin\theta_{-q}\chi_{2\pi+q})(\cos\theta_q\chi_q^\dagger + \sin\theta_q\chi_{2\pi-q})\Big] + \\
&- \frac{J}{2}\sum_{q\in\Gamma^+} \sin q \Big[(\cos\theta_q\chi_q + \sin\theta_q\chi_{2\pi-q}^\dagger)(\cos\theta_{-q}\chi_{-q} + \sin\theta_{-q}\chi_{2\pi+q}^\dagger)\Big]
\end{aligned}
$$

From the Bogoliubov transformation, we get $\cos\theta_{2\pi\pm q} = \cos\theta_{\pm q} = \cos\theta_q$, $\sin\theta_{2\pi\pm q} = \sin\theta_{\pm q} = \pm\sin\theta_q$ and $\chi_{2\pi\pm q} = \chi_{\pm q}$. This works because a shift of 2π or a reflection of q still span the set $\Gamma^{(\pm)}$, so in other words we are working with an equivalence class of q under those two operations. Thus, we rewrite the Hamiltonian as:

$$
\begin{aligned}
H^{(+)} = &-J\sum_{q\in\Gamma^+}(h-\cos q)\Big[\cos^2\theta_q\chi_q^\dagger\chi_q + \sin^2\theta_q\chi_{-q}\chi_{-q}^\dagger\Big] + \\
&+ J\sum_{q\in\Gamma^+}\Big[(h-\cos q)\cos\theta_q\sin\theta_q - \frac{1}{2}\sin\theta_q(\cos^2\theta_q - \sin^2\theta_q)\Big]\chi_{-q}^\dagger\chi_q^\dagger + \text{h.c.} + \\
&- \frac{J}{2}\sum_{q\in\Gamma^+}\sin q\,(-2\sin\theta_q\cos\theta_q)\,\chi_q\chi_q^\dagger - \frac{J}{2}\sum_{q\in\Gamma^+} 2\sin q\sin\theta_q\cos\theta_q\chi_{-q}^\dagger\chi_{-q} = \\
= &-J\sum_{q\in\Gamma^+}[(h-\cos q)\cos 2\theta_q + \sin q\sin 2\theta_q]\chi_q^\dagger\chi_q + \\
&+ \frac{J}{2}\sum_{q\in\Gamma^+}[(h-\cos q)\sin 2\theta_q - \sin\theta_q\cos 2\theta_q]\,\chi_{-q}^\dagger\chi_q^\dagger + \text{h.c.} + \\
&- J\sum_{q\in\Gamma^+}\Big[(h-\cos q)\sin^2\theta_q - \frac{1}{2}\sin q\sin 2\theta_q\Big].
\end{aligned}
$$

To get a diagonal Hamiltonian we choose the paramenter θ_q such that the coefficients of the superconducting terms are zero:

$$
(h-\cos q)\sin 2\theta_q - \sin\theta_q\cos 2\theta_q = 0 \to \tan 2\theta_q = \frac{\sin q}{h-\cos q}.
$$

Thus, by defining $\epsilon(q) = \sqrt{(h-\cos q)^2 + \sin^2 q}$ we get the relations:

$$
\begin{aligned}
\sin 2\theta_q &= \frac{\sin q}{\epsilon(q)} \\
\cos 2\theta_q &= \frac{h-\cos q}{\epsilon(q)},
\end{aligned}
$$

which we can plug in the Hamiltonian (reintroducing the constant term), thus obtaining

$$
\begin{aligned}
H^{(+)} &= -J \sum_{q\in\Gamma^+} \epsilon(q)\chi_q^\dagger \chi_q - J \sum_{q\in\Gamma^+} \left[\frac{h-\cos q}{2}\left(1-\frac{h-\cos q}{\epsilon(q)}\right) - \frac{\sin^2 q}{2\epsilon(q)} - \frac{h}{2}\right] = \\
&= -J \sum_{q\in\Gamma^+} \epsilon(q)\left(\chi_q^\dagger \chi_q - \frac{1}{2}\right) + \frac{J}{2}\sum_{q\in\Gamma^+}\cos q = -J \sum_{q\in\Gamma^+} \epsilon(q)\left(\chi_q^\dagger \chi_q - \frac{1}{2}\right),
\end{aligned}
$$

where the sum of cosines vanishes because of the presence of simmetric terms. A similar discussion can be carried out for $H^{(-)}$, but we must be careful when we handle the zero-momentum term because of the sign change in the energy. Keeping this in mind we reach the result:

$$
H^{(-)} = -J \sum_{q\in\Gamma^-, q\neq 0} \epsilon(q)\left(\chi_q^\dagger \chi_q - \frac{1}{2}\right) + J\epsilon(0)\left(\chi_0^\dagger \chi_0 - \frac{1}{2}\right).
$$

3 Results

After rotating the fields, we can now identify the lowest energy eigenvalue state for each of the eight cases: even and odd Hamiltonian, with an even or odd number of sites, for positive and negative values of the magnetic field.

- for an even number of sites, with $h > 0$, the lowest energy state of the even Hamiltonian is obtained by filling all the energy levels $E = -\frac{J}{2}\sum_q \epsilon(q)$
- for an even number of sites, with $h > 0$, the lowest energy state of the odd Hamiltonian is obtained by filling all the energy levels except for the one with positive energy $E = -\frac{J}{2}\sum_{q\neq 0} \epsilon(q)$
- for an even number of sites, with $h < 0$, the lowest energy state of the even Hamiltonian is again obtained as in the previous case $E = -\frac{J}{2}\sum_q \epsilon(q)$
- for an even number of sites, with $h < 0$, the lowest energy state of the odd Hamiltonian is obtained in the same way $E = -\frac{J}{2}\sum_{q\neq 0} \epsilon(q)$
- for an odd number of sites, with $h > 0$, the lowest energy state of the even Hamiltonian is obtained by filling all the energy levels except the one with the lowest modulus (energies are all negative) $E = -\frac{J}{2}\sum_q \epsilon(q) + J\epsilon(\pi/N)$

- for an odd number of sites, with $h > 0$, the lowest energy state of the odd Hamiltonian is obtained by filling all the energy levels $E = -\frac{J}{2}\sum_q \epsilon(q) + J\epsilon(0)$
- for an odd number of sites, with $h < 0$, the lowest energy state of the even Hamiltonian is obtained in the same way as before $E = -\frac{J}{2}\sum_q \epsilon(q) + J\epsilon(\pi)$ (notice that now the energy with the smallest modulus is in $q = \pi$ because the spectrum changes)
- for an odd number of sites, with $h < 0$, the lowest energy state of the odd Hamiltonian is obtained by leaving empty the state with $q = 0$ and the one whith $q = p$ where p is the element nearest to π in Γ^- (notice that we are excluding the positive contribution in 0 and the one which is the lowest in modulus.) It is now straightforward to show that

  $$\frac{\partial E^+_{h>0,odd}}{\partial h} - \frac{\partial E^+_{h<0,odd}}{\partial h} = -2J$$

  i.e. the ground state energy is not smoothly connected between $h < 0$ and $h > 0$ (this is a first order quantum phase transition that happens only for odd N).