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Tutorial 1: 1D Transverse Field Ising Model

1 Mean field theory for TFIM

Consider the transverse field Ising model, given by

$$\hat{H} = -J \sum_{i=1}^{N} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - g \sum_{i=1}^{N} \hat{\sigma}_i^x, \tag{1}$$

where periodic boundary conditions are assumed. The relevant symmetry operator is $U = \prod_i \hat{\sigma}_i^x$, which generates the symmetry group $\mathbb{Z}_2$.

As we have seen in the lecture, there are two distinct groundstate phases as a function of g; for $g \ll 1$ we have spontaneous symmetry breaking and for $g \gg 1$ we have a "disordered" paramagnetic state, which are separated by a quantum phase transition. In this tutorial, we will try to understand this phase diagram through other approaches: namely mean field theory, and exact diagonaliztion by fermionization.

a) Consider the mean field ansatz, where the ground state is given by a product state, $|vac\rangle = \prod_i |\phi\rangle_i$, where $|\phi\rangle_i$ is some arbitrary normalized single spin state on site i. Assuming translational invariance, express the energy of this trial state with the TFIM hamiltonian.

b) Now minimize the variational energy to obtain the variational estimate for the ground state energy as a function of g/J. Characterize the variational ground state in terms of its symmetry. Identify the location of the phase transition.

2 Solving 1D TFIM with Fermions:

In this part of the tutorial, we solve the TFIM model in 1D using a method developed by Jordan and Wigner. Here, we also assume periodic boundary conditions. As a first step, we will begin by making a 90^o rotation about the y-axis:

$$\hat{\sigma}^z \to -\hat{\sigma}^x, \qquad \hat{\sigma}^x \to \hat{\sigma}^z \tag{2}$$

to get

$$\hat{H} = -J \sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x - g \sum_i \hat{\sigma}_i^z. \tag{3}$$

Here we've also rewritten the sum over nearest neighbors to be specific to a 1D system. Does this transformation affect the phase diagram?

Then we can introduce the Jordan-Wigner transformation, which involves writing the spin operators as "strings" of fermionic operators:

$$\begin{aligned}
\hat{\sigma}_i^z &= 1 - 2c_i^\dagger c_i, \\
\hat{\sigma}_i^+ \equiv (\hat{\sigma}_i^x + i\hat{\sigma}_i^y)/2 &= \left[\prod_{j<i} \left(1 - 2\hat{c}_j^\dagger \hat{c}_j\right)\right] \hat{c}_i, \\
\hat{\sigma}_i^- \equiv (\hat{\sigma}_i^x - i\hat{\sigma}_i^y)/2 &= \left[\prod_{j<i} \left(1 - 2\hat{c}_j^\dagger \hat{c}_j\right)\right] \hat{c}_i^\dagger,
\end{aligned} \tag{4}$$

where the notation $j < i$ means that the product is taken over all sites j that are located to the left of i, and $\hat{c}^\dagger$ and $\hat{c}$ are operators for spinless fermions and satisfy the anti-commutation relations:

$$\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \delta_{ij}, \qquad \{\hat{c}_i, \hat{c}_j\} = \left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} = 0. \tag{5}$$

a) The fermionic occupation number operator, is given by

$$\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i, \tag{6}$$

and has eigenvalues 0 and 1 in the occupation number basis. From the commutation relations, show that

$$\hat{n}_i^k = \hat{n}_i, \tag{7}$$

for all natural numbers k.

b) From here we get that

$$1 - 2\hat{c}_i^\dagger \hat{c}_i = \exp\left(i\pi \hat{c}_i^\dagger \hat{c}_i\right). \tag{8}$$

Using this expression, show that

$$\begin{aligned}
\exp\left(i\pi\hat{c}_i^\dagger\hat{c}_i\right)\hat{c}_i &= \hat{c}_i \\
\hat{c}_i\exp\left(i\pi\hat{c}_i^\dagger\hat{c}_i\right) &= -\hat{c}_i \\
\exp\left(i\pi\hat{c}_i^\dagger\hat{c}_i\right)\hat{c}_i^\dagger &= -\hat{c}_i^\dagger \\
\hat{c}_i^\dagger\exp\left(i\pi\hat{c}_i^\dagger\hat{c}_i\right) &= \hat{c}_i^\dagger.
\end{aligned} \tag{9}$$

The above identities can be used to ensure the correct canonical commutation relations for spin operators, given by

$$\left[\hat{\sigma}_i^+, \hat{\sigma}_j^-\right] = \delta_{ij}\hat{\sigma}_i^z, \qquad \left[\hat{\sigma}_i^z, \hat{\sigma}_j^\pm\right] = \pm 2\delta_{ij}\hat{\sigma}_i^\pm. \tag{10}$$

(You don't have to show (10), only (9)).

c) Using the Jordan-Wigner transformation and the fact that $\hat{\sigma}^x = (\hat{\sigma}^+ + \hat{\sigma}^-)$, show that the Hamiltonian in (3) can be written as

$$\begin{aligned}
\hat{H} = &- J\sum_{i=1}^{N-1}\left[\hat{c}_i^\dagger\hat{c}_{i+1}^\dagger - \hat{c}_i\hat{c}_{i+1} - \hat{c}_i\hat{c}_{i+1}^\dagger + \hat{c}_i^\dagger\hat{c}_{i+1}\right] \\
&+ (-1)^{\mathcal{N}_f} J\left[\hat{c}_N^\dagger\hat{c}_1^\dagger - \hat{c}_N\hat{c}_1 - \hat{c}_N\hat{c}_1^\dagger + \hat{c}_N^\dagger\hat{c}_1\right] \\
&- \sum_{i=1}^{N} g\left(1 - 2\hat{c}_i^\dagger\hat{c}_i\right),
\end{aligned} \tag{11}$$

where $\mathcal{N}_f = \sum_{i=1}^N \hat{c}_i^\dagger\hat{c}_i$ is the total number of fermions.

d) What is the symmetry operator in the fermionic language? What are its quantum numbers?

e) By now, you should have recognized that the Hamiltonian (and the eigenstates) split into two parity sectors. We have to separately diagonalize the Hamiltonian in the $\mathcal{N}_f$ = even and odd sectors separately, and to find the ground state, we must choose the lowest energy.

Let us now introduce Fourier-transformed operators $\hat{c}_k$ and $\hat{c}_k^\dagger$, which are related to $\hat{c}_i$ and $\hat{c}_i^\dagger$ through the expressions

$$\hat{c}_i = \frac{1}{\sqrt{N}}\sum_k \hat{c}_k e^{ikx_i}, \qquad \text{and} \qquad \hat{c}_i^\dagger = \frac{1}{\sqrt{N}}\sum_k \hat{c}_k^\dagger e^{-ikx_i}, \tag{12}$$

where

$$k = \begin{cases} 2n\pi/(Na), & \text{if } \mathcal{N}_f \text{ is odd}, \\ \pm(2n-1)\pi/(Na), & \text{if } \mathcal{N}_f \text{ is even}, \end{cases} \tag{13}$$

and

$$n = -\frac{N}{2}+1, -\frac{N}{2}+1, ..., 0, 1, \ldots, \frac{N}{2} \quad \text{if } \mathcal{N}_f \text{ is odd},$$
$$n = 1, \ldots, \frac{N}{2} \quad \text{if } \mathcal{N}_f \text{ is even},$$

where we assume an even N number of sites.

Explain why the different parity sectors result in distinct boundary conditions: for $\mathcal{N}_f$ is odd (odd parity), we have periodic boundary conditions (PBC) in the fermionic language and for $\mathcal{N}_f$ is even (even parity), we have antiperiodic boundary conditions (ABC). Why are these the relevant boundary conditions and quantization of momenta in these parity sectors?

f) These new fermionic operators $\hat{c}_k$ and $\hat{c}_k^\dagger$ satisfy the fermionic anti-commutation relations such that

$$\left\{\hat{c}_k, \hat{c}_{k'}^\dagger\right\} = \delta_{kk'}, \qquad \{\hat{c}_k, \hat{c}_{k'}\} = \left\{\hat{c}_k^\dagger, \hat{c}_{k'}^\dagger\right\} = 0. \tag{14}$$

Show that the Hamiltonian can be written as

$$\hat{H} = \begin{cases} -gN + \sum_{k>0} \underbrace{\left[(2g - 2J\cos(ka))\,\hat{c}_k^\dagger \hat{c}_k + iJ\sin(ka)\left(\hat{c}_{-k}^\dagger \hat{c}_k^\dagger + \hat{c}_{-k}\hat{c}_k\right)\right]}_{H_k}, \text{if ABC} \\ -gN + \sum_{k>0} H_k - 2J(n_0 - n_\pi) + 2g(n_0 + n_\pi - 1), \text{ if PBC}, \end{cases} \tag{15}$$

where a is the lattice spacing, and $n_{ka} = c_k^\dagger c_k$. The difference in the ABC and PBC sectors arises because of the differences in the quantized momenta. Note, that in PBC, the momenta $k = 0, \pi$ appear with no negative counterparts, and hence appear separately in the momentum space Hamiltonian.

g) The last step to diagonalize the Hamiltonian H_k involves the Bogoliubov transformation that maps $\hat{c}_k$ and $\hat{c}_k^\dagger$ onto $\hat{\gamma}_k$ and $\hat{\gamma}_k^\dagger$ according to

$$\hat{c}_k^\dagger = u_k \hat{\gamma}_k^\dagger - iv_k \hat{\gamma}_{-k}, \qquad \hat{c}_k = u_k \hat{\gamma}_k + iv_k \hat{\gamma}_{-k}^\dagger, \tag{16}$$

where u_k and v_k are real numbers that satisfy $u_k^2 + v_k^2 = 1$, $u_{-k} = u_k$ and $v_{-k} = -v_k$. The operators $\hat{\gamma}_k$ and $\hat{\gamma}_k^\dagger$ satisfy the fermionic anti-commutation relations.

One can then write $u_k = \cos(\theta_k/2)$ and $v_k = \sin(\theta_k/2)$, and set θ_k such that the terms proportional to $\hat{\gamma}_k^\dagger \hat{\gamma}_{k'}^\dagger$ and $\hat{\gamma}_k \hat{\gamma}_{k'}$ are equal to zero. This results in the relation

$$\tan\theta_k = \frac{J\sin(ka)}{g - J\cos(ka)}, \tag{17}$$

and then the Hamiltonian can finally be written in terms of these new operators $\hat{\gamma}_k$ and $\hat{\gamma}_k^\dagger$ as

$$\hat{H}_k = \epsilon_k(\hat{\gamma}_k^\dagger \hat{\gamma}_k - \hat{\gamma}_{-k}\hat{\gamma}_{-k}^\dagger) = \epsilon_k(\hat{\gamma}_k^\dagger \hat{\gamma}_k + \hat{\gamma}_{-k}^\dagger \hat{\gamma}_{-k} - 1), \tag{18}$$

where H_0 is a constant, and

$$\epsilon_k = 2\sqrt{(g - J\cos ka)^2 + J^2 \sin^2 ka}. \tag{19}$$

(Check the algebra until this point.)

Describe the ground states of this Hamiltonian (in each momenta sector) in terms of the γ fermions.

Hint: What choice of $\langle vac|\hat{\gamma}_k^\dagger \hat{\gamma}_k|vac\rangle$ *minimizes the energy?*

h) Now, consider the many-body ground state of the fermionized TFIM hamiltonian. Which fermion parity sector does the global ground state belong to? What is the ground state energy?

Note: to actually determine the global ground state, you should consider the analytical expressions for the ground state energies in the two sectors separately, and then plot them numerically using Mathematica. This is a subtle point, and the comparison is difficult analytically since the domains of the momenta are different in the ABC and PBC cases: there are $N/2$ *momenta points between* $(0, \pi)$ *in ABC, and* $N/2 - 1$ *momenta points between* $(0, \pi)$ *in ABC. You can also consult Sec. 3.1 of [1].*

i) What is the energy of the lowest excited state(in the thermodynamic limit)? Where does the many-body spectral gap close?

j) Does the transition match with the answer you obtained using mean field theory? Explain your answer physically.

[1] G. B. Mbeng, A. Russomanno, G. E. Santoro, `https://arxiv.org/pdf/2009.09208.pdf`