3.1 The Transverse Field Ising Model

Consider the Hamiltonian of the Transverse Field Ising Model (TFIM)

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^x \hat{\sigma}_j^x - h \sum_j \hat{\sigma}_j^z$$

where $J, h > 0$ with PBC $\hat{\sigma}_L^x \hat{\sigma}_{L+1}^x = \hat{\sigma}_L^x \hat{\sigma}_1^x$.

1. We could try to map spins to bosonic operators

$$\begin{cases} \hat{\sigma}_j^x = \hat{b}_j + \hat{b}_j^\dagger \\ \hat{\sigma}_j^y = i(\hat{b}_j^\dagger - \hat{b}_j) \\ \hat{\sigma}_j^z = 1 - 2\hat{b}_j^\dagger \hat{b}_j \end{cases} \quad \Leftrightarrow \quad \begin{cases} \hat{b}_j = \hat{\sigma}_j^+ = \frac{1}{2}\hat{\sigma}_j^x + \frac{i}{2}\hat{\sigma}_j^y \\ \hat{b}_j^\dagger = \hat{\sigma}_j^- = \frac{1}{2}\hat{\sigma}_j^x - \frac{i}{2}\hat{\sigma}_j^y \end{cases}$$

(a) Bosons as define above are «hard-core bosons». We know that

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 0 \text{ with } i \neq j, \qquad \left[\hat{\sigma}^a, \hat{\sigma}^b\right] = 2i\varepsilon_{abc}\hat{\sigma}^c, \qquad \left\{\hat{\sigma}^a, \hat{\sigma}^b\right\} = 2\delta_{ab}.$$

So bosons commute at different sites, but

$$\{\hat{b}_j, \hat{b}_j^\dagger\} = \tfrac{1}{2}\hat{\sigma}_i^x\hat{\sigma}_i^x + \tfrac{1}{2}\hat{\sigma}_j^y\hat{\sigma}_j^y = \mathbb{1}, \qquad \hat{b}_j^\dagger\hat{b}_j^\dagger = \tfrac{1}{4}\hat{\sigma}_j^x\hat{\sigma}_j^x - \tfrac{1}{4}\hat{\sigma}_j^y\hat{\sigma}_j^y + \tfrac{1}{4}\{\hat{\sigma}_j^x, \hat{\sigma}_j^y\} = 0,$$

thus at most one boson is allowed on each site.

(b) In 1D it's useful to modify bosons to spinless fermions by *Jordan Wigner transformation*

$$\hat{b}_j = \hat{K}_j \hat{c}_j = \hat{c}_j \hat{K}_j, \qquad \hat{K}_j = \prod_{i=1}^{j-1}(1 - 2\hat{n}_i) = \pm 1,$$

where non-local string operator $\hat{K}_j$ corresponds just to a sign and $\hat{K}_j = \hat{K}_j^\dagger = \hat{K}_j^{-1}$. So if $\hat{c}$ are fermions then $\hat{b}$ satisfies the commutation and anticommutation relations

$$\begin{aligned} &[\hat{b}_i, \hat{b}_j] = 0, \quad [\hat{b}_i, \hat{b}_j^\dagger] = 0, \quad [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0, \\ &\{\hat{b}_j, \hat{b}_j\} = 0, \quad \{\hat{b}_j, \hat{b}_j^\dagger\} = 0, \quad \{\hat{b}_j^\dagger, \hat{b}_j^\dagger\} = 0. \end{aligned} \tag{1}$$

Second row could be proven using

$$\hat{b}_j^\dagger\hat{b}_j = \hat{c}_j^\dagger\hat{K}_j^\dagger\hat{K}_j\hat{c}_j = \hat{c}_j^\dagger\hat{c}_j, \quad \hat{b}_j^\dagger\hat{b}_j^\dagger = \hat{c}_j^\dagger\hat{K}_j^\dagger\hat{K}_j^\dagger\hat{c}_j^\dagger = \hat{c}_j^\dagger\hat{c}_j^\dagger, \quad \hat{b}_j\hat{b}_j = \hat{c}_j\hat{K}_j\hat{K}_j\hat{c}_j = \hat{c}_j\hat{c}_j.$$

And without loss of generality for $j > i$

$$\hat{b}_i\hat{b}_j^\dagger = \hat{c}_i\hat{K}_{i,j}\hat{c}_j^\dagger, \quad \hat{b}_j^\dagger\hat{b}_i = \hat{c}_j^\dagger\hat{K}_{i,j}\hat{c}_i \overset{1}{=} -\hat{K}_{i,j}\hat{c}_i\hat{c}_j^\dagger \overset{2}{=} \hat{c}_i\hat{K}_{i,j}\hat{c}_j^\dagger, \quad \Rightarrow \quad [\hat{b}_i, \hat{b}_j^\dagger] = 0,$$

with $\hat{K}_{i,j} = \prod_{k=i}^{j}(1 - 2\hat{n}_k)$. It was used in $\overset{1}{=}$ that $\{\hat{c}_i, \hat{c}_j^\dagger\} = 0$ and in $\overset{2}{=}$ that $\hat{c}_i$ changes parity for $\hat{K}_{i,j}$. The operators conjugation does not change the calculations, so we have proved (1). We need carefully work with PBS

$$\hat{b}_L^\dagger\hat{b}_1 = \hat{K}_L\hat{c}_L^\dagger\hat{c}_1 \overset{3}{=} -\left(\prod_{i=1}^{L}(1 - 2\hat{c}_i^\dagger\hat{c}_i)\right)\hat{c}_L^\dagger\hat{c}_1 = -(-1)^{\hat{N}}\hat{c}_L^\dagger\hat{c}_1, \qquad \hat{N} = \sum_{j=1}^{L}\hat{c}_j^\dagger\hat{c}_j,$$

where we used in $\overset{3}{=}$ that j-site occupied and we could complete to $-(-1)^{\hat{N}}$.

(c) Summarising, spins are mapped into fermions using

$$\begin{aligned} \hat{\sigma}_x &= \hat{K}_j(\hat{c}_j^\dagger + \hat{c}_j), \\ \hat{\sigma}_y &= \hat{K}_j i(\hat{c}_j^\dagger - \hat{c}_j), \\ \hat{\sigma}_z &= 1 - 2\hat{c}_j^\dagger\hat{c}_j, \end{aligned} \qquad \hat{K}_j = \prod_{i=1}^{j-1}(1 - 2\hat{c}_i^\dagger\hat{c}_i).$$

This is the Jordan Wigner transformation of the TFIM

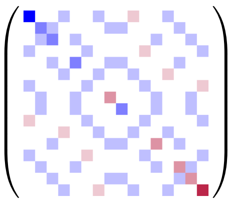
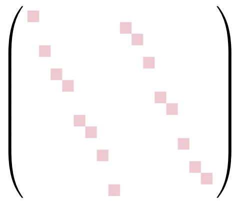
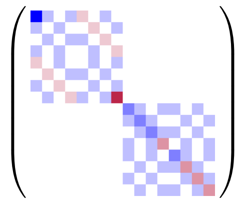
$$\begin{aligned} \hat{H} = hL - J\sum_{j=1}^{L-1}\left(\hat{c}_j^\dagger\hat{c}_{j+1} + \hat{c}_j^\dagger\hat{c}_{j+1}^\dagger + \text{h.c.}\right) + 2h\sum_{j=1}^{L}\hat{c}_j^\dagger\hat{c}_j \\ + J\,(-1)^{\hat{N}}\left(\hat{c}_L^\dagger\hat{c}_1 + \hat{c}_L^\dagger\hat{c}_1^\dagger + \text{h.c.}\right). \end{aligned}$$

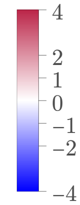
The number of fermions is not conserved, because of terms $\hat{c}^\dagger\hat{c}^\dagger$, but $[(-1)^{\hat{N}}, \hat{H}] = 0$, so parity is constant. With $(-1)^{\hat{N}} = 1$ we have antiperiodic boundary conditions and periodic otherwise.

2. We could separate Hilbert space as $\mathcal{H} = \mathcal{H}_{\text{even}} \oplus \mathcal{H}_{\text{odd}}$, and conserving parity of fermions $\hat{H}$ as

$$\hat{H} = \hat{P}_0 \hat{H} \hat{P}_0 + \hat{P}_1 \hat{H} \hat{P}_1 = \begin{pmatrix} \hat{H}_0 & 0 \\ 0 & \hat{H}_1 \end{pmatrix}, \qquad \hat{P}_{0,1} = \tfrac{1 \pm (-1)^{\hat{N}}}{2}.$$

Consider $L = 4$, than we could visualize such transform for $J = h = 1$ as

$\hat{H} =$ , $\hat{U} =$ , $\hat{U}^\dagger \hat{H} \hat{U} =$ .



where $\hat{U}$ represents reordering basis from

$$|0000\rangle, |0001\rangle, |0010\rangle, |0011\rangle, |0100\rangle, |0101\rangle, |0110\rangle, |0111\rangle,$$
$$|1000\rangle, |1001\rangle, |1010\rangle, |1011\rangle, |1100\rangle, |1101\rangle, |1110\rangle, |1111\rangle$$

to

$$|0000\rangle, |0011\rangle, |0101\rangle, |0110\rangle, |1001\rangle, |1010\rangle, |1100\rangle, |1111\rangle,$$
$$|0001\rangle, |0010\rangle, |0100\rangle, |0111\rangle, |1000\rangle, |1011\rangle, |1101\rangle, |1110\rangle.$$

(a) To diagonalize $\hat{H}$ we could start from Fourier Transform

$$\hat{c}_k = \frac{1}{\sqrt{L}} \sum_j e^{ikj} \hat{c}_j, \qquad \hat{c}_j = \frac{1}{\sqrt{L}} \sum_k e^{-ikj} \hat{c}_k.$$

Consider L is even. If we want $\hat{c}_{L+1} = \hat{c}_1$ we have H_1 and

$$\mathcal{K}_{p=1} = \left\{ k = \frac{\pi}{L} 2n \;\middle|\; n = -\tfrac{1}{2}L + 1, \ldots, 0, \ldots, \tfrac{1}{2}L \right\},$$

otherwise $\hat{c}_{L+1} = -\hat{c}_1$ in H_0 and

$$\mathcal{K}_{p=0} = \left\{ k = \frac{\pi}{L}(2n-1) \;\middle|\; n = -\tfrac{1}{2}L + 1, \ldots, 0, \ldots, \tfrac{1}{2}L \right\}.$$

And rewriting in terms of $\mathcal{K}_p$ hamiltonian we have

$$\hat{H}_p = -\sum_{k \in \mathcal{K}_p} (J \cos k + h) \left(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k} \hat{c}_{-k}^\dagger \right) - J \sum_{k \in \mathcal{K}_p} \left(e^{ik} \hat{c}_k^\dagger \hat{c}_{-k}^\dagger + \text{h.c.} \right)$$

(b) It is useful to combine $k = 0$ and $k = \pi$ for $p = 1$

$$\hat{H}_{k=0,\pi} = -2J(\hat{n}_0 - \hat{n}_\pi) + 2h(\hat{n}_0 + \hat{n}_\pi - 2).$$

The remaining terms come into pairs $(k, -k)$, so we could go to the positive k:

$$\mathcal{K}_1^+ = \left\{ k = \frac{\pi}{L} 2n \;\middle|\; n = 1, \ldots, \tfrac{1}{2}L - 1 \right\},$$
$$\mathcal{K}_0^+ = \left\{ k = \frac{\pi}{L}(2n-1) \;\middle|\; n = 1, \ldots, \tfrac{1}{2}L \right\}.$$

The $\hat{H}$ can be expressed as

$$\hat{H}_0 = \sum_{k \in \mathcal{K}_0^+} \hat{H}_k, \qquad \hat{H}_1 = \hat{H}_{k=0,\pi} + \sum_{k \in \mathcal{K}_1^+} \hat{H}_k,$$

with

$$\hat{H}_k = -2(J \cos k + h) \left(\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k} \hat{c}_{-k}^\dagger \right) - 2iJ \sin k \left(\hat{c}_k^\dagger \hat{c}_{-k}^\dagger - \hat{c}_{-k} \hat{c}_{-k} \right).$$

Introducing $\hat{\Psi}_k^\dagger = (\hat{c}_k^\dagger,\ \hat{c}_{-k})$ we could simplify $\hat{H}_k$ to the

$$\hat{H} = \hat{\Psi}_k^\dagger H_k \hat{\Psi}_k, \qquad H_k = -2J \begin{pmatrix} -\frac{h}{J} + \cos k & i \sin k \\ -i \sin k & \frac{h}{J} - \cos k \end{pmatrix}.$$

Great, we have reduced the Hamiltonian to quadratic form and ready for the *Bogolyubov transform*:

$$\hat{\Psi}_k = U \hat{\Phi}_k, \quad \Rightarrow \quad \hat{H}_k = \hat{\Phi}_k^\dagger D_k \hat{\Phi}_k, \qquad D_k = U^\dagger H_k U = \begin{pmatrix} \varepsilon_k & 0 \\ 0 & -\varepsilon_k \end{pmatrix},$$

where $\hat{\Phi}_k^\dagger \overset{\text{def}}{=} (\hat{\gamma}_k^\dagger,\ \hat{\gamma}_{-k})$ – our new operators. Diagonalizing H_k we have

$$U_k = \begin{pmatrix} u_k & -\bar{v}_k \\ v_k & u_k \end{pmatrix} = \frac{1}{\sqrt{\varepsilon_k(\varepsilon_k + z_k)}} \begin{pmatrix} \varepsilon_k + z_k & iy_k \\ iy_k & \varepsilon_k + z_k \end{pmatrix}, \qquad \boxed{\varepsilon_k = 2J\sqrt{\left(\cos k - \tfrac{h}{J}\right)^2 + \sin(k)^2}} \tag{2}$$

where we introduced new parameters

$$u_k = \frac{\varepsilon_k + z_k}{\sqrt{\varepsilon_k(\varepsilon_k + z_k)}}, \qquad v_k = \frac{iy_k}{\sqrt{\varepsilon_k(\varepsilon_k + z_k)}}, \qquad \begin{aligned} z_k &= 2(h - J\cos k), \\ y_k &= 2J\sin k. \end{aligned}$$

We could show that still

$$\{\hat{\gamma}_k, \hat{\gamma}_k^\dagger\} = \{\bar{u}_k \hat{c}_k + \bar{v}_k \hat{c}_{-k}^\dagger,\ u_k \hat{c}_k^\dagger + v_k \hat{c}_{-k}\} = |u_k|^2 + |v_k|^2 = 1,$$

so $\hat{\gamma}$ is a fermion. Calculate commutators? But they are fermions!

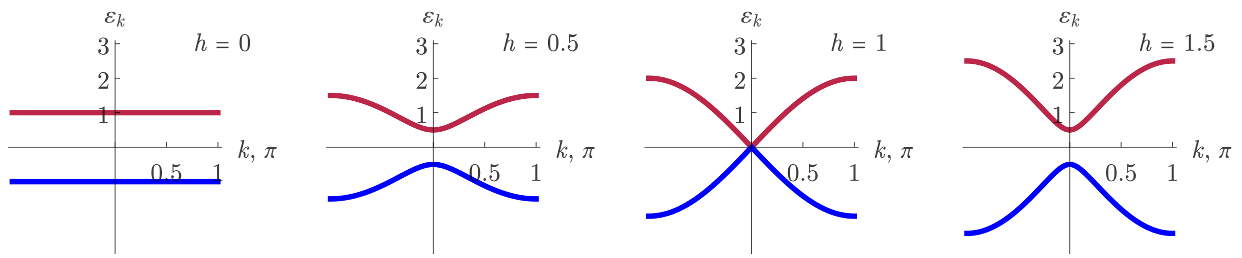


Figure 1: TFIM dispersion with different magnetic fields h with $J = 1$

3. (a) Ground state we could find in $\hat{H}_0$ such that $\hat{\gamma}_k |\text{gs}\rangle = 0\ \forall k$. As in BCS theory we could start from some state (not orthogonal $|\text{gs}\rangle$), apply $\hat{\gamma}_k$ and normalize, coming to the

$$|\text{gs}\rangle = \frac{\prod_k \hat{\gamma}_{-k}\hat{\gamma}_k}{\|\prod_k \hat{\gamma}_{-k}\hat{\gamma}_k |0\rangle\|} |0\rangle = \prod_{k \in \mathcal{K}_0^+} \left(u_k + v_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger\right)|0\rangle, \qquad E_0 = -\sum_{k\in\mathcal{K}_0^+} \varepsilon_k,$$

with $|0\rangle \sim |\downarrow \ldots \downarrow\rangle$ – vacuum for the original fermions $\hat{c}_k |0\rangle = 0\ \forall k$. If we want to continue exist in separated Hilbert space, than elementary excitation should save parity

$$\hat{\gamma}_{k_1}^\dagger \hat{\gamma}_{k_2}^\dagger |\text{gs}\rangle = \hat{c}_{k_1}^\dagger \hat{c}_{k_2}^\dagger \prod_{k \neq |k_1|, |k_2|}^{K_0^+} \left(\bar{u}_k - \bar{v}_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger\right)|0\rangle .$$

Going to the even amount of fermions we could apply even amount of $\hat{\gamma}_k$ to the $|\text{gs}\rangle$.

(b) Gap between minimal exitation and $|\text{gs}\rangle$ is $\varepsilon_{k=0}$, and gap in ε_k disappear at $h/J = 1$ (fig. 1). Interesting to plot all $\hat{H}$ eigenvalues and see what is happening in the same values of h (fig. 2).

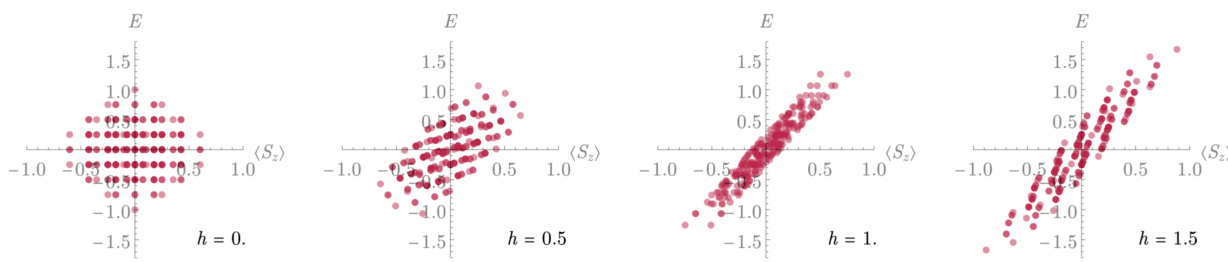


Figure 2: Eigenvalues of $\hat{H}$ as a function of $\langle S_z \rangle$

4. Consider ξ as
$$f(r) = \left\langle \sigma_j^z \sigma_{j+r} \right\rangle \propto e^{-r/\xi},$$
so we could estimate it numerically (fig. 3). We have finite L that strongly affects ξ estimation, but definitely something interesting happens at $h = h_\mathrm{c} = 1$.

   We know that
$$\frac{1}{E_\mathrm{gap}} \propto \frac{1}{\varepsilon_{k=0}} \propto \xi^z \propto (h - h_\mathrm{c})^{-\nu z},$$
and from (2) at $k = 0$ we have $E_\mathrm{gap} \propto h - 1$, than $h_\mathrm{c} = 1$ and $\nu z = 1$.

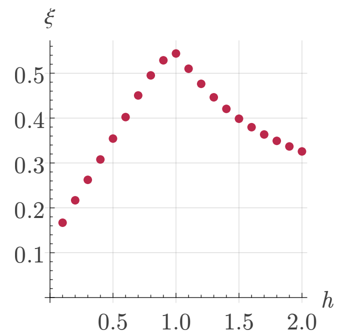


Figure 3: Correlation radius ξ as a function of external magnetic field h at $L = 20$, ground state