Some Majumdar-Ghosh Notes

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1 Majumdar-Ghosh Model

1.1 Clebsch-Gordan Preliminaries

Setup: 1-dimensional spin-1/2 $D^{(1/2)}$ chain. The Hamiltonian is given for a real parameter $J \in \mathbb{R}$:

$$\begin{aligned} H &= J \sum_{j=1}^{N-2} h^{(MG)}_{j,j+1,j+2} \\ &= J \sum_{j=1}^{N-2} 2\vec{S}_j \cdot \vec{S}_{j+1} + \vec{S}_j \cdot \vec{S}_{j+2} \end{aligned} \tag{1.1}$$

We recall a useful fact from the Heisenberg interaction (see Quantum Spin Systems: Proving things to myself (Chap. 10)). Note that we define spin matrices S^i by taking a representation π of the Lie algebra $\mathfrak{su}_2$ and scaling the standard Pauli matrices $\sigma^1, \sigma^2, \sigma^3$:

$$\pi\left(\frac{1}{2}\sigma^i\right) = S^i, \qquad i = 1, 2, 3$$

This tells us that the Heisenberg interaction $\vec{S}_j \cdot \vec{S}_{j+1}$ can be expressed as

$$h = \left(\frac{1}{2}\vec{\sigma}_j\right) \cdot \left(\frac{1}{2}\vec{\sigma}_{j+1}\right) = \frac{1}{4}(2T_{j,j+1} - \mathbb{1}) \tag{1.2}$$

where $T_{j,j+1}$ denotes the transposition operator on sites $j, j+1$: $T_{j,j+1}(u \otimes v) = v \otimes u$. It is worth pausing to note something about this interaction: Clebsch-Gordan decomposition of two neighboring spin-1/2 sites $\mathbb{C}^2 \otimes \mathbb{C}^2$ has

$$D^{(1/2)} \otimes D^{(1/2)} \cong D^{(1)} \oplus D^{(0)}, \qquad \Big(= \mathrm{Sym}(\mathbb{C}^2 \otimes \mathbb{C}^2) \oplus \mathrm{Alt}(\mathbb{C}^2 \otimes \mathbb{C}^2)\Big)$$

i.e. $D^{(1)} = \mathrm{Sym}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ consists of symmetric vectors $\{\left|\uparrow\uparrow\right\rangle, \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right), \left|\downarrow\downarrow\right\rangle\}$ and $D^{(0)} = \mathrm{Alt}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ consists of the singlet vector, the antisymmetric $\phi = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$. Observe that the transposition operator T is block-diagonalized by the decomposition $D^{(1)} \oplus D^{(0)}$, and if we let $P^{(1)}$ be the orthogonal projection on $D^{(1)}$ and $P^{(0)}$ for $D^{(0)}$,

$$\begin{aligned} T|_{D^{(0)}} &= T|_{\mathrm{Alt}(\mathbb{C}^2 \otimes \mathbb{C}^2)} = -P^{(0)} \\ T|_{D^{(1)}} &= T|_{\mathrm{Sym}(\mathbb{C}^2 \otimes \mathbb{C}^2)} = P^{(1)} \end{aligned}$$

So we can block-diagonalize the Heisenberg interaction on $D^{(1)} \oplus D^{(0)}$ so that

$$\begin{aligned} h_{j,j+1} &= \frac{1}{4}\left(2T_{j,j+1} - \mathbb{1}\right) \\ &= \frac{1}{4}\Big(2(P^{(1)} - P^{(0)}) - (P^{(1)} + P^{(0)})\Big) \\ &= \frac{1}{4}P^{(1)} - \frac{3}{4}P^{(0)} \end{aligned}$$

Can we do somthing similar for the Majumdar-Ghosh Hamiltonian? We consider the Clebsch-Gordan decomposition:

$$\begin{aligned} D^{(1/2)} \otimes D^{(1/2)} \otimes D^{(1/2)} &\cong D^{(1/2)} \otimes \left(D^{(1)} \oplus D^{(0)}\right) \\ &\cong \left(D^{(1/2)} \otimes D^{(1)}\right) \oplus \left(D^{(1/2)}\right) \\ &\cong D^{(3/2)} \oplus D^{(1/2)} \oplus D^{(1/2)} \end{aligned}$$

Let's think a bit about this decomposition and find bases for these subspaces in terms of tensor products of $|\uparrow\rangle, |\downarrow\rangle$ (which are eigenspaces of the spin operator $J_3 = \text{diag}(3/2, 1/2, -1/2, -3/2)$ which counts total spin, and the lowering operator J_- allows us to move within these eigenspaces). We opt to not normalize.

$$\begin{aligned} \text{Spin-3/2 } D^{(3/2)} &: \{|\uparrow\uparrow\uparrow\rangle,\ \ |\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle,\ \ |\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle,\ \ |\downarrow\downarrow\downarrow\rangle\} \\ \text{Spin-1/2 } D^{(1/2)} &: \{|\uparrow\uparrow\downarrow\rangle - 2\,|\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle,\ \ -|\downarrow\downarrow\uparrow\rangle + 2\,|\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\rangle\} \\ \text{Spin-1/2' } D'^{(1/2)} &: \{|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle,\ \ |\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\rangle\} \end{aligned} \tag{1.3}$$

1.2 Transposition operators: the key to MG

1.2.1 Transposition operators on $D^{(1/2)} \otimes D^{(1/2)} \otimes D^{(1/2)} \cong D^{(3/2)} \oplus D^{(1/2)} \oplus D^{(1/2)}$

We now study how the transposition operators act on these spaces by studying their action on the bases (1.3). Here are the most important findings, in short:

$$\begin{aligned} \text{Spin-3/2 } D^{(3/2)} &: T_{j,j+1}\Big|_{D^{(3/2)}} = \mathbb{1}, \qquad T_{j+1,j+2}\Big|_{D^{(3/2)}} = \mathbb{1}, \qquad T_{j,j+2}\Big|_{D^{(3/2)}} = \mathbb{1} \\ \text{Spin-1/2 } D^{(1/2)} &: T_{j,j+1} + T_{j+1,j+2} + T_{j,j+2}\Big|_{D^{(1/2)}} = 0 \\ \text{Spin-1/2' } D'^{(1/2)} &: T_{j,j+1} + T_{j+1,j+2} + T_{j,j+2}\Big|_{D'^{(1/2)}} = 0 \end{aligned} \tag{1.4}$$

Taken together, this means that

$$3P^{(3/2)}_{j,j+1,j+2} = T_{j,j+1} + T_{j+1,j+2} + T_{j,j+2} \tag{1.5}$$

We will compute this in a moment. But note that while transposition operators are block-diagonal with respect to $D^{(3/2)} \oplus (V)$ where $V = D^{(1/2)} \oplus D^{(1/2)}$, they do not respect the decomposition $D^{(1/2)} \oplus D^{(1/2)}$: for instance, see that $T_{j,j+1}\left(|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle\right) = |\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle \notin D^{(1/2)}$. Only their sum does. Let's compute to see this, choosing to look at the Hilbert space of 3 adjacent spins labeled 1,2,3 (so $j = 1, j+1 = 2, j+2 = 3$)

The spin-3/2 subspace $D^{(3/2)}$. It is clear just by looking at these basis elements that on this space, transposition operators act as the identity due to symmetry.

The spin-1/2 subspace $D^{(1/2)}$. On the first basis element:

$$\begin{aligned} \left(T_{1,2} + T_{2,3} + T_{1,3}\right)&\left(|\uparrow\uparrow\downarrow\rangle - 2\,|\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle\right) \\ &= |\uparrow\uparrow\downarrow\rangle - 2\,|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle \\ &\quad + |\uparrow\downarrow\uparrow\rangle - 2\,|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle \\ &\quad + |\downarrow\uparrow\uparrow\rangle - 2\,|\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle \\ &= 0 \end{aligned}$$

and the other element is basically the same, after flipping all the spins.

The spin-1/2' subspace $D'^{(1/2)}$. On the first basis element:

$$\begin{aligned}\big(T_{1,2}+T_{2,3}+T_{1,3}\big)\big(|\uparrow\uparrow\downarrow\rangle-|\downarrow\uparrow\uparrow\rangle\big)\\ &=|\uparrow\uparrow\downarrow\rangle-|\uparrow\downarrow\uparrow\rangle\\ &\quad+|\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\rangle\\ &\quad+|\downarrow\uparrow\uparrow\rangle-|\uparrow\uparrow\downarrow\rangle\\ &=0\end{aligned}$$

and the other element is basically the same, after flipping all the spins.

Altogether, this will show us that the Majumdar-Ghosh hamiltonian is a sum of projectors onto spin-3/2 subspaces, after subtracting a scalar multiple of the identity to make the the ground state energy zero and noting the role of boundary terms. To see why, we do a quick computation using (1.2) to relate spin matrices and transposition operators

$$\begin{aligned}\vec{S}_1\cdot\vec{S}_2+\vec{S}_1\cdot\vec{S}_3+\vec{S}_2\cdot\vec{S}_3&=\frac{1}{4}\left(2T_{1,2}-\mathbb{1}+2T_{1,3}-\mathbb{1}+2T_{2,3}-\mathbb{1}\right)\\ &=\frac{1}{2}(T_{1,2}+T_{1,3}+T_{2,3})-\frac{3}{4}\mathbb{1}\\ (1.5)\qquad &=\frac{3}{2}P^{(3/2)}_{1,2,3}-\frac{3}{4}\mathbb{1}\end{aligned}\tag{1.6}$$

Plugging this into a small example chain, say $N=5$, we can use (1.1) and ignore the J scalar out front and compute:

$$\begin{aligned}H&=\sum_{j=1}^{3}2\vec{S}_j\cdot\vec{S}_{j+1}+\vec{S}_j\cdot\vec{S}_{j+2}\\ &=2\vec{S}_1\cdot\vec{S}_2+\vec{S}_1\cdot\vec{S}_3+2\vec{S}_2\cdot\vec{S}_3+\vec{S}_2\cdot\vec{S}_4+2\vec{S}_3\cdot\vec{S}_4+\vec{S}_3\cdot\vec{S}_5\\ &=\vec{S}_1\cdot\vec{S}_2+\left(\vec{S}_1\cdot\vec{S}_2+\vec{S}_1\cdot\vec{S}_3+\vec{S}_2\cdot\vec{S}_3\right)+\left(\vec{S}_2\cdot\vec{S}_3+\vec{S}_2\cdot\vec{S}_4+\vec{S}_3\cdot\vec{S}_4\right)+\left(\vec{S}_3\cdot\vec{S}_4+\vec{S}_3\cdot\vec{S}_5+\vec{S}_4\cdot\vec{S}_5\right)-\vec{S}_4\cdot\vec{S}_5\\ (1.6)\qquad&=\vec{S}_1\cdot\vec{S}_2+\left(\frac{3}{2}P^{(3/2)}_{1,2,3}-\frac{3}{4}\mathbb{1}+\frac{3}{2}P^{(3/2)}_{2,3,4}-\frac{3}{4}\mathbb{1}+\frac{3}{2}P^{(3/2)}_{3,4,5}-\frac{3}{4}\mathbb{1}\right)-\vec{S}_4\cdot\vec{S}_5\\ &=\vec{S}_1\cdot\vec{S}_2-\vec{S}_4\cdot\vec{S}_5+\sum_{j=1}^{3}\left(\frac{3}{2}P^{(3/2)}_{j,j+1,j+2}-\frac{3}{4}\mathbb{1}\right)\end{aligned}$$

Thus, our Hamiltonian for finite chains is

$$\begin{aligned}H_{[1,N]}&=\sum_{j=1}^{N-2}2\vec{S}_j\cdot\vec{S}_{j+1}+\vec{S}_j\cdot\vec{S}_{j+2}\\ &=\vec{S}_1\cdot\vec{S}_2-\vec{S}_{N-1}\cdot\vec{S}_N+\sum_{j=1}^{N-2}\left(\frac{3}{2}P^{(3/2)}_{j,j+1,j+2}-\frac{3}{4}\mathbb{1}\right)\end{aligned}\tag{1.7}$$

We can adjust the ground state energy to be zero and make this Hamiltonian nonnegative definite by translating the spectrum up by adding $\frac{3}{4}\mathbb{1}$ factors to each term in the sum:

$$\widetilde{H}_{[1,N]}=(\textit{boundary terms})+\frac{3}{2}\sum_{j}^{N-2}P^{(3/2)}_{j,j+1,j+2}$$

Punchline: We can study the Majumdar-Ghosh Hamiltonian by studying $\widetilde{H}$, which amounts to studying sums of $P^{(3/2)}_{j,j+1,j+2}$.

Note: Since the transposition operator $T_{i,j}$ commutes with on-site representations of $GL(n)$, it commutes with operators $R_g\otimes\cdots\otimes R_g$, i.e. if $R_g\in GL(n)$ a representation of an element $g\in G$, $[T_{1,2},R_g\otimes R_g]=0$. In particular $O(n)$, this model has $O(n)$ symmetry.

1.2.2 Casimir: Another way to see MG as a sum of spin-3/2 projectors

For greater understanding, we consider a more Lie-algebraic view of the Majumdar-Ghosh Hamiltonian. The result will be exactly the same as in the section on transposition operators (1.2). Again, for readability, let's do everything on three sites $j = 1, j+1 = 2, j+2 = 3$, but it works more generally.

First, recall from Clebsch-Gordan theory (see AKLT notes) that the quadratic Casimir $\mathbf{S}^2$ on an irreducible spin-s representation $D^{(s)}$ commutes with the generators of the Lie Algebra and so by Schur (and some commutator shenanigans):

$$\begin{aligned}\mathbf{S}^2 &= (S^1)^2 + (S^2)^2 + (S^3)^2 \\ &= s(s+1)\mathbb{1}\end{aligned} \tag{1.8}$$

We will now compute the Casimir C in two ways, inspired by a useful expression in Caspers, Emmett, Magnus 1984. Recall to perform this computation that spins at different sites commute: $[S_i^{(\cdot)}, S_j^{(\cdot)}] = 0$ for $i \neq j$, and don't forget the notation, e.g. $S_3^1 = \mathbb{1} \otimes \mathbb{1} \otimes S^1$, so the generators of the spin-1/2 tensor product representation on 3 sites are the sums $S_1^i + S_2^i + S_3^i = S^i \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes S^i \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes S^i$:

$$\begin{aligned} C &:= (S_1^1 + S_2^1 + S_3^1)^2 + (S_1^2 + S_2^2 + S_3^2)^2 + (S_1^3 + S_2^3 + S_3^3)^2 \\ &= \mathbf{S}_1^2 + \mathbf{S}_2^2 + \mathbf{S}_3^2 + 2\vec{S}_1 \cdot \vec{S}_2 + 2\vec{S}_2 \cdot \vec{S}_3 + 2\vec{S}_1 \cdot \vec{S}_3 \\ (*) \qquad &= \frac{3}{4}\mathbb{1} + \frac{3}{4}\mathbb{1} + \frac{3}{4}\mathbb{1} + 2(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_3) \\ &= \frac{9}{4}\mathbb{1} + 2(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_3) \end{aligned} \tag{1.9}$$

where $(*)$ holds since $\mathbf{S}^2$ is the Casimir element for the irreducible representation $D^{(1/2)}$, and we apply it using (1.8) to individual tensor factors, e.g.

$$\mathbf{S}_2^2 = \mathbb{1} \otimes \mathbf{S}^2 \otimes \mathbb{1} = \mathbb{1} \otimes \left[\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right)\mathbb{1}\right] \otimes \mathbb{1}$$

Note before proceeding to the second computation that the final term $\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_3$ is the term we computed before and saw was the spin-3/2 projector.

Now, to the other computation, which recognizes C as the Casimir operator on the full spin-1/2 tensor product representation on three sites $D^{(1/2)} \otimes D^{(1/2)} \otimes D^{(1/2)}$ and then applies (1.8) to each irreducible subrepresentation from Clebsch-Gordan in $D^{(3/2)} \oplus D^{(1/2)} \oplus D'^{(1/2)}$:

$$\begin{aligned} C &= \frac{3}{2}\left(\frac{3}{2}+1\right)P^{(3/2)} + \frac{1}{2}\left(\frac{1}{2}+1\right)P^{(1/2)} + \frac{1}{2}\left(\frac{1}{2}+1\right)P'^{(1/2)} \\ &= \frac{15}{4}P^{(3/2)} + \frac{3}{4}P^{(1/2)} + \frac{3}{4}P'^{(1/2)} \\ &= \frac{12}{4}P^{(3/2)} + \frac{3}{4}\mathbb{1} \end{aligned} \tag{1.10}$$

Now, we can combine (1.9) and (1.10):

$$\frac{9}{4}\mathbb{1} + 2(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_3) = \frac{12}{4}P^{(3/2)} + \frac{3}{4}\mathbb{1}$$

and do a bit of algebra to obtain:

$$\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_1 \cdot \vec{S}_3 = \frac{3}{2}P^{(3/2)} - \frac{3}{4}\mathbb{1}$$

1.3 Ground states for chains of length 3 and 4

Now, as a step to uncovering the ground states of the Majumdar-Ghosh Hamiltonian, we focus our attention to this decomposition, which will allow us to show frustration-freeness (*CHECK THIS*)

1.3.1 Ground states of 3-site chain

We will show that the 3-site chain Hamiltonian (after ignoring boundary terms, so just $P^{(3/2)}_{j,j+1,j+2}$) has a 4-dimensional kernel. We begin by observing the following decomposition, hinted at earlier:

$$\begin{aligned} D^{(1/2)} \otimes D^{(1/2)} \otimes D^{(1/2)} &\cong D^{(1/2)} \otimes (D^{(1)} \oplus D^{(0)}) \cong (D^{(1)} \oplus D^{(0)}) \otimes D^{(1/2)} \\ &\cong \left(D^{(1/2)} \otimes D^{(1)}\right) \oplus \left(D^{(1/2)} \otimes D^{(0)}\right) \\ &\cong \left(D^{(1)} \otimes D^{(1/2)}\right) \oplus \left(D^{(0)} \otimes D^{(1/2)}\right) \end{aligned}$$

We will find that the

In the decomposition $D^{(1/2)} \otimes D^{(1/2)} \cong D^{(1)} \oplus D^{(0)}$, we refer to the symmetric elements of $D^{(1)}$ as triplets and the antisymmetric element of $D^{(0)}$ as a singlet. Let ϕ denote the singlet, eg $\phi = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \in D^{(0)}$. Consider the action of the projector $P^{(3/2)}_{j,j+1,j+2}$ on the subspace contained within three adjacent sites $\mathbb{C}^2 \otimes D^{(0)} \subseteq D^{(1/2)} \otimes \left(D^{(1)} \oplus D^{(0)}\right)$:

$$\begin{aligned} 3P^{(3/2)}_{j,j+1,j+2}\left(|\uparrow\rangle \otimes \phi\right) &= (T_{j,j+1} + T_{j,j+2} + T_{j+1,j+2})(|\uparrow\rangle \otimes \phi) \\ &= \frac{1}{\sqrt{2}}(T_{j,j+1} + T_{j,j+2} + T_{j+1,j+2})\left(|\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle\right) - \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle\right) \\ &= 0 \\ 3P^{(3/2)}_{j,j+1,j+2}\left(|\downarrow\rangle \otimes \phi\right) &= (T_{j,j+1} + T_{j,j+2} + T_{j+1,j+2})(|\downarrow\rangle \otimes \phi) \\ &= 0 \end{aligned}$$

So, $P^{(3/2)}_{j,j+1,j+2}$ is 0 on $\mathbb{C}^2 \otimes D^{(0)}$, and we can similarly show that $P^{(3/2)}_{j,j+1,j+2}$ is 0 on $D^{(0)} \otimes \mathbb{C}^2$. Taken together, this means that

$$\operatorname{span}\left[\{\mathbb{C}^2 \otimes \phi\} \cup \{\phi \otimes \mathbb{C}^2\}\right] \subseteq \ker(P^{(3/2)}_{j,j+1,j+2})$$

But in fact, the set on the left is 4-dimensional, which can be seen by looking at explicit bases and noting that all constituent vectors are mutually orthogonal:

$$\begin{aligned} \operatorname{span}\{\mathbb{C}^2 \otimes \phi\} &= \operatorname{span}\{|\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle\,,\ \ |\downarrow\uparrow\downarrow\rangle - |\downarrow\downarrow\uparrow\rangle\} \\ \operatorname{span}\{\phi \otimes \mathbb{C}^2\} &= \operatorname{span}\{|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle\,,\ \ |\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle\} \end{aligned}$$

and since $\ker P^{(3/2)}_{j,j+1,j+2} \cong D^{(1/2)} \oplus D^{(1/2)}$, the kernel is 4-dimensional as well. Thus,

$$\ker(P^{(3/2)}_{j,j+1,j+2}) = \operatorname{span}\left[\{\mathbb{C}^2 \otimes \phi\} \cup \{\phi \otimes \mathbb{C}^2\}\right] \tag{1.11}$$

So the Hamiltonian for the chain of length 3 (ignoring boundary terms) has a 4-dimensional kernel.

1.3.2 Ground states of 4-site chain

Now, we will show that the 4-site chain Hamiltonian $P^{(3/2)}_{1,2,3} + P^{(3/2)}_{2,3,4}$ has a 5-dimensional kernel, spanned by $\phi \otimes \phi$ and $\mathbb{C}^2 \otimes \phi \otimes \mathbb{C}^2$.

$$
\begin{aligned}
\sqrt{2}\left(3P^{(3/2)}_{1,2,3}+3P^{(3/2)}_{2,3,4}\right)(\phi\otimes\phi) &= \sqrt{2}(T_{1,2}+T_{1,3}+2T_{2,3}+T_{2,4}+T_{3,4})(\phi\otimes\phi)\\
&= (T_{1,2}+T_{1,3}+2T_{2,3}+T_{2,4}+T_{3,4})(|{\uparrow\downarrow\uparrow\downarrow}\rangle-|{\downarrow\uparrow\uparrow\downarrow}\rangle-|{\uparrow\downarrow\downarrow\uparrow}\rangle+|{\downarrow\uparrow\downarrow\uparrow}\rangle)\\
&= \ \ |{\downarrow\uparrow\uparrow\downarrow}\rangle-|{\uparrow\downarrow\uparrow\downarrow}\rangle-|{\downarrow\uparrow\downarrow\uparrow}\rangle+|{\uparrow\downarrow\downarrow\uparrow}\rangle\\
&\quad+|{\uparrow\downarrow\uparrow\downarrow}\rangle-|{\uparrow\uparrow\downarrow\downarrow}\rangle-|{\downarrow\downarrow\uparrow\uparrow}\rangle+|{\downarrow\uparrow\downarrow\uparrow}\rangle\\
&\quad+2\left(|{\uparrow\uparrow\downarrow\downarrow}\rangle-|{\downarrow\uparrow\uparrow\downarrow}\rangle-|{\uparrow\downarrow\downarrow\uparrow}\rangle+|{\downarrow\downarrow\uparrow\uparrow}\rangle\right)\\
&\quad+|{\uparrow\downarrow\uparrow\downarrow}\rangle-|{\downarrow\downarrow\uparrow\uparrow}\rangle-|{\uparrow\uparrow\downarrow\downarrow}\rangle+|{\downarrow\uparrow\downarrow\uparrow}\rangle\\
&\quad+|{\uparrow\downarrow\downarrow\uparrow}\rangle-|{\downarrow\uparrow\downarrow\uparrow}\rangle-|{\uparrow\downarrow\uparrow\downarrow}\rangle+|{\downarrow\uparrow\uparrow\downarrow}\rangle\\
&= 0
\end{aligned}
$$

Now for the 4-dimensional one: (NEED TO VERIFY, BUT PRELIMINARY COMPUTATIONS SUGGEST IT WORKS)

$$
\begin{aligned}
\left(3P^{(3/2)}_{1,2,3}+3P^{(3/2)}_{2,3,4}\right)(\mathbb{C}^2\otimes\phi\otimes\mathbb{C}^2) &= (T_{1,2}+T_{1,3}+2T_{2,3}+T_{2,4}+T_{3,4})(\mathbb{C}^2\otimes\phi\otimes\mathbb{C}^2)\\
&=
\end{aligned}
$$

1.4 Ground states of k-sites: Frustration freeness

We will now use frustration-freeness to prove that for a chain with k-sites, the Hamiltonian has a 4-dimensional kernel for odd k and a 5-dimensional kernel for even k. Recall that since $P^{(3/2)}_{j,j+1,j+2}$ is a positive semidefinite operator, and so is $P^{(3/2)}_{j,j+1,j+2}\otimes\mathbb{1}$, we have that

$$
\ker\left(\sum_{j=1}^{N-2}P^{(3/2)}_{j,j+1,j+2}\right)=\bigcap_{j=1}^{N-2}\ker(P^{(3/2)}_{j,j+1,j+2})
$$

So we can study the ground states of the full chain by studying

1.5 Dimerization: example in a chain of length 4

The signature of dimerization is the expectation of the projection operator $P^{(0)}_{j,j+1}$, which detects singlets on neighboring sites, which is sensible since we can decompose as following:

$$
\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2\cong\mathbb{C}^2\otimes\left(D^{(1)}\oplus D^{(0)}\right)\otimes\mathbb{C}^2
$$

There will be two weak-$*$ limits of ground states, and this expectation will be different between the two.

Consider for sake of example the chain of length 4, with sites labeled $-1,0,1,2$. As we described before, there are 5 ground state vectors

$$
\ker H_{[-1,2]}=\operatorname{span}\left[\{\phi\otimes\phi\}\cup\{\mathbb{C}^2\otimes\phi\otimes\mathbb{C}^2\}\right]
$$

We can pictorially see that the two ground states will correspond to $\phi\otimes\phi$ and $\{\mathbb{C}^2\otimes\phi\otimes\mathbb{C}^2\}$, with the only reason for their dimensional difference being the open boundary conditions: bonds correspond to singlets ϕ, and unconnected sites to copies of $\mathbb{C}^2$. If we use $[i,i+1]$ to denote a singlet bond between sites $i,i+1$,

First, $\phi\otimes\phi=[-1,0][1,2]$:

Now, $\mathbb{C}^2\otimes\phi\otimes\mathbb{C}^2=\mathbb{C}^2\otimes[0,1]\otimes\mathbb{C}^2$:

We wish to compute the expectations of $P_{0,1}^{(0)}$ for any state in these subspaces. We choose this observable because $P^{(0)}$, below, is the rank-1 projector on the singlet ϕ:

$$\begin{aligned} P^{(0)} &= \frac{1}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\left(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right) \\ &= \frac{1}{2}\left(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\right) \end{aligned} \tag{1.12}$$

and so $P_{0,1}^{(0)}$ detects a singlet bond between sites 0 and 1.

Towards calculating the expectation, let's decompose the Hilbert space into $\mathcal{H} = \mathcal{H}_{-1} \otimes \mathcal{H}_{[0,1]} \otimes \mathcal{H}_2$ and compute reduced density matrices restricted to the subsystem on sites $\{0,1\}$ for these two pure states ρ and σ, corresponding respectively to the unit vectors $\phi \otimes \phi$ and $|\alpha\rangle \otimes \phi \otimes |\beta\rangle \in \mathbb{C}^2 \otimes \phi \otimes \mathbb{C}^2$:

$$\begin{aligned} \rho_{[0,1]} &= \mathrm{Tr}_{\{-1\}\cup\{2\}}\left(|\phi\rangle \otimes |\phi\rangle\right)\left(\langle\phi| \otimes \langle\phi|\right) \\ &= \sum_{i,j\in\{\uparrow,\downarrow\}} \langle i| \otimes \mathbb{1}_2 \otimes \langle j| \; \frac{1}{4}\Big(\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right] \otimes \left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right] \Big)\Big(\left[\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right] \otimes \left[\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right] \Big) \; |i\rangle \otimes \mathbb{1}_2 \otimes |j\rangle \\ &= \frac{1}{4}\Big(\left[|\downarrow\rangle \otimes -|\downarrow\rangle\right]\left[\langle\downarrow| \otimes -\langle\downarrow|\right] \Big) + \frac{1}{4}\Big(\left[|\downarrow\rangle \otimes |\uparrow\rangle\right]\left[\langle\downarrow| \otimes \langle\uparrow|\right] \Big) \\ &\quad + \frac{1}{4}\Big(\left[-|\uparrow\rangle \otimes -|\downarrow\rangle\right]\left[-\langle\uparrow| \otimes -\langle\downarrow|\right] \Big) + \frac{1}{4}\Big(\left[-|\uparrow\rangle \otimes |\uparrow\rangle\right]\left[-\langle\uparrow| \otimes \langle\uparrow|\right] \Big) \\ &= \frac{1}{4}\left(|\downarrow\downarrow\rangle\langle\downarrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\uparrow\uparrow\rangle\langle\uparrow\uparrow|\right) \\ &= \frac{1}{4}\left(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\right) \end{aligned} \tag{1.13}$$

And now for σ (which depends on $\alpha, \beta \in \mathbb{C}^2$, but these will wash out in the partial trace)

$$\begin{aligned} \sigma_{[0,1]} &= \mathrm{Tr}_{\{-1\}\cup\{2\}} |\alpha\rangle\langle\alpha| \otimes |\phi\rangle\langle\phi| \otimes |\beta\rangle\langle\beta| \\ &= |\phi\rangle\langle\phi| \end{aligned} \tag{1.14}$$

Now that we have the reduced density matrices, we can compute expectations in these ground states:

$$\begin{aligned} \left\langle \phi \otimes \phi, P_{0,1}^{(0)} \phi \otimes \phi \right\rangle &= \mathrm{Tr}\rho P_{0,1}^{(0)} \\ &= \mathrm{Tr}\rho_{[0,1]} P^{(0)} \\ \text{(1.13)} \qquad &= \frac{1}{4}\left(\langle\uparrow\uparrow| P^{(0)} |\uparrow\uparrow\rangle + \langle\uparrow\downarrow| P^{(0)} |\uparrow\downarrow\rangle + \langle\downarrow\uparrow| P^{(0)} |\downarrow\uparrow\rangle + \langle\downarrow\downarrow| P^{(0)} |\downarrow\downarrow\rangle \right) \\ \text{(1.12)} \qquad &= \frac{1}{4}\left(0 + \frac{1}{2} + \frac{1}{2} + 0\right) \\ &= \frac{1}{4} \\ \left\langle \alpha \otimes \phi \otimes \beta, P_{0,1}^{(0)}(\alpha \otimes \phi \otimes \beta) \right\rangle &= \mathrm{Tr}\sigma P_{0,1}^{(0)} \\ &= \mathrm{Tr}\sigma_{[0,1]} P^{(0)} \\ &= \mathrm{Tr}\,|\phi\rangle\langle\phi| \; |\phi\rangle\langle\phi| \\ &= 1 \end{aligned} \tag{1.15}$$

This is really where we see dimerization–this "singlet detecting" observable.

1.6 Proving there are exactly two ground states for thermodynamic limit

We found the ground states for even and odd chain lengths, so now we will take limits to populate the weak-* limits

1.6.1 Correlation functions and the Thermodynamic Limit

We wish to pin down the ground states in the thermodynamic limit. Since any ground state is uniquely determined by its value on the algebra of local observables, we will take limits as ground states from above get arbitrarily long for fixed local observables. (*note: Bruno says that in this model, all ground states arise as weak-* limits of finite chain ground states. You may wonder whether there are infinite volume ground states that don't arise in this way–Bruno says it varies from case to case, with some easier than others. The formal definition of a state is a bit clumsy. Look at Naaijken's "Infinite lattices quantum spin systems" for GNS representations, which should address the core issue*)

Before proceeding, note that the product structure makes two point correlations between observables at sites i, j on the bases for ground states trivial any time i and j are not nearest neighbors (if they are, then it depends on whether they share a bond. Sharing a bond will generally lead to correlation). For instance, if we let $A_k \in M_2(\mathbb{C})$ and consider $\psi = \alpha \otimes \phi \in \text{span}(\mathbb{C}^2 \otimes \phi)$, a ground state for the chain $[1, 3]$, the correlation between sites 1 and 3 is 0:

$$\begin{aligned} R_{1,3} &= \langle\psi| A_1 \otimes \mathbb{1} \otimes A_3 |\psi\rangle - \langle\psi| A_1 \otimes \mathbb{1} \otimes \mathbb{1} |\psi\rangle \langle\psi| \mathbb{1} \otimes \mathbb{1} \otimes A_3 |\psi\rangle \\ &= \langle\alpha \otimes \phi| A_1 \otimes \mathbb{1} \otimes A_3 |\alpha \otimes \phi\rangle - \langle\alpha| A_1 |\alpha\rangle \langle\phi| \mathbb{1} \otimes A_3 |\phi\rangle \\ &= \langle\alpha| A_1 |\alpha\rangle \langle\phi| \mathbb{1} \otimes A_3 |\phi\rangle - \langle\alpha| A_1 |\alpha\rangle \langle\phi| \mathbb{1} \otimes A_3 |\phi\rangle \\ &= 0 \end{aligned}$$

But this is not the case if we take linear combinations of these ground states–we get cross terms that introduce correlations between the ends of the chain. It will turn out that these correlations decay exponentially fast, leaving only two infinite volume ground states: the one as a product of singlets between sites $i, i+1$ for i odd, and the one with products of singlets between $i, i+1$ for i even.

We can get a sufficient picture just by looking at odd chains.

1.6.2 Odd length chains

:

The general odd-n length chain ground state is $\psi = a \left|\alpha \otimes \phi^{\otimes(2l+n+2r)-1}\right\rangle + b \left|\phi^{\otimes(2l+n+2r)-1} \otimes \beta\right\rangle$, where $\alpha, \beta \in \mathbb{C}^2$ are unit vectors and $a, b \in \mathbb{C}$ with $|a|^2 + |b|^2 = 1$. Then if we consider the observable

$$A = \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r}, \qquad A_i \in M_2(\mathbb{C})$$

we can quickly compute the expectation in the state $|\psi\rangle$:

$$\begin{aligned} \langle\psi| A |\psi\rangle =& |a|^2 \left\langle \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \right\rangle \\ &+ \bar{a}b \left\langle \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \phi^{\otimes(2l+n+2r)-1} \otimes \beta \right\rangle \\ &+ a\bar{b} \left\langle \phi^{\otimes(2l+n+2r)-1} \otimes \beta \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \right\rangle \\ &+ |b|^2 \left\langle \phi^{\otimes(2l+n+2r)-1} \otimes \beta \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \phi^{\otimes(2l+n+2r)-1} \otimes \beta \right\rangle \\ =& \left\langle \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \right\rangle \\ &+ \left\langle \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \phi^{\otimes(2l+n+2r)-1} \otimes \beta \right\rangle \\ (FIXME - INDEXING) \qquad &+ |a|^2 \left\langle \phi^{\otimes(2l+n+2r)-1} \otimes \beta \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \alpha \otimes \phi^{\otimes(2l+n+2r)-1} \right\rangle \\ &+ \left\langle \phi^{\otimes(2l+n+2r)-1} \otimes \beta \middle| \mathbb{1}^{2l} \otimes A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}^{2r} \middle| \phi^{\otimes(2l+n+2r)-1} \otimes \beta \right\rangle \end{aligned}$$

Let's restrict our attention to the special observable $A_1 \otimes \cdots \otimes A_n = \mathbb{1}^{\otimes n}$, so we're just taking inner products. Moving from this observable to the others will be easy once we understand the correlation structure. The key difficulty is the cross terms between α and β–the first and last terms are product states, and so expectations of local observables can be computed exactly. The cross terms will decay exponentially, and the product states will survive, yielding our result.

First, a fundamental computation for chains of length 3. Let $\psi = a\left|\alpha \otimes \phi\right\rangle + b\left|\phi \otimes \beta\right\rangle$, $a, b \in \mathbb{C}$ with $|a| + |b| = 1$. Mimicking the above expression and splitting the inner product,

$$\begin{aligned}\left\langle\psi\right| \mathbb{1} \left|\psi\right\rangle = &|a|^2 \left\langle\alpha \otimes \phi\right| \mathbb{1} \left|\alpha \otimes \phi\right\rangle \\ &+ a\bar{b} \left\langle\phi \otimes \beta\right| \mathbb{1} \left|\alpha \otimes \phi\right\rangle \\ &+ \bar{a}b \left\langle\alpha \otimes \phi\right| \mathbb{1} \left|\phi \otimes \beta\right\rangle \\ &+ |b|^2 \left\langle\phi \otimes \beta\right| \mathbb{1} \left|\phi \otimes \beta\right\rangle\end{aligned} \tag{1.16}$$

The first and last terms split into products–this makes computing expectations of arbitrary observables puresl

Lemma 1.1.

$$\langle\alpha \otimes \phi|\phi \otimes \beta\rangle = -\frac{1}{2}\langle\alpha|\beta\rangle$$

Applying this to the reduced density matrix for either ground state, we see that they are orthogonal for any finite length! See Naaijkens to understand GNS stuff better