

AN INTRODUCTION TO QUANTUM SPIN SYSTEMS¹
NOTES FOR MA5020 (JOHN VON NEUMANN GUEST LECTURES)
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11.2. Frustration free spin chains with a unique Matrix Product ground state. We begin our discussion of general frustration free models in one dimension by stating a result about the structure of the ground states of frustration free spin chains. This will serve as motivation to analyzing in some detail the spin chains with unique MPS ground states and also set the stage for studying some interesting generalizations, such as models with multiple ground states, examples of frustration free chains for which the product structure is not expressed in terms of matrices but in terms of operators on an infinite-dimensional Hilbert space, and frustration free models in more than one dimension.

We start by considering spin systems on $\mathbb{Z}^+ = \{1, 2, \dots\}$, i.e., a half-infinite chain, with a d -dimensional Hilbert space $\mathcal{H}_x = \mathbb{C}^d$, at each site $x \in \mathbb{Z}^+$. We assume that $0 \leq h \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$ is a frustration free nearest neighbor interaction. By this we mean that the finite-volume Hamiltonians

$$H_{[1,L]} = \sum_{x=1}^{L-1} h_{x,x+1},$$

where $h_{x,x+1} = h \in \mathcal{A}_{[x,x+1]}$, have a non-trivial kernel for all $L \geq 2$. Let $\mathcal{G} = \ker h \subset \mathbb{C}^d \otimes \mathbb{C}^d$. Then the frustration free property is equivalent to

$$(11.20) \quad \bigcap_{x=1}^{L-1} \underbrace{\mathbb{C}^d \otimes \dots \otimes \mathbb{C}^d}_{x-1} \otimes \mathcal{G} \otimes \underbrace{\mathbb{C}^d \otimes \dots \otimes \mathbb{C}^d}_{L-1-x} \neq \{0\}, \text{ for all } L \geq 2.$$

The set of states η on $\mathcal{A}_{\mathbb{Z}^+}$ such that $\eta(h_{x,x+1}) = 0$, for $x = 1, \dots, L-1$, has weak-* limit points. Any such limiting state ω satisfies $\omega(h_{x,x+1}) = 0$ for all $x \in \mathbb{Z}^+$. We will call such states zero-energy states and, since they are defined as limits of finite-volume ground states, they are ground states in the sense of Definition 6.2. The set of zero-energy states is a face in the set of all states, meaning that any pure states appearing in the decomposition of a zero-energy state are also zero-energy states. This shows that the set of pure zero-energy states on $\mathcal{A}_{\mathbb{Z}^+}$ for a nearest neighbor interaction $h \geq 0$ such that $\mathcal{G} = \ker h$ satisfies (11.20), is non-empty. We have the following theorem about the structure of such states.

Theorem 11.3 ([22]). *Let $0 \leq h \in \mathcal{B}(\mathbb{C}^d \otimes \mathbb{C}^d)$ such that $\mathcal{G} = \ker h$ satisfies (11.20), and suppose ω is a pure state on $\mathcal{A}_{\mathbb{Z}^+}$ such that $\omega(h_{x,x+1}) = 0$, for all $x \geq 1$. Then, given an orthonormal basis $\{|i\rangle \mid i = 1, \dots, d\}$ of \mathbb{C}^d , there exists a Hilbert space \mathcal{K} , a unit vector $\Omega \in \mathcal{K}$, and a set of operators $V_1, \dots, V_d \in \mathcal{B}(\mathcal{K})$ for which:*

i) \mathcal{K} is the closed linear span of

$$\{V_{i_1} \cdots V_{i_n} \Omega \mid i_1, \dots, i_n \in \{1, \dots, d\} \text{ and } n \geq 0\}$$

ii) $\sum_{\alpha=1}^d V_{\alpha}^* V_{\alpha} = \mathbb{1}$.

iii) For all $n \geq 1, i_1, \dots, i_n, j_1, \dots, j_n \in \{1, \dots, d\}$, we have

$$(11.21) \quad \omega(|i_1, \dots, i_n\rangle \langle j_1, \dots, j_n|) = \langle V_{i_n} \cdots V_{i_1} \Omega, V_{j_n} \cdots V_{j_1} \Omega \rangle$$

iv) For every $\psi = \sum_{i,j=1}^d \psi_{i,j} |i, j\rangle \in \mathcal{G}^{\perp}$, we have

$$(11.22) \quad \sum_{i,j=1}^d \overline{\psi_{i,j}} V_j V_i = 0.$$

v) Define the operator $\hat{\mathbb{E}} : \mathcal{B}(\mathcal{K}) \rightarrow \mathcal{B}(\mathcal{K})$ by

$$(11.23) \quad \hat{\mathbb{E}}(X) = \sum_{i=1}^d V_i^* X V_i, \quad \text{for all } X \in \mathcal{B}(\mathcal{K}).$$

Then, for any $X \in \mathcal{B}(\mathcal{K})$, $\hat{\mathbb{E}}(X) = X$ if and only if $X = \lambda \mathbb{1}$ for some $\lambda \in \mathbb{C}$.

In order to make the connection with the structure of the ground states we found for the AKLT model in the previous section, consider $\mathcal{K} = \mathbb{C}^2$, and define the maps $E_A : \mathcal{B}(\mathcal{K}) \rightarrow \mathcal{B}(\mathcal{K})$, for $A \in M_d$, by

$$\mathbb{E}_A(X) = \sum_{i,j=1}^d \langle i|A|j\rangle V_i^* X V_i = V^*(A \otimes X)V, \quad \text{for all } X \in \mathcal{B}(\mathcal{K}),$$

where $V : \mathcal{K} \rightarrow \mathbb{C}^d \otimes \mathcal{K}$ is the isometry defined by

$$V\varphi = \sum_{i=1}^d |i\rangle \otimes V_i\varphi.$$

Then,

$$(11.24) \quad \omega(A_1 \otimes \cdots \otimes A_n) = \text{Tr}|\Omega\rangle\langle\Omega|\mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n}(\mathbb{1}).$$

Since the space \mathcal{K} for the AKLT model is finite-dimensional, the operators V_i and the transfer operator $\hat{\mathbb{E}}$ are represented by matrices. Properties very similar to the ones we proved for the AKLT model in Section 11.1, follow from the product structure whenever $\dim \mathcal{K} < \infty$ without further assumptions. This will be shown in the next section. We will also prove a general result about the spectral gap of models with matrix product ground state.

11.3. Some properties of translation invariant matrix product states. In this section we derive some general properties of states of a form very similar to (11.24) under the additional assumption that $k = \dim \mathcal{K} < \infty$. This is the case of Matrix Product States (MPS). The operators V_i are now $k \times k$ matrices. Under the assumptions of Theorem 11.3 the transfer matrix $\hat{\mathbb{E}}$ has a simple eigenvalue 1. Its transpose, $\hat{\mathbb{E}}^T$ then also has a simple eigenvalue 1 and the Perron-Frobenius theory for completely positive maps (see Appendix ??) then implies that there is a unique density matrix $\rho \in M_k$ such that $\hat{\mathbb{E}}^T(\rho) = \rho$. Regarding ρ as a positive linear functional on M_k , we can express this by the relation

$$(11.25) \quad \rho(\hat{\mathbb{E}}(B)) = \rho(B), \quad B \in M_k.$$

By replacing $|\Omega\rangle\langle\Omega|$ by ρ in (11.24), we get expectations $\omega(A_1 \otimes \cdots \otimes A_n)$ that are translation invariant. Indeed, using $\hat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$ and (11.25) it is straightforward to verify that

$$(11.26) \quad \omega(A_1 \otimes \cdots \otimes A_n) = \omega(\mathbb{1} \otimes A_1 \otimes \cdots \otimes A_n) = \omega(A_1 \otimes \cdots \otimes A_n \otimes \mathbb{1}).$$

The positivity and normalization also follow directly from the definition. Therefore, the finite chain expressions

$$(11.27) \quad \omega(A_1 \otimes \cdots \otimes A_n) = \text{Tr}\rho\mathbb{E}_{A_1} \circ \cdots \circ \mathbb{E}_{A_n}(\mathbb{1}).$$

define a unique translation invariant state on $\mathcal{A}_{\mathbb{Z}}$.

In addition to the assumption that 1 is a simple eigenvalue of $\hat{\mathbb{E}}$, we will also assume in this section that all other eigenvalues of $\hat{\mathbb{E}}$ have modulus strictly less than one. This situation is referred as a transfer matrix with *trivial peripheral spectrum* or, equivalently, that $\hat{\mathbb{E}}$ is *primitive*. (see [71]). Eigenvalues of absolute value 1 other than a simple eigenvalue 1, in general correspond to states that are not pure but have a non-trivial decomposition into pure states.

If ρ is not faithful and has support projection P , then one can construct the same translation-invariant pure state by replacing V_i with Pv_iP , $i = 1, \dots, d$ (see [21]). In the sequel we will assume that $P = \mathbb{1}$, i.e., that $\rho > 0$, or work with the modified v_i if, originally, $P \neq \mathbb{1}$. In particular, the smallest eigenvalue of ρ is then strictly positive.

For any faithful state ρ , i.e., a density matrix with trivial kernel, we can define a non-degenerate inner product on M_k by

$$(11.28) \quad \langle A, B \rangle_\rho = \text{Tr} \rho A^* B \quad \text{for all } A, B \in M_k,$$

and let $\|\cdot\|_\rho$ denote the corresponding norm. Let $\rho_{\min} = \min \text{spec}(\rho)$. Since ρ is finite-dimensional, we have $\rho_{\min} > 0$. It follows that the norm $\|\cdot\|_\rho$ is equivalent to the Hilbert-Schmidt norm on M_k , $\|A\|_2 = \sqrt{\text{Tr} A^* A}$, i.e.

$$(11.29) \quad \|A\|_2^2 = \text{Tr}[A^* A] \leq \text{Tr} \left[\frac{\rho}{\rho_{\min}} A^* A \right] = \frac{1}{\rho_{\min}} \|A\|_\rho^2 \quad \text{for any } A \in M_k.$$

As in the case of the AKLT model, the trivial peripheral spectrum of $\hat{\mathbb{E}}$ implies that there exists $C > 0$ and $\lambda \in (0, 1)$ such that

$$(11.30) \quad a(n) := \left\| \hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho| \right\| \leq C\lambda^n.$$

Since $\hat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$, we have

$$(11.31) \quad \left\| \hat{\mathbb{E}}^{n+1} - |\mathbb{1}\rangle\langle\rho| \right\| = \left\| \hat{\mathbb{E}} \circ (\hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho|) \right\| \leq \left\| \hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho| \right\|$$

and therefore $a(n)$ is monotone decreasing in n .

The following maps $\Gamma_n : M_k \rightarrow \mathcal{H}_{[1,n]}$ generalize the maps $\psi^{(n)}(\cdot)$ of the AKLT model:

$$(11.32) \quad \Gamma_n(B) = \sum_{i_1, \dots, i_n} \text{Tr}[B v_{i_n} \cdots v_{i_1}] |i_1, \dots, i_n\rangle, \quad B \in M_k.$$

These are the Matrix Product Ground states for finite chains of length n . We will now study the vectors $\Gamma_n(B)$ and the linear subspace spanned by them in some detail. We begin with a lemma that estimates the inner product of two such vectors.

Lemma 11.4. *For any $B, C \in M_k$,*

$$(11.33) \quad |\langle \Gamma_n(B), \Gamma_n(C) \rangle - \langle B, C \rangle_\rho| \leq k a(n) \|B^*\|_2 \|C^*\|_2 \leq \frac{k}{\rho_{\min}} a(n) \|B\|_\rho \|C\|_\rho$$

Proof. Recall (11.32).

$$\begin{aligned} \langle \Gamma_n(B), \Gamma_n(C) \rangle &= \sum_{i_1, \dots, i_n} \overline{\text{Tr}[B v_{i_n} \cdots v_{i_1}]} \cdot \text{Tr}[C v_{i_n} \cdots v_{i_1}] \\ &= \sum_{i_1, \dots, i_n} \text{Tr}[v_{i_1}^* \cdots v_{i_n}^* B^*] \text{Tr}[C v_{i_n} \cdots v_{i_1}] \\ &= \sum_{\alpha, \beta} \sum_{i_1, \dots, i_n} \langle \alpha | v_{i_1}^* \cdots v_{i_n}^* B^* | \alpha \rangle \cdot \langle \beta | C v_{i_n} \cdots v_{i_1} | \beta \rangle \\ &= \sum_{\alpha, \beta} \langle \alpha | \hat{\mathbb{E}}^n (B^* | \alpha \rangle \langle \beta | C) | \beta \rangle \\ (11.34) \quad &= \sum_{\alpha, \beta} \langle \alpha | \mathbb{1} \rangle \langle \rho | (B^* | \alpha \rangle \langle \beta | C) | \beta \rangle + \sum_{\alpha, \beta} \langle \alpha | \left(\hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho| \right) (B^* | \alpha \rangle \langle \beta | C) | \beta \rangle, \end{aligned}$$

where we have used the indices α and β to denote summation over the orthonormal basis of \mathbb{C}^k . Now the first term above is clearly

$$(11.35) \quad \sum_{\alpha, \beta} \langle \alpha | \mathbb{1} | \beta \rangle \text{Tr}[\rho (B^* | \alpha \rangle \langle \beta | C)] = \text{Tr}[\rho B^* C] = \langle B, C \rangle_\rho$$

and the remainder can then be estimated by

$$(11.36) \quad \sum_{\alpha, \beta} \left\| \left| \hat{\mathbb{E}}^n - |\mathbb{1}\rangle\langle\rho| \right\| \|B^*|\alpha\rangle\| \|C^*|\beta\rangle\| \leq a(n)k \|B\|_2 \|C\|_2 \leq \frac{a(n)k}{\rho_{\min}} \|B\|_\rho \|C\|_\rho$$

where we have used both (11.29) and (11.42). \square

It is clear that in the special case of $C = B$, the above lemma yields:

$$(11.37) \quad \left| \|\Gamma_n(B)\|^2 - \|B\|_\rho^2 \right| \leq \frac{k}{\rho_{\min}} a(n) \|B\|_\rho^2$$

and if $\|B\|_\rho \neq 0$, then

$$(11.38) \quad \left| \frac{\|\Gamma_n(B)\|^2}{\|B\|_\rho^2} - 1 \right| \leq \frac{k}{\rho_{\min}} a(n)$$

Thus, if $k\rho_{\min}^{-1}a(n) < 1$, Γ_n is injective. Let us set $b(n) = k\rho_{\min}^{-1}a(n)$.

Let n_0 be the smallest integer such that Γ_n is injective for all $n \geq n_0$. We will refer to n_0 as the *injectivity length*.

As the ρ inner product is non-degenerate, a simple consequence of this bound is that Γ_n is eventually injective. In fact, the following corollary is immediate.

Corollary 11.5. *For any $B \in M_k$, the bound*

$$(11.39) \quad \|B\|_\rho \sqrt{1 - b(n)} \leq \|\Gamma_n(B)\| \leq \|B\|_\rho \sqrt{1 + b(n)}$$

holds for n sufficiently large. Here $\rho_{\min}b(n) = ka(n)$ and n large means $b(n) < 1$.

Proof of Corollary 11.5. The bound

$$(11.40) \quad \left| \|\Gamma_n(B)\|^2 - \|B\|_\rho^2 \right| \leq b(n) \|B\|_\rho^2$$

follows immediately from (??). If $B = 0$, there is nothing to prove. Otherwise, this bound can be re-written as

$$(11.41) \quad -b(n) \leq \frac{\|\Gamma_n(B)\|^2}{\|B\|_\rho^2} - 1 \leq b(n)$$

from which the above claim readily follows. \square

This result shows that Γ_n is injective for sufficiently large n , *i.e.* that there exists n_0 such that for all $n \geq n_0$, we have $\dim \text{ran} \Gamma_n = k^2$. One can also show that, if $\hat{\mathbb{E}}$ is primitive, regardless of the values of λ and ρ_{\min} , Γ_n is injective for $n \geq k^4$ [71].

Let $\alpha_1, \dots, \alpha_k$ be an orthonormal basis of \mathbb{C}^k . Using Cauchy-Schwarz, we then have the following pair of inequalities, which we will use to prove the next lemma:

$$(11.42) \quad \sum_{j=1}^k \|B^*\alpha_j\| \leq \sqrt{k} \sqrt{\sum_j \|B^*\alpha_j\|^2} = \sqrt{k} \|B^*\|_2 = \sqrt{k} \|B\|_2 \leq \sqrt{\frac{k}{\rho_{\min}}} \|B\|_\rho$$

for any $B \in M_k$.

Now consider three consecutive intervals (organized left-middle-right) with lengths ℓ , m , and r respectively. We wish to estimate the inner product of vectors $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C}^d)^{\otimes r}$ and $\psi \in (\mathbb{C}^d)^{\otimes \ell} \otimes \mathcal{G}_{m+r}$. If $m \geq n_0$, the maps Γ_{m+r} and $\Gamma_{\ell+m}$ are injective. Therefore there exist unique matrices $B_\varphi(k_1, \dots, k_r), B_\psi(i_1, \dots, i_\ell) \in M_k$, such that

$$(11.43) \quad \varphi = \sum_{k_1, \dots, k_r} \Gamma_{\ell+m}(B_\varphi(k_1, \dots, k_r)) \otimes |k_1, \dots, k_r\rangle$$

and similarly,

$$(11.44) \quad \psi = \sum_{i_1, \dots, i_\ell} |i_1, \dots, i_\ell\rangle \otimes \Gamma_{m+r}(B_\psi(i_1, \dots, i_\ell)).$$

It will be convenient to define

$$(11.45) \quad C_\varphi = \sum_{k_1, \dots, k_r} B_\varphi(k_1, \dots, k_r) \rho v_{k_1}^* \cdots v_{k_r}^* \rho^{-1}$$

and

$$(11.46) \quad D_\psi = \sum_{i_1, \dots, i_\ell} v_{i_1}^* \cdots v_{i_\ell}^* B_\psi(i_1, \dots, i_\ell)$$

It will be useful to use the following notations: $\mathbf{i} = (i_1, \dots, i_\ell)$, $\mathbf{j} = (j_1, \dots, j_m)$, $\mathbf{k} = (k_1, \dots, k_r)$, where each individual index takes value in $\{1, \dots, k\}$. We also define $v_{\mathbf{i}} = v_{i_\ell} \cdots v_{i_1}$, $v_{\mathbf{i}}^* = v_{i_1}^* \cdots v_{i_\ell}^*$, etc.

Lemma 11.6. *Suppose that m is large enough so that $b(m) < 1$. (Thus $m \geq n_0$.) Let $\ell \geq 0$ and $r \geq 0$. For every $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C}^d)^{\otimes r}$ and $\psi \in (\mathbb{C}^d)^{\otimes \ell} \otimes \mathcal{G}_{m+r}$, we have the estimate*

$$(11.47) \quad |\langle \varphi, \psi \rangle - \langle C_\varphi, D_\psi \rangle_\rho| \leq \frac{b(m)}{1 - b(m)} \|\varphi\| \|\psi\|.$$

Proof.

$$(11.48) \quad \begin{aligned} \langle \varphi, \psi \rangle &= \sum_{\mathbf{i}, \mathbf{j}, \mathbf{k}} \text{Tr}[v_{\mathbf{i}}^* v_{\mathbf{j}}^* B_\varphi(\mathbf{k})^*] \text{Tr}[B_\psi(\mathbf{i}) v_{\mathbf{k}} v_{\mathbf{j}}] \\ &= \sum_{\mathbf{i}, \mathbf{k}} \langle \Gamma_m(v_{\mathbf{i}} B_\varphi(\mathbf{k})), \Gamma_m(B_\psi(\mathbf{i}) v_{\mathbf{k}}) \rangle \end{aligned}$$

Now we apply Lemma 11.4. See that

$$(11.49) \quad \begin{aligned} \left| \langle \varphi, \psi \rangle - \sum_{\mathbf{i}, \mathbf{k}} \langle v_{\mathbf{i}}^* B_\varphi(\mathbf{k}), B_\psi(\mathbf{i}) v_{\mathbf{k}} \rangle_\rho \right| &\leq b(m) \sum_{\mathbf{i}, \mathbf{k}} \|v_{\mathbf{i}} B_\varphi(\mathbf{k})\|_\rho \|B_\psi(\mathbf{i}) v_{\mathbf{k}}\|_\rho \\ &\leq b(m) \sqrt{\sum_{\mathbf{i}, \mathbf{k}} \|v_{\mathbf{i}} B_\varphi(\mathbf{k})\|_\rho^2} \sqrt{\sum_{\mathbf{i}, \mathbf{k}} \|B_\psi(\mathbf{i}) v_{\mathbf{k}}\|_\rho^2} \end{aligned}$$

by an application of Cauchy-Schwarz.

One now sees that

$$(11.50) \quad \begin{aligned} \sum_{\mathbf{i}, \mathbf{k}} \|v_{\mathbf{i}} B_\varphi(\mathbf{k})\|_\rho^2 &= \sum_{\mathbf{i}, \mathbf{k}} \text{Tr}[\rho B_\varphi(\mathbf{k})^* v_{\mathbf{i}}^* v_{\mathbf{i}} B_\varphi(\mathbf{k})] \\ &= \sum_{\mathbf{k}} \text{Tr}[\rho B_\varphi(\mathbf{k})^* B_\varphi(\mathbf{k})] = \sum_{\mathbf{k}} \|B_\varphi(\mathbf{k})\|_\rho^2 \end{aligned}$$

where we have used that

$$(11.51) \quad \sum_{\mathbf{i}} v_{\mathbf{i}}^* v_{\mathbf{i}} = \mathbb{1}$$

By (11.38), it is clear that

$$(11.52) \quad \sum_{\mathbf{k}} \|B_\varphi(\mathbf{k})\|_\rho^2 \leq \frac{1}{1 - b(\ell + m)} \sum_{\mathbf{k}} \|\Gamma_{m+\ell}(B_\varphi(\mathbf{k}))\|^2$$

and by the orthonormality of the basis $|\mathbf{k}\rangle$, we have

$$(11.53) \quad \sum_{\mathbf{k}} \|\Gamma_{m+\ell}(B_\varphi(\mathbf{k}))\|^2 = \|\varphi\|^2$$

The other factor is seen to be:

$$(11.54) \quad \begin{aligned} \sum_{\mathbf{i}, \mathbf{k}} \|B_\psi(\mathbf{i})v_{\mathbf{k}}\|_\rho^2 &= \sum_{\mathbf{i}, \mathbf{k}} \text{Tr} [\rho v_{\mathbf{k}}^* B_\psi(\mathbf{i})^* B_\psi(\mathbf{i}) v_{\mathbf{k}}] \\ &= \sum_{\mathbf{i}} \text{Tr} \left[\left(\hat{\mathbb{E}}^t \right)^r (\rho) B_\psi(\mathbf{i})^* B_\psi(\mathbf{i}) \right] \\ &= \sum_{\mathbf{i}} \|B_\psi(\mathbf{i})\|_\rho^2 \\ &\leq \frac{1}{1-b(m+r)} \sum_{\mathbf{i}} \|\Gamma_{m+r}(B_\psi(\mathbf{i}))\|^2 = \frac{\|\psi\|^2}{1-b(m+r)} \end{aligned}$$

where we used that $\hat{\mathbb{E}}^t(\rho) = \rho$.

Thus the right-hand-side of (11.49) is bounded by

$$(11.55) \quad b(m) \frac{1}{\sqrt{1-b(\ell+m)}} \frac{1}{\sqrt{1-b(m+r)}} \|\varphi\| \|\psi\| \leq \frac{b(m)}{1-b(m)} \|\varphi\| \|\psi\|$$

where we have used the monotonicity property that follows from (11.31).

Note also that

$$(11.56) \quad \begin{aligned} \sum_{\mathbf{i}, \mathbf{k}} \langle v_{\mathbf{i}} B_\varphi(\mathbf{k}), B_\psi(\mathbf{i}) v_{\mathbf{k}} \rangle_\rho &= \sum_{\mathbf{i}, \mathbf{k}} \text{Tr} [\rho B_\varphi(\mathbf{k})^* v_{\mathbf{i}}^* B_\psi(\mathbf{i}) \rho \rho^{-1} v_{\mathbf{k}}] \\ &= \text{Tr} \left[\rho \left(\sum_{\mathbf{k}} \rho^{-1} v_{\mathbf{k}} \rho B_\varphi(\mathbf{k})^* \right) \left(\sum_{\mathbf{i}} v_{\mathbf{i}}^* B_\psi(\mathbf{i}) \right) \right] \\ &= \langle C_\varphi, D_\psi \rangle_\rho \end{aligned}$$

as claimed. \square

11.4. The commutation property. Consider a frustration free quantum spin chain with MPS ground states such as, e.g., the AKLT chain. To start, we assume that $\hat{\mathbb{E}}$ is primitive with a unique density matrix ρ that is an eigenvector with eigenvalue 1 of $\hat{\mathbb{E}}^T$, and WLOG we can assume that $\ker \rho = \{0\}$, the smallest eigenvalue of ρ , ρ_{\min} , is non-zero. Let $G_n \in M_d^{\otimes n}$ denote the orthogonal projections onto \mathcal{G}_n .

Proposition 11.7 (Commutation Property). *For all $m \geq 1, \ell \geq 0, r \geq 0$, we have*

$$(11.57) \quad \left\| (G_{\ell+m} \otimes \mathbb{1}^{\otimes r}) (\mathbb{1}^{\otimes \ell} \otimes G_{m+r}) - G_{\ell+m+r} \right\| \leq \epsilon_m,$$

where

$$(11.58) \quad \epsilon_m = \frac{b(m)}{(1-b(m))^2}.$$

Proof. Since $G_{\ell+m+r}$ projects onto a subspace of the ranges of both $G_{\ell+m} \otimes \mathbb{1}^{\otimes r}$ and $\mathbb{1}^{\otimes \ell} \otimes G_{m+r}$, we have the identity

$$(G_{\ell+m} \otimes \mathbb{1}^{\otimes r}) (\mathbb{1}^{\otimes \ell} \otimes G_{m+r}) - G_{\ell+m+r} = (G_{\ell+m} \otimes \mathbb{1}^{\otimes r} - G_{\ell+m+r}) (\mathbb{1}^{\otimes \ell} \otimes G_{m+r} - G_{\ell+m+r}).$$

From this it is easy to see that to prove (11.57) is equivalent to showing that for all $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C}^{\otimes r})$, $\psi \in \mathbb{C}^{\otimes \ell} \otimes \mathcal{G}_{m+r}$, such that $G_{\ell+m+r} \varphi = G_{\ell+m+r} \psi = 0$, they have the following bound

$$(11.59) \quad |\langle \varphi, \psi \rangle| \leq \epsilon_m \|\varphi\| \|\psi\|.$$

The inner product can be estimated by applying Lemma 11.6 and using the extra information we have about the vectors φ and ψ . Since $\varphi \in \mathcal{G}_{\ell+m} \otimes (\mathbb{C})^{\otimes r}$, there exists $A \in M_k$ such that $B_\varphi(\mathbf{k}) = Av_{\mathbf{k}}$, which allows us to determine C_φ :

$$(11.60) \quad C_\varphi = \sum_{\mathbf{k}} Av_{\mathbf{k}} \rho v_{\mathbf{k}}^* \rho^{-1} = A(\hat{\mathbb{E}}^T)^r(\rho)\rho^{-1} = A.$$

Now, $G_{\ell+m+r}\psi = 0$ implies

$$(11.61) \quad \langle \Gamma_{\ell+m+r}(A), \psi \rangle = 0, \text{ for all } A \in M_k.$$

In combination with Lemma 11.6 this gives

$$(11.62) \quad |\langle A, D_\psi \rangle_\rho| \leq \frac{b(m)}{1-b(m)} \|\psi\| \|A\|_\rho,$$

and hence

$$(11.63) \quad \|D_\psi\|_\rho \leq \frac{b(m)}{1-b(m)} \|\psi\|.$$

By a similar reasoning, we find

$$(11.64) \quad \|C_\varphi\|_\rho \leq \frac{b(m)}{1-b(m)} \|\varphi\|.$$

Combining this information with Lemma 11.6 proves the proposition. \square

Proposition 11.7 is referred to as the Commutation Property of the the ground states projections because it directly implies a bound on the commutator:

$$\begin{aligned} \left\| [G_{\ell+m} \otimes \mathbb{1}^{\otimes r}, \mathbb{1}^{\otimes \ell} \otimes G_{m+r}] \right\| &\leq \left\| (G_{\ell+m} \otimes \mathbb{1}^{\otimes r})(\mathbb{1}^{\otimes \ell} \otimes G_{m+r}) - G_{\ell+m+r} \right\| \\ &\quad + \left\| G_{\ell+m+r} - (\mathbb{1}^{\otimes \ell} \otimes G_{m+r})(G_{\ell+m} \otimes \mathbb{1}^{\otimes r}) \right\| \\ &\leq 2\epsilon_m. \end{aligned}$$

This property is closely related to the Factorization Property proved in [36] which, in turn, can be seen to underly the Area Law for the entanglement entropy [33].

11.5. The martingale method and proof of non-vanishing spectral gap for quantum chains with MPS ground states. The Commutation Property of Proposition 11.7 in combination with the frustration freeness of the spin chains with MPS ground states we are considering in this chapter, can be seen to imply a uniform lower bound for the spectral gap of these models. See, e.g., [21] or [65]. The martingale method is a simple argument that relates the quantity ϵ_m to a lower bound for the spectral gap in an efficient way [49] and is based on an idea that has been very useful in the context of classical interacting particle models [45] and other many-body systems [12, 13].

To present the martingale method in a transparent way, it is useful to identify the crucial properties that make it work in the context of quantum spin systems.

The ground state space of a finite chain is the intersection of the ground state spaces of shorter chains. We will describe this as a sequence of decreasing subspaces $\mathcal{H}_N \supset \mathcal{G}_1 \supset \mathcal{G}_2 \cdots \supset \mathcal{G}_N$, which are the null spaces of a corresponding increasing sequence of non-negative Hamiltonians. For $n = 1, \dots, N$, $H_n \in \mathcal{B}(\mathcal{H}_N)$, $\mathcal{G}_n = \ker H_n$, $H_1 \leq H_2 \cdots \leq H_N$. Note however, that although the sequence H_n , $n = 1, \dots, N$, will typically be associated with the system on an increasing sequence of finite volumes, the H_n do not have to coincide with the finite-volume Hamiltonians in terms of which the model is defined. In general, we will have constants $c, C > 0$ such that

$$(11.65) \quad cH_N \leq H_{\Lambda_N} \leq CH_N,$$

where H_{Λ_N} is the finite-volume Hamiltonian of which we want the estimate the spectral gap.

Define

$$(11.66) \quad h_n = \begin{cases} H_1 & \text{if } n = 1 \\ H_n - H_{n-1} & \text{if } n = 2, \dots, N \end{cases}$$

and let G_n and $g_n \in \mathcal{B}(\mathcal{H})_N$ be the orthogonal projection onto $\ker H_n$ and $\ker h_n$, respectively. Of course, (11.66) is equivalent to assuming that $H_n = \sum_{k=1}^n h_k$, and H_n will be increasing if we require $h_k \geq 0$. Furthermore, define

$$(11.67) \quad E_n = \begin{cases} \mathbb{1} - G_1 & \text{if } n = 0 \\ G_n - G_{n+1} & \text{if } 1 \leq n \leq N-1 \\ G_N & \text{if } n = N \end{cases}$$

It is easily verified that the E_n are mutually orthogonal orthogonal projections forming a resolution of the identity: $\sum_{n=0}^N E_n = \mathbb{1}$ and $E_n E_m = \delta_{n,m} E_n$.

Assumptions for the Martingale Method:

- (i) There is a constant $\gamma > 0$ such that $h_n \geq \gamma(\mathbb{1} - g_n)$, $n = 1 \dots N$.
- (ii) There are integers $\ell \geq 0, r \geq 1$, such that $E_k g_n = g_n E_k$, if $k \notin [n - \ell, n + r]$.
- (iii) There exists $\epsilon \in [0, \sqrt{\ell + r}]$, such that $E_n g_{n+1} E_n \leq \epsilon^2 E_n$, $n = 1, \dots, N-1$.

Theorem 11.8. *In the setup described immediately here above, assume the Assumption (i)–(iii) hold. Let $\psi \in \mathcal{H}_N$ such that $G_N \psi = 0$. Then*

$$\langle \psi, H_N \psi \rangle \geq \frac{\gamma}{2} (1 - \epsilon \sqrt{1 + \ell + r})^2 \|\psi\|^2.$$

Proof. By assumption $E_N \psi = G_N \psi = 0$. Hence

$$(11.68) \quad \|\psi\|^2 = \sum_{n=0}^{N-1} \|E_n \psi\|^2.$$

Using this, for all $n = 0, \dots, N-1$, we have

$$(11.69) \quad \begin{aligned} \|E_n \psi\|^2 &= \langle \psi, (\mathbb{1} - g_{n+1}) E_n \psi \rangle + \langle \psi, g_{n+1} E_n \psi \rangle \\ &= \langle \psi, (\mathbb{1} - g_{n+1}) E_n \psi \rangle + \langle \psi, \left(\sum_{m=0}^{N-1} E_m \right) g_{n+1} E_n \psi \rangle. \end{aligned}$$

By Assumption (ii) and the mutual orthogonality of the projections E_m , the summation in the last term can be reduced and we obtain

$$(11.70) \quad \|E_n \psi\|^2 \leq \langle \psi, (\mathbb{1} - g_{n+1}) E_n \psi \rangle + \langle \psi, \left(\sum_{k=n-\ell}^{n+r} E_k \right) g_{n+1} E_n \psi \rangle.$$

After applying the inequality

$$(11.71) \quad |\langle \varphi_1, \varphi_2 \rangle| \leq \frac{1}{2c} \|\varphi_1\|^2 + \frac{c}{2} \|\varphi_2\|^2, \quad \varphi_1, \varphi_2 \in \mathcal{H}, c > 0,$$

two each of the two terms in (11.70), we find

$$\begin{aligned} \|E_n \psi\|^2 &\leq \frac{1}{2c_1} \langle \psi, (\mathbb{1} - g_{n+1}) \psi \rangle + \frac{c_1}{2} \langle \psi, E_n \psi \rangle \\ &\quad + \frac{1}{2c_2} \langle \psi, E_n g_{n+1} E_n \psi \rangle + \frac{c_2}{2} \langle \psi, \left(\sum_{k=n-\ell}^{n+r} E_k \right)^2 \psi \rangle. \end{aligned}$$

To estimate the first term of the RHS, we use Assumption (i). The second term can be combined with the LHS. For the third term we use Assumption (iii). In the fourth term we can use the mutual orthogonality of the E_m . This gives

$$(11.72) \quad \left(1 - \frac{c_1}{2} - \frac{\epsilon^2}{2c_2}\right) \|E_n \psi\|^2 - \frac{c_2}{2} \sum_{k=n-\ell}^{n+r} \|E_k \psi\|^2 \leq \frac{1}{2c_1 \gamma} \langle \psi, h_{n+1} \psi \rangle.$$

We now sum over $n = 0, \dots, N-1$, use the fact the $\{E_n \mid n = 0, \dots, N\}$ is a resolution of the identity, and recall that $E_n \psi = G_N \psi = 0$. The result is

$$(11.73) \quad \langle \psi H_N \psi \rangle \geq 2c_1 \gamma \left[1 - \frac{c_1}{2} - \frac{\epsilon^2}{2c_2} - \frac{c_2(1+\ell+r)}{2} \right] \|\psi\|^2.$$

We can maximize the constant in the RHS by choosing $c_1 = 1 - \epsilon/\sqrt{1+\ell+r}$ and $c_2 = \epsilon/\sqrt{1+\ell+r}$. This yields the inequality stated in the theorem. \square

Let us now apply this theorem to the spin chains with a unique pure MPS ground state, such as the AKLT chain. For simplicity of the notation, assume that the model is defined in terms of a frustration-free nearest neighbor interaction $0 \leq h \in M_d \otimes M_d$. Then, let $m \geq 1$ and define

$$(11.74) \quad h_n = \sum_{x=(n-1)m+1}^{(n+1)m-1} h_{x,x+1}.$$

Then, we have

$$\begin{aligned} H_n &= \sum_{k=1}^n h_k \\ H_{[1,(n+1)m]} &\leq H_n \leq 2H_{[1,(n+1)m]} \\ E_n &= G_{(n+1)m} \otimes \mathbb{1}^{\otimes(N-n)m} - G_{(n+2)m} \otimes \mathbb{1}^{\otimes(N-n-1)m} \\ g_n &= \mathbb{1}^{\otimes(n-1)m} \otimes G_{2m} \otimes \mathbb{1}^{\otimes(N-n)m}. \end{aligned}$$

Assumption (i) is satisfied with γ given by the spectral gap of $H_{[(n-1)m+1,(n+1)m]}$. Since m is fixed, and the model is translation invariant this gap is positive and independent of n . Assumption (ii) is satisfied with $\ell = 0, r = 1$. For the spin chains with a unique pure MPS ground states (iii) follows from the Commutation Property (Proposition 11.7), To see this, it suffices to express the quantities E_n and g_{n+1} in terms of the ground state projection operators:

$$(11.75) \quad \|g_{n+1} E_n\| = \|(\mathbb{1}^{\otimes(n-1)m} \otimes G_{2m})(G_{(n+1)m} \otimes \mathbb{1}^{\otimes m} - G_{(n+2)m})\| \leq \epsilon_m$$

where ϵ_m is the quantity estimate in Proposition 11.7. It then suffices to note that, for two orthogonal projections G and E , one has

$$(11.76) \quad \|GE\| \leq \epsilon \Leftrightarrow EGE \leq \epsilon^2 E.$$

Other choices for the sequence H_n are possible and may provide more precise information in some cases. E.g., if one is interested in estimating the spectral gap for finite systems with periodic boundary conditions, it is useful to let H_{N-1} be comparable to the Hamiltonian of the chain with open boundary conditions and H_N the Hamiltonian for the system with the same Hilbert space but with the additional term(s) that corresponds to considering periodic boundary conditions. Further refinements of the method exist. See, e.g., [61].

The method can also be applied to some quantum spin models in higher dimensions as long as one can find sequences of finite volumes and associate Hamiltonians such that the Assumptions (i)-(iii) are satisfied. See, e.g., [7, 9] for a few examples in two and more dimensions.

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