Note: Knabe's Method

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Abstract

This is a proof memo on the method known as Knabe's method [1], which uses the spectral gap of an n-site finite system with OBC to bound the spectral gap of an $N > 2n$ site system with PBC.

First we show the following.

- The statement that the first excited energy ϵ_1 of a Hamiltonian H satisfies $\epsilon_1 \geq \epsilon$ is equivalent to $H^2 \geq \epsilon H$.

Indeed, if

$$H = \sum_{\epsilon_i > 0} \epsilon_i P_i \tag{1}$$

is the spectral decomposition of H, then

$$H^2 - \epsilon H = \sum_{\epsilon_i > 0} \epsilon_i (\epsilon_i - \epsilon) P_i. \tag{2}$$

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Consider a 2-local frustration-free Hamiltonian

$$H = \sum_{i=1}^{N} P_{i,i+1} \tag{3}$$

with periodic boundary conditions. Here $P_{i,i+1}$ is a projection operator. The frustration-free condition means that, if P_0 denotes the projection onto the ground states of H, then

$$(1 - P_0) P_{i,i+1} P_0 = 0, \quad i = 1, \ldots, N. \tag{4}$$

Since $P_{i,i+1} \geq 0$, this is equivalent to the ground-state energy of H being zero:

$$H P_0 = 0. \tag{5}$$

Consider H^2:

$$\begin{aligned} H^2 &= \sum_{i,j=1}^{N} P_{i,i+1} P_{j,j+1} && (6) \\ &= \sum_{i=1}^{N} P_{i,i+1} + \sum_{i=1}^{N} (P_{i,i+1} P_{i+1,i+2} + P_{i+1,i+2} P_{i,i+1}) && (7) \\ &\quad + \sum_{2 \leq |i-j|_N \leq \lfloor N/2 \rfloor} 2 P_{i,i+1} P_{j,j+1}. && (8) \end{aligned}$$

The first and third terms are positive semidefinite, but the second term need not be. We have introduced

$$|i-j|_N := \min_{k\in\mathbb{Z}} |i-j+kN|. \tag{9}$$

For $2 \le n \le \lfloor N/2 \rfloor$, focus on a subinterval $[i, i+n]$ of the circle and define the OBC Hamiltonian on this interval by

$$h_{n,i} := \sum_{j=i}^{i+n-1} P_{j,j+1}. \tag{10}$$

Here $P_{j+N,j+1+N} = P_{j,j+1}$. Its square is

$$h_{n,i}^2 = \sum_{j=i}^{i+n-1} P_{j,j+1} + \sum_{j=i}^{i+n-2} (P_{j,j+1}P_{j+1,j+2} + P_{j+1,j+2}P_{j,j+1}) \tag{11}$$

$$+ \sum_{2\le|j-k|_N,\ i\le j,k\le i+n-1} 2P_{j,j+1}P_{k,k+1}. \tag{12}$$

Then, in $\sum_{i=1}^N h_{n,i}^2$,

- the first term of (8) appears n times,
- the second term of (8) appears $n-1$ times,
- for the third type of terms, the term with distance $|i-j|_N = l$ appears $n-l$ times for $l = 2, \dots, n-1$.

Therefore

$$H^2 - \frac{1}{n-1}\sum_{i=1}^N h_{n,i}^2 = -\frac{1}{n-1}H + \sum_{l=2}^{n-1} \frac{l-1}{n-1} \sum_{|i-j|_N=l} 2P_{i,i+1}P_{j,j+1} \tag{13}$$

$$+ \sum_{l=n}^{\lfloor N/2 \rfloor} \sum_{|i-j|_N=l} 2P_{i,i+1}P_{j,j+1}. \tag{14}$$

The second and third terms in the last line are positive semidefinite, so

$$H^2 \ge \frac{1}{n-1}\sum_{i=1}^N h_{n,i}^2 - \frac{1}{n-1}H. \tag{15}$$

Assume the following.

- The OBC Hamiltonian $h_{n,i}$ has a spectral gap $\epsilon_n > 0$ that does not depend on i, i.e.

$$h_{n,i}^2 \ge \epsilon_n h_{n,i}. \tag{16}$$

Under this assumption,

$$H^2 \ge \frac{1}{n-1}\sum_{i=1}^N \epsilon_n h_{n,i} - \frac{1}{n-1}H = \frac{n}{n-1}\left(\epsilon_n - \frac{1}{n}\right)H. \tag{17}$$

Thus we have shown the following.

- If there exists $n \in \{2, \dots, \lfloor N/2 \rfloor\}$ such that the OBC Hamiltonian $h_{n,i}$ has a uniform spectral gap

$$\epsilon_n > \frac{1}{n}, \tag{18}$$

  independent of i, then H has spectral gap

$$\frac{n}{n-1}\left(\epsilon_n - \frac{1}{n}\right). \tag{19}$$

- In particular, for a translation-invariant Hamiltonian, if for some $n \geq 2$ the OBC Hamiltonian h_n on $n+1$ sites has spectral gap

$$\epsilon_n > \frac{1}{n}, \tag{20}$$

then for every $N > 2n$, the PBC Hamiltonian H on N sites has spectral gap

$$\frac{n}{n-1}\left(\epsilon_n - \frac{1}{n}\right). \tag{21}$$

Therefore, in the frustration-free and translation-invariant case, proving numerically that the OBC Hamiltonian on $n+1$ sites has spectral gap $\epsilon_n > 1/n$ proves the existence of a PBC spectral gap in the limit $N \to \infty$.

References

[1] Stefan Knabe, "Energy gaps and elementary excitations for certain VBS-quantum antiferromagnets," Journal of Statistical Physics 52 (1988), 627–638.