Chapter 1

Ground energy of spin systems

We reduce Frustration-Free Bose-Hubbard Hamiltonian to an eigenvalue problem for a class of 2-local Hamiltonians defined by graphs. The reduction is based on a well-known mapping between hard-core bosons and spin systems, which we now review.

We define the subspace $\mathcal{W}_N(G) \subset \mathcal{Z}_N(G)$ of N hard-core bosons on a graph G to consist of the states where each vertex of G is occupied by either 0 or 1 particle, i.e.,

$$\mathcal{W}_N(G) = \mathrm{span}\{\mathrm{Sym}(|i_1, i_2, \ldots, i_N\rangle) \colon i_1, \ldots, i_N \in V,\ i_j \neq i_k \text{ for distinct } j,k \in [N]\}.$$

A basis for $\mathcal{W}_N(G)$ is the subset of occupation-number states (**??**) labeled by bit strings $l_1 \ldots l_{|V|} \in \{0,1\}^{|V|}$ with Hamming weight $\sum_{j\in V} l_j = N$. The space $\mathcal{W}_N(G)$ can thus be identified with the weight-N subspace

$$\mathrm{Wt}_N(G) = \mathrm{span}\{|z_1, \ldots, z_{|V|}\rangle :\ z_i \in \{0,1\},\ \sum_{i=1}^{|V|} z_i = N\}$$

of a $|V|$-qubit Hilbert space. We consider the restriction of H_G^N to the space $\mathcal{W}_N(G)$, which can equivalently be written as a $|V|$-qubit Hamiltonian O_G restricted to the space $\mathrm{Wt}_N(G)$. In particular,

$$H_G^N\big|_{\mathcal{W}_N(G)} = O_G\big|_{\mathrm{Wt}_N(G)} \tag{1.1}$$

where

$$\begin{aligned} O_G &= \sum_{\substack{A(G)_{ij}=1\\ i\neq j}} \big(|01\rangle\langle 10| + |10\rangle\langle 01|\big)_{ij} + \sum_{A(G)_{ii}=1} |1\rangle\langle 1|_i \\ &= \sum_{\substack{A(G)_{ij}=1\\ i\neq j}} \frac{\sigma_x^i\sigma_x^j + \sigma_y^i\sigma_y^j}{2} + \sum_{A(G)_{ii}=1} \frac{1-\sigma_z^i}{2}. \end{aligned}$$

Note that the Hamiltonian O_G conserves the total magnetization $M_z = \sum_{1=1}^{|V|} \frac{1-\sigma_z^i}{2}$ along the z axis.

We define $\theta_N(G)$ to be the smallest eigenvalue of (**??**), i.e., the ground energy of O_G in the sector with magnetization N. We show that approximating this quantity is QMA-complete.

Problem 1 (XY Hamiltonian). We are given a K-vertex graph G, an integer $N \leq K$, a real number c, and a precision parameter $\epsilon = \frac{1}{T}$. The positive integer T is provided in unary; the graph is specified by its adjacency matrix, which can be any $K \times K$ symmetric 0-1 matrix. We are promised that either $\theta_N(G) \leq c$ (yes instance) or else $\theta_N(G) \geq c + \epsilon$ (no instance) and we are asked to decide which is the case.

1.1 Relation between spins and particles

1.1.1 The transform

1.2 Hardness reduction from frustration-free BH model

Theorem 1. *XY Hamiltonian is QMA-complete.*

Proof. An instance of XY Hamiltonian can be verified by the standard QMA verification protocol for the Local Hamiltonian problem [**?**] with one slight modification: before running the protocol Arthur measures the magnetization of the witness and rejects unless it is equal to N. Thus the problem is contained in QMA.

To prove QMA-hardness, we show that the solution (yes or no) of an instance of Frustration-Free Bose-Hubbard Hamiltonian with input G, N, ϵ is equal to the solution of the instance of XY Hamiltonian with the same graph G and integer N, with precision parameter $\frac{\epsilon}{4}$ and $c = N\mu(G) + \frac{\epsilon}{4}$.

We separately consider yes instances and no instances of Frustration-Free Bose-Hubbard Hamiltonian and show that the corresponding instance of XY Hamiltonian has the same solution in both cases.

Case 1: no instances

First consider a no instance of Frustration-Free Bose-Hubbard Hamiltonian, for which $\lambda_N^1(G) \geq \epsilon + \epsilon^3$. We have

$$\begin{aligned}
\lambda_N^1(G) &= \min_{\substack{|\phi\rangle \in \mathcal{Z}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|H_G^N - N\mu(G)|\phi\rangle && (1.2)\\
&\leq \min_{\substack{|\phi\rangle \in \mathcal{W}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|H_G^N - N\mu(G)|\phi\rangle && (1.3)\\
&= \min_{\substack{|\phi\rangle \in \mathrm{Wt}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|O_G - N\mu(G)|\phi\rangle && (1.4)\\
&= \theta_N(G) - N\mu(G) && (1.5)
\end{aligned}$$

where in the inequality we used the fact that $\mathcal{W}_N(G) \subset \mathcal{Z}_N(G)$. Hence

$$\theta_N(G) \geq N\mu(G) + \lambda_N^1(G) \geq N\mu(G) + \epsilon + \epsilon^3 \geq N\mu(G) + \frac{\epsilon}{2},$$

so the corresponding instance of XY Hamiltonian is a no instance.

Case 2: yes instances

Now consider a yes instance of Frustration-Free Bose-Hubbard Hamiltonian, so $0 \leq \lambda_N^1(G) \leq \epsilon^3$.

We consider the case $\lambda_N^1(G) = 0$ separately from the case where it is strictly positive. If $\lambda_N^1(G) = 0$ then any state $|\psi\rangle$ in the ground space of H_G^N satisfies

$$\langle\phi|\sum_{w=1}^{N}(A(G)-\mu(G))^{(w)} + \sum_{k\in V}\widehat{n}_k(\widehat{n}_k - 1)|\phi\rangle = 0.$$

Since both terms are positive semidefinite, the state $|\phi\rangle$ has zero energy for each of them. In particular, it has zero energy for the second term, or equivalently, $|\phi\rangle \in \mathcal{W}_N(G)$. Therefore

$$\lambda_N^1(G) = \min_{\substack{|\phi\rangle\in\mathcal{W}_N(G)\\ \langle\phi|\phi\rangle=1}}\langle\phi|H_G^N - N\mu(G)|\phi\rangle = \min_{\substack{|\phi\rangle\in\mathrm{Wt}_N(G)\\ \langle\phi|\phi\rangle=1}}\langle\phi|O_G - N\mu(G)|\phi\rangle = \theta_N(G) - N\mu(G),$$

so $\theta_N(G) = N\mu(G)$, and the corresponding instance of XY Hamiltonian is a yes instance.

Finally, suppose $0 < \lambda_N^1(G) \leq \epsilon^3$. Then $\lambda_N^1(G)$ is also the smallest *nonzero* eigenvalue of $H(G,N)$, which we denote by $\gamma(H(G,N))$. (Here and throughout this paper we write $\gamma(M)$ for the smallest nonzero eigenvalue of a positive semidefinite matrix M.) Note that $\lambda_N^1(G) > 0$ also implies (by the inequalities (**??**)–(**??**)) that $\theta_N(G) - N\mu(G) > 0$, so

$$\theta_N(G) - N\mu(G) = \gamma\left((O_G - N\mu(G))\big|_{\mathrm{Wt}_N(G)}\right).$$

To upper bound $\theta_N(G)$ we use the Nullspace Projection Lemma (Lemma **??**). We apply this Lemma using the decomposition $H(G,N) = H_A + H_B$ where

$$H_A = \sum_{k\in V}\widehat{n}_k(\widehat{n}_k - 1)\big|_{\mathcal{Z}_N(G)} \qquad H_B = \sum_{w=1}^{N}(A(G)-\mu(G))^{(w)}\big|_{\mathcal{Z}_N(G)}.$$

Note that H_A and H_B are both positive semidefinite, and that the nullspace S of H_A is equal the space $\mathcal{W}_N(G)$ of hard-core bosons. To apply the Lemma we compute bounds on $\gamma(H_A)$, $\|H_B\|$, and $\gamma(H_B|_S)$. We use the bounds $\gamma(H_A) = 2$ (since the operators $\{\widehat{n}_k \colon k \in V\}$ commute and have nonnegative integer eigenvalues),

$$\|H_B\| \leq N\|A(G)-\mu(G)\| \leq N(\|A(G)\| + \mu(G)) \leq 2N\|A(G)\| \leq 2KN \leq 2K^2$$

(where we used the fact that $\|A(G)\|$ is at most the maximum degree of G, which is at most the number of vertices K), and

$$\begin{aligned}\gamma(H_B|_S) &= \gamma\left(\sum_{w=1}^{N}(A(G)-\mu(G))^{(w)}\big|_{\mathcal{W}_N(G)}\right)\\ &= \gamma\left((O_G - N\mu(G))\big|_{\mathrm{Wt}_N(G)}\right)\\ &= \theta_N(G) - N\mu(G).\end{aligned}$$

Now applying the Lemma, we get

$$\lambda_N^1(G) = \gamma(H(G,N)) \geq \frac{2(\theta_N(G) - N\mu(G))}{2 + (\theta_N(G) - N\mu(G)) + 2K^2}.$$

Rearranging this inequality gives

$$\theta_N(G) - N\mu(G) \leq \lambda_N^1(G)\frac{2(K^2+1)}{2-\lambda_N^1(G)} \leq 4K^2\lambda_N^1(G) \leq 4K^2\epsilon^3$$

where in going from the second to the third inequality we used the fact that $1 \leq K^2$ in the numerator and $\lambda_N^1(G) \leq \epsilon^3 < 1$ in the denominator. Now using the fact (from the definition of Frustration-Free Bose-Hubbard Hamiltonian) that $\epsilon \leq \frac{1}{4K}$, we get

$$\theta_N(G) \leq N\mu(G) + \frac{\epsilon}{4},$$

i.e., the corresponding instance of XY Hamiltonian is a yes instance. $\square$