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Contents

1 Introduction	1
2 Introduction to quantum information theory	2
3 Relevant classical methods	5
4 Approximation algorithms for the groundstate energy of traceless 2-local-Hamiltonians	8
5 Testing specific models	14
6 Generalization to qutrits	18
Bibliography	21

Chapter 1

Introduction

Approximating quantum systems with product states is a relevant method to several fields. In chemistry, it is called the Hartree-Fock method, in quantum many-body physics we call it mean-field theory. It is successful in approximating a solution to the Schrödinger equation of atoms, molecules and nanostructures [1].

In this thesis I will give an introduction to a paper by Bravyi *et al.* [2], introducing the reader to the basic concepts. The paper demonstrates an efficient algorithm for approximating the ground state energy of traceless 2-local Hamiltonians. Finding the ground state of such a system is also highly relevant to classical and quantum complexity theory, since it generalizes the max- k -sat problem, where we are given a set of Boolean constraints on k variables each and try to satisfy as many constraints as possible. In this sense, the topic of this thesis is a beautiful intersection, since in its theory it combines physics, mathematics and computer science, while in its application it is useful for multiple subfields of chemistry, physics and computer science.

Chapter 2

Introduction to quantum information theory

I will first give an introduction to quantum information theory, which uses quantum mechanical concepts to perform information processing and transmission of information. In quantum mechanics, we can associate a Hilbert space \mathbb{H} with every quantum system. Quantum states are operators $\rho : \mathbb{H} \rightarrow \mathbb{H}$, which we can represent as density matrices. In general, a complex $M \times M$ matrix is a density matrix if it is:

1. Hermitian, $\rho = \rho^\dagger$,
2. positive, $\rho \geq 0$,
3. normalized, $\text{Tr}\rho = 1$.

The set of density matrices is a convex set and its pure states obey $\rho^2 = \rho$. In quantum computing, we mostly deal with N 2-level systems called qubits, the composite space of which is $H = H_1 \otimes H_2 \otimes \dots \otimes H_N$. In this space, there are states ρ which can not be expressed through a tensor product of states in the subsystems $\rho = \rho_1 \otimes \rho_2 \dots \otimes \rho_N$. We call these states entangled states. States which can be expressed as such are called separable or product states. We can represent a qubit state as

$$\rho = \frac{1}{2} \left(\mathbb{I} + \sum_{i=1}^3 \sigma_i \tau_i \right).$$

This is called the Bloch representation of the state, and is associated with the Bloch-vector $\boldsymbol{\tau}$. The σ_i are generators of $SU(2)$, in our case the Pauli matrices:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

For qubits, the positivity property is equivalent to $\text{Tr}\rho^2 \leq \text{Tr}\rho$, which implies $|\boldsymbol{\tau}| \leq 1$ and characterizes the Bloch-vector-space as a solid Ball with Radius 1, which is called the Bloch sphere.

Suppose $|0\rangle$ and $|1\rangle$ form an orthogonal basis for the 2-dimensional one qubit state space. An arbitrary vector in the space can then be written

$$|\psi\rangle = a|0\rangle + b|1\rangle.$$

where a and b are complex numbers. The normalization condition of quantum states is equivalent to $\langle\psi|\psi\rangle = 1$ and $|a|^2 + |b|^2 = 1$. The orthogonal basis vectors of the state space are called computational basis.

The basic model of transmitting quantum information has three steps: We send a state ρ through a quantum channel \mathcal{N} and the receiver has to measure the outcome in order to extract information. Quantum channels can be understood either as geometrical transformations associated with the Bloch representation, or as completely positive, trace preserving maps. A quantum channel has to be trace preserving i.e. $Tr(\mathcal{N}(\rho)) = Tr(\rho)$ in order for the outcome state to be normalized. It must be completely positive, i.e., the map $\mathbb{I} \otimes \mathcal{N}$ maps positive semidefinite hermitian matrices to positive semidefinite hermitian matrices for any identity matrix \mathbb{I} , in order for the outcome state to be positive. A completely positive map is trace preserving if and only if $\sum_i A_i^\dagger A_i = \mathbb{I}$.

By the Kraus representation Theorem [3] a linear map Ψ is completely positive if and only if there exist operators $\{A_i\}$ such that

$$\Psi(\rho) = \sum_i A_i \rho A_i^\dagger.$$

Maps that are both completely positive and trace preserving are called CPT maps. We discern between unital and non-unital maps. Unital maps map the identity to itself. Geometrically, we can interpret this as the image of the map having the same center as the Bloch sphere. Unital maps can be expressed as convex combinations of the Pauli operators and the identity. Their action in the Bloch sphere are different rotations with shrinking parameters, since the Pauli matrices are unitary.[4]

The most commonly used model for quantum computation is the quantum circuit model, which generalizes its classical analogue. To classify quantum algorithms we use, in parallel to classical complexity theory, quantum complexity classes. The two prominent complexity classes in classical computation are P and NP. P is the set of problems which can be solved by a deterministic Turing machine in polynomial time, while NP is the set of problems which can be solved by a nondeterministic Turing machine in polynomial time. The class QMA is the quantum analogue of NP in a probabilistic setting, the class of all problems which can be solved by a quantum verifier probabilistically in polynomial time.[5] We call a problem complete, if any other problem in its class can be reduced to it. Reduction means that for predicates L_1 and L_2 there is a polynomial f , such that $L_1(x) = L_2(f(x))$. We say that f reduces L_1 to L_2 polynomially.[6]

The Hamiltonian of a system corresponds to its energy, the spectrum of the operator being the set of possible outcomes when measuring the total energy. A k -local-Hamiltonian is a hermitian matrix acting on N qubits, which can be written as a sum of Hamiltonians where each acts on at most k qubits. Physically, this corresponds to system, where the interaction energy between more than k qubits is negligible. Specifically, we look at 2-local-Hamiltonians on qubits of the form

$$H = H_1 + H_2.$$

where

$$H_1 = \sum_{j=1}^{3n} D_j P_j, \quad H_2 = \sum_{i,j=1}^{3n} C_{i,j} P_i P_j \quad (2.1)$$

with the Pauli-operators

$$P_{3a-2} = X_a, \quad P_{3a-1} = Y_a, \quad P_{3a} = Z_a.$$

The minimal eigenvalue of such a systems corresponds to its ground state. Since the quantum state achieving this optimal value might be an entangled state which might not be computable in polynomial time, we are interested in finding the product state that achieves the best approximation. It is equivalent to finding the best approximation to the maximal eigenvalue, because $\lambda_{\max}(-H) = \lambda_{\min}(H)$. [7]

In the local Hamiltonian problem, we are to determine, whether the groundstate energy of a given k -local Hamiltonian is below one threshold or above another. It is equivalent to the maximum constraint satisfaction problem from classical computation. The 2-local Hamiltonian problem is QMA complete.[5] Specifically, we look at *traceless* 2-local Hamiltonians, as these are the quantum generalization of binary quadratic functions of the form

$$F(x) = x^T B x + v^T x, \quad x \in \{\pm 1\}^n, .$$

where $B \in \mathbb{R}^{n \times n}$ is a matrix with zero diagonal and $v \in \mathbb{R}^n$ a vector.

Chapter 3

Relevant classical methods

For productstate approximation algorithms, many techniques from classical computing are used and generalized. Finding the maximal eigenvalue of a traceless 2-local hamiltonian is the quantum analogue to maximizing a binary quadratic program (MaxQP): Given a matrix A with $a_{ii} = 0$ maximize

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} x_i x_j \quad \text{s.t.} \quad x_i \in \{-1, 1\} \quad \forall i.$$

An important tool for solving such problems is the relaxation of a semidefinite program (SDP), which has been pioneered by Goemans and Williamson.

In semidefinite programming we try to maximize a linear function, such that an affine combination of symmetric matrices is positive semidefinite. An affine combination is a linear combination $\sum_{i=1}^n a_i x_i$ where x_i are elements of a vector space, such that $\sum_{i=1}^n a_i = 1$. Semidefinite programs are very useful, as they can be solved efficiently both in theory and in practice.[8] We can write a general SDP as:

$$\begin{aligned} &\text{minimize} && C \cdot X \\ &\text{s.t.} && A_i \cdot X = b_i, \quad i = 1, \dots, m \\ &&& X \geq 0 \end{aligned}$$

where C and A_i are symmetric matrices and $b_i \in \mathbb{R}^m$ a vector. This is called the primal problem. The dual of a SDP is its reformulated version, such that instead of minimizing (maximizing) an objective function, we maximize (minimize) another:

$$\begin{aligned} &\text{maximize} && \sum_{i=1}^m y_i b_i \\ &\text{s. t.} && C - \sum_{i=1}^m y_i A_i \geq 0 \end{aligned}$$

If the optimal value of the primal and the dual problem are the same, we say that *strong duality* holds. While this is not the case in general, it usually holds for SDPs.

For SDPs we can use Slaters condition for strong duality, which states that if there is an x^* that is strictly feasible (i.e. all constraints are satisfied and inequalities hold), then the problem is strictly dual.[9]

The relaxation of a SDP was first proposed by Goemans and Williamson in [10] as part of an approximation algorithm for the max-cut problem, which is a special case of MaxQP. In max-cut, we are given a graph and are to find a partition of the vertices into two sets, such that the number of edges between the two sets is as large as possible. Goemans and Williamson start by formulating the problem into a semidefinite program. Given a vertex set $V = \{1, \dots, n\}$ and non-negative weights $w_{i,j} = w_{j,i}$, maximize the objective function $\frac{1}{2} \sum_{i < j} w_{i,j} (1 - y_i y_j)$ such that $y_i \in S = \{-1, 1\} \quad \forall i \in V$. As this is in NP, we need to relax the constraints, which is accomplished by extending the objective function to a larger space, namely $S^n = \{-1, 1\}^n$. We then have to consider vectors v_i and look at the inner product $v_i \cdot v_j$. The algorithm proposed by Goemans and Williamson proceeds by partitioning the vertices of the graph based on randomized rounding. The rounding is based on a random hyperplane cut of the vectors. It has a approximation ratio of 0.878.

The first algorithm for approximating an optimal solution of MaxQP was proposed by Charikar and Wirth and has a $\Omega\left(\frac{1}{\log n}\right)$ approximation ratio. [11] Since the algorithm described in the next chapter uses a similar approach, I will now lay out the ideas of arriving at the classical result. It also uses relaxation of a SDP and randomized rounding, but instead of partitioning based on a random hyperplane cut through the origin, it takes into account the size of the projections of a random vector onto the solution vectors. For this, the relaxed semidefinite program is

$$\begin{aligned} \max \quad & \sum_{i,j} a_{ij} v_i \cdot v_j \\ \text{s.t.} \quad & v_i \cdot v_i = 1 \quad \forall i \\ & v_i \in \mathbb{R}^n \end{aligned}$$

Using this, the algorithm, which can be solved in polynomial time is:

1. Obtain an optimal solution $\{v_i\}$ to the SDP
2. Create vector r in which the r_i are independently distributed over the normal distribution
3. Let $z_i = v_i \cdot r / T$, where $T = \sqrt{4 \log n}$
4. If $|z_i| > 1$ then $y_i = \text{sgn}(z_i)$, otherwise $y_i = z_i$
5. Round the y_i to ± 1

Step 4 truncates any values outside $[-1, +1]$. The last rounding step is based on the size of the $y_i \in [-1, 1]^n$:

$$x_i = \begin{cases} -1, & \text{with probability } \frac{1-y_i}{2} \\ +1, & \text{with probability } \frac{1+y_i}{2} \end{cases}.$$

The result then clearly lies in $[-1, +1]$. The proof that this algorithm indeed has an approximation ratio of $\Omega(\frac{1}{\log n})$ exploits the spherical symmetry of the distribution of the vector r to show that

$$T^2 \mathbb{E}[z_i z_j] = v_i \cdot v_j.$$

Therefore, if every $|z_i|$ would be at most one, the approximation ratio would be $\frac{1}{T^2}$. Since this isn't the case, we have to prove that the expected value of $\Delta_{ij} = z_i z_j - y_i y_j$ is small in magnitude. In this case

$$|\mathbb{E}(\Delta_{ij})| < 8e^{-\frac{T^2}{2}}.$$

This can be used to finally show that the x_i are a good approximation to the y_i . This algorithm also efficiently solves max-cut and can therefore be seen as a generalization of [10]. In the next chapter, we will see the techniques used here to tackle the problem of approximating the maximal value of a traceless 2-local Hamiltonian.

Chapter 4

Approximation algorithms for the groundstate energy of traceless 2-local-Hamiltonians

The algorithm discussed here is able to efficiently find a product state approximation for a general traceless 2-local Hamiltonian with an approximation ratio $\Omega(\frac{1}{\log n})$ [2]. I will explain the algorithm and the central results that enable and validate it. Before looking at the algorithm itself, there is a preliminary lemma we have to look at. Hamiltonians of the kind $H = H_1 + H_2$ as defined in (2.1) have terms that are linear in Pauli operators. The following lemma will let us reduce this Hamiltonian to a purely quadratic one, for the theorems presented in this paper. We form a new $n + 1$ -qubit Hamiltonian:

$$H' = H_2 + Z_{n+1}H_1.$$

Lemma 1. $\lambda_{\max}(H') = \lambda_{\max}(H)$. Moreover, given any $(n + 1)$ -qubit state ω we can efficiently compute an n -qubit state ϕ such that

$$\langle \phi | H | \phi \rangle \geq \langle \omega | H' | \omega \rangle.$$

If ω is a tensor product of single qubit stabilizer states then so is ϕ .

The idea is, that for any n -qubit traceless 2-local Hamiltonian with linear terms, there is a purely quadratic $(n + 1)$ -qubit traceless 2-local Hamiltonian that has the same maximal eigenvalue and has an at best equally good product state approximation. Therefore, the bounds that we proof for quadratic Hamiltonians are valid also for Hamiltonians with linear terms. This enables us to set $H_1 = 0$. To proof this, we first show that all eigenvalues of H' are either eigenvalues of $H_2 - H_1$ or $H_1 + H_2$. This is the case because H' commutes with Z_{n+1} and therefore they share a common set of eigenvectors $|\psi\rangle$:

$$Z_{n+1}H_1|\psi\rangle = \lambda(Z_{n+1})\lambda(H_1)|\psi\rangle = \pm\lambda(H_1)|\psi\rangle = \lambda(Z_{n+1}H_1)|\psi\rangle.$$

$H_2 - H_1$ can be obtained from $H_1 + H_2$ by the time reversal map:

$$(Y^{\otimes n}(H_2 + H_1)Y^{\otimes n})^T = H_2 - H_1.$$

To see why this is true, we need the following properties of the Pauli matrices σ_i :

$$\sigma_a \sigma_b = \delta_{ab} \mathbb{I} + i \epsilon_{abc} \sigma_c.$$

and

$$X^T = X, \quad Y^T = -Y, \quad Z^T = Z..$$

We can see that the map takes any Pauli operator P_a to $-P_a$. This means it takes H_1 to $-H_1$ and leaves H_2 unchanged since it is quadratic in Pauli operators. Both the matrix transpose and the conjugation by a unitary operator conserve the spectrum, so we have proven that H and H' have the same spectrum and also the same maximal eigenvalue. Using similar arguments, we can then choose the product state $|\phi\rangle$ according to $|\omega\rangle$, such that its eigenvalues will always be at least equal.

The last statement in the lemma refers to an elegant concept that is very useful to quantum error correction. We say an operator A stabilizes a state $|\psi\rangle$ if $A|\psi\rangle = |\psi\rangle$. Conversely, a state is called a stabilizer state of an operator, if it is in its $+1$ -eigenspace. For practicality, we look at operators from the n -qubit Pauli group. This is favorable because they are unitary and their eigenvalues (± 1) differ significantly from another, such that we can easily perform phase estimations to find out the eigenvalue. If we are given a set of operators $S = \{A, B, C \dots\}$, we know that any errors (which are also from the Pauli group) either commute or anticommute with elements in S . One can correct any error E that anticommutes with S , and if the error lies in S it is correctable if they commute with S . [12] We say an operator commutes with a group, or is in the normalizer of the group, if for some $A, B \in S$: $EA = BE$ with possibly $A \neq B$. This criterion is very easy to check and gives us a useful mathematical toolbox. For choosing the product state $|\phi\rangle$, we use operations on $|\omega\rangle$ that take eigenvectors of matrices from the Pauli group to eigenvectors of matrices from the Pauli group. Therefore, if ω is a tensor product of single qubit stabilizer states, ϕ is, too.

The following Theorem is the main result of the part of the publication described here.

Theorem 1. *There is an efficient classical algorithm which, given H of the form (2.1), outputs a product state $|\phi\rangle = |\phi_1\rangle \otimes \dots \otimes |\phi_n\rangle$ such that with probability at least $\frac{2}{3}$*

$$\langle \phi | H | \phi \rangle \geq \frac{\lambda_{\max}(H)}{O(\log n)}.$$

Moreover, each single-qubit state ϕ_i in an eigenstate of one of the Pauli operators X , Y or Z

The algorithm largely mirrors the MaxQP algorithm by Charikar and Wirth presented earlier. I will first present the semidefinite program, explain the algorithm

and then demonstrate the ideas of proving Theorem 1. In our case, the semidefinite program is:

$$\begin{aligned} \max \quad & \text{Tr}(CM) \\ \text{s.t.} \quad & M_{i,i} = 1 \\ & M \geq 0 \end{aligned}$$

where M is a hermitian matrix. The ideal solution M is connected to our state in the following way:[7]

$$M_{i,j} = \text{tr}(\rho P_i P_j) \quad i, j = 1 \dots 3n.$$

We can set M as a real symmetric matrix without loss of generality, because if the Pauli operators act on different matrices they commute, and therefore the matrix entry is real in this case. If they act on the same qubit, the matrix entry is purely imaginary because the operators anticommute. We can eliminate these terms using $M' = \frac{M+M^*}{2}$ because they represent linear terms. This does not change the outcome of the objective function and is therefore fully without loss of generality.

From this perspective the constraints can be understood in the following way:

$$\begin{aligned} M_{i,i} &= \text{tr}(\rho P_i P_i) = \text{tr}(\rho) = 1 \quad \text{since} \quad P_i P_i = 1 \\ M \geq 0 &\Leftrightarrow x^T M x = \text{tr}(\rho (\sum_i^{3n} x_i P_i) (\sum_j^{3n} x_j P_j)) = \text{tr}(\rho X^2) \geq 0 \end{aligned}$$

where $X = \sum_i^{3n} x_i P_i$ and since $X^2, \rho \geq 0$. Since M is real and symmetric, we can express any matrix element as $M_{i,j} = \langle v^i | v^j \rangle$ for some unit vectors $v^1, v^2, \dots, v^{3n+1}$. The vectors have unit norm, since $M_{i,i} = 1$.

After solving the SDP, we choose a random vector $|r\rangle$, the components of which are drawn from the normal distribution and project our solution vectors on it. This is identical to the MaxQP algorithm discussed earlier, except for the constant T which has to be chosen differently. We can build a good geometrical intuition for the truncation step. Since we will project our optimal vectors obtained from the semidefinite program to the random vector $|r\rangle$, we have to make sure that the projections correspond to valid bloch vector components. We ask the following question: What is the maximal value that a component of a valid bloch vector can have, if all three components have the same value? In other words, if we pick every value without knowing the others, what is the maximal value that we can assign to it such that the vector is part of the unit sphere?

$$\|z\| = \sqrt{z_1^2 + z_2^2 + z_3^2} = \sqrt{3z_1^2} = 1.$$

Therefore the maximal value, above which we should round down is $\frac{1}{\sqrt{3}}$. If we truncate such that no bloch vector component can be above this value, we will

always have a valid state. Visually, this is the same as fitting a cube inside the bloch sphere and reducing our state space to inside the cube. The projections are $z_i = \langle r | v^i \rangle / T$ with $T = c\sqrt{\log n}$ and $c = O(\log n)$. This constant will be discussed later. The algorithm looks like this:

1. Solve the relaxed semidefinite program, obtaining an optimal set of vectors v_i
2. Let $|r\rangle$ be a vector of $3n$ indepently and identically distributed $N(0, 1)$ random variables
3. If $|z_i| > \frac{1}{\sqrt{3}}$, we round down: $y_i = \frac{\text{sgn}(z_i)}{\sqrt{3}}$. Otherwise $y_i = z_i$.

As output we take $\rho = \rho_1 \otimes \dots \otimes \rho_n$ where:

$$\rho_a = \frac{1}{2} (\mathbb{I} + y_{3a-2}P_{3a-2} + y_{3a-1}P_{3a-1} + y_{3a}P_{3a}) ..$$

We want to show that this algorithm fullfils the approximation ratio $\Omega(\frac{1}{\log n})$ with probability $\frac{2}{3}$.

First we demonstrate that the approximation ratio is bounded below by a constant.[13]

Theorem 2. *Suppose H is traceless 2-local Hamiltonian. then*

$$\lambda_{sep}(H) \geq \frac{1}{9} \lambda_{max}(H).$$

Where we call λ_{sep} the highest eigenvalue achievable by a product state:

$$\lambda_{sep}(H) = \max_{\phi_1, \dots, \phi_n} \langle \phi_1 \otimes \phi_2 \otimes \dots \otimes \phi_n | H | \phi_1 \otimes \phi_2 \otimes \dots \otimes \phi_n \rangle.$$

We can proof this using entanglement-breaking depolarizing channels. Depolarizing channels are a simple model for noise in quantum information theory. [14] They are implemented by a map Δ_λ , which maps a state ρ onto a linear combination of itself and the identity matrix:[15]

$$\Delta_\lambda(\rho) = \lambda\rho + \frac{1-\lambda}{d}\mathbb{I},$$

where d is the dimension of state. The parameter λ must satisfy

$$-\frac{1}{d^2-1} \leq \lambda \leq 1.$$

This channel maps pure states to mixed states. For $\lambda = 0$ we get the maximally noisy channel, for $\lambda = 1$ the identity. In our case we look at entanglement breaking

channels. These are channels for which the output state is always separable, i.e. if any entangled density matrix is mapped to a separable one.[16] Here, the relevant map \mathcal{E}_δ is defined by its action on the Pauli group:

$$\mathcal{E}_\delta(I) = I \quad \mathcal{E}_\delta(P) = \delta P \quad P \in \{X, Y, Z\}.$$

Therefore, the action on a qubit state in Bloch representation is:

$$\mathcal{E}_\delta(\rho) = \frac{1}{2}\mathbb{I} + \delta \sum_{i=1}^3 \tau_i P_i.$$

Geometrically, this reduces the length of any Bloch vector by a factor δ . Generally, a CPT map Φ can be written as $\Phi(\rho) = \frac{1}{2}(\mathbb{I} + (\mathbf{t} + T\boldsymbol{\tau})P_i)$ where \mathbf{t} is a vector and T a matrix.[17] We can write this as $\mathbf{T} = \begin{pmatrix} 1 & 0 \\ \mathbf{t} & T \end{pmatrix}$, where we can assume without loss of generality that T is diagonal, which follows directly from the Kraus representation Theorem. \mathbf{T} has then the canonical form

$$\mathbf{T} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ t_1 & \lambda_1 & 0 & 0 \\ t_2 & 0 & \lambda_2 & 0 \\ t_3 & 0 & 0 & \lambda_3 \end{pmatrix}.$$

If $\mathbf{t} = 0$, this channel is unital. Unital qubit channels are entanglement breaking if and only if $\sum_j |\lambda_j| \leq 1$ (after T was diagonalized)[17] This implies that qubit channels of the form we look at in the paper are entanglement breaking for $\delta \leq \frac{1}{3}$ as we have $\lambda_1 = \lambda_2 = \lambda_3 = \delta$. Using our definition of \mathcal{E} , we see

$$\text{Tr}(\sigma P_{j_1} P_{j_2} \dots P_{j_L}) = \frac{1}{3^L} \text{Tr}(\rho P_{j_1} P_{j_2} \dots P_{j_L})$$

Where $\sigma = \mathcal{E}_{\frac{1}{3}}^{\otimes n}(\rho)$. With this, we can proof the Theorem due to Lieb.

We consider the n -qubit state ψ satisfying $\langle \psi | H | \psi \rangle = \lambda_{\max}(H)$ With the identity shown above, the depolarized state

$$\sigma = \mathcal{E}_{\frac{1}{3}}^{\otimes n}(|\psi\rangle\langle\psi|).$$

is separable and

$$\lambda_{\text{sep}}(H) \geq \text{Tr}(\sigma H) = \frac{1}{9} \langle \psi | H | \psi \rangle.$$

which is the wanted statement.

It is then shown that the y_i are a good approximation to the z_i , i.e. that the expectation value of $\Delta_{ij} = z_i z_j - y_i y_j$ is sufficiently small. Specifically,



$$\mathbb{E}_r |\Delta_{i,j}| \leq e^{-\Omega(T^2)} \quad 0 \leq i < j \leq 3n.$$

Using this, one can show that the approximation ration holds. To find out more about the constant T , we can look at a recent publication by Harrow and Montanaro [18]. An algorithm is presented which gives an product state approximation ratio to traceless k -local Hamiltonians with respect to the 1-norm of the coefficients of the Hamiltonian, $C_{i,j}$ and D_j in our case. This result uses a different notion of approximation ratio but is concerned with the same kind of Hamiltonians. We use the following equation which is proven in the paper:

$$\sum_{i,j=1}^{3n} |C_{i,j}| \leq Kn\lambda_{max}(H).$$

$K > 0$ is an absolute constant, that we can use to shwow that the approximation ratio $\Omega(\frac{1}{\log n})$ holds, if we choose T and c as described. For 2-local Hamiltonians, Harrow and Montanaro show that

$$\lambda_{min}(H) \leq -\|\hat{H}\|_1/(24l)$$

where l is the maximal number of terms that each qubit participates in and $\|\hat{H}\|_1$ the 1-norm of the coefficients. Another relevant recent result is an algorithm by Ghabarian and Parekh [7],  which finds a constant approximation ratio for the quantum Heisenberg model. 

Chapter 5

Testing specific models

I will now discuss the results of my implementation of the algorithm and the implemented Hamiltonians. The code is written in Python, while for the semidefinite program the interface picos is used. To produce informative plots, the implementation executes the algorithm with output y , and computes the ratio $r = y^T C y / \lambda_{max}$. It does this o times per number of qubits n . The average of the o ratios per n is plotted, where a logarithmic scale is used for the x -axis. I have chosen to plot in the range of $n = 4$ to $n = 5200$ in equidistant steps on the logarithmic scale, using $o = 20$.

The Ising model with a transverse field has physical relevance because it can be used to study quantum phase transitions of ferroelectrics with a tunneling effect or systems of interacting magnetic spins with an outer field. The Hamiltonian,

$$H = \alpha \sum_i Z_i + \beta \sum_i X_i X_{i+1}$$

has been exactly solved in one dimension in [19]. One way to do this by transforming the Hamiltonian into a quadratic form of Fermi operators via the Jordan-Wigner transformation [20]. To diagonalize this Hamiltonian one can use the Bogoliubov transformation which is an isomorphism in the canonical commutation or anticommutation relation algebra.[21]

The parameter α corresponds to the tunneling energy and β to the nearest neighbour interaction. We here look at a closed chain, meaning $1 \leq i \leq n$, $X_{n+1} = X_1$. I have first implemented the model with $\alpha = 0$, $\beta = 1$. This is a model of a one-dimensional chain with nearest neighbor interaction with out an outer field. The state that is stabilized by all terms simultaneously is the state achieving the maximal eigenvalue. In this case, it is the n -fold tensor product of the $+1$ -eigenvector of X :

$$|\psi\rangle = |+X_1\rangle \otimes \dots \otimes |+X_n\rangle,$$

where

$$|+X_i\rangle = \frac{|0\rangle_i + |1\rangle_i}{\sqrt{2}}.$$

The maximal eigenvalue of the Hamiltonian is therefore $\lambda_{max} = n$, since it has n terms. Fig. 5.1 shows the result of computing numeric values of the approximation ratio over a range of n qubit Hamiltonians of this kind.

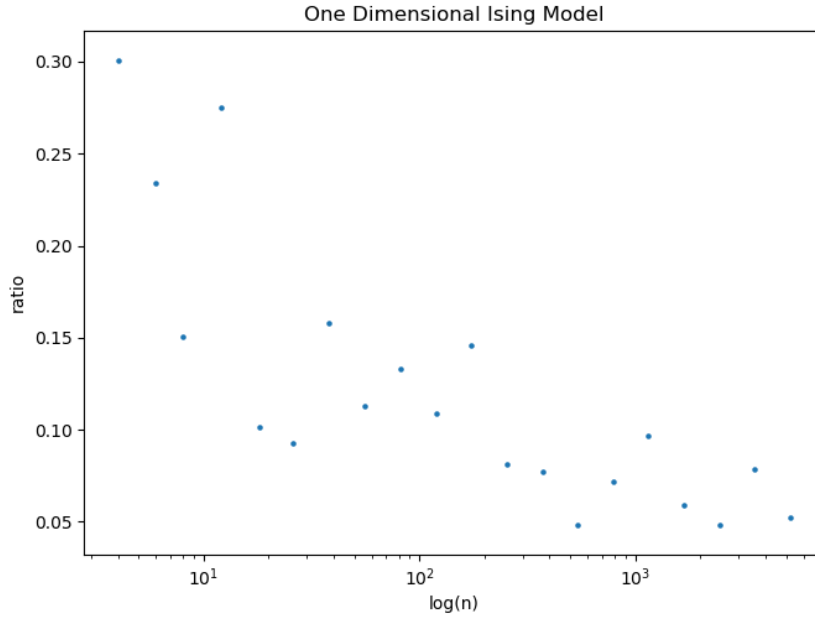


Figure 5.1: The average of 20 approximation ratios per n , plotted from 4 to 5200 qubits with logarithmic scale on the x -axis for the one dimensional Ising model with no transverse field.

It exhibits the expected behaviour of $\Omega(\frac{1}{\log n})$. I have also implemented the transverse field Ising model for non-zero α . Since this Hamiltonian has terms that are linear in Pauli operators, we have to transform it as discussed in chapter 4. The Hamiltonian that was implemented is

$$H = H_2 + Z_{n+1}H_1 = \alpha Z_{n+1} \sum_i Z_i + \beta \sum_i X_i X_{i+1}.$$

Fig. 5.2 shows the result of implementing this model.

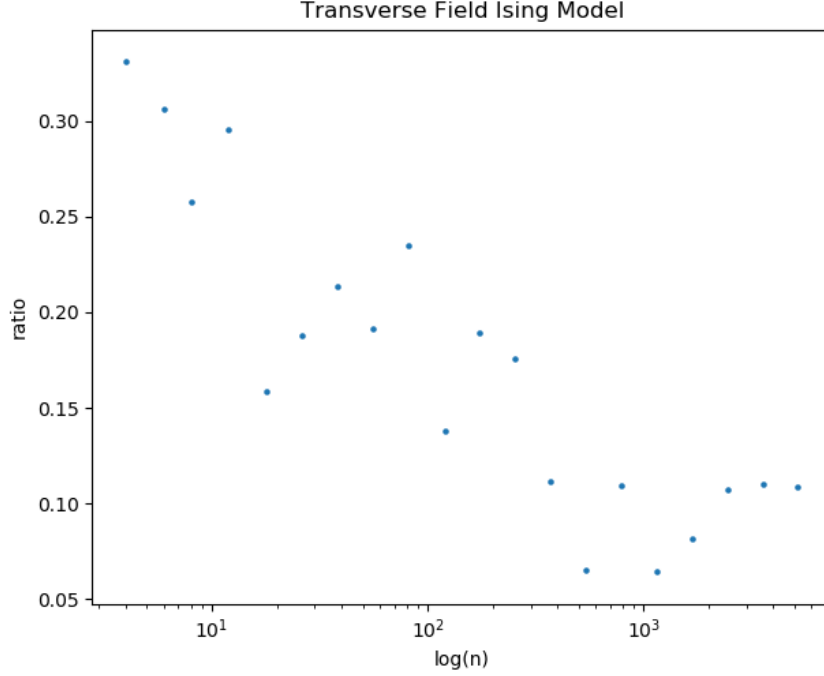


Figure 5.2: The average of 20 approximation ratios per n , plotted from 4 to 5200 qubits with logarithmic scale on the x -axis for the transverse field Ising model. For testing I have chosen $\alpha = 2$ and $\beta = 3$.

The second Hamiltonian implemented is

$$H = \sum_{i=1}^{\frac{n}{4}} X_i X_{i+1} + Z_i Z_{i+1} + X_{i+2} + X_{i+3},$$

where we restrict n to be a multiple of 4. In contrast to the Ising model without a transverse field, the maximal eigenvalue can not be achieved by a product state in this case. To find out the maximal eigenvalue let's look at the first two quadratic terms:

$$H_2 = X_1 X_2 + Z_1 Z_2.$$

The state achieving the maximal eigenvalue $\lambda_{\max}(H_2) = 2$ is the EPR-state $|\text{EPR}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$. This is a maximally entangled state. To find out the product state which approximates this the best, look at a general product state and maximize the overlap.

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = (a_1 |0\rangle + b_1 |1\rangle) \otimes (a_2 |0\rangle + b_2 |1\rangle)$$

with $a_1^2 + b_1^2 = a_2 + b_2^2 = 1$.

$$\max_{\psi_1, \psi_2} \left(|\langle \text{EPR} | \psi \rangle|^2 \right) = \max \left(\left| \frac{1}{\sqrt{2}} (a_1 a_2 + b_1 b_2) \right|^2 \right) = \frac{1}{2}$$

with either $a_1 = a_2 = 1$ and $b_1 = b_2 = 0$ or $b_1 = b_2 = 1$ and $a_1 = a_2 = 0$. Therefore, the product states with the maximal overlap are $|00\rangle$ and $|11\rangle$ with maximal eigenvalue $\lambda_{sep}(H_2) = 1$, the approximation ratio being $\frac{\lambda_{sep}H(2)}{\lambda_{max}(H_2)} = 0.5$.

In general the maximal product state of the Hamiltonian is therefore $\lambda_{max}(H) = n$, and the best achievable eigenvalue by a product state is $\lambda_{sep}(H) \frac{3}{4}n$. Fig. 5.3 shows the expected $\Omega\left(\frac{1}{\log n}\right)$ approximation ratio.

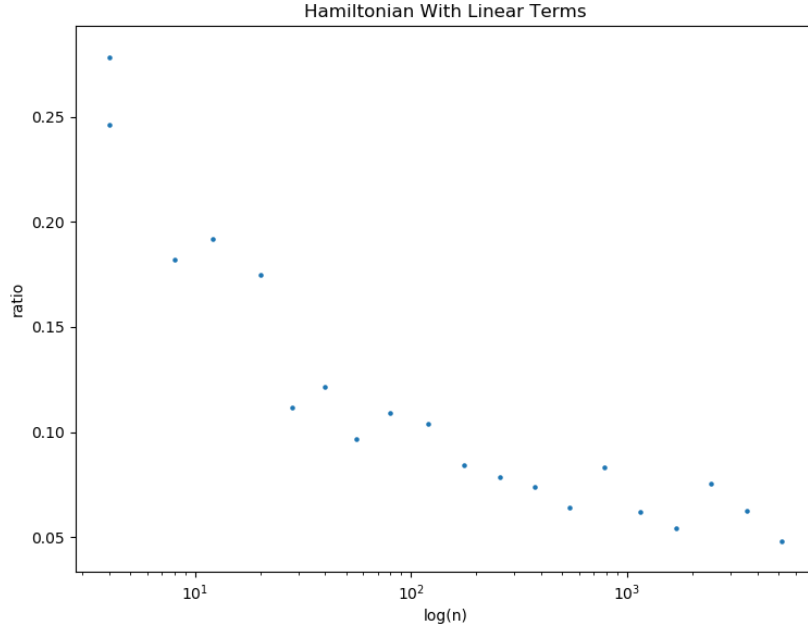


Figure 5.3: The average of 20 approximation ratios per n , plotted from 4 to 5200 qubits with logarithmic scale on the x -axis for a chain with linear terms

Chapter 6

Generalization to qutrits

Most quantum processors are currently based on qubits. Quantum computing based on 3-level systems is known to offer many advantages over qubit-based quantum computing. As an example, error correction can be done more efficiently [22] and quantum cryptography is more robust [23]. A qutrit processor has also recently been used to thermalization in closed quantum systems [24]. In this chapter I will introduce the reader to the basic concepts of 3-level systems and discuss the generalization of the algorithm discussed in chapter 4 to qutrit systems.

First, we will look at the generalization of the Bloch representation to d -level systems. We represent a state ρ with the help of a $d^2 - 1$ -dimensional Bloch vector $\boldsymbol{\tau}$. We call the Bloch space the space of states that fulfill the conditions presented in chapter 1. A state ρ can be represented in the following way:

$$\rho = \frac{1}{d}\mathbb{I} + \sum_{i=1}^{d^2-1} \tau_i \sigma_i$$

where σ_i are generators of $SU(d)$ obeying

$$\sigma_i \sigma_j = \frac{2}{d} \delta_{ij} + d_{ijk} \sigma_k + i f_{ijk} \sigma_k \quad (6.1)$$

The f_{ijk} and d_{ijk} are the structure constants of the Lie-Algebra. f_{ijk} is totally antisymmetric and equals the Levi-Civita-Symbol for $d = 2$, d_{ijk} is totally symmetric and vanishing for $d = 2$. We can construct the generators as follows:[25]

$$\{\sigma_i\}_{i=1}^{d^2-1} = \{u_{jk}, v_{jk}, w_l\}.$$

where

$$\begin{aligned} u_{jk} &= |k\rangle \langle k| + |k\rangle \langle j|, \quad v_{jk} = -i(|j\rangle \langle k| - |k\rangle \langle j|), \\ w_l &= \sqrt{\frac{2}{l(l+1)}} \sum_{j=1}^l (|j\rangle \langle j| - l|l+1\rangle \langle l+1|), \\ 1 &\leq j \leq k \leq d, 1 \leq l \leq d-1 \end{aligned}$$

The τ_i are the components of the Bloch vector and are the expectation values of the σ_i :

$$\tau_i = \text{Tr}(\rho \sigma_i)$$

The center of the Bloch space is the maximally mixed state $\rho_* = \frac{1}{d}\mathbb{I}$. For $d \geq 3$ there are Bloch vectors with $|\tau| \leq 1$ which do not correspond to a positive semi-definite matrix. The space spanned by the Bloch-vectors is therefore not a solid ball with radius 1. We can deduce using (6.1) the following conditions that we have to put on the Bloch vector for the density matrix to describe a pure state [26]:

$$\rho = \rho^2 \Leftrightarrow \begin{cases} \tau^2 = \frac{d-1}{2d} \\ d_{ijk}\tau_j\tau_k = \frac{d-2}{d}\tau_i \end{cases}.$$

The first condition implies the Bloch vector of a pure state being confined to a $d^2 - 1$ dimensional outsphere. The second condition says that the vectors of the pure states are a well defined subset of the surface of the outsphere. The generators of $SU(3)$ are the Gell-Mann-matrices λ_i :

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \end{aligned}$$

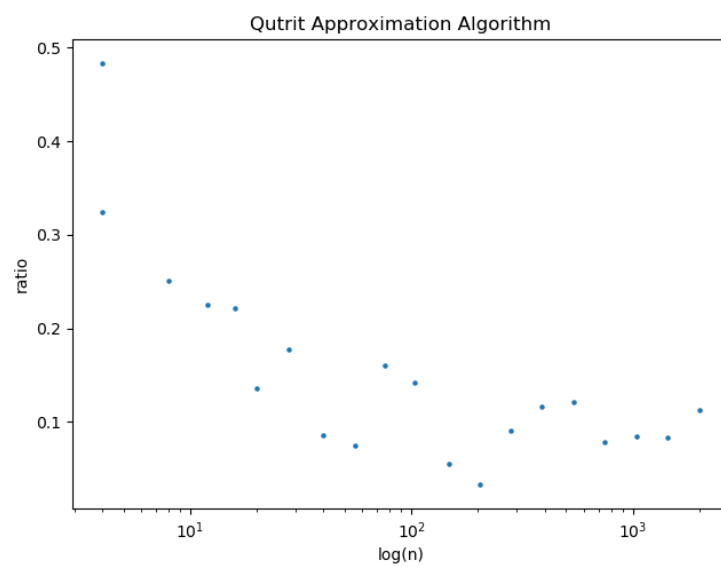


Figure 6.1: My qutrit plot

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