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Bounding Spectral Properties of Many-Body Quantum Systems

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Simulating quantum many-body systems with large size is a considerable challenge in physics. Often, understanding complex many-body phenomena requires information about the spectrum of their Hamiltonian. Apart from performing the exact diagonalisation, which is not possible for systems with tens of particles, there are some scalable methods for obtaining information about specific energy regions (e.g., ground state properties, spectral gap). The main methods that address the problem of characterising properties of the spectrum are variational methods and quantum Monte Carlo methods. These methods were mostly used for low energy states, performing poorly for excited states. On the other hand, semidefinite programming is emerging as a complementary tool, able to yield certified results for quantities of interest. In this thesis, we explore the capabilities of semidefinite programming in the context of quantum many-body systems. Recent works regarding the ground state [WSF⁺24], [WJF⁺26] showcased the potential of these programs and we proceed to focus on their performance in the context of highly entangled states. The proposed semidefinite program can determine parts of the spectrum with no eigenstate and provide bounds for the expectation values of a target eigenstate.

Keywords: Quantum many-body physics, moment matrix, relaxation methods, semidefinite programming, optimisation

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1 Introduction

One of the main challenges in physics is understanding the complex behaviour of systems made up of multiple quantum particles, commonly known as quantum many-body systems. Some of the problems in this subfield involve a N -particle system that lies in a Hilbert space of dimension d . The behaviour of the system is described by the Hamiltonian that acts on the Hilbert space of the whole system $\mathbb{C}^{d^N}$. Some main questions in the field concern system evolution, the minimal energy state (ground state), thermal states and the spectral gap. There is one aspect about these systems that is slowing progress in this field. To obtain complete information about the spectrum, one needs to perform an exact diagonalisation of the Hamiltonian. Since it acts on a Hilbert space $\mathbb{C}^{d^N}$, the size of the operator is $d^N \times d^N$, which grows exponentially with the number of particles. A major consequence is that the full characterisation of the spectrum becomes intractable for systems beyond tens of particles.

There are several alternatives to the memory consumption issue, each of them with a drawback. Tensor network solutions provide upper bounds for the ground state energy, but they fail to maintain the performance for highly entangled states. Quantum Monte Carlo methods solve the scaling issue by using stochastic sampling, but they suffer from the sign problem. Other alternatives are relaxation methods in semidefinite programming (SDP). By relaxing the physical constraints, this approach searches for a solution in a superset of valid quantum states. Relaxation methods SDPs provide lower bounds on the ground state energy, since the optimisation is done over a superset. Therefore, by combining with a variational method, one can confine the true energy [WSF⁺24]. The method provides bounds for observables and these programs might become more complex compared to the previous alternatives.

This work revolves around relaxation methods applied to SDPs, which were introduced almost 20 years ago [NPA07]. This approach manages to address the question of whether a set of expectation values could belong to a quantum state. Initially, they were proposed for bounding the violation of Bell inequalities, but later on, these methods were also adapted for studying many-body quantum systems. Most of the works using relaxed SDPs for quantum many-body systems focus on properties regarding the ground state, entering into direct competition with tensor network methods that provide extremely good results in this case. Our work proposes to explore with similar techniques different areas of the spectrum: the spectral gap and excited states. Characterising these properties provides knowledge about macroscopic phenomena like phase transitions and about some potential correlation with thermal states. Apart from the physical motivation, there is a need for tools designed for the high-energy regime, since none of the alternative scalable methods provide good results in this context.

The structure of this work is the following: In Section 2 we provide a more detailed description of the key concepts of the work, then we proceed to present the proposed SDP relaxation in Section 3. All the numerical findings and the performance of the method are presented in Section 4 and Section 5 concludes the work with the final remarks and future directions.

2 Background

2.1 Semidefinite Programming

Convex optimisation is a branch of mathematics solving problems that arise in various fields like physics, signal processing, finance and control systems. In standard form, a

convex optimisation problem reads

$$\begin{aligned} & \underset{\mathbf{x} \in \mathcal{A}}{\text{minimize}} && f_o(\mathbf{x}) \\ & \text{subject to} && f_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, p, \\ & && h_j(\mathbf{x}) = 0 \quad j = 1, \dots, q. \end{aligned} \tag{1}$$

It consists of a linear convex function $f_o(\mathbf{x})$ to be minimised/maximised, usually called cost function, inequality constraints $f_i(\mathbf{x})$ and linear equality constraints $h_j(\mathbf{x})$. The optimisation is done over a convex set $\mathcal{A}$ which contains optimisation variables $\mathbf{x}$. The set of variables that fulfil all the constraints is called the feasible set. Depending on the cardinality of the feasible set, a convex optimisation problem can have different statuses. If there is at least one element in the feasible set, the program status is feasible. When the feasible set is empty, the SDP status is infeasible.

A semidefinite program (SDP) is a particular case of a convex optimisation problem, which has matrix positivity constraints instead of scalar inequality constraints and has symmetric matrices as optimisation variables. The standard form of a SDP is

$$\begin{aligned} & \underset{X \in \mathcal{A}}{\text{minimize}} && \text{Tr}\{CX\} \\ & \text{subject to} && X \succeq 0, \\ & && \text{Tr}\{A_i X\} = b_i \quad i = 1, \dots, p, \end{aligned} \tag{2}$$

where $\text{Tr}\{CX\}$ is the cost function, $X \succeq 0$ the matrix positivity constraint, $\text{Tr}\{A_i X\} = b_i$ are the equality constraints, X is the optimisation variable and $\mathcal{A} = \mathbb{C}^{n \times n}$ is the convex set, with C, A_i, X hermitian matrices and $b_i \in \mathbb{R}$.

Optimising a convex function over a convex set ensures that each local minimum/maximum is a global minimum/maximum. This represents one of the strong points of this family of optimisation problems. We will proceed to prove this for a general SDP.

Proof:

For a function to be convex, it has to fulfil the following:

$$f((1 - \alpha)X + \alpha Y) \leq (1 - \alpha)f(X) + \alpha f(Y), \quad \alpha \in [0, 1]. \tag{3}$$

One can note that this applies to the cost function from (2), by simply using the properties of the trace.

$$\text{Tr}\{(1 - \alpha)CX + \alpha CY\} = (1 - \alpha) \text{Tr}\{CX\} + \alpha \text{Tr}\{CY\}, \quad \alpha \in [0, 1]. \tag{4}$$

A set is convex if the segment between any two points from the set is also contained in the set

$$X, Y \in \mathcal{A} \implies (1 - \alpha)X + \alpha Y \in \mathcal{A}, \quad \alpha \in [0, 1], \tag{5}$$

where $\mathcal{A}$ is the convex set. In the context of a SDP, the subset of all the positive semidefinite matrices that obey the linear equality constraint is the feasible set. For $X, Y \in \mathbf{P}$, where $\mathbf{P}$ is the set of positive semidefinite matrices, one can note that the following holds:

$$(1 - \alpha)X + \alpha Y \in \mathbf{P}, \quad \alpha \in [0, 1], \tag{6}$$

since the convex combination of two positive semidefinite matrices is positive semidefinite. To prove that any local minimum/maximum is global when optimising over a convex cost function and a convex set, one can use the proof by contradiction. Let X^* be a local minimum, meaning that

$$\text{Tr}\{CX^*\} < \text{Tr}\{CX\}, \quad X^*, X \in \mathbf{P}, \tag{7}$$

such that

$$\|X - X^*\|_1 = \text{Tr}\left\{\sqrt{(X - X^*)^\dagger(X - X^*)}\right\} < \epsilon, \quad (8)$$

for an arbitrary small ϵ and let $Y \in \mathbf{P}$ be the global minimum, therefore

$$\text{Tr}\{CY\} < \text{Tr}\{CX\}, \forall X \in \mathbf{P}. \quad (9)$$

Because the feasible set is convex, the segment between any two feasible points is also part of the set. Let

$$Z = (1 - \alpha)X^* + \alpha Y \quad (10)$$

be a point on the segment determined by the local minimum and the global minimum. For any convex function, (3) holds and combining this with the fact that Y is the global minimum, one can write

$$\text{Tr}\{(1 - \alpha)CX^* + \alpha CY\} < (1 - \alpha)\text{Tr}\{CX^*\} + \alpha\text{Tr}\{CX^*\} = \text{Tr}\{CX^*\}, \quad (11)$$

therefore

$$\text{Tr}\{CZ\} < \text{Tr}\{CX^*\}. \quad (12)$$

Now, if one sets α such that Z is a point within ϵ distance from X^* , it is clear that X^* is not the minimum from that surrounding, which contradicts the initial assumption that X^* is a local minimum. $\square$

Because of this property, which ensures that any local minimum/maximum is actually global in this setting, the algorithm solving a SDP problem has the certainty that once it finds a solution, it is the optimal one.

Each SDP has two possible formulations: the primal problem (2) and the dual problem. One can transform one to the other by writing the Lagrangian and manipulating the terms [BV04]. An important property is the concept of strong duality. Let p^* be the solution of the primal problem and d^* be the solution of the dual problem. Weak duality always holds and implies

$$p^* \geq d^*, \quad (13)$$

while strong duality implies

$$p^* = d^*. \quad (14)$$

In some SDP problems, one formulation may require fewer variables and constraints, making it easier to model analytically. In those cases, strong duality is a crucial property that allows the interchange between formulations.

There are several numerical solvers for SDP problems. Out of all the available options, two main classes of solvers are commonly used: interior-point methods (e.g., Mosek [MOS26]) and splitting methods (e.g., SCS [OCPB24]). Depending on the size and the number of optimisation variables involved in the SDP, one might prefer the solver from Mosek, which is faster but needs more memory resources, or SCS, which is slower but requires less memory. Any of these solvers has the same approach when it comes to solving a SDP problem. They are iterative algorithms and solve both the primal and the dual problem in parallel. They monitor convergence criteria at each iteration, until either they find a feasible/unfeasible status of the problem or they hit the maximum number of iterations. Some examples of metrics used in the convergence criteria are the cost function and the duality gap $|p^* - d^*|$.

2.2 Many-Body quantum physics

Many-body quantum physics studies the complex behaviour of systems of interacting quantum particles (e.g., a 1-dimensional spin chain). The complete description of the state of the system is encoded in a linear positive semidefinite Hermitian operator called the density matrix, which acts on the Hilbert space of the system.

The efforts of the many-body physics community are focused on understanding the behaviour of systems made up of many quantum particles. One example would be a spin system, which is a collection of spin- $\frac{1}{2}$ particles. The objective is to understand the complexity of such systems or design algorithms to get information numerically about their behaviour. One step in this direction is the study of simplified spin models in 1, 2 or 3 dimensions (e.g., Heisenberg model, Ising model). A notorious problem in this area is the ground state problem. Each different configuration of the spins represents a state and it is associated with a specific density matrix operator. The ground state problem implies finding the spin configuration with the lowest energy, called the ground state. Another area of interest is related to the spectral gap. This is the difference in energy from the ground state to the first excited state. The interest arises because there are some correlations between the size of the gap and some other characteristics of the system, with implications for criticality, emerging phenomena, and adiabatic quantum algorithms.

Fully understanding the behaviour of many-body systems is an ambitious objective for the physics community, but it requires overcoming a considerable issue. For a N -particle spin system, the Hilbert space is $\mathbb{C}^{2^N}$. It is now straightforward to notice that for a system with N particles, one requires $4^N - 1$ elements to fully write down the density matrix operator. This exponential scaling is the main issue regarding many-body quantum systems, since the problem becomes intractable for systems of large size.

2.3 Relaxation methods

Relaxation methods are a workaround for the exponential growth of the Hilbert space size in many-body systems. This approach transforms the original problem into a more general one, which requires less computational effort. To further explain the concept of a relaxation method, we will proceed with an example. Take an arbitrary local many-body Hamiltonian for qubits

$$H = \sum_{i=1}^{N-1} h_{i,i+1}. \quad (15)$$

If we are interested in computing the ground-state energy, the goal is to find the lowest energy configuration, therefore, solve the following optimisation problem

$$\begin{aligned} & \underset{\rho \in \mathbb{C}^{2^N \times 2^N}}{\text{minimize}} && \text{Tr}\{H\rho\} \\ & \text{subject to} && \rho \succeq 0, \\ & && \text{Tr}\{\rho\} = 1, \end{aligned} \quad (16)$$

As mentioned before, for large sizes of N , the problem becomes intractable. However, one can take advantage of the local structure of the Hamiltonian and write a different optimisation problem, the relaxation of (16) as

$$\begin{aligned}
& \underset{\rho_{i,i+1} \in \mathbb{C}^{4 \times 4}}{\text{minimize}} && \sum_{i=1}^{N-1} \text{Tr}\{h_{i,i+1} \rho_{i,i+1}\} \\
& \text{subject to} && \rho_{i,i+1} \succeq 0, \quad i = 1, \dots, N-1, \\
& && \text{Tr}\{\rho_{i,i+1}\} = 1, \quad i = 1, \dots, N-1,
\end{aligned} \tag{17}$$

where

$$\rho_{i,i+1} = \text{Tr}_{1,\dots,i-1,i+2,\dots,N}\{\rho\}. \tag{18}$$

and $\text{Tr}_i\{\cdot\}$ is the partial trace over the i -th subsystem. One can notice that the size of the reduced density matrices is constant. Hence, the relaxed problem has a different memory scaling, which makes it tractable. The SDP (17) is a relaxation of (16) because the implication goes only one way. For any density matrix $\rho \in \mathbb{C}^{2^N \times 2^N}$, there exists a set of well-defined reduced density matrices $\{\rho_{i,i+1}\}_{i=1,\dots,N-1}$, where $\rho_{i,i+1} \in \mathbb{C}^{4 \times 4}$, but from one set of reduced density matrices is not guaranteed to construct a well-defined density matrix.

The relaxation method provides a lower bound for the lowest energy. Let E_0^* be the actual ground state energy, the solution of (16), and E_1^* be the solution of the relaxed problem (17). Because in (17) the solution is obtained by minimising each local subsystem energy independently, there is no guarantee that by combining all the resulting local configurations one will get a physical global state. Therefore, there is the following relation between the two solutions

$$E_1^* \leq E_0^*. \tag{19}$$

The same thing happens for a maximisation problem. As long as one performs a relaxation, the allowed solutions would lie in a larger set than the solution of the original problem, resulting in obtaining lower bounds for a minimisation problem and upper bounds for a maximisation problem.

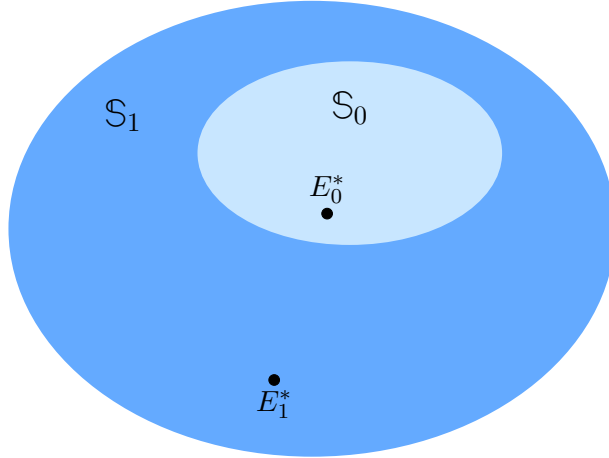


Figure 1: Schematic representation displaying that the set of solutions $\mathbb{S}_0$ from the original problem (16) is a subset of $\mathbb{S}_1$, the one from the relaxed problem (17).

2.4 Relaxation methods in many-body quantum physics

The moment matrix is a concept first introduced in [NPA07]. Having a quantum state ρ , one can always build a corresponding moment matrix

$$M_{ab} = \text{Tr}\{O_a^\dagger O_b \rho\}, \quad a, b = 1 \dots m, \tag{20}$$

which is a positive semidefinite Hermitian matrix. The entries are expectation values of observables, often referred to as moments.

Proof: The matrix M is positive semidefinite if and only if

$$v^\dagger M v \geq 0 \quad (21)$$

By writing the expression of $v^\dagger M v$ element-wise, one can notice that M is positive semidefinite

$$\begin{aligned} v^\dagger M v &= \sum_{a,b}^m v_a^* M_{ab} v_b, \\ &= \sum_{a,b}^m v_a^* \text{Tr}\{O_a^\dagger O_b \rho\} v_b, \\ &= \text{Tr}\left\{\left(\sum_a^m v_a O_a\right)^\dagger \sum_b^m v_b O_b \rho\right\} \geq 0. \end{aligned} \quad (22)$$

To check if the matrix is Hermitian, one has to check if $M = M^\dagger$.

$$\begin{aligned} (M^\dagger)_{ab} &= (M_{ba})^*, \\ &= \left(\text{Tr}\{O_b^\dagger O_a \rho\}\right)^*, \\ &= \text{Tr}\{(O_b^\dagger O_a \rho)^\dagger\}, \\ &= \text{Tr}\{\rho O_a^\dagger O_b\}, \\ &= M_{ab}. \end{aligned} \quad (23)$$

□

As stated before, one can build a moment matrix from a well-defined state ρ . However, from a moment matrix, one cannot determine a density matrix operator for a physical state. Because the implication is unidirectional, one can use the moment matrix formalism as a relaxation of the density matrix. Thus, by replacing it with the moment matrix in a SDP, one builds a relaxed version of the problem.

In [NPA07], the authors introduced the concept of NPA hierarchy. It states that one can build a family of SDPs to get monotonically tighter bounds on the desired quantity and it is proven that by increasing the size of the list $\{O_a\}_{a=1\dots m}$, meaning that the moment matrix increases in size, the bounds become tighter. These concepts were later on adapted for spin- $\frac{1}{2}$ systems. The authors from [WSF⁺24] designed a SDP to bound the ground state energy. This work introduced new constraints that rely on some preliminary bounds for the ground state energy, the upper bound being computed with a variational method and the lower bound with a relaxed SDP. Having these, the authors added the following linear constraints to reduce the feasible set of the SDP

$$\begin{aligned} E_{GS} &\leq E_{UB}, \\ E_{GS} &\geq E_{LB}. \end{aligned} \quad (24)$$

Another relaxation regarding ground state is presented in the work from [KSDN24]. It uses the renormalisation group and applies a series of relaxation methods, including establishing a hierarchy of constraints for local reduced density matrices. In the following years, the authors in [JFM⁺26] introduced a method to use the NPA hierarchy of SDPs to map the phase transition diagram of a spin system. Relaxation methods SDPs were

utilised for open quantum systems as well, obtaining certification of steady-state properties [MFDB⁺25]. Later on, in [WJF⁺26], the authors from [WSF⁺24] continued the work by exploiting the structure of the systems to enhance the scalability of the SDPs. After the display of the success of the additional constraints, two other works introduce some novel constraints based on the commutation and anti-commutation properties of the Hamiltonian with respect to ground and thermal equilibrium states [FFS24], [AKG⁺26].

3 Method

The objective of this work is to introduce a novel method that allows one to bound the properties of a many-body system when its energy is constrained to an arbitrary interval in the spectrum. From the technical point of view, this work focuses on studying the performance of a pair of novel SDP constraints. To benchmark the power of the method, we use it to inspect the spectrum properties of the Ising Hamiltonian with transverse and longitudinal fields

$$H = -J \sum_{i=1}^N \sigma_i^z \sigma_{i+1}^z - g \sum_{i=1}^N \sigma_i^x - h \sum_{i=1}^N \sigma_i^z \quad (25)$$

and periodic boundary conditions, defined on a Hilbert space $\mathbb{C}^{2^N}$, where d is the dimension of the model and

$$\mathbb{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (26)$$

$$\sigma_i^\alpha = \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \cdots \otimes \mathbb{1}_{i-1} \otimes \sigma_i^\alpha \otimes \mathbb{1}_{i+1} \otimes \cdots \otimes \mathbb{1}_N, \quad (27)$$

$$(\sigma_i^\alpha)^\dagger \sigma_j^\beta = \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \cdots \otimes \mathbb{1}_{i-1} \otimes (\sigma_i^\alpha)^\dagger \otimes \mathbb{1}_{i+1} \otimes \cdots \otimes \mathbb{1}_{j-1} \otimes \sigma_j^\beta \otimes \mathbb{1}_{j+1} \otimes \cdots \otimes \mathbb{1}_N, \quad (28)$$

$\alpha, \beta \in \{x, y, z\}$.

The main interest is to observe the impact of the new constraints on the tasks of obtaining information about the properties of the spectral gap and excited states. To introduce the novel constraints of this work, we will start by analysing the exact problem. The objective is to design a SDP to compute expectation values for a target eigenstate of energy E . The brute force approach is the following SDP:

$$\begin{aligned} & \text{minimize/maximize} && \text{Tr}\{O\rho\} \\ & \text{subject to} && \rho \succeq 0, \\ & && \text{Tr}\{\rho\} = 1, \\ & && [\rho, H] = 0, \\ & && H\rho = E\rho. \end{aligned} \quad (29)$$

The constraints

$$\rho \succeq 0 \quad (30)$$

$$\text{Tr}\{\rho\} = 1 \quad (31)$$

allow the feasible set to contain only well-defined quantum states,

$$[\rho, H] = 0 \quad (32)$$

restricts the possible solutions to those of the form

$$\rho = \sum_{k=1}^{2^N} p_k |E_k\rangle \langle E_k|, \quad (33)$$

where $|E_k\rangle \langle E_k|$ are eigenstates from the spectral decomposition of the Hamiltonian

$$H = \sum_{k=1}^{2^N} E_k |E_k\rangle \langle E_k|. \quad (34)$$

The constraint

$$H\rho = E\rho \quad (35)$$

leaves in the feasible set only eigenstates of the Hamiltonian that have the desired energy E . Unfortunately, this SDP requires exponentially more memory as the system increases in size. Moreover, knowing an arbitrary eigenvalue of the Hamiltonian precisely is not realistic. To fix the latter issue, we will rewrite the SDP such that it looks for a range of values, which we will call an energy shell.

$$\begin{aligned} & \text{minimize/maximize} && \text{Tr}\{O\rho\} \\ & \text{subject to} && \rho \succeq 0, \\ & && \text{Tr}\{\rho\} = 1, \\ & && [\rho, H] = 0, \\ & && H\rho \leq (E + \delta E)\rho, \\ & && H\rho \geq (E - \delta E)\rho, \end{aligned} \quad (36)$$

where the shell has a thickness of $2\delta E$. The states from the feasible set of this SDP are of the form

$$\rho = \sum_{E_k \in [E - \delta E, E + \delta E]} p_k |E_k\rangle \langle E_k|, \quad p_k \in [0, 1], \quad (37)$$

where E_k is the eigenvalue associated to the state $|E_k\rangle \langle E_k|$ from the spectral decomposition of the Hamiltonian (34).

Proof: The spectral decomposition of a state ρ in the Hamiltonian eigenbasis reads

$$\rho = \sum_{k,k'=1}^{2^N} a_{k,k'} |E_k\rangle \langle E_{k'}|. \quad (38)$$

Now inspect the expression of the commutator $[H, \rho]$

$$\begin{aligned} [H, \rho] &= \sum_{i,k,k'=1}^{2^N} E_i a_{k,k'} |E_i\rangle \langle E_i| |E_k\rangle \langle E_{k'}| - \sum_{i,k,k'=1}^{2^N} E_i a_{k,k'} |E_k\rangle \langle E_{k'}| |E_i\rangle \langle E_i|, \\ &= \sum_{k,k'=1}^{2^N} E_k a_{k,k'} |E_k\rangle \langle E_{k'}| - \sum_{k,k'=1}^{2^N} E_{k'} a_{k,k'} |E_k\rangle \langle E_{k'}|, \\ &= \sum_{k,k'=1}^{2^N} [(E_k - E_{k'}) a_{k,k'}] |E_k\rangle \langle E_{k'}|, \end{aligned} \quad (39)$$

and by imposing (32) one can note that the only allowed states are

$$\rho = \sum_{k=1}^{2^N} p_k |E_k\rangle \langle E_k|, \quad (40)$$

where $p_k > 0$ and $\sum_k p_k = 1$. One can rewrite the first energy shell constraint

$$H\rho \leq (E + \delta E)\rho \quad (41)$$

as

$$[H - (E + \delta E)]\rho \leq 0 \quad (42)$$

The expression of the left-hand side term from the inequality reads

$$\begin{aligned} [H - (E + \delta E)]\rho &= \sum_{i=1}^{2^N} E_i |E_i\rangle \langle E_i| \sum_{k=1}^{2^N} p_k |E_k\rangle \langle E_k| - (E + \delta E) \sum_{k=1}^{2^N} p_k |E_k\rangle \langle E_k|, \\ &= \sum_{k=1}^{2^N} E_k p_k |E_k\rangle \langle E_k| - (E + \delta E) \sum_{k=1}^{2^N} p_k |E_k\rangle \langle E_k|, \\ &= \sum_{k=1}^{2^N} [E_k - (E + \delta E)] p_k |E_k\rangle \langle E_k|, \end{aligned} \quad (43)$$

then (42) holds if and only if

$$E_k \leq E + \delta E. \quad (44)$$

Repeating the same steps for

$$H\rho \geq (E - \delta E)\rho \quad (45)$$

yields

$$E_k \geq E - \delta E, \quad (46)$$

thus, the feasible set contains only states of this form (37). $\square$

Now the SDP has some realistic requirements regarding the targeted state, yet the scaling problem still holds. To address the scalability issue, we use the moment matrix relaxation. Instead of using the density matrix, we use the moment matrix, with its elements as a list of optimisation variables.

Before formulating the relaxed SDP, there are some preliminary objects to be defined: The relaxation in this work focuses on the following observables

$$O_a \in \{\mathbb{1}, \sigma_i^x, \sigma_i^y, \sigma_i^z, \}_{i=1, \dots, N}, \quad (47)$$

where N is the number of particles in the system. Let $\mathcal{B}$ be a list of such observables

$$\mathcal{B} = \{O_a^\dagger O_b\}_{a,b=1, \dots, m}, \quad (48)$$

acting as a basis to build the set of moments $\langle O_a^\dagger O_b \rangle$ that serve as optimisation variables,

We build the moment matrix using the elements of $\mathcal{B}$ in the following manner:

$$M = \begin{bmatrix} \langle O_1^\dagger O_1 \rangle & \langle O_1^\dagger O_2 \rangle & \cdots & \langle O_1^\dagger O_m \rangle \\ \langle O_2^\dagger O_1 \rangle & \langle O_2^\dagger O_2 \rangle & \cdots & \langle O_2^\dagger O_m \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle O_m^\dagger O_1 \rangle & \langle O_m^\dagger O_2 \rangle & \cdots & \langle O_m^\dagger O_m \rangle \end{bmatrix},$$

To formulate the relaxed SDP in terms of the moment matrix, we need to translate the constraints from the density matrix context to the moment matrix one. The relaxation of the positivity constraint (30) is the positivity of the moment matrix

$$M \succeq 0, \quad (49)$$

since for any valid quantum state, the associated moment matrix is always positive. The counterpart of the normalisation of the state (31) is

$$\langle \mathbb{1} \rangle = 1. \quad (50)$$

Starting from the property of an eigenstate (32), one can note that

$$\text{Tr}\{O[H, \rho]\} = 0, \quad (51)$$

which is equivalent to

$$\text{Tr}\{[O, H]\rho\} = 0, \quad (52)$$

by using the properties of the trace. Therefore,

$$\langle [O, H] \rangle = 0 \quad (53)$$

holds for an arbitrary operator O and for all states that are diagonal in the energy eigenbasis. The equation (53) serves as a constraint for the relaxed SDP. To restrict the feasible set similarly to the energy shell constraint from (36), we start from the family of states (37) and inspect the following expression

$$\begin{aligned} \left| \text{Tr}\{O_a^\dagger O_b (H - E\mathbb{1})\rho\} \right| &= \left| \text{Tr}\left\{ \sum_{E_k \in [E-\delta E, E+\delta E]} p_k O_a^\dagger O_b (H - E\mathbb{1}) |E_k\rangle \langle E_k| \right\} \right|, \\ &= \left| \sum_{E_k \in [E-\delta E, E+\delta E]} (E_k - E) p_k \text{Tr}\{O_a^\dagger O_b |E_k\rangle \langle E_k|\} \right|, \\ &= \left| \sum_{E_k \in [E-\delta E, E+\delta E]} (E_k - E) p_k \langle E_k | O_a^\dagger O_b | E_k \rangle \right|, \\ &\leq \sum_{E_k \in [E-\delta E, E+\delta E]} |(E_k - E)| p_k |\langle E_k | O_a^\dagger O_b | E_k \rangle|, \\ &\leq \delta E \|O_a^\dagger O_b\|_{\text{op}}, \end{aligned} \quad (54)$$

where

$$\|O_a^\dagger O_b\|_{\text{op}} = \sup_{\langle \psi | \psi \rangle = 1} \sqrt{\langle \psi | O_b^\dagger O_a O_a^\dagger O_b | \psi \rangle}. \quad (55)$$

Since we work with elements of the Pauli basis, $\|O_a^\dagger O_b\|_{\text{op}} = 1, \forall O_a, O_b \in \mathcal{B}$.

Furthermore, $\left| \text{Tr}\{O_a^\dagger O_b (H - E\mathbb{1})\rho\} \right|$ can be written in the moment matrix context as follows:

$$\begin{aligned} \left| \text{Tr}\{O_a^\dagger O_b (H - E\mathbb{1})\rho\} \right| &= \langle O_a^\dagger O_b (H - E\mathbb{1}) \rangle, \\ &= \left| \langle O_a^\dagger O_b H \rangle - E \langle O_a^\dagger O_b \rangle \right|. \end{aligned} \quad (56)$$

Finally, the relaxed energy shell constraint takes the form:

$$-\delta E \leq \langle O_a^\dagger O_b H \rangle - E \langle O_a^\dagger O_b \rangle \leq \delta E \quad (57)$$

By combining all the equivalent constraints, one can formulate the SDP proposed by this work

$$\begin{aligned} & \text{minimize/maximize} \quad \langle O \rangle \\ & \text{subject to} \quad M \succeq 0, \\ & \quad \langle \mathbb{1} \rangle = 1, \\ & \quad \langle [O_a, H] \rangle = 0, \quad \forall O_a \in \mathcal{B}, \\ & \quad -\delta E \leq \langle O_a^\dagger O_b H \rangle - E \langle O_a^\dagger O_b \rangle \leq \delta E, \quad \forall O_{a,b} \in \mathcal{B}. \end{aligned} \quad (58)$$

4 Results

This work inspected spectral properties of the Hamiltonian (25) with $J = 1$, $g = 1.3$ and $h = 0.5$, which displays chaotic behaviour. To numerically analyse the properties of this model, we used the solver from Mosek and all the simulations that produced the results of this work were run on a standard desktop workstation having an Intel Core i5-12500 3.00 GHz processor and 16 GB of RAM. As stated before, this solver converges to the solution in a small number of iterations, but has a larger memory consumption. This issue was mitigated by exploiting a common symmetry in local periodic boundary condition spin systems, the translational invariance. As the name suggests, translational invariance implies that by shifting the spins along the D-dimensional lattice, the properties remain unchanged. This reduces the number of unique entries in the moment matrix, hence reducing the number of optimisation variables. The translational invariance in the context of moments reads

$$\begin{cases} \langle \sigma_i^\alpha \rangle = \langle \sigma_{i+k}^\alpha \rangle, & \forall k \in \mathbb{Z}, \\ \langle \sigma_i^\alpha \sigma_j^\beta \rangle = \langle \sigma_k^\gamma \sigma_l^\delta \rangle, & \text{if } |i-j| = |k-l|, \quad \alpha, \beta, \gamma, \delta \in \{x, y, z\} \end{cases} \quad (59)$$

The SDP from (58) is a numerical tool with several applications. It can be used to inspect the energy gap between the ground state and the first excited state. However, the main application of the tool is to provide non-trivial bounds for properties of excited states.

4.1 Spectral gap results

A tool that certifies the absence of an eigenstate is convenient in the context of many-body quantum physics. Because of the novel shell constraints (57), the proposed SDP manages to successfully conclude the absence of an eigenstate in the chosen energy shell $[E - \delta E, E + \delta E]$. If there is no eigenstate contained in that range and the problem is constrained enough, the feasible set is empty and the SDP returns the infeasible status for the problem. In this work, we used this particular aspect of the SDP to design a routine that scans a part of the spectrum and provides an energy interval with no eigenstate within the scanned region.

The spectrum scanning routine can only provide certain information about the absence of an eigenstate. The SDP returning a feasible problem status is an inconclusive scenario, since it can occur because there are too few observables in $\mathcal{B}$, meaning that the problem is too relaxed, or because indeed there is an eigenstate in the energy shell. The routine reads:

1. Choose a basis $\mathcal{B}$ that scales polynomially with the system size N ,
2. Fix the value for δE ,
3. Choose an initial energy level E ,
4. Run the SDP with the energy shell $[E - \delta E, E + \delta E]$,
5. Shift the energy level E with exactly $2\delta E$,
6. Repeat steps 4 and 5 until the desired part of the spectrum has been scanned.

As a result, the user will have a list with all the problem statuses returned by the SDPs and their corresponding energy shells. Each sequence of consecutive infeasible problem statuses allows the user to concatenate the corresponding energy shells and obtain the interval without an eigenstate.

One of our work priorities was to test this novel approach and provide a proof of concept. We focused on utilising this routine in obtaining information about the spectral gap. Our choice of parameters was

$$\delta E = 0.1 \quad (60)$$

and

$$\mathcal{B} = \{\mathbb{1}, \sigma_i^x, \sigma_i^y, \sigma_i^z, \sigma_i^\alpha \sigma_{i+d}^\beta\}_{i=1\dots N; d=1,\dots, \lceil \frac{N-3}{2} \rceil; \alpha, \beta \in x, y, z} \quad (61)$$

as basis for the set of moments, where N is the system size and $\lceil \cdot \rceil$ is the ceiling function. In Fig. 2, one can notice that the routine successfully identified a considerable part of the spectral gap for small system sizes. From the figure, we can state that some system sizes are more difficult to certify than others and that there is no visible dependence on system size.

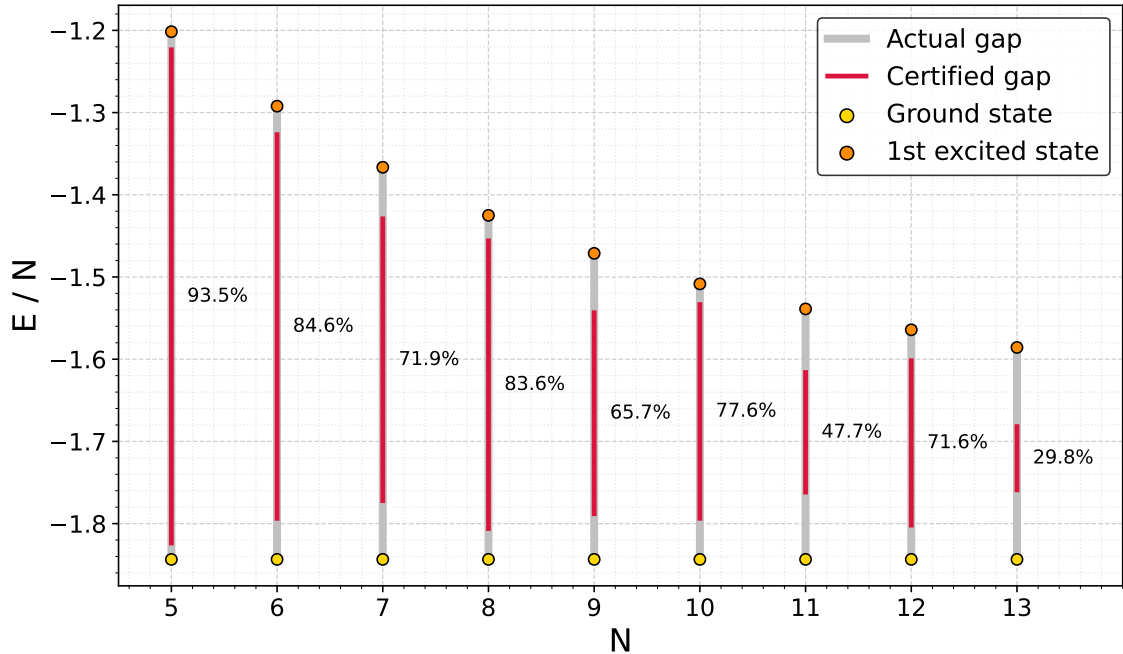


Figure 2: Proof of concept results for the spectrum scanning routine applied for the spectral gap of the mixed field Ising model (25) with $J = 1$, $g = 1.3$ and $h = 0.5$ displaying the percentage of the gap that was certified to lack eigenstates.

4.2 Excited states results

One of the use cases of the tool proposed by the work is bounding properties of excited states. The tool allows the user to establish a connection between local expectation values and an energy range $[E - \delta E, E + \delta E]$. Note that the energy range is the user's choice.

We will now present the behaviour of the tool in the context of bounding properties of excited states. Starting from the fact that the feasible set of the proposed SDP has entries that could be expectation values compatible with physical states of the form (37), one can write the cost function for those states as

$$\sum_{E_k \in [E - \delta E, E + \delta E]} p_k \langle E_k | O | E_k \rangle, \quad p_k \in [0, 1]. \quad (62)$$

Let

$$\mathbb{E} = \{E_k\}_{E_k \in [E - \delta E, E + \delta E]} \quad (63)$$

be the set of all the eigenstates in the energy shell. Depending on $\mathbb{E}$, there are three main scenarios:

$$|\mathbb{E}| = 0, \quad (64)$$

$$|\mathbb{E}| = 1, \quad (65)$$

$$|\mathbb{E}| > 1, \quad (66)$$

where $|\mathbb{E}|$ is the cardinality of $\mathbb{E}$. We will now analyse each scenario in the context of high-energy eigenstates.

The scenario (64) is unlikely to occur if the energy shell targets a part of the spectrum that has high energy. This happens because the spectrum of this model spans a region $[A, B]$, where A, B are proportional to the system size N , and the number of states inside the spectrum is 2^N . There is an exponential number of states distributed across an interval whose length grows linearly. Hence, the average spacing between energy levels gets exponentially smaller as the system grows.

The ideal case would be (65). This occurs if and only if the SDP has successfully isolated an excited state in the energy shell. By minimising and maximising (62), one will obtain non-trivial bounds on the desired quantity.

A more common scenario is (66). If this happens, the solver will maximise the weight p_k of the term that minimises/maximises (62). Therefore, the results of the optimisation provide a lower bound of $\langle O \rangle$, corresponding to the state

$$\rho_{min} = |E_k^{min}\rangle \langle E_k^{min}|, \quad (67)$$

that minimises the cost function and an upper bound of $\langle O \rangle$ corresponding to the state

$$\rho_{max} = |E_k^{max}\rangle \langle E_k^{max}|, \quad (68)$$

that maximises the cost function. The states ρ_{min} and ρ_{max} do not coincide unless all the states in $\mathbb{E}$ are degenerate. Thus, the bounds are not as tight as possible since they usually are not associated with the same state.

To pinpoint the performance of our proposed solution, we chose to compare it to similar methods from the literature. One of these methods has been proposed in [WSF⁺24]. Initially, it was designed for bounding ground state properties, but in this work, we looked

into its performance in bounding properties of excited states. The SDP of this method reads

$$\begin{aligned}
& \text{minimize/maximize} && \langle O \rangle \\
& \text{subject to} && M \succeq 0, \\
& && E_{LB} - \langle H \rangle \leq 0, \\
& && \langle H \rangle - E_{UB} \leq 0, \\
& && \langle \mathbb{1} \rangle = 1.
\end{aligned} \tag{69}$$

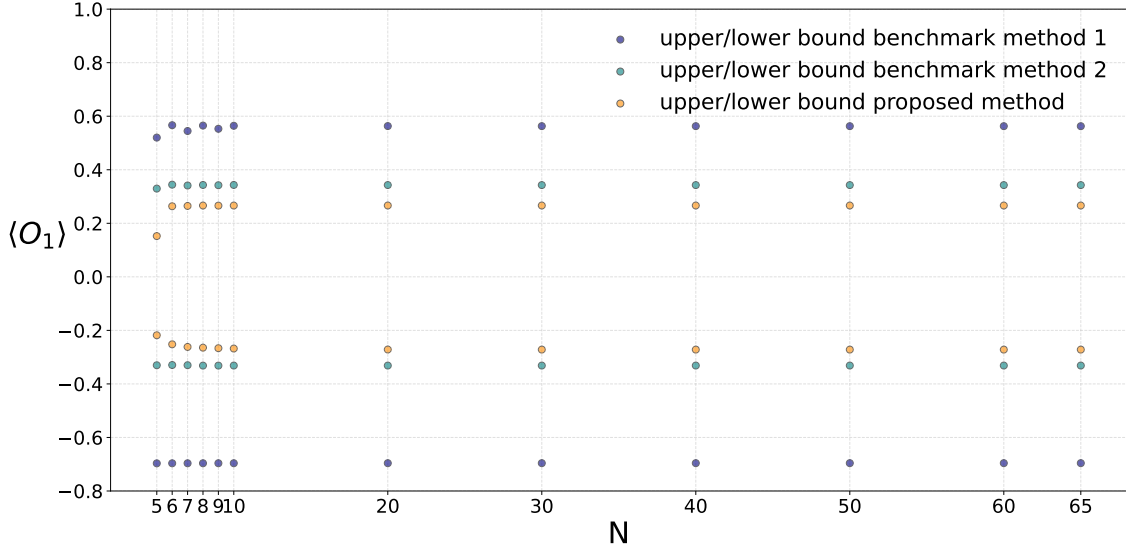
Another method chosen for benchmarking the performance of our SDP is a variation of (69). To this, we added the constraint (53) to have a clear perspective of the improvements added by each constraint. The second benchmarking SDP reads

$$\begin{aligned}
& \text{minimize/maximize} && \langle O \rangle \\
& \text{subject to} && M \succeq 0, \\
& && E_{LB} - \langle H \rangle \leq 0, \\
& && \langle H \rangle - E_{UB} \leq 0, \\
& && \langle \mathbb{1} \rangle = 1. \\
& && \langle [O_a, H] \rangle = 0, \quad \forall O_a \in \mathcal{B},
\end{aligned} \tag{70}$$

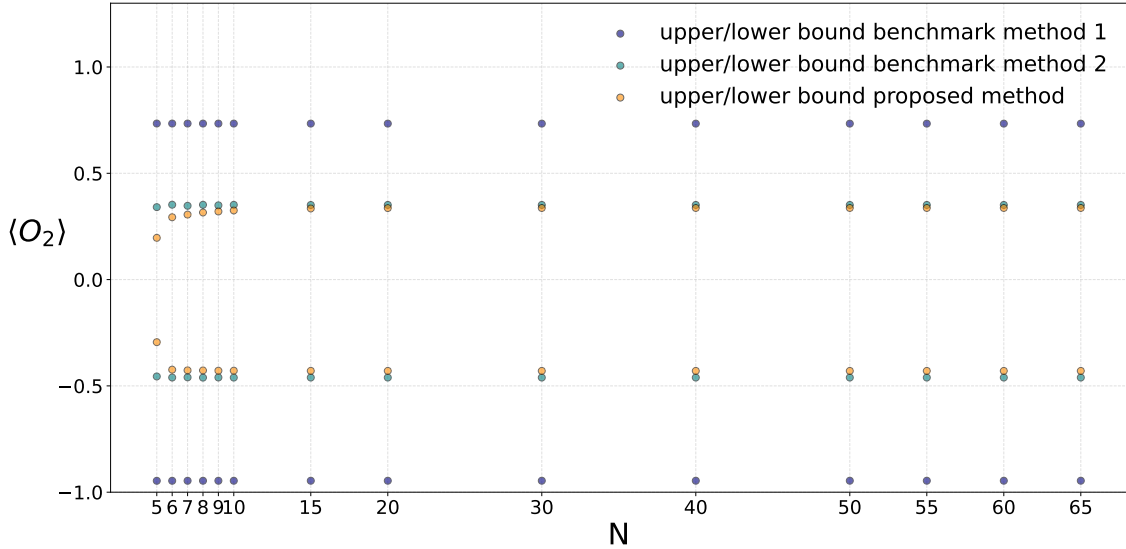
In order to keep the comparison fair, the results from all the methods were produced by the same $\mathcal{B}$ and we set $E_{LB} = E - \delta E$, $E_{UB} = E + \delta E$. We choose to study the bounds for the following quantities

$$\begin{aligned}
O_1 &= \sigma_{N/2}^x, \\
O_2 &= \sigma_{N/2}^z.
\end{aligned} \tag{71}$$

In Fig. 3a, Fig. 3b one can see the obtained bounds of $\langle O_1 \rangle$ and $\langle O_2 \rangle$ for a range of system sizes. We can see that all methods provided non-trivial bounds for both observables, meaning they return intervals strictly contained in $[-1, 1]$, the largest possible interval for quantum states. There is a clear hierarchy that stands out from the figure: the method (69) produces the loosest bounds, then (70) and the method (58) manages to find the tightest bounds. We noticed a significant drop in the bound difference when adding the constraint (53). As expected, this addition to the SDP improves the results considerably because the constraint drastically shrinks the feasible set. Building on this considerable improvement, our method further restricts the feasible set, thereby producing tighter bounds.



(a) Results for $\langle O_1 \rangle$



(b) Results for $\langle O_2 \rangle$

Figure 3: Comparison between benchmark method 1 (69), benchmark method 2 (70) and proposed method (58) in bounding the expectation value of (71) for excited states in the energy interval $[-0.01, 0.01]$ and $\mathcal{B} = \{1, \sigma_i^x, \sigma_i^y, \sigma_i^z, \sigma_i^\alpha \sigma_{i+1}^\beta\}_{i=1\dots N, \alpha, \beta \in \{x, y, z\}}$.

5 Conclusion

Quantum many-body physics problems are notoriously difficult to solve, because of the exponential scaling of the associated Hilbert space, which makes the exact characterisation of their properties a hard task. However, there are some scalable alternatives. One of these is represented by relaxation methods SDPs, which are a fundamental component of this work. The objective was to design a SDP to bound properties of many-body quantum systems in a scalable manner. We worked towards achieving this goal by using the moment matrix relaxation method. This approach meant replacing the optimisation variable of the

SDP with the elements of a moment matrix that has a size growing polynomially with the number of particles. Another crucial aspect, in terms of scalability, was the exploitation of translational invariance of the Hamiltonian (25), which drastically reduced the number of optimisation variables. After we established an efficient use of the resources, we introduced a new pair of linear constraints that, combined with other proposals from the literature, manage to provide non-trivial information about the spectrum of a spin system model.

The work introduced two possible applications of the novel constraints. We first presented a proof-of-concept routine for scanning the spectrum of a spin Hamiltonian and certifying regions that contain no eigenstates. The other application of the proposed SDP was bounding expectation values of excited states. In Section 4, we showed the performance of our proposed method. It successfully proved that the SDP can certify a large region of the spectral gap and it provided the tightest pair of upper and lower bounds for the two analysed observables among the three SDPs of interest. One observation regarding the results is that the gap scanning requires a number of optimisation variables that grows quadratically with the system size in order to mark the problem as infeasible. On the other hand, bounding properties of excited states requires a number of variables that grows linearly with the number of particles.

Like the other scalable methods used in quantum many-body physics, SDP relaxations have some limitations. Even though our proposed approach does not use a density matrix as an optimisation variable, the solver still has to assess the positivity of a matrix, in this case, the moment matrix. This process represents a bottleneck of these methods. In this work, we used the solver from Mosek, which is known for requiring substantial memory resources. In future work, we would like to observe the performance of the tool coupled with another solver (e.g., SCS). Apart from this goal, we would like to further investigate the robustness of the spectrum scanning routine and improve the methodology such that it becomes applicable for larger systems.

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