Delft University of Technology

Constructing Bell inequalities from the Hydrogen molecule

B.M. La Rivière (43848399)

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Contents

1 Introduction

Nonlocality is a fundamental property of nature in which local measurements performed on some entangled quantum states can result in correlations which are irreproducible by any local hidden variable model [11]. Such correlations are called nonlocal and can be detected through the violation of a so-called Bell inequality [13, 11], which are linear inequalities formulated in terms of conditional probabilities resulting from local measurements performed by some observers, also called parties, on a composite quantum state [43]. Not only does do nonlocal quantum states lie at the heart of questions about the fundamental nature of the universe [16], it is also a resource for device-independent (DI) quantum information tasks, with the most prominent examples being DI key distribution [1, 17, 10, 9], DI entanglement detection [8, 23], self testing [7, 24] and generation and amplification of randomness [32, 41]. Hence, searching for optimal Bell inequalities which reveal these nonlocal correlations in a given quantum state has been one of the central objectives in the field of quantum information theory [30].

Quantum states which produce nonlocal correlations are also necessarily entangled; these states are not separable and are irrepresentable as mixtures of projections onto product state [21]. The opposite is not always true, there exist entangled quantum states that are not nonlocal [5]. Or inn other words, entanglement is a weaker property than nonlocality. Despite it being a weaker property, entanglement still proves to be a useful tool in characterizing the nature of quantum phase transitions and properties of many-body systems [36, 4, 31]. Nonetheless, the main focus of these studies in many-body systems has been the detection of entanglement while leaving the detection of nonlocality, which is accomplished by constructing multipartite Bell inequalities consisting of many-body correlations [47, 49, 15], rather unexplored. This is caused by a multitude of reasons; many-body correlations present in these systems make these inequalities impossible to measure [41], the characterization of the nonlocal correlations is a NP hard problem [6] and multipartite quantum states often grow exponentially with the system size, making the analysis of quantum correlations in larger systems near impossible. To overcome part of these problems, recently it has been shown that for some many-body systems, nonlocality can be detected using only one- and two-body correlation functions [41, 43], opening up the path to the detection of nonlocality in spin systems. In addition, a recent study by J. Tura *et al.* [44] demonstrated that for some quantum spin Hamiltonians in one spatial dimension, families of Bell inequalities can be assigned in a natural way and nonlocality is revealed in its ground state. Moreover, in the same study an algorithm was presented to speed up the determination of the optimal set of classical correlations, allowing for the construction of Bell inequalities in a wider range of spin systems without being limited to only one- and two-body correlation functions.

In turn, using the ground state energy of a spin Hamiltonian to detect nonlocality opens up the study of this in a wide range of systems, from which molecular structures could possibly be particularly interesting. However, Hamiltonians describing molecular structures are often expressed in terms of anti-commuting fermionic creation and annihilation operators acting on numbered basis states while Bell inequalities are formulated in terms of commuting spin operators acting on qubits. Partially as a result of recent advances in solving the Hamiltonian of these structures on a quantum computer [37, 48, 35, 27], there exist multiple transformations which effectively do this while still preserving the anti-commuting properties of the fermionic operator algebra, with two key examples being the Jordan-Wigner [48, 22] and the Bravyi-Kitaev transformation [37, 12]. Mapping these fermionic Hamiltonians and their ground states to spin operators acting on qubits not only allows for it to be solved on a quantum computer, the resulting spin Hamiltonians and their ground states also make it possible for the study of nonlocality in these molecular structures. But, some questions arise. Despite being isospectral, mapping a fermionic Hamiltonian to a spin Hamiltonian with the two transformation mentioned above results in two different different spin Hamiltonians and ground states. Naturally, the question then arises whether construction of Bell inequalities from these spin Hamiltonians also results in the same family of Bell inequalities. Moreover, since the ground states are also different, can both tailored optimal Bell inequalities reveal nonlocality in the respective ground state of these spin Hamiltonians?

In this report we try to answer these questions for one of the simplest molecular structures; the Hydrogen molecule H_2. We map the fermionic Hamiltonian describing molecular Hydrogen to spin Hamiltonians with both the Jordan-Wigner and the Bravyi-Kitaev transformation, construct Bell inequalities from these Hamiltonians, optimize them and study whether these optimal inequalities are able to reveal nonlocal correlation in the ground state of the spin Hamiltonians. Moreover, we also investigate which of these transformation allows for the best detection of nonlocality in the ground state of the Hydrogen molecule. The structure of the report is the following: In Section 2 we discuss the general form of a fermionic Hamiltonian describing molecular structures and how it can be mapped to a spin Hamiltonian using either the Jordan-Wigner or the Bravyi-

Kitaev transformations. Subsequently, in the same section, we also give an explanation on how to construct families of Bell inequalities from spin Hamiltonians and how they can reveal nonlocality in the ground state. We then given the fermionic Hamiltonian describing molecular Hydrogen and the resulting spin Hamiltonians in Section 3 alongside with a dictionary on how to construct families of Bell inequalities from these Hamiltonian and optimize them. Moreso, we describe how we numerically implemented these in the same section. Lastly, in Section 4 we show the results of the simulation and in Section 5 we conclude.

2 Theoretical background

In this section we present the theoretical background used throughout the report. We first discuss the general form of a fermionic Hamiltonian describing molecular structures in Section 2.1, after which we describe the Jordan-Wigner [48, 22] and the Bravyi-Kitaev transformation [37, 12] used to map the fermionic Hamiltonian to spin Hamiltonians in Section 2.2. In Section 2.3 we illustrate the construction of Bell inequalities from a spin Hamiltonian, obtained through mapping the fermionic Hamiltonian, and how it can be used to detect nonlocality in its ground state. Lastly, o reveal these nonlocal correlations, two properties are calculated; the ground state energy of the Hamiltonian and the so-called classical bound [44], which comes down to determining the optimal set of classical correlations. Since this is a computationally ineffective task in general [13], being it scaling exponentially, we present the dynamical programming algorithm from [44] to speed up this process in Section 2.4. We present Section 2.3 and 2.4 in a similar fashion to that described in [44]. Throughout this report, we provide all expressions and results in atomic units (a.u.) unless stated otherwise. For simplicity, we leave out all identity matrices and tensor products from equations. E.g. $\sigma_x^{(0)} \otimes \sigma_y^{(1)} \otimes \sigma_y^{(2)} \otimes \mathbb{I}^{(4)}$ is written as $\sigma_x^{(0)}\sigma_y^{(1)}\sigma_z^{(2)}$.

2.1 Describing molecular structures

The physical properties and dynamics of many-body systems, such as molecular structures, are governed by the Hamiltonian describing these systems and the form of the corresponding electronic wavefunctions, which is obtained through solving the Schrödinger equation. These wavefunctions are often very complex in nature and their description scales exponentially with the system size [40]. Expressing these wavefunctions in terms of Slater determinants, which are anti-symmetric products of single electron basis functions that approximate the electrons spin orbitals, reduces the resources needed to simulate these systems. However, as a result of the strong electron correlations present in the Hamiltonian, expressing the wavefunction as a single Slater fails to describe these correlation effects and thus the wavefunction is often expressed in terms of a linear combination of Slater determinants [25], making their description a formidable task. To further compress the resources needed to describe these wavefunctions, we express the Hamiltonian and its wavefunction in its second quantized form, requiring the Hamiltonian to be projected onto a set of orthogonal basis functions [28]. A common choice for this set of functions for molecular structures are the molecular spin orbitals [39], which we denote by ϕ_p. Projecting the electronic Hamiltonian onto these molecular spin orbitals allows for it to be written as [25]

$$\mathcal{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_r a_s, \tag{2.1}$$

where the indices p, q, r and s run over all n molecular spin orbitals captured in the so called molecular basis. The Hamiltonian elements

$$h_{pq} := \int d\sigma \phi_p^*(\sigma) \left(-\frac{\nabla^2}{2} - \sum_k \frac{Z_k}{|R_k - r|} \right) \phi_q(\sigma) \tag{2.2}$$

and

$$v_{pqrs} := \int d\sigma_1 d\sigma_2 \frac{\phi_p^*(\sigma_1)\, \phi_q^*(\sigma_2)\, \phi_s(\sigma_1)\, \phi_r(\sigma_2)}{|r_1 - r_2|} \tag{2.3}$$

are the one and two electron integrals respectively, with Z_k and R_k being the charge and the position of the kth nucleus and r_i the location of the ith electron and both of these elements are integrated over the spatial and the spin degrees of freedom. Writing the Hamiltonian described above in its second quantized form, makes it so it is defined in terms of the (Dirac) fermionic creation ($a_j^\dagger$) and annihilation (a_j) operators (CAPs) acting on numbered basis states. Or in other words, these are the previously mentioned fermionic Hamiltonians. The fermionic annihilation operator is defined as

$$\begin{aligned} a_j \left|\ldots, f_j, \ldots\right\rangle &= (-1)^{\sum_{i=1}^{j-1} f_i} \left|\ldots, f_j - 1, \ldots\right\rangle, \\ a_j \left|\ldots, 0_j, \ldots\right\rangle &= 0, \end{aligned} \tag{2.4}$$

and the creation operator is given by

$$\begin{aligned} a_j^\dagger \left|\ldots, f_j, \ldots\right\rangle &= (-1)^{\sum_{i=1}^{j-1} f_i} \left|\ldots, f_j + 1, \ldots\right\rangle, \\ a_j^\dagger \left|\ldots, 1_j, \ldots\right\rangle &= 0. \end{aligned} \tag{2.5}$$

Both of these operators act on the numbered basis states $|\ldots, f_j, \ldots\rangle$, with f_j being the occupancy of the jth molecular spin orbital and the states are extended by linearity to the whole Fock space. The term $(-1)^{\sum_{i=1}^{j-1} f_i}$ accounts for a phase factor of ± 1 in order to preserve the anti-symmetric nature of fermionic wavefunctions under the exchange of two disjoint CAPs [28]. As a result of this anti-symmetry, the fermionic CAPs obey the following anti-commutation relations:

$$\{a_i, a_j^\dagger\} = \delta_{i,j}, \qquad \{a_i^\dagger, a_j^\dagger\} = \{a_i, a_j\} = 0. \tag{2.6}$$

2.2 From fermionic to spin Hamiltonians

We use the Hamiltonian described in (2.1) to model molecular structures. Directly constructing Bell inequalities from this Hamiltonian is not possible since the Hamiltonian is described in anti-commuting fermionic CAPs acting on numbered basis states while Bell inequalities are often formulated in terms of commuting spin operators acting on qubits [13]. Tailoring Bell inequalities to these fermionic Hamiltonians thus requires the fermionic operators and numbered basis states to be mapped to spin operators and qubits respectively in order to overcome the algebraic differences. There exist multiple methods that do so while preserving the anti-commuting properties of fermionic CAPs [45, 38, 37, 48, 25]. We limit ourselves to the usage of the Jordan-Wigner [22] and the Bravyi-Kitaev [12] transformation for mapping fermionic Hamiltonians describing molecular structures to spin Hamiltonians. Below we briefly outline them for the sake of completeness.

2.2.1 Jordan-Wigner transformation

Mapping fermionic CAPs and numbered basis states to spin operators and qubits requires two types of information to be mapped; the occupation of the molecular spin orbital to which we apply a fermionic operator and the parity of the set of orbitals with a lower index than the targeted orbital [37]. One method of mapping the occupation of the molecular spin orbitals is by directly storing the occupation directly in the state of the qubits, such that

$$|f_0, \ldots, f_{n-1}\rangle \to |q_0, \ldots, q_{n-1}\rangle\,, \tag{2.7}$$

with $f_j = q_j \in \{0, 1\}$, f_j denoting the occupancy of the jth molecular spin orbital and q_j being the state of the jth qubit. The same one-to-one correspondence can not be used to map the fermionic CAPs to spin operators due to the algebraic differences between these operators. One way to preserve the anti-commutation relation of fermionic CAPs is by expressing them in terms of spin operators as

$$a_j = \left(\prod_{i=0}^{j-1} \sigma_z^{(i)}\right) \sigma_-^{(j)}, \qquad a_j^\dagger = \left(\prod_{i=0}^{j-1} \sigma_z^{(i)}\right) \sigma_+^{(j)}, \tag{2.8}$$

where $\sigma_+^{(j)} = \frac{1}{2}\left(\sigma_x^{(j)} - i\sigma_y^{(j)}\right)$ is the raising operator, $\sigma_-^{(j)} = \frac{1}{2}\left(\sigma_x^{(j)} + i\sigma_y^{(j)}\right)$ is the lowering operator and $\sigma_x^{(j)}$, $\sigma_y^{(j)}$ and $\sigma_z^{(j)}$ are the Pauli spin operators acting on the jth qubit. The chain of $\sigma_z^{(i)}$ operators accounts for an added phase of -1 if the parity of all qubits before the pth qubit is odd, similar to the action of fermionic CAPS on numbered basis states [28]. The correspondence between fermionic CAPs and spin operators shown in (2.8) is called the Jordan-Wigner transformation [22, 37, 48].

2.2.2 Bravy-Kitaev transformation

Despite the Jordan-Wigner transformation being a very simple mapping of fermionic CAPs to spin operators due to the one-to-one correspondence between occupation of the molecular spin orbitals and the state of the qubits, it does have the downside of mapping the parity in a nonlocal manner. This results in the number of qubit operators required to simulate a single fermionic operator to scale as $\mathcal{O}(j)$ [37], where j is the index of the jth molecular spin orbital to which we apply a fermionic operator. Another method to map the fermionic CAPs to spin operators is with the parity basis [37]. As the name suggests, the parity is now a local mapping, while the occupation of the molecular spin orbitals is mapped in a nonlocal manner. Due to this nonlocal mapping of the occupation, this transformation still does not overcome the unfavourable scaling of the number of qubits required to simulate a single fermionic operator. There is also a middle ground between the Jordan-Wigner transformation and the parity basis which is called the Bravyi-Kitaev transformation [12]. Similar to what was done for the Jordan-Wigner transformation, we start of by defining the correspondence between the occupation of the molecular spin orbitals and the state of the qubits, which is now in terms of the so-called Bravi-Kitaev basis [12]:

$$|f_0, \ldots, f_{n-1}\rangle \to |b_0, \ldots, b_{n-1}\rangle\,, \tag{2.9}$$

with

$$b_j = \left[\sum_{q=0}^{j} \beta_{jq} f_q \right] \pmod 2, \tag{2.10}$$

and where β is the Bravyi-Kitaev matrix [12]. This matrix is built up recursively via

$$\begin{aligned} \beta_1 &= [1], \\ \beta_{2^{x+1}} &= \begin{pmatrix} \beta_{2^x} & \mathbf{0} \\ \mathbf{A} & \beta_{2^x} \end{pmatrix}, \end{aligned} \tag{2.11}$$

where $\mathbf{A}$ is a $(2^x \times 2^x)$ matrix of zeros with the bottom row filled by ones and the matrix $\mathbf{0}$ is a $(2^x \times 2^x)$ matrix with zeros only. Since we are dealing with a basis different from the qubit basis, it useful that we first define three sets of operators involved in the Bravyi-Kitaev transformation, which are the parity set, the update set and the flip set.

The Jordan-Wigner transformation accounts for a phase factor of -1 through a chain of σ_z gates acting on qubits with an index lower than that with an arbitrary index j to which the fermionic operator are applied. Unfortunately, knowing which qubits need to acquire this phase factor is less straightforward for the Bravyi-Kitaev transformation due to the state of qubits being expressed in terms of the Bravyi-Kitaev basis. Qubits, with an index lower than the index j, that require this phase factor with the of -1 Bravyi-Kitaev transformation can be captured in the so-called parity set, which we will call $P(j)$. To obtain the elements of this set, it is convenient to start of by considering the parity operator in the qubit basis:

$$p_i = \sum_j \pi_{ij} f_j, \tag{2.12}$$

where

$$\pi_{ij} = \begin{cases} 1, & i < j \\ 0, & i \geq j. \end{cases} \tag{2.13}$$

In terms of the Bravy-Kitaev basis, which is defined in (2.10), the parity operator becomes

$$p_i = \sum_k \left[\pi \beta^{-1} \right]_{ik} b_k, \tag{2.14}$$

with β^{-1} being the inverse of the Bravyi-Kitaev matrix defined in (2.11), which has an analytically closed form [37]. The elements of the matrix $\left[\pi\beta^{-1}\right]$ are ones and zeros, with the ones denoting the indices which require a phase factor of -1. Next, we discuss the update set, which we denote by $U(j)$ and it contains the indices of the qubits which must be updated if the occupation of the jth orbital changes. Since the matrix β contains described the mapping of the occupation of the molecular spin orbitals to the Bravyi-Kitaev basis, its elements describe which qubits change when we change the occupation of some orbital and thus $U(j)$ is determined by the Bravyi-Kitaev matrix β. Lastly, we define the flip set $F(j)$ that describes whether a qubit with an arbitrary index j has the same or an inverted parity with respect to the occupation of the jth molecular spin orbitals and its indices can be obtained by through the inverse of the Bravyi-Kitaev matrix β^{-1}.

With these three sets described above, we now define the relation between fermionic CAPs and spin operator through the Bravyi-Kitaev transformation. The fermionic CAPs are mapped to spin operators according to

$$\begin{aligned} a_j^\dagger &= \frac{1}{2} \left(X_{U(j)} X_j Z_{P(j)} - i X_{U(j)} Y_j Z_{\rho(j)} \right) \\ a_j &= \frac{1}{2} \left(X_{U(j)} X_j Z_{P(j)} + i X_{U(j)} Y_j Z_{\rho(j)} \right), \end{aligned} \tag{2.15}$$

where

$$\rho(j) \equiv \begin{cases} P(j), & \text{if } j \text{ is even} \\ P(j)/F(j), & \text{if } j \text{ is odd.} \end{cases} \tag{2.16}$$

The operators $X_{U(j)}$ and $Z_{(\rho(j))}$ denote a chain of σ_x and σ_z respectively for the qubits present in the sets $U(j)$ and $\rho(j)$.

One of the reasons why the Bravyi-Kitaev transformation is particularly interesting for mapping fermionic operators is because of the scaling of the number of spin operators required to simulate a single fermionic operator. Both the Jordan-Wigner transformation and the parity basis had an unfavourable scaling for this; both scaled as $\mathcal{O}(j)$, where j is the molecular spin orbital to which we apply the fermionic operator. The Bravyi-Kitaev transformation on the other hand, requires less operators to simulate a fermionic operator since it scales as $\mathcal{O}(\log(j))$ [37], effectively reducing the number of spin operators requires to simulate fermionic operators and thus also fermionic Hamiltonians describing molecular structures. Despite this unfavourable scaling of the Jordan-Wigner transformation, we will still using it alongside with the Bravyi-Kitaev transformation to map the fermionic Hamiltonian describing the Hydrogen molecule to two distinct isospectral spin Hamiltonians.

2.3 Constructing a Bell inequality

After mapping the fermionic Hamiltonian to spin operators, we construct families of Bell inequalities from them. The family of Bell inequalities that we consider are those, for some set of quantum observables, such that the corresponding Bell operator $\mathcal{B}$ coincides with the Hamiltonian [44]:

$$\mathcal{B} := \beta_C \mathbb{I} + \mathcal{H}, \tag{2.17}$$

where $\beta_C \in \mathcal{R}$ is the classical bound and $\mathcal{H}$ is a spin Hamiltonian in one spatial dimension. Ultimately, we aim to find Bell inequalities of the $I + \beta_C \geq 0$ which can detect nonlocal correlations in the ground state ρ of the spin Hamiltonian, in which I corresponds to the spin Hamiltonian and it is a linear combination of conditional probabilities obtained through measurements performed by some observers with coefficients in front of them [13]. If these coefficients are known, the problem is to find the classical bound β_C, which geometrically means to make the Bell inequality tangent to the local polytope:

$$\beta_C = -\min_{\text{LHVM}} I, \tag{2.18}$$

where the minimum is taken over all local hidden variable models (LHVM) [13]. Since I corresponds to the Hamiltonian, we find that it is minimized by the ground state of the spin Hamiltonian. In other words, the largest possible violation is caused by the ground state and it is said to be nonlocal is $\text{Tr}(\mathcal{B}\rho) < 0$.

Before diving into the construction of Bell inequalities from spin Hamiltonians in one spatial dimension, we will first sketch the general picture of the Bell experiment performed by some observers. We consider Bell inequalities with n observers, often called parties, which is the same number of molecular spin orbitals (and thus qubits) present in the system. Each party can choose one out of m dichotomic quantum observables, we also regularly call them measurements, with outcomes ± 1. We denote the vector containing the measurement choices of each party by $\mathbf{k} = (k_0, \cdots, k_{n-1})$, with $0 \leq k_i < m$. Performing the Bell experiment results in the outcomes $\mathbf{a} = (a_0, \cdots, a_{n-1})$ for the measurement vector $\mathbf{k}$, with $a_i = \pm 1$. The Bell inequalities naturally tailored to the Bell operator of the form of (2.17) can be written as $I + \beta_C \geq 0$, with, in its most general form,

$$I = \sum_{i=0}^{n-1} \sum_{r=0}^{R} \sum_{\mathbf{k}=\mathbf{0}}^{m^r-1} \gamma_{\mathbf{k}}^{(i,r)} M_{\mathbf{k}}^{(i,r)}, \tag{2.19}$$

where the index i runs over all n molecular spin orbitals, r denotes the number of nearest neighbouring interactions with a maximum of R neighbours, $\gamma_{\mathbf{k}}^{(i,r)}$ are real-valued coefficients that are a linear combination of the Hamiltonian elements h_{pq} and v_{pqrs} ((2.2) and (2.3)) and the elements $M_{\mathbf{k}}^{(i,r)}$ are the so-called correlators.

There is one ambiguity that is left for us to elaborate on to define the full picture of this specific Bell experiment. Spin Hamiltonians obtained through mapping a fermionic Hamiltonian with either the Jordan-Wigner or the Bravyi-Kitaev transformations contain Pauli strings consisting of σ_x, σ_y and σ_z gates. Often, the measurements $0 \leq k_i < m$ are only performed in the xy-plane and add an extra measurement m is added in the z-direction. We include this measurement in the choice of measurements the observers can choose from such that $0 \leq k_i \leq m$ unless stated otherwise.

2.4 Classical optimization

As mentioned earlier, the ground state ρ of a spin Hamiltonian is nonlocal if the ground state energy $\text{Tr}(\mathcal{H}\rho)$ is lower than the classical bound β_C. The classical bound is obtained through optimization of I over all local hidden

variable models (see equation (2.18)). By Fine's theorem [18], it suffices to optimize I over all deterministic local strategies instead, in which the correlators $M_{\mathbf{k}}^{(i,r)}$ factorize as

$$M_{\mathbf{k}}^{(i,r)} = \prod_{j=0}^{r+1} M_{k_j}^{(i+j)}, \tag{2.20}$$

where $M_{\mathbf{k}}^{(i,r)} \in \{-1, +1\}$. This allows for the classical bound β_C to be obtained through optimizing I through

$$\beta_C = - \min_{M_{k_j}^{(i)} = \pm 1} I, \tag{2.21}$$

in which the minimum is now taken over all possible configurations of $M_{k_j}^{(i)}$, $\forall i \in [0, n-1] \cap \mathbb{Z}$ and $0 \leq k_j \leq m$. The determination of β_C through minimizing over all of these configurations is a computationally ineffective task since the number of possible configurations for all local deterministic strategies $M_{k_j}^{(i)}$ scales exponentially with the number of observers and the number of measurements [13]. In [44] an dynamic programming algorithm was presented which splits this minimization into nested parts through a recursive algorithm, allowing for an up-to exponential speed up of the determination of β_C for spin Hamiltonians in one spatial dimension with local interactions only. To make usage of this algorithm, is convenient to express the set of local deterministic strategies as a $m \times n$ matrix $\mathbf{M}$ where the column correspond to the different observers and the rows to the measurements performed by these observers. In other words, for a given matrix index (k, i), we have the local deterministic strategy of the kth measurement from the ith party which can take values ± 1. We denote the matrix $\mathbf{M}^{(i,R)}$ to be a sub-matrix of the matrix $\mathbf{M}$, consisting of the columns i to $i + R - 1$. The goal is to find the optimal $\mathbf{M}$ in order to determine the classical bound β_C, which is now done through a recursive algorithm. For this algorithm we start of with defining the function h_i acting on the matrix $\mathbf{M}^{(i-1,R+1)}$, such that

$$h_i\left(\mathbf{M}^{(i-1,R+1)}\right) := \sum_{r=0}^{R} \sum_{\mathbf{k}=\mathbf{0}}^{m^r-1} \gamma_{\mathbf{k}}^{(i-1,r)} M_{\mathbf{k}}^{(i-1,r)}, \tag{2.22}$$

for $i > 0$. Using this function, we define the recursive function E_i to be

$$\begin{aligned} E_0\left(\mathbf{M}^{(0,R)}\right) &:= 0, \\ E_i\left(\mathbf{M}^{(i,R)}\right) &:= \min_{M_k^{(i-1)}} \left\{ E_{i-1}\left(\mathbf{M}^{(i-1,R)}\right) + h_i\left(\mathbf{M}^{(i-1,R+1)}\right) \right\}, \end{aligned} \tag{2.23}$$

which, once again, holds for $i > 0$. For each iteration of the algorithm, the function E_i optimizes the local deterministic strategies of the $i-1$th party by comparing all 2^m possible configurations of the local deterministic strategy $M_k^{(i-1)}$. The classical bound β_C can be obtained through this algorithm as the final iteration of the algorithm, such that

$$\beta_C := -E_n\left(\mathbf{M}^{(n,R)}\right). \tag{2.24}$$

This algorithm is efficient for one-dimensional geometries, whereas it becomes exponentially expensive in general Bell inequalities. However, since the Hamiltonians we find in nature are local, this may also yield good results if we get qubit interactions that are close to one-dimensional.

3 Numerical methods

In this section we present the numerical steps taken to implement the fermionic Hamiltonian describing the Hydrogen molecule H_2, map it to spin Hamiltonians and construct Bell inequalities from these. We start of by describing the fermionic Hamiltonian of the Hydrogen molecule in its minimal basis in Section 3.1. Moreover, in the same section we also show the acquired isospectral spin Hamiltonians obtained through mapping the fermionic Hamiltonian of molecular Hydrogen with the Jordan-Wigner and the Bravyi-Kitaev transformation. After that, we discuss the algorithm used to construct Bell inequalities from these spin Hamiltonians in Section 3.2. In addition, we also present that general measurement setting that we use to perform the Bell experiment in the same section. Since changing the possible choices of measurements the observes can use directly alter the shape of the corresponding Bell inequality [44], we present a model to find the optimal Bell inequality from this family of Bell inequalities in Section 3.3.

3.1 The Hydrogen molecule

In Section 2.1 we presented the general form of a fermionic Hamiltonian describing molecular structures, alongside with the corresponding Hamiltonian elements h_{pq} and v_{pqrs}. We use this general Hamiltonian to build up the fermionic Hamiltonian describing the Hydrogen molecule in its so-called minimal basis, which consists of a single $1s$ atomic orbital per atom [40]. Despite the atomic p-orbitals causing a small correction to the molecular orbitals, the minimal basis still reaches chemical accuracy while requiring less molecular spin orbitals to model the molecule [39] and therefore the minimal basis is the basis of our choice. From the overlap of the $1s$ orbitals of these atoms two different molecular orbitals form; the bonding orbital $|\phi_g\rangle$ and the anti-bonding orbital $|\phi_u\rangle$, which are given by

$$\begin{aligned} |\varphi_g\rangle &= \frac{1}{\sqrt{1+\langle\varphi_{H_1}|\varphi_{H_2}\rangle}}\left(|\varphi_{H_1}\rangle + |\varphi_{H_2}\rangle\right), \\ |\varphi_u\rangle &= \frac{1}{\sqrt{1-\langle\varphi_{H_1}|\varphi_{H_2}\rangle}}\left(|\varphi_{H_1}\rangle - |\varphi_{H_2}\rangle\right), \end{aligned} \tag{3.1}$$

where $|\phi_{H_i}\rangle$ denotes the $1s$ orbital of the ith Hydrogen atom and the normalisation factor is a result of the atomic $1s$ orbitals not being orthogonal. In terms of these molecular orbitals, the minimal basis of the Hydrogen molecule is defined as [48, 37]

$$\begin{aligned} |\phi_0\rangle &= |\varphi_g\rangle|\uparrow\rangle \qquad |\phi_1\rangle = |\varphi_g\rangle|\downarrow\rangle \\ |\phi_2\rangle &= |\varphi_u\rangle|\uparrow\rangle \qquad |\phi_3\rangle = |\varphi_u\rangle|\downarrow\rangle . \end{aligned} \tag{3.2}$$

With the molecular spin orbitals in shown in the minimal basis, we calculate the Hamiltonian elements h_{pq} and v_{pqrs}. Unfortunately, these integrals are not analytically solvable for Slater type orbitals (STOs), such as the atomic $1s$ orbitals and thus the molecular spin orbitals [40]. Therefore, we introduce a finite sized basis set $|\chi_i\rangle$ and express the atomic $1s$ orbitals as a linear combination of this finite basis set, such that

$$|\phi_{H_i}\rangle = \sum_j C_{i,j}|\chi_j\rangle . \tag{3.3}$$

The optimal basis strongly depends on the types of orbitals included into the atomic basis. We use the STO-3G basis, which approximates STO-like orbitals as a linear combination of three Gaussians, causing the integrals

Table 1: Hamiltonian elements h_{pq} and v_{pqrs} computed with a restricted Hartree-Fock calculation with the OpenFermionPyscf package [26] at an interatomic distance $R = 1.401$ a.u. and the atomic $1s$ orbitals approximated by the STO-3G basis.

Integral	Value [a.u]
$h_{00} = h_{11}$	-1.252477
$h_{22} = h_{33}$	-0.475934
$v_{0110} = v_{1001}$	0.674493
$v_{2332} = v_{3223}$	0.697397
$v_{0220} = v_{0330} = v_{1221} = v_{1331}$ $= v_{2002} = v_{3003} = v_{2112} = v_{3113}$	0.663472
$v_{0202} = v_{1313} = v_{2130} = v_{2310}$ $= v_{0312} = v_{0132}$	0.181287

to become analytically solvable [39]. We compute these integrals through a restricted Hartree-Fock calculation using the OpenFermionPyscf package [26] and show the resulting nonzero Hamiltonian elements h_{pq} and v_{pqrs} for an interatomic distance of $R = 1.401$ a.u. in Table 1. In terms of the minimal basis and the corresponding calculated Hamiltonian elements, the fermionic Hamiltonians describing the Hydrogen molecule is given by

$$\begin{aligned}\mathcal{H} = &\sum_{i=0}^{3} h_{ii}\hat{n}_i + h_{0110}\hat{n}_0\hat{n}_1 + v_{2332}\hat{n}_2\hat{n}_3 + v_{0330}\hat{n}_0\hat{n}_3 + v_{1221}\hat{n}_1\hat{n}_2 + \\ &+ (v_{0220} - h_{0202})\,\hat{n}_0\hat{n}_2 + (v_{1331} - v_{1313})\,\hat{n}_1\hat{n}_3 + \\ &+ v_{0123}(a_0^\dagger a_1^\dagger a_3 a_2 + \text{h.c.}) + v_{0312}(a_0^\dagger a_3^\dagger a_1 a_2 + \text{h.c.}),\end{aligned} \tag{3.4}$$

where h.c. denotes the hermitian conjugate.

3.1.1 Spin Hamiltonians of the Hydrogen molecule

We map this fermionic Hamiltonian describing the Hydrogen molecule to two different isospectral spin Hamiltonians with the Jordan-Wigner and the Bravyi-Kitaev transformation, for which we use the OpenFermion package [26]. The resulting spin Hamiltonian obtained with the Jordan-Wigner transformation is given by

$$\begin{aligned}\mathcal{H}_{JW} = &-0.81261\mathbb{I} + 0.171201\left(\sigma_z^{(0)} + \sigma_z^{(1)}\right) - 0.2227965\left(\sigma_z^{(2)} + \sigma_z^{(3)}\right) + 0.16862325\sigma_z^{(0)}\sigma_z^{(1)} \\ &+ 0.12054625\sigma_z^{(0)}\sigma_z^{(2)} + 0.1658688\left(\sigma_z^{(0)}\sigma_z^{(3)} + \sigma_z^{(1)}\sigma_z^{(2)}\right) + 0.12054625\sigma_z^{(1)}\sigma_z^{(3)} + 0.17434925\sigma_z^{(2)}\sigma_z^{(3)} \\ &- 0.04532175\left(-\sigma_y^{(0)}\sigma_y^{(1)}\sigma_x^{(2)}\sigma_x^{(3)} + \sigma_x^{(0)}\sigma_y^{(1)}\sigma_y^{(2)}\sigma_x^{(3)} + \sigma_y^{(0)}\sigma_x^{(1)}\sigma_x^{(2)}\sigma_y^{(3)} - \sigma_x^{(0)}\sigma_x^{(1)}\sigma_y^{(2)}\sigma_y^{(3)}\right)\end{aligned} \tag{3.5}$$

and the spin Hamiltonian acquired through the Bravyi-Kitaev transformation is defined as

$$\begin{aligned}\mathcal{H}_{BK} = &-0.81261\mathbb{I} + 0.171201\sigma_z^{(0)} + 0.16862325\sigma_z^{(1)} - 0.2227965\sigma_z^{(2)} + 0.171201\sigma_z^{(0)}\sigma_z^{(1)} \\ &+ 0.12054625\sigma_z^{(0)}\sigma_z^{(2)} + 0.17434925\sigma_z^{(1)}\sigma_z^{(3)} + 0.04532175\left(\sigma_x^{(0)}\sigma_z^{(1)}\sigma_x^{(2)} + \sigma_y^{(0)}\sigma_z^{(1)}\sigma_y^{(2)}\right) \\ &+ 0.165868\sigma_z^{(0)}\sigma_z^{(1)}\sigma_z^{(2)} + 0.12054625\sigma_x^{(0)}\sigma_z^{(2)}\sigma_x^{(3)} - 0.2227965\sigma_x^{(1)}\sigma_z^{(2)}\sigma_x^{(3)} \\ &+ 0.04532175\left(\sigma_x^{(0)}\sigma_z^{(1)}\sigma_x^{2}\sigma_z^{3} + \sigma_y^{(0)}\sigma_z^{(1)}\sigma_y^{(2)}\sigma_z^{(3)}\right) + 0.165868\sigma_z^{(0)}\sigma_z^{(1)}\sigma_z^{(2)}\sigma_z^{(3)}.\end{aligned} \tag{3.6}$$

3.2 Constructing Bell inequalities from spin Hamiltonians

We construct Bell inequalities from both of these spin Hamiltonians, requiring the calculation of the unknown set of coefficients $\gamma_{\mathbf{k}}^{(i,r)}$ and the determination of the corresponding classical bound β_C. As a quick reminder, the family of Bell inequalities that we consider are those such that the Bell operator coincides with a spin Hamiltonian (see equation (2.17)). In order to achieve this, we calculate the coefficients $\gamma_{\mathbf{k}}^{(i,r)}$ that allow for this to happen. Below we define a dictionary that allows for the computation of these coefficients $\gamma_{\mathbf{k}}^{(i,r)}$ and use them to determine the classical bound β_C. We start of with defining the quantum observables used by the observables in the Bell experiment, which we define as

$$M_k^{(i)} := \begin{cases} \cos\theta_k^{(i)}\sigma_x^{(i)} + \sin\theta_k^{(i)}\sigma_y^{(i)}, & 0 \le k < m \\ \sigma_z^{(i)}, & k = m, \end{cases} \tag{3.7}$$

and we substitute these into the factorized correlators $M_{\mathbf{k}}^{(i)}$ expressed in (2.20), such that

$$M_{\mathbf{k}}^{(i,r)} \to \bigotimes_{j=0}^{r+1} \mathcal{M}_{k_j}^{(i,r)}. \tag{3.8}$$

By substituting these in the general expression for I, defined (2.19), we obtain an operator which we denote by $\mathcal{I}$. This operator still contain the unknown set of coefficients $\gamma_{\mathbf{k}}^{(i,r)}$ that are yet to be determined. To find these, we make use of the criterion that the Bell operator coincides with the Hamiltonian, or in other words, $\mathcal{I} = \mathcal{H}$. In order to achieve this, we extract a system of equations from $\mathcal{I}$ and $\mathcal{H}$ through

$$\text{Tr}\left(\mathcal{I}\mathcal{P}\right) = \text{Tr}\left(\mathcal{H}\mathcal{P}\right), \tag{3.9}$$

where $\mathcal{P}$ is a projector, with $\mathcal{P} \in \{\mathbb{I}, \sigma_x, \sigma_y, \sigma_z\}^{\otimes n}$. Here the identity matrix $\mathbb{I}$ corresponds to the case in which an observer does not perform a measurement, corresponding to the lower-order correlators. In other words, it accounts for the possibility to extract the coefficients of correlations from the spin Hamiltonians with a length less than the number of qubits. Calculating (3.9) for all possible projectors $\mathcal{P}$ results in a system with 4^n equations, which we solve for the set of coefficients $\gamma_{\mathbf{k}}^{(i,r)}$. Since the number of equations is not necessarily equal to the number of unknown coefficients, exact diagonalization of the corresponding matrix equation is not possible and we therefore resort to approximating the solution to the system of equations by using a least-squares method [33].

We use the calculated coefficients $\gamma_{\mathbf{k}}^{(i,r)}$ to determine the classical bound β_C. In Section 2.4 we presented the dynamical programming algorithm from [44] to determine β_C through a recursive function, allowing for an up-to exponential speedup over comparing all possible configurations of the local deterministic strategies. To use this algorithm effectively, the spin Hamiltonians should consist out of local interactions only. However, the spin Hamiltonians defined in (3.5) and (3.6), and thus the corresponding family of Bell inequalities, show many-body correlations of the same size as the number of qubits. Even though some spin systems allow for the detection of nonlocality with only one- and two-body correlations [41, 43, 42], omitting these higher-order many-body correlations from the spin Hamiltonian defined in (3.5) and (3.6), such that the resulting Hamiltonians consist only of one- and two-body correlations, is not an option since it will result in both spin Hamiltonians to only contain σ_z operators, making the detection of nonlocality in its ground state ρ impossible. Therefore, we do not use this dynamic programming algorithm to determine β_C, but instead determine it by brute force through calculating all 2^{nm} possible configurations of the local deterministic strategies and comparing them with each other. Despite this being computationally ineffective for most many-body systems, it is still relatively fast due to the small number of qubits required to describe the Hydrogen molecule in its minimal basis.

3.3 Calculating an optimal Bell inequality

Constructing Bell inequalities from spin Hamiltonians with the dictionary described above would result in just a single Bell inequality out of a whole family of explorable Bell inequalities. Changing these measurement settings defined in (3.7), for example by changing the angles $\theta_k^{(i)}$, will result in a different system of equations and thus different solutions for the set of coefficients $\gamma_{\mathbf{k}}^{(i,r)}$. This in turn would lead to a different classical bound β_C. In other words, changing the measurement settings of the obersvers performing the Bell experiment will result in a different Bell inequality. It is possible that for some configurations of the angles $\theta_k^{(i)}$ the constructed Bell inequality is incapable of revealing nonlocal correlations in a round state ρ, while in essence, ρ could be nonlocal. To overcome this, we aim at finding the optimal measurement settings to find the optimal Bell inequality. This comes down to finding the minimal classical bound, such that $\mathrm{Tr}\,(\mathcal{B}\rho)$ is the smallest. To do this, we minimize β_C with the Nelder-Mead algorithm [29], in which we treat the angles $\theta_k^{(i)}$ as variational parameters. For each minimization step, we create a new set of quantum observables $\mathcal{M}_{k_j}^{(i,r)}$ for the new set of angles $\theta_k^{(i)}$. We use these quantum observable to obtain a new set of equations for the set of coefficients $\gamma^{(i,r)}$ and solve them, after which we determine the new classical bound β_C. These steps are repeated until the algorithm converges towards a minimum.

To reduce the overall computation time needed to obtain the optimal set of angles $\theta_k^{(i)}$, we introduce some constraints on them. Without these constraints, we would have to optimize $\sum_{i=0}^{n-1} m_i - 1$ different angles, where m_i is the number of measurements per observer and the factor -1 stems from the first measurement of the zeroth observer to always be fixed in order to prevent infinite global minima. But if we fix the angles of the zeroth observer to be [41]

$$\theta_k^{(0)} = \frac{k\pi}{m} \tag{3.10}$$

and then use

$$\theta_k^{(i)} = \frac{k\pi}{m} + \theta^{(i)} \tag{3.11}$$

for all other observers, where $\theta^{(i)}$ is the angle between the zeroth measurement of the zeroth and ith observer, we essentially reduce the number of angles needed to be optimized. More specifically, instead of optimizing $\sum_{i=0}^{n-1} m_i - 1$ angles, we know only need to optimize $n-1$ angles, reducing the overall computation time needed to find these optimal angles.

3.4 Simulation parameters

Having defined the methods of obtaining optimal Bell inequalities, we now specify the parameters we use during the simulations. In the results section, we use these parameters unless stated otherwise. Because are fairing a highly non-convex functional landscape of β_C, we employ the Nelder-Mead minimization scheme alongside with the basinhopping algorithm to overcome the problem of convergence towards local minima [46]. For this, we use five basinhopping steps for each simulation, as it proved to be able to find the optimal Bell inequality in every simulation while also keeping the minimization of the classical bound β_C at a relatively low computational cost. Moreover, we initialize the relative angles $\theta^{(1)}$, $\theta^{(2)}$ and $\theta^{(3)}$ to be random, with $\theta^{(i)} \in [0, \pi], \quad \text{for } i \in \{1, 2, 3\}$.

4 Results and discussion

In this section we provide the results of the construction and optimization of Bell inequalities for the spin Hamiltonians describing the Hydrogen molecule, which are defined in (3.5) and (3.6). Prior to showing our findings and elaborating on them, we first test whether dictionary provided in the previous section is capable of effectively tailoring Bell inequalities to spin Hamiltonians and optimizing them. We do this for a toy Hamiltonian and present the results in Section 4.1. After testing the dictionary, we use it to construct Bell inequalities from the spin Hamiltonians (3.5) and (3.6) and optimize them. In Section 4.2 we provide the results of this. Lastly, we discuss possible further outlooks in Section 4.3.

4.1 Testing the model

Before using the dictionary to construct optimal Bell inequalities for the Hydrogen molecule, we first we first test its effectiveness of constructing optimal Bell inequalities on a toy spin Hamiltonian. For this, we use the following bipartite Hamiltonian:

$$\mathcal{H} = \sqrt{2}\left(\sigma_x^{(0)}\sigma_x^{(1)} + \sigma_z^{(0)}\sigma_z^{(1)}\right). \tag{4.1}$$

Presumably, the optimal Bell inequality tailored to this Hamiltonian is the CHSH inequality. The settings for the corresponding Bell experiment are as follows: Since there are only two qubits in the system, there are two observers, which we will call Alice and Bob. Both Alice and Bob can choose from $m = 2$ dichotomic measurements. Since the Hamiltonian only consists out of σ_x and σ_z gates, Alice and Bob do not measure in the σ_y basis and are only allowed to measure in the xz-plane, for which they are allowed to pick one of the following quantum observables

$$\mathcal{M}_k^{(i)} = \cos\theta_k^{(i)}\sigma_x^{(i)} + \sin\theta_k^{(i)}\sigma_z^{(i)}, \tag{4.2}$$

where $k \in \{0, 1\}$. Similar to what we described in Section 3.3, we fix the angles to be that of (3.11), for which $\theta^{(0)}$ is taken as zero for Alice. This not only causes the umber of angles to be optimized to be reduced to one, it makes it so the quantum observables of Alice are given by

$$A_0 = \sigma_x^{(0)}, \quad \text{and} \quad A_1 = \sigma_z^{(0)}. \tag{4.3}$$

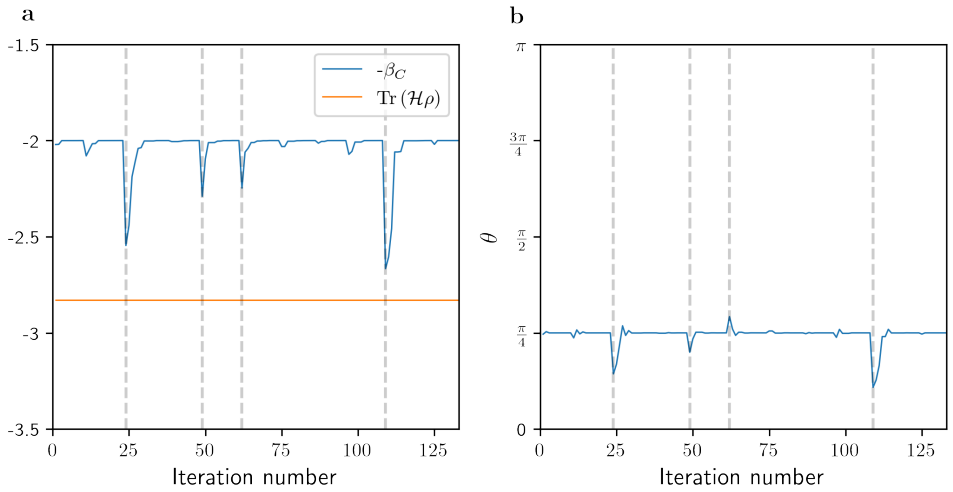

Figure 1: Results of the minimization of the classical bound β_C obtained through construction of optimal Bell inequalities from the Hamiltonian described in (4.1), for which the two observers Alice and Bob used the measurements settings given in (4.3) and (4.4) respectively. The minimization was done through optimization of the relative angle θ, which is the angle between the measurements of Alice and Bobs, with the Nelder-Mead minimization algorithm in combination with the Basinhopping algorithm for five Basinhopping steps. The iteration number denotes the number of iterations of the Nelder-Maed algorithm and the vertical dotted lines indicate the start of a new basinhopping step. β_C is shown as negative for visual clarity. **a**: $-\beta_C$ and the ground state energy $\mathrm{Tr}\,(\mathcal{H}\rho)$ as a function of the number of iterations. **b**: Values of the angle θ as a function of the number of iterations.

and those of Bob are defined as

$$B_0 = \cos(\theta)\,\sigma_x^{(1)} + \sin(\theta)\,\sigma_z^{(1)}, \quad \text{and} \quad B_1 = \cos\left(\frac{\pi}{2}+\theta\right)\sigma_x^{(1)} + \sin\left(\frac{\pi}{2}+\theta\right)\sigma_z^{(1)}, \tag{4.4}$$

where $\theta \in [0,\pi]$ is the relative angle between the quantum observables of Alice and Bob. It is this angle which we aim to optimize to find the minimal classical bound β_C, or in other words, the CHSH inequality. This inequality is given by [14]

$$|\langle A_0B_0\rangle + \langle A_0B_1\rangle + \langle A_1B_0\rangle - \langle A_1B_1\rangle| \leq 2, \tag{4.5}$$

where the minimal classical bound is shown to be $\beta_C = 2$ and this is obtainable for an optimal relative angle of $\theta = \frac{\pi}{2}$. We minimize the the classical bound β_C, and subsequently optimize the angle θ, and show the resulting in Fig. 1. We show the negative of the determined classical bound, for visual clarity, as a function of the iteration number for multiple basinhopping steps alongside with the ground state energy $\mathrm{Tr}(\mathcal{H}\rho)$ of the Hamiltonian described in (4.1) in Fig. 1**a** . We observe that for each basinhopping step the classical bound converges towards $\beta_C = 2$, while the ground state energy $\mathrm{Tr}(\mathcal{H}\rho) = -2\sqrt{2}$. To see whether the resulting inequality is thus able to detect the nonlocal correlations present in the ground state of this Hamiltonian, it being one the Bell states and is thus nonlocal [13], we compute $\mathrm{Tr}(\mathcal{B}\rho)$ to be $\mathrm{Tr}(\mathcal{B}\rho) = -2\sqrt{2}+2 < 0$ and thus revealing that ρ is nonlocal. This shows that the dictionary is capable of detecting nonlocal correlations in the ground state. Moreover, in Fig. 1**b** we show the angle θ as a function of the iteration number of all basinhopping steps. We observe that for each basinhopping step, the angle θ converges towards $\theta = \frac{\pi}{4}$, for which we find that the set of coefficients $\gamma_k^{(i,r)}$ to be $\gamma_k^{(i,0)} = 0$ for $i \in \{0,1\}$ and $k \in \{0,1\}$ and $\gamma_{00}^{0,1} = -\gamma_{01}^{0,1} = \gamma_{10}^{0,1} = \gamma_{11}^{0,1} = 1$. Therefore, we find that under optimal measurement settings, the Bell inequality $I + \beta_C \geq 0$ becomes

$$\langle A_0B_0\rangle - \langle A_0B_1\rangle + \langle A_1B_0\rangle + \langle A_1B_1\rangle + 2 \geq 0, \tag{4.6}$$

which is nearly the same inequality as the CHSH inequality given by (4.5). This indicates that the dictionary is capable of not only constructing correct optimal Bell inequalities to spin Hamiltonians, but also to detect nonlocal correlations present in the ground state of these Hamiltonians.

4.2 Applying the algorithm to the Hydrogen molecule

Having found that the dictionary correctly constructs optimal Bell inequalities from the toy Hamiltonian described in (4.1), we now use it to try to do the same for the two isospectral spin Hamiltonians obtained through mapping the fermionic Hamiltonian describing the Hydrogen molecule with either the Jordan-Wigner or the Bravyi-Kitaev transformation, which are shown in (3.5) and (3.6) respectively. We start of by using the simplest isomorphism for this Bell experiment, which consists of using the measurement setting described in (3.7) for all four observers, each of which can choose one of three ($m = 2$) quantum observables. Once again, we fix the measurement settings of the zeroth observer to be those of (3.10), such that the angle $\theta_0^{(0)} = 0$ and $\theta_1^{(0)} = \frac{\pi}{2}$. Or in other words, the quantum observables from which the zeroth observer can choose are $\mathcal{M}_0^{(0)} = \sigma_x^{(0)}$, $\mathcal{M}_1^{(0)} = \sigma_y^{(0)}$ and $\mathcal{M}_1^{(0)} = \sigma_z^{(0)}$. The measurement settings of the three other observer are given by (3.11), in which the angles $\theta^{(1)}$, $\theta^{(2)}$ and $\theta^{(3)}$ are relative to the quantum observables of the zeroth observer. We aim at finding the optimal relative angles such that the classical bound β_C is minimal. For this we again use the simulation parameter given in Section 3.4 and treat these angles as variational parameters. In Fig.2 we show the results of this minimization of the classical bound β_C for both the spin Hamiltonians (3.5) and (3.6).

Fig.2**a** and Fig.2**b** show $-\beta_C$ and the ground state energy $\mathrm{Tr}(\mathcal{H}\rho)$ for the spin Hamiltonians obtained through mapping the fermionic Hamiltonian with the Jordan-Wigner and the Bravyi-Kitaev transformations respectively as a function of the iteration number of the Nelder-Mead algorithm. We observe two things: First of all, the dictionary seems to find the global minimum of the classical bound for both constructed optimal Bell inequalities since the same minimal classical bound is found for multiple Basinhopping iterations, which was also observed for the testing done on the toy Hamiltonian (Fig. 1**a**). Secondly, both constructed optimal Bell inequalities have the negative of the minimal classical bound to be lower than the ground state energy of the respective spin Hamiltonians. This results in $\mathrm{Tr}(\mathcal{B}\rho)$ to be equal to $\mathrm{Tr}(\mathcal{B}\rho) \approx -1.851024 + 1.921083 = 0.070059 \geq 0$ for the optimal Bell inequality constructed from the spin Hamiltonian obtained through the Jordan-Wigner transformation and $\mathrm{Tr}(\mathcal{B}\rho) \approx -1.851024 + 1.958629 = 0.107605 \geq 0$ for the optimal Bell inequality tailored to the spin Hamiltonian obtained through the Bravyi-Kitaev transformation. Therefore, in both cases we find that that the ground state does not violate the constructed optimal Bell inequalities for both spin Hamiltonians. We do however observe that the minimal classical bound are not the same for the constructed optimal Bell inequalities, indicating that the Jordan-Wigner and the Bravyi-Kitaev transformation result in spin Hamiltonian that do

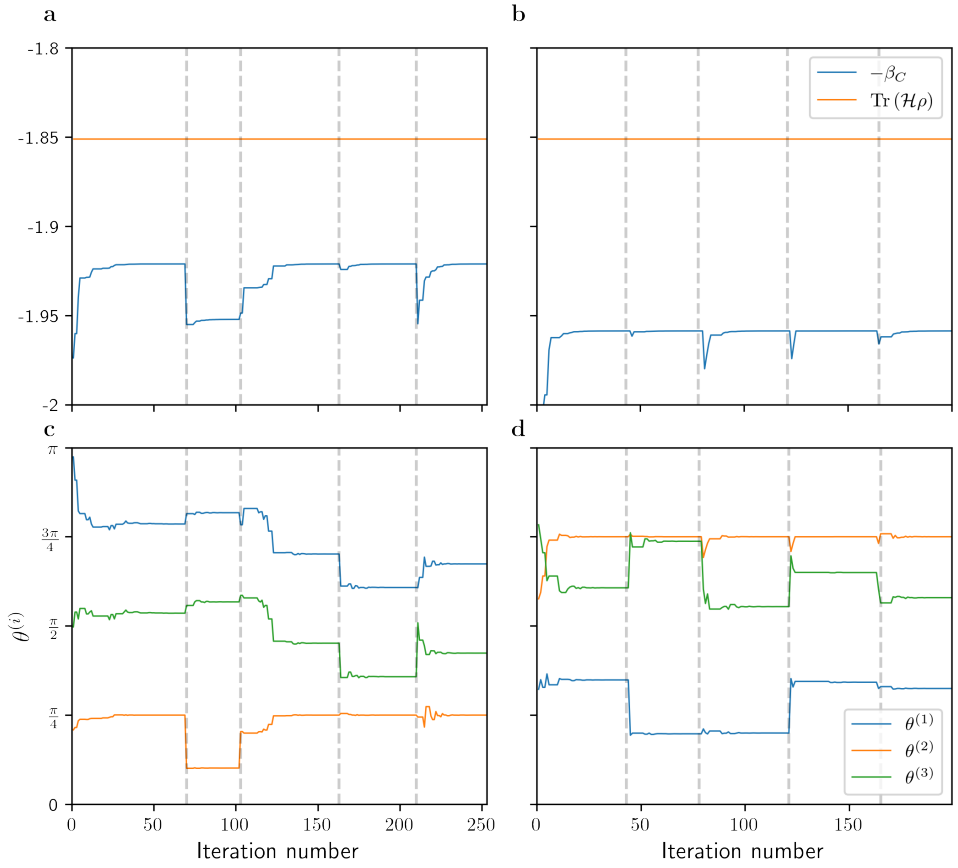

Figure 2: Results of the minimization of the classical bound β_C obtained through the construction of optimal Bell inequalities from the Hamiltonians shown in (3.5) and (3.6), for which the observers can choose quantum observables from the measurement setting (3.7) for $m = 2$ and the measurement angles shown in (3.11). The minimization was done through optimization of the relative angles $\theta^{(1)}$, $\theta^{(2)}$ and $\theta^{(3)}$. The iteration number denotes the number of iterations of the Nelder-Maed algorithm and the vertical dotted lines indicate the start of a new basinhopping step. β_C is shown as negative for visual clarity. **a**: $-\beta_C$ and the ground state energy $\mathrm{Tr}\,(\mathcal{H}\rho)$ as a function of the number of iterations for the spin Hamiltonian obtained with the Jordan-Wigner transformation. **b**: $-\beta_C$ and the ground state energy $\mathrm{Tr}\,(\mathcal{H}\rho)$ as a function of the number of iterations for the spin Hamiltonian obtained with the Bravyi-Kitaev transformation. **c**: Relative angles $\theta^{(1)}$, $\theta^{(2)}$ and $\theta^{(3)}$ as a function of the number of iterations for spin Hamiltonian acquired through the Jordan-Wigner transformation. **d**: Relative angles $\theta^{(1)}$, $\theta^{(2)}$ and $\theta^{(3)}$ as a function of the number of iterations for spin Hamiltonian acquired through the Bravyi-Kitaev transformation.

not produce the same family of Bell inequalities.

Both optimal Bell inequalities not detecting nonlocal correlations in the ground states of the respective spin Hamiltonians does not means that these ground states are not nonlocal. To illustrate this, we first consider the ground state of the spin Hamiltonian obtained through mapping the fermionic Hamiltonian of molecular Hydrogen (for the fermionic ground state see [20]) with the Jordan-Wigner transformation:

$$|\psi_G\rangle_{\mathrm{JW}} = 0.11282737\,|0011\rangle - 0.99361461\,|1100\rangle\,. \tag{4.7}$$

This state is a pure entangled state and all pure entangled states violate a Bell inequality [34], indicating that ground state of this spin Hamiltonian is in fact nonlocal. The ground state of the spin Hamiltonian obtained through the Bravyi-Kitaev transformation is given by

$$|\psi_G\rangle_{\mathrm{BK}} = 0.11282737\,|0010\rangle - 0.99361461\,|1000\rangle\,, \tag{4.8}$$

which is a pure state, but it is not fully entangled, nor fully separable. In fact, this state is 3-separable [19] since it can be written as

$$|\psi_G\rangle_{\mathrm{BK}} = \left(0.11282737\,|01\rangle_{0,2} - 0.99361461\,|10\rangle_{0,2}\right) \otimes |0\rangle_1 \otimes |0\rangle_3\,, \tag{4.9}$$

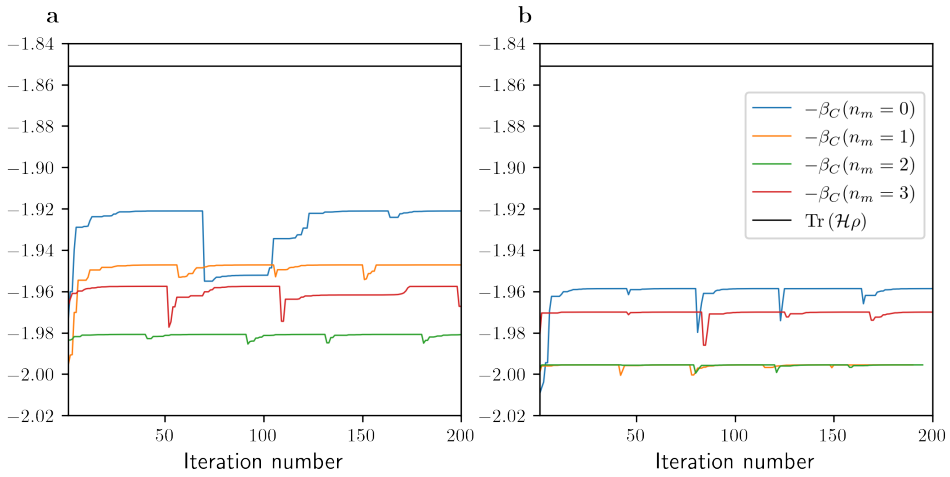

Figure 3: Results of the minimization of the classical bound β_C obtained through the construction of optimal Bell inequalities from the Hamiltonians shown in (3.5) and (3.6), for which the observers can choose quantum observables from the measurement setting (3.7) for either $m = 2$ or $m = 3$ and the measurement angles shown in (3.11). The minimization was done through optimization of the relative angles $\theta^{(1)}$, $\theta^{(2)}$ and $\theta^{(3)}$. We performed this simulation for the case in which zero, one, two or three observers can choose from one of $m = 3$ quantum observables instead of $m = 2$ observables. The iteration number denotes the number of iterations of the Nelder-Maed algorithm and the vertical dotted lines indicate the start of a new basinhopping step. β_C is shown as negative for visual clarity. **a**: $-\beta_C$ and the ground state energy $\mathrm{Tr}(\mathcal{H}\rho)$ as a function of the number of iterations for the spin Hamiltonian obtained with the Jordan-Wigner transformation. **b**: $-\beta_C$ and the ground state energy $\mathrm{Tr}(\mathcal{H}\rho)$ as a function of the number of iterations for the spin Hamiltonian obtained with the Bravyi-Kitaev transformation.

where the indices denote the respective qubits f the observers. We observe that this state is partially separable and thus also only partially entangled, meaning that the qubits 1 and 3 are not nonlocal since separable quantum states are not entangled and thus not nonlocal [19]. However, the qubits 0 and 2 form a pure entangled state and thus these qubits could yield nonlocal correlations when performing a Bell experiment on the entire ground state, possibly allowing for violating of a Bell inequality [3]. Despite this state still being possibly partially nonlocal, it does show us that the spin Hamiltonian obtained through the Jordan-Wigner transformation might be more optimal for the detection of nonlocality since its corresponding ground state is a pure entangled state, which is not the case for the spin Hamiltonian acquired with the Bravyi-Kitaev transformation.

Since the ground state of spin Hamiltonian obtained through the Jordan-Wigner transformation should violate a Bell inequality and the ground state of the spin Hamiltonian mapped found with the Bravyi-Kitaev transformation could possibly could be nonlocal as a result of the partial entanglement present in this state, we aim at extending the family of Bell inequalities constructed from these Hamiltonians. We achieve this through the addition of extra quantum observables for either one, two, three or all four observers. For this we still use the measurement settings denoted in (3.7), but now we simply change m from $m = 2$ to $m = 3$. This is first done for just a single observer and we construct the optimal Bell inequalities from the two spin Hamiltonians defined in (3.5) and (3.6) and calculate $\mathrm{Tr}(\mathcal{B}\rho)$ to see whether the new optimal Bell inequality is able to detect the nonlocal correlations present in the respective ground states. We then do the exact same, but now instead of only having one observer with four quantum observables, we now have two with three observables, after which we repeat this but now for three and four observers with three quantum observables. In Fig.3 we show the minimal classical bound β_C resulting from these simulations for both spin Hamiltonians. We observe that for both spin Hamiltonians, the minimal classical bound increases as we increase the number of quantum observables for the observers with respect to the simple isomorphism in which each observers can only choose from two quantum observables. This indicates that we will not be able to violate the Bell inequalities by adding one measurement to each party since $\mathrm{Tr}(\mathcal{B}\rho)$ only increases and drifts away from a possible violation. Whether the addition of even more measurements brings us closer to the violation of these family of Bell inequalities is yet to be determined for these specific spin Hamiltonians obtained through mapping fermionic Hamiltonians. Moreover, it is also possible that the families of Bell inequalities that we are considering do not cause the ground state to violate it and that these nonlocal correlations can only be revealed through other type of Bell inequalities.

There is one additional thing we can conclude from our simulations. In Fig. 2**c** and Fig. 2**d** we show the optimal angles $\theta^{(0)}$, $\theta^{(1)}$ and $\theta^{(2)}$ corresponding to the minimum of β_C for the two spin Hamiltonians obtained through the Jordan-Wigner and the Bravyi-Kitaev transformation shown in Fig. 2**a** and Fig. 2**b** respectively. We observe that there are multiple configurations of these optimal angles corresponding to the respective minimal classical bounds for both optimal Bell inequalities, indicating that there are multiple global minima present in the functional landscape of β_C. This can be explained by the fact that the dictionary does not make a distinction between the separate observers. Besides the relative angles, the different observers are simply labelled in an arbitrary way that are interchangeable with each other, resulting in the possibility of having multiple global minima of β_C.

4.3 Improvements and further outlooks

Despite us not having found an optimal Bell inequality from the family of Bell inequalities constructed from the spin Hamiltonians described in (3.5) and (3.6) for both the simplest isomporphism and the case in which the observers have the choice of one additional quantum observable, there should be a Bell inequality that is violated by the ground states of the spin Hamiltonian obtained through the Jordan-Wigner transformation and possibly also one for the spin Hamiltonian acquired with the Bravyi-Kitaev transformation. Therefore, we should extend on the family of Bell inequalities tailored to these spin Hamiltonian through either the addition of measurements or through other means. One of such is by adding more atomic orbitals to the atomic basis from which we construct the molecular spin orbitals. So far we have only considered the fermionic Hamiltonian, and thus also the spin Hamiltonians, of molecular Hydrogen in the minimal basis, consisting of only a single $1s$ orbital per atomic. As early mentioned earlier, the p-like orbitals cause a small change to the shape of the molecular orbitals [40]. By including these orbitals into the basis, we ultimately get a more accurate description of the ground state of the system and, which is more important for us, it causes for extra molecular spin orbitals to be added to the basis in which we express the Hamiltonians of molecular Hydrogen. This results in a new family of Bell inequality due to a different structure and number of qubits of the resulting spin Hamiltonians obtained through the Jordan-Wigner and the Bravyi-Kitaev transformation and more family of Bell inequalities increases the probability of finding an optimal Bell inequality which is violated. There is however a problem with doing this: the dictionary proposed in Section (3) calculates the classical bound by comparing all 2^{mn} possible configurations of the local deterministic strategies. If we would add more qubits, the overall computation time would exponentially increase. One way to possibly overcome this problem is by omitting higher-body correlation terms from the corresponding spin Hamiltonians. For example, if we were to use the 3-21G basis to simulate the Hydrogen molecule, which contains an additional atomic p-orbital per atom, we would have a total of eight molecular spin orbitals in our basis [39]. By omitting the higher-order correlations, such that the spin Hamiltonians only contain up to four- or five-body correlators, we can use the recursive algorithm described in Section 2.4 to speed up the determination of β_C, proving an up-to exponential speed.

Another method that could help in finding optimal Bell inequalities that are violated by the ground states of these spin Hamiltonians is by considering isometric states to these ground states for which an optimal Bell inequality is already known. To illustrate this, we can find a state isometric to the ground state shown in (4.7) by making the substitution $|0_i 0_{i+1}\rangle \to |\tilde{0}_{\lfloor i/2 \rfloor}\rangle$ and $|1_i 1_{i+1}\rangle \to |\tilde{1}_{\lfloor i/2 \rfloor}\rangle$, where $\lfloor x \rfloor$ denotes the floor of x, resulting in this isometric state to be

$$\left|\tilde{\psi}_G\right\rangle_{\text{JW}} = 0.11282737 \left|\widetilde{01}\right\rangle - 0.99361461 \left|\widetilde{10}\right\rangle. \tag{4.10}$$

This bipartite state is much easier to analyze and to find a corresponding optimal Bell inequality for. The corresponding general bipartite Bell inequality has the form of

$$I = \sum_i \alpha_i \langle A_i \rangle + \sum_j \beta_j \langle B_j \rangle + \sum_i \sum_j \gamma_{i,j} \langle A_i B_j \rangle, \tag{4.11}$$

where the coefficients α_i, β_j and $\gamma_{i,j}$ are to optimized to find the largest possible violation and the observers Alice and Bob can choose from i and j quantum observables respectively. Despite there still needing to be found an optimal Bell inequality, the overall size of the set of unknown coefficients is much smaller in comparison to the Bell inequality to be tailored to the spin Hamiltonians of the entire Hydrogen molecule. Moreso, there has been a lot of research on Bell inequalities that are similar to this one [2], possibly allowing to deduce the optimal coefficients. Besides the Bell inequality being easier to optimize, it could also reveal more about the underlying structure of the original non-isometric Bell inequality. This could be useful for the ground state of

the spin Hamiltonian obtained through the BK transformation. We observe that the isometric state described above is precisely the same as the partially entangled part of the ground state shown in (4.8). Finding the optimal Bell inequality for the isometric state could reveal the structure of the optimal Bell inequality for the two observers measuring the entangled qubits of the ground state (4.8), effectively reducing the complexity of finding the optimal Bell inequality of the entire ground state.

5 Conclusion

In this report we investigated if mapping the fermionic Hamiltonian describing the Hydrogen molecule to two isopectral spin Hamiltonian with the Jordan-Wigner and the Bravyi-Kitaev transformation results in the same tailored family of Bell inequalities and whether the optimal inequalities from these families are violated by the ground state of the respective spin Hamiltonians. For this we presented a dictionary that described how to construct families of Bell inequalities from spin Hamiltonians, requiring the calculation of the set of coefficients $\gamma_{\mathbf{k}}^{(i,r)}$, such that the Bell operator coincides with the spin Hamiltonian, and the determination of the classical bound β_C through the comparison of all possible local deterministic strategies. Moreover, we gave a method to obtain the optimal inequality from the family of Bell inequalities through the minimization of β_C with the Nelder-Mead minimization scheme in combination with the Basinhopping algorithm in which we treated the relative angles between the measurements of different observers as variational parameters and optimized them.

Prior to using this dictionary to construct optimal Bell inequalities from the spin Hamiltonians representing the Hydrogen molecule, we first tested the capabilities of this dictionary in doing so on a bipartite toy spin Hamiltonian with observers Alice and Bob. Under optimal measurement settings for Alice and Bob, the optimal Bell inequality tailored to the Hamiltonian should be the CHSH inequality. We tailored Bell inequalities to this spin Hamiltonian, optimized them and determined that the proposed dictionary was indeed fully capable of retaining the CHSH inequality from the Hamiltonian. Moreover, it did this by obtaining the exact same optimal measurement settings as theoretically derived for the CHSH inequality. Therefore, we concluded that the dictionary seems to work correctly.

Having tested the dictionary, we used it to construct optimal Bell inequalities from the spin Hamiltonian obtained from mapping the fermionic Hamiltonians describing molecular Hydrogen with the Jordan-Wigner and the Bravyi-Kitaev transformation. We first did this for the simplest isomorphism in which all four observers could choose from one of three quantum observables ($m = 2$) and found that for both spin Hamiltonians, the respective ground state did not violate the constructed optimal Bell inequalities. Despite them not being violated, we did find that the minimal classical bound was different for the two spin Hamiltonians, possibly indicating that the families of Bell inequalities tailored to these spin Hamiltonians are different from one another. To test if the addition of extra quantum observables would result in the optimal Bell inequalities getting closer to a possible violation, we performed the same simulations, but now with an additional quantum observable for only one, two, three or all four observers. We observe that the addition of these extra quantum observables did not bring the constructed optimal Bell inequalities closer to a violation. In fact, it shifted the inequalities further away from a violation, similar to [44]. Despite us not having found an optimal Bell inequalities that is violated by the ground states of both respective spin Hamiltonians, we did find that the spin Hamiltonian obtained through mapping the fermionic Hamiltonian describing molecular Hydrogen with Jordan-Wigner and the Bravyi-Kitaev do possibly results in different families of Bell inequalities.

This does not allow us to conclude that the ground states of the respective spin Hamiltonians do not show nonlocal correlations since the ground state of the spin Hamiltonian obtained through the Jordan-Wigner transformation is a pure entangled state and thus always violates a Bell inequality [34] and the ground state of the spin Hamiltonian acquired with the Bravyi-Kitaev transformation is a partially entangled state, possibly allowing for the violation of a Bell inequality. From this we conclude one of two things. that in order to obtain a Bell inequality from the spin Hamiltonian representations of the Hydrogen molecule, one must explore beyond the simplest isomorphism considered here. This implies either increasing the number of molecular spin orbitals through the addition of atomic orbitals to the minimal basis or possibly through the addition of more than $m = 3$ measurements per party.

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