Anderson Bound for an Antiferromagnetic Kagome Lattice

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1 Introduction

The general form of the antiferromagnetic Heisenberg model in the basis of the single-qubit Pauli gates is given as follows:

$$H = \sum_{<i,j>} X_i X_j + Y_i Y_j + Z_i Z_j, \tag{1}$$

where the summation runs over the nearest neighbors of the lattice under study. In our case, we will focus on the Kagome lattice, which is defined using a hexagonal unit cell and a basis consisting of 3 atoms (see Fig. 1). Thus, the ground state energy of the antiferromagnetic Heisenberg model for the Kagome lattice is the lowest eigenvalue of the Hamiltonian of Eq. 1 when defined over the lattice shown in Fig. 1. Our task is to compute this ground state energy using a variational quantum eigensolver (VQE) as accurately as possible for a finite 12-site cluster within the otherwise periodically repeating Kagome lattice (see Fig. 1). In this work, we propose an approach for computing this ground state energy by shifting our focus on instead deriving a highly accurate lower bound for this ground state energy using VQE. We will then show that our approach for estimating the lower bound for the ground state energy of the 12-site cluster of the problem statement is exact in principle as long as the VQE-based estimation of the lower bound is exact.

As a first step in our approach, we redefine the construction of the Kagome lattice using unit cells of 4 rectangular sublattices (see Fig. 2). In this way, any finite cluster within the Kagome lattice can be constructed by specifying four pairs of integers, i.e., (x_n, y_n), where $n = 1$ to 4 represents each of the 4 rectangular sublattices and each pair represents the corresponding number of repeat units along the x and y directions. Hence, the 12-site Kagome cluster of the problem statement is easily constructed using $(x_1, y_1) = (1, 1), (x_2, y_2) = (2, 1), (x_3, y_3) = (2, 1)$ and $(x_4, y_4) = (1, 1)$.

We now show how this sublattice decomposition allows us to easily define a lower bound for the ground state energy of any finite-sized Kagome cluster using the idea of Anderson bound estimation [1, 2]. The approach translates to the

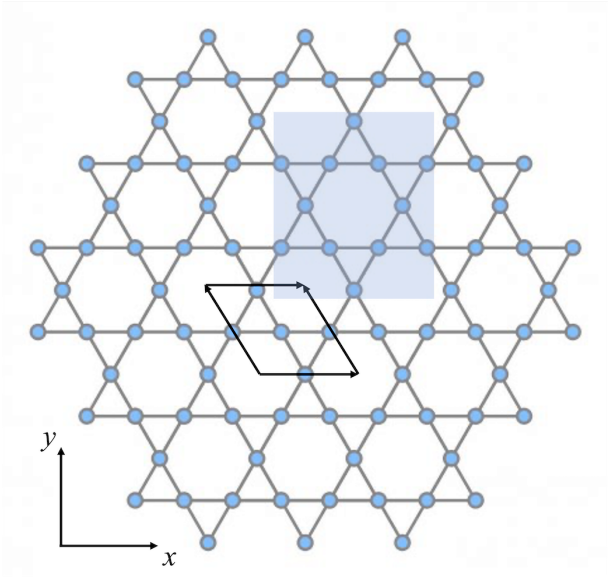

Figure 1: Kagome crystal lattice with its hexagonal primitive unit cell indicated using solid black lines. The 12-site cluster of the problem statement is indicated in blue. Cartesian directions are anotated.

simple observation that the ground state energy of any N-site finite cluster of any lattice model is lower bounded by the sum of m-site overlapping subclusters of the same lattice model. The proof of this is straightforward and is detailed elsewhere [2]. The requirements for applying this approach for lower bound estimation is that the Hamiltonian of the lattice model under study must be translationally invariant and one should be able to decompose this Hamiltonian into site-specific Hamiltonians, which are themselves translationally invariant as well. Since all of these requirements are met by the antiferromagnetic Heisenberg model on a Kagome lattice, we can apply this approach for estimating a lower bound for its ground state energy.

We focus on our rectangular sublattice decomposition of the Kagome lattice to estimate this lower bound. Based on the idea described above, a lower bound for a Kagome cluster of size $\{(x_n, y_n)\}$ is simply given as:

$$E_{lb} = (x_1 y_1)e_1 + (x_2 y_2)e_2 + (x_3 y_3)e_3 + (x_4 y_4)e_4, \tag{2}$$

where e_n is the ground state energy of the same antiferromagnetic Heisenberg model of Eq. 1 defined over the unit cell of the rectangular sublattice n. Therefore, the true ground state energy for this cluster obeys:

$$E_{lb} \leq E_0. \tag{3}$$

The lower bound estimate of Eq. 2 can be further simplified by observing that each of the four rectangular sublattice unit cells will share the same ground

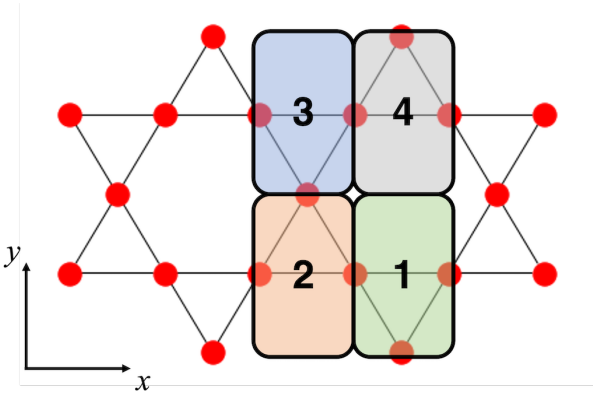

Figure 2: A finite portion of the Kagome lattice showing the four-fold rectangular sublattice decomposition used in this work. The four rectangular sublattice unit cells are highlighted in green, orange, blue and grey and are indexed as $n = 1, 2, 3$ and 4 respectively as annotated. Cartesian directions are annotated as well.

state energy, i.e., $e_1 = e_2 = e_3 = e_4 = e_0$. This is because the four rectangular sublattice unit cells are equivalent to each other by a set of appropriate mirror reflections and the Hamiltonian of Eq. 1 is invariant with respect to such symmetry operations. With this simplification, we rewrite our estimate for the lower bound as:

$$E_{lb} = (x_1y_1 + x_2y_2 + x_3y_3 + x_4y_4)e_0. \tag{4}$$

As long as this lower bound is exact, we can directly estimate the true ground state energy of any Kagome cluster by simply using the exact value for e_0.

We test the performance of this lower bound for linear and bilinear chains of the 12-site Kagome cluster using the classically computed exact value of $e_0 = -3$ (see Fig. 3 and Tables 1-2). We observe that the true ground state energy is always higher than the estimated lower bound, validating the bound estimation approach. More importantly, the lower bound is exact for the 12-site Kagome cluster of the problem statement. **Therefore, in our approach, we focus on an accurate estimation of e_0 using VQE, which will provide us with an accurate value of E_0 using its lower bound estimate from Eq. 4.**

We now comment on the theoretical performance of our approach based on the two quantitative judging criteria. Firstly, the accuracy of our approach is limited only by the accuracy of the estimation of e_0. This is where devising an accurate and robust VQE algorithm for its estimation will be crucial. Secondly, the scalability of our solution is of $O(1)$ with respect to both larger qubit devices as well as larger Kagome lattices, solely because our approach relies only on performing VQE for a fixed 3-site subcluster. A disadvantage of our approach is the obvious inexactness of the lower bound. For instance, the linear chain comprising two 12-site Kagome clusters leads to an inexact lower bound, albeit

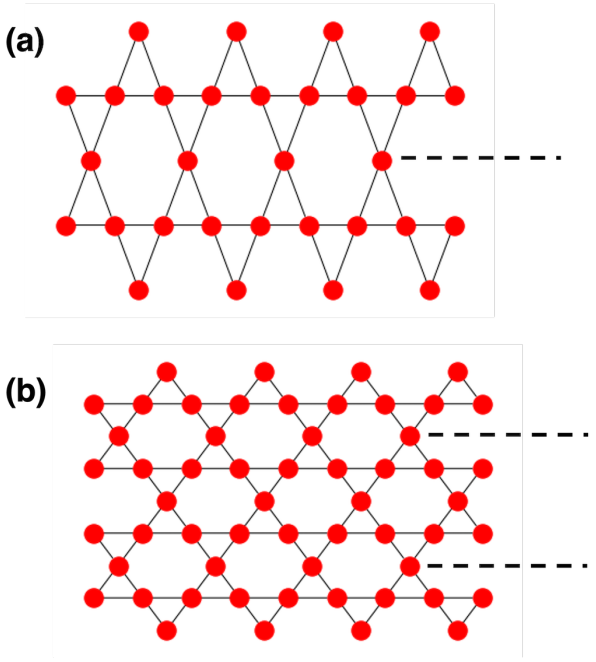

Figure 3: (a) Linear chain of 12-site Kagome clusters. (b) Bilinear chain of 12-site Kagome clusters.

having an error of only 2.85%. Thus, the bound itself gives a nearly accurate result but not an exact one in the case of this cluster. However, it is worth noting that the bound estimation is exact for an infinitely large cluster. *Note: please double check this last statement*.

References

[1] PW Anderson, *Limits on the energy of the antiferromagnetic ground state*, Physical Review **83** (1951), no. 6, 1260.

[2] J Eisert, *A note on lower bounds to variational problems with guarantees*, arXiv preprint arXiv:2301.06142 (2023).

Table 1: Performance testing of the Anderson lower bound on linear chains of antiferromagnetic 12-site Kagome clusters

Chain Size	Exact E_0	E_{lb}
1	-18	-18
2	-29.1462	-30
3	N/A	-42
4	N/A	-54
5	N/A	-66
6	N/A	-78

Table 2: Performance testing of the Anderson lower bound on bilinear chains of antiferromagnetic 12-site Kagome clusters

Chain Size	Exact E_0	E_{lb}
1	-35.1445	-36
2	N/A	-60
3	N/A	-84
4	N/A	-108
5	N/A	-132
6	N/A	-156