Inquiry into Quantum Walk Graph Hamiltonians for Sudoku

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I. INTRODUCTION

This note was originally inspired by the intuitive realization that the Rydberg blockade can be used to find solutions to the NP-Hard Maximal Independent Set (MIS) problem more efficiently than classical computers. I attempted three approaches to this problem: an adiabatic algorithm that dynamically configures the lattice geometry of a system of hard-core bosons, a circuit of controlled root swap gates, and a continuous time quantum walk (CTQW) using a Hamiltonian with embedded kinetic constraints on dipole moments. In this note I focus on the latter approach. I describe two Hamiltonians that host kinetically constrained, continuous time quantum walks which may be used to more efficiently search for solutions to NP-Complete problems like Sudoku — the PXP model and a more general model which exhibits the symmetries of such problems more transparently. These models implement continuous "quantum backtracking" without the need for complicated unitary circuits. My aim is to provide intuitive "driving" Hamiltonians that can compactly represent and generate the MIS and Sudoku state trees, which can then be used in existing CTQW algorithms.

II. BACKGROUND

The Maximal Independent Set (MIS) of a graph is the largest set of vertices such that no two vertices in the set are connected; i.e. no two vertices in the set are in the same clique for any clique. It is easy to see how this could be solved for a planar graph using adiabatic evolution by arranging Rydberg atoms on a 2D lattice. Sudoku is more difficult to solve since its representation as an MIS problem is non-planar, and it is NP-Complete, making it a valuable case study. I represent Sudoku as a cube of N^3 atoms where any two atoms in the same row, column, or vertical are connected (a mapping from N color graph coloring to binary MIS). Then, each layer of the cube is a different Sudoku number. We ignore the subgrid constraint for simplicity. Notice that solving MIS on this graph solves Sudoku since our $3N^2$ constraints are

1. One Sudoku number per 2D puzzle cell (3D vertical) (N^2 constraint cliques).

2. No repeated Sudoku numbers per 2D puzzle row/column ($2 * N^2$ constraint cliques).

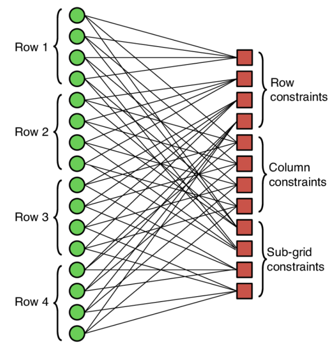

FIG. 1. Sudoku Hopping Pathways Cross-Section. The full graph of modes is 3D to account for multiple Sudoku numbers, with vertical edges connecting each plane cross-section.

III. MODEL

Take any graph G with a set V of N vertices and a minimal set C of M cliques that cover the graph. We define a clique as any group of vertices where each vertex is connected to every other vertex in the clique. Define $D_i = \{C_j | V_i \in C_j, 1 \leq j \leq M\}$, i.e. the set of cliques that contain the vertex V_i for any $1 \leq i \leq N$.

The PXP model embodies all constraints of Sudoku using the cubic graph I described earlier. We can define the PXP model for G as follows:

$$P_j = \prod_{k \in C_j} P_k \tag{1}$$

$$H = \sum_{i \in V} X_i \prod_{C_j \in D_i} P_j. \tag{2}$$

To more intuitively see the constraints via conservation laws and symmetries in a more compact format, I propose a more general particle hopping model that conserves the dipole moments of groups of constraints assigned to individual vertices.

Let our system contain M modes corresponding to each clique and N modes corresponding to each vertex. Define a bosonic creation operator $c_i^\dagger$ that excites any clique mode, and a creation operator $v_i^\dagger$ that excites any vertex mode. By defining the clique hopping Hamiltonian as follows, each v_i is effectively a $|D_i|$ level system. We have

$$H = \sum_{i \in V} (v_i^\dagger)^{|D_i|} \prod_{C_j \in D_i} c_j + h.c. \tag{3}$$

which conserves total particle number and the dipole moment of each clique C_i. Under the Schroedinger equation, at most one vertex will be occupied in each clique. In Sudoku, H conserves the dipole moment of row, column, subgrid, and vertical constraints ($|D_i| = 4$). Then, when a Sudoku cell is filled in, these constraint particles are annihilated and none can be reused by a different vertex (Fig 2). The hopping pathways of H happen to mimic the classical factor or Tanner bipartite graph (Fig 1) with the constraints on one side (red) and the solution sites on the other (green).

IV. PHASE TRANSITIONS

In an initial state with no initial conditions, $\psi_0 = \otimes_M |1\rangle \otimes_N |0\rangle$ respects this constraint with the c_i modes each containing a single excitation $|1\rangle$ and the v_i modes in the vacuum state $|0\rangle$; i.e. where the total particle number equals M. ψ_0 then defines a Krylov subspace that is closed under the action of H. Each such subspace corresponds to a different level of constraint. For example, suppose we start with a state $\psi_0 = \otimes_M |n\rangle \otimes_N |0\rangle$ for some density of particles per clique $n >> 1$ in the thermodynamic limit. In this case, there is no constraint and the subspace is a free boson gas, which is classically easy to solve.

As we reduce n to 1, we achieve the Sudoku model, containing all solutions to Sudoku with equal probability. The hard-boson constraint is then an emergent property of this constrained, low density regime, occurring sharply at $n = 1$ giving a first-order phase transition. To see this, suppose we add a defect such that there are $nM = M + 1$ particles and n is now just over 1. Regardless of the clique mode it started in, the defect destabilizes all of the constraints, since it can diffuse across the entire lattice because the hopping pathway graph is connected.

For specific instances of $n < 1$ we achieve the NP-Complete partially solved Sudoku puzzle where there is only a single state where all cells are filled and the constraints are satisfied. Note that this only applies for specific instances where a solution exists, and that the initial state of the clique modes fully specifies the Sudoku initial state and constrained subspace. For example, suppose there was a reverse defect where one clique site initially had 0 particles. To fill this site at some time $t > 0$, a Sudoku cell would need to transfer its 3 excitations to the clique modes and one of these excitations would have to go to the initially empty site. But this is only possible if the initially empty site contributed a particle to the Sudoku cell at some time $t' < t$. This is impossible, so the initial condition remains fixed for all time and the search space is minimal.

If we further reduce $n << 1$, we achieve an over-constrained model which is classically easy to solve.

Thus, H hosts transitions between classical hardness and quantum hardness between $n << 1$ and $n < 1$. If quantum advantage is to be observed in a CTQW performed on this model, it will exist in this range. Furthermore, it is known that a high degree of symmetry and constraint leads to quantum scarring; an interesting question is whether the hardness transition corresponds to the transition between quantum scars and eigenstate thermalizing behavior.

A large number of initial conditions ($n << 1$) corresponds to a high degree of symmetry, classical feasibility, and quantum scarring behavior — but this all disappears when n increases to the NP-Complete region (characterized by an exponential growth of "dead branches" in the solution tree (Fig 3), because H does not contain all Sudoku symmetries).

V. QUESTIONS

1. Does the change in constraint-particle density n represent phase transitions between NP and P? Are the transitions smooth (quantum scars tend to disappear sharply)? How is this transition related to the emergence of quantum scarring behavior? How do symmetries emerge and fade during this transition?

2. Aside from computational prospects, I discussed how the model transitions from a free-boson model to a model with an exclusion constraint. What are the low temperature behaviors of each level of constraint, and how does this relate to computational difficulty and/or symmetries?

3. We can extend the hopping structure to other types of constraints (e.g. parity constraint). Idea: study how graph Hamiltonians can be created from general constraints corresponding to each clique.

4. Can we present this model as a novel compact, intuitive way to generate driving Hamiltonians that host subspaces with different levels of more precise constraints than existing models?

5. The Sudoku state graph (e.g. Fig 2, 3) contains a bulk in the center that obstructs the flow of probability current from the initial state to the solution state. Furthermore, NP dead-end states act as "cavity walls" that prevent transmission to the solution (Fig 3). Idea: compute scattering parameters to study how probability current flows through NP-Complete state graphs.

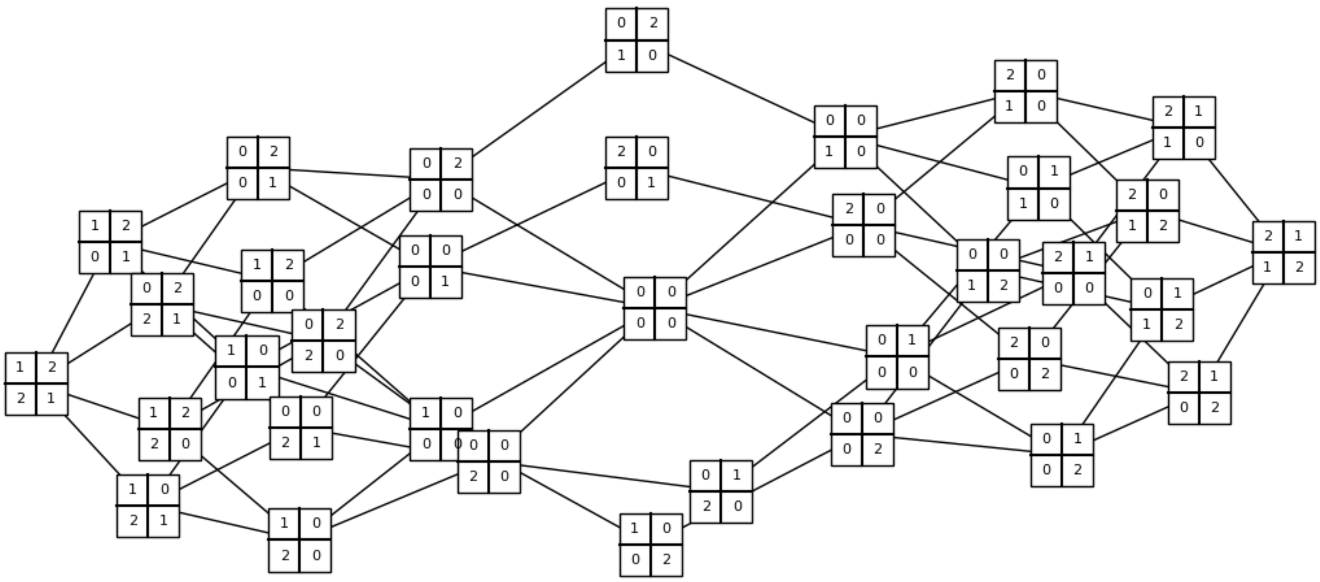

FIG. 2. 2x2 Sudoku Hamiltonian Adjacency Graph. Standard representations of Sudoku states rather than cubes for simplicity.

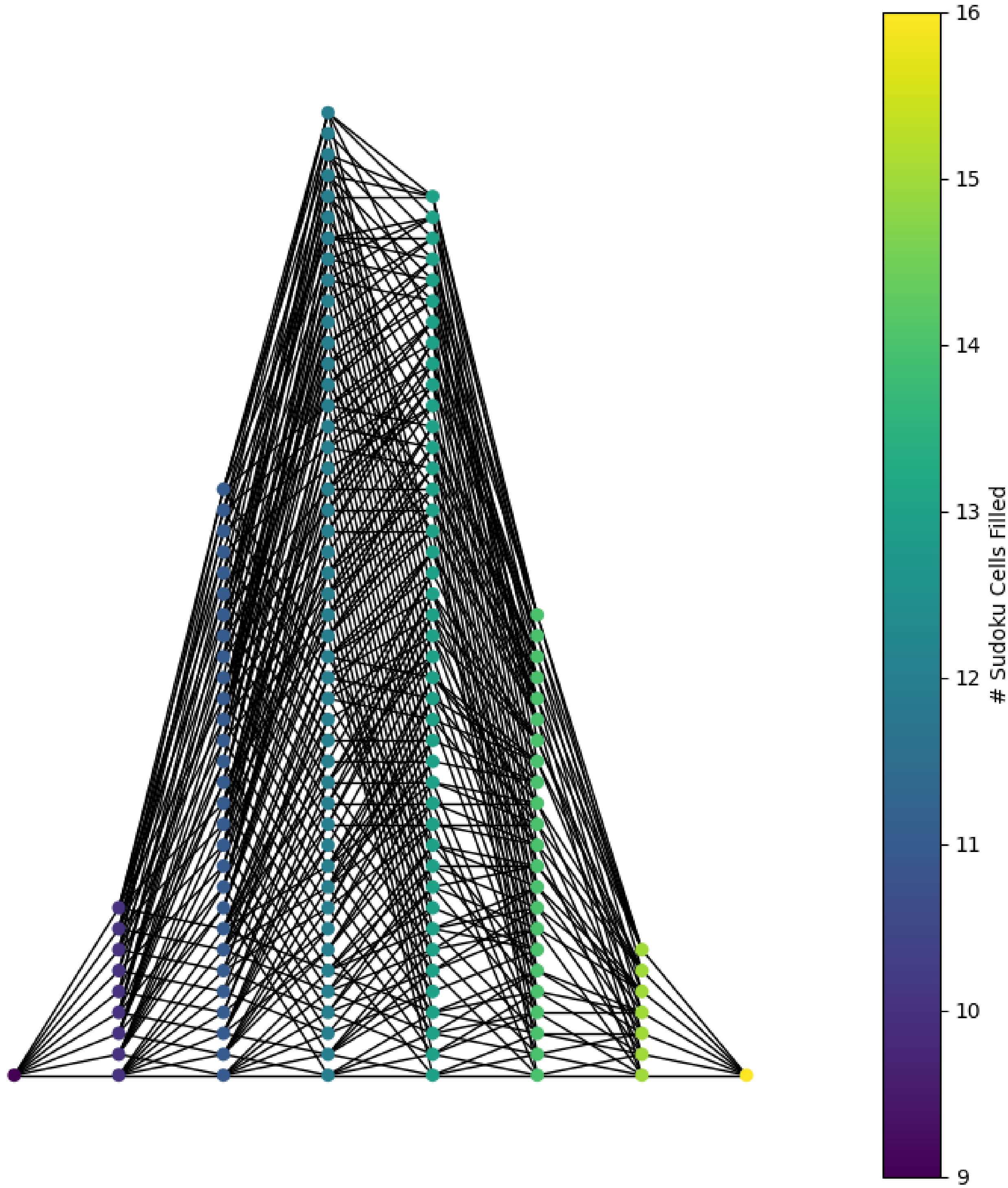

FIG. 3. 4x4 Sudoku Hamiltonian Adjacency Graph. The leftmost state is the initial state with 9 cells filled, and the rightmost state is the solution.