Simulation of the Ground State of 2D Rydberg Arrays using a Convolutional Neural Network

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Introduction

Rydberg atom arrays, which are cold atoms trapped in a 2D lattice that interact into Rydberg states, are a source of great interest. They have been associated with quantum information processing, realization of exotic many-body states and quantum simulation among many other areas of research. Thus, solving for these arrays would lead to progress in those fields.
With the advent of machine learning, it has become even more possible to simulate these arrays and calculate their ground states with increasing accuracy. Different machine learning models have been applied to this problem including but not limited to Graph Neural Networks and Convolutional Neural Networks.
The goal of this project is to investigate the fidelity of the method shown in [1] that uses Convolutional Neural Networks (CNNs) coupled with Monte Carlo methods to solve for the ground state of these Rydberg Arrays

Rydberg Arrays

The long-range interactions possible with Rydberg atoms create frustration in any lattice structure even uncomplicated structures like square lattices. That coupled with other factors including the Rydberg Blockade radius (R_b), lattice spacing(a), the laser detuning(δ) for the optical tweezers used to create these lattices in experiment and the Rabi frequency(Ω)play into the energy calculations. According to [2] the agreed upon Hamiltonian of a Rydberg Array is:

$$\hat{H} = \sum_{i=1}^{N}\left[\frac{\Omega}{2}\hat{\sigma}_i^x - \delta\hat{n}_i\right] + \sum_{i\neq j}\frac{V}{(|\vec{r}_i - \vec{r}_j|/a)^6}\,\hat{n}_i\hat{n}_j$$

$\hat{\sigma}_i^x = |0_i\rangle\langle 1_i| + |1_i\rangle\langle 0_i|$ and $\hat{n}_i = |1_i\rangle\langle 1_i|$. We take $|0_i\rangle, |1_i\rangle$ to be the ground state and Rydberg state of atom i in the lattice, respectively. V represents the interaction strength and can be expressed in terms of R_b :

$$\frac{V}{\left(\frac{R_b}{a}\right)^6} \equiv \Omega$$

where we take the structure $\Omega = a = 1$.
This project first focused on proving the fidelity of the method, named Convolutional Quantum Neural State(CQNS), on square lattices compared to the results in [2].

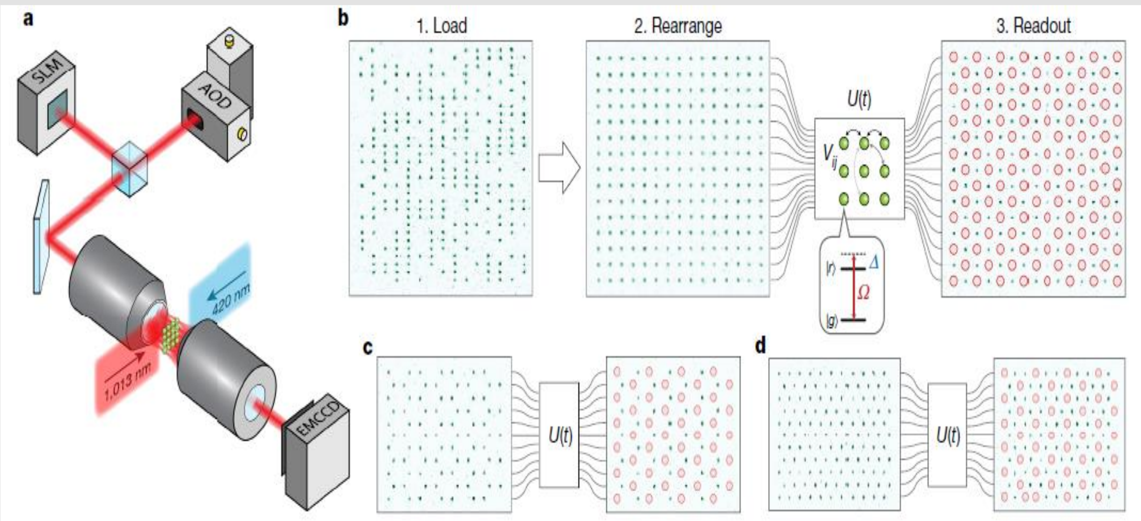


Fig 1: Rydberg Atom Arrays in Experiment[3]. **a.** Atoms are loaded into a 2D array of optical tweezer traps and rearranged into defect-free patterns by a second set of tweezers. **b.** Fluorescence image of initial random loading of atoms, followed by rearrangement to a defect-free square array. After this initialization, the atoms evolve coherently under laser excitation with Rabi frequency Ω(t) and detuning Δ(t), and long-range interactions V. Finally, the state of each atom is read out, with atoms excited detected as loss and marked with red circles. Shown on the far right is an example measurement following quasi-adiabatic evolution into the checkerboard phase. **c, d.** Similar evolution on honeycomb and triangular lattices result in analogous ordered phases of Rydberg excitations with filling 1/2 and 1/3, respectively.

Methodology

Simulation of Ground States

To simulate these Rydberg arrays, we use an Ising model where we take '1' to be the Rydberg state and '-1' to be the ground state. The Rydberg Array is represented by a matrix with the same dimensions as the lattice to be simulated. A starting lattice with a random configuration of 'atoms' in ground and Rydberg states is produced and used to begin the optimization towards its ground state.

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix}$$

Fig 2: Example 4 x 4 Rydberg Array Matrix Representation

The state of the array can be represented as $|\psi\rangle = \sum_S w(S)|S\rangle$. $|S\rangle$ represents the configuration of the lattice and $w(S)$ represents the coefficient for that configuration. Given a configuration CQNS returns the coefficient. That coefficient is used to calculate the energy of the system. The total energy of the system can be represented as:

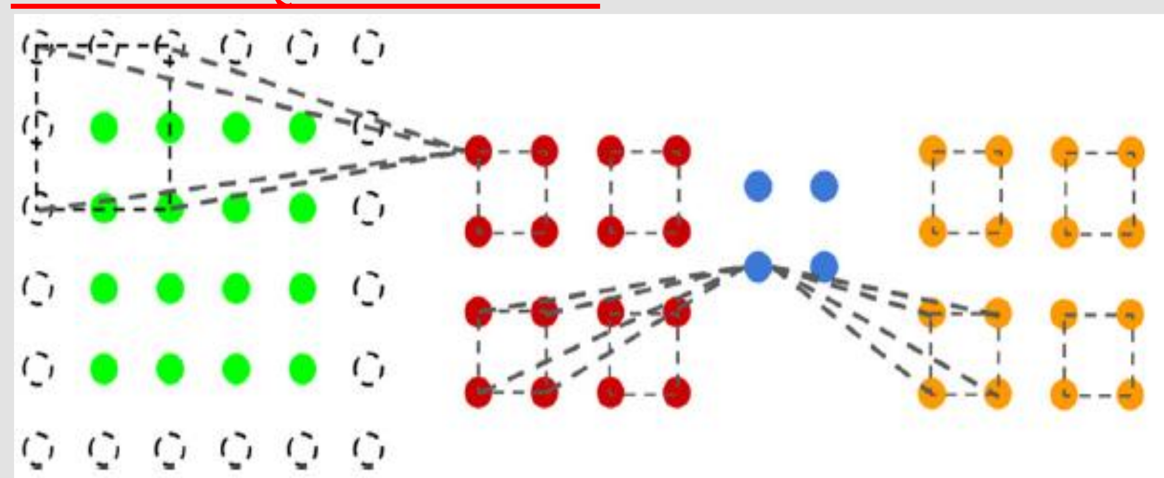
$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\sum_S w_S^2}\sum_S w_S^2 \sum_{S'}\frac{w_{S'}}{w_S}H_{S'S}$$

Where $H_{S'S} = \langle S|H|S'\rangle$.
The goal is to gradually minimize the energy calculated using the stochastic gradient method[1], where the energy E and gradients G can be represented as:

$$E = \langle E_s\rangle$$
$$G = \langle O_s E_s\rangle - \langle E_s\rangle\langle O_s\rangle$$

Where $E_s = \sum_S \frac{w_{S'}}{w_S}H_{S'S}$ and $O_s = \frac{1}{w_S}\frac{\partial w_S}{\partial a_i}$. Here a_i is all the parameters in the CQNS.

Basic 2D CQNS Structure



First, a simulated Rydberg Array with Periodic Boundary Conditions to avoid loss of information at the edge of the lattice

Second, the results of convolution layer of CNN that occurs on lattice. The convolution filter in the above example is 3 x 3 but this can be adjusted.

Third, the results of maxpooling layer. This reduces the output dimensions and introduces position invariance [1]. This allows a smaller amount of convolution filters to be used.

Lastly, the outputs of transpose convolution layer, which restores the original dimension. The product of these outputs is *w(S).*

Results

Convergence to Ground State Energy

The first requirement was to see if the CQNS, when applied to a simulated square Rydberg array, would converge to a ground state energy. It was already assured that the method would converge[1];

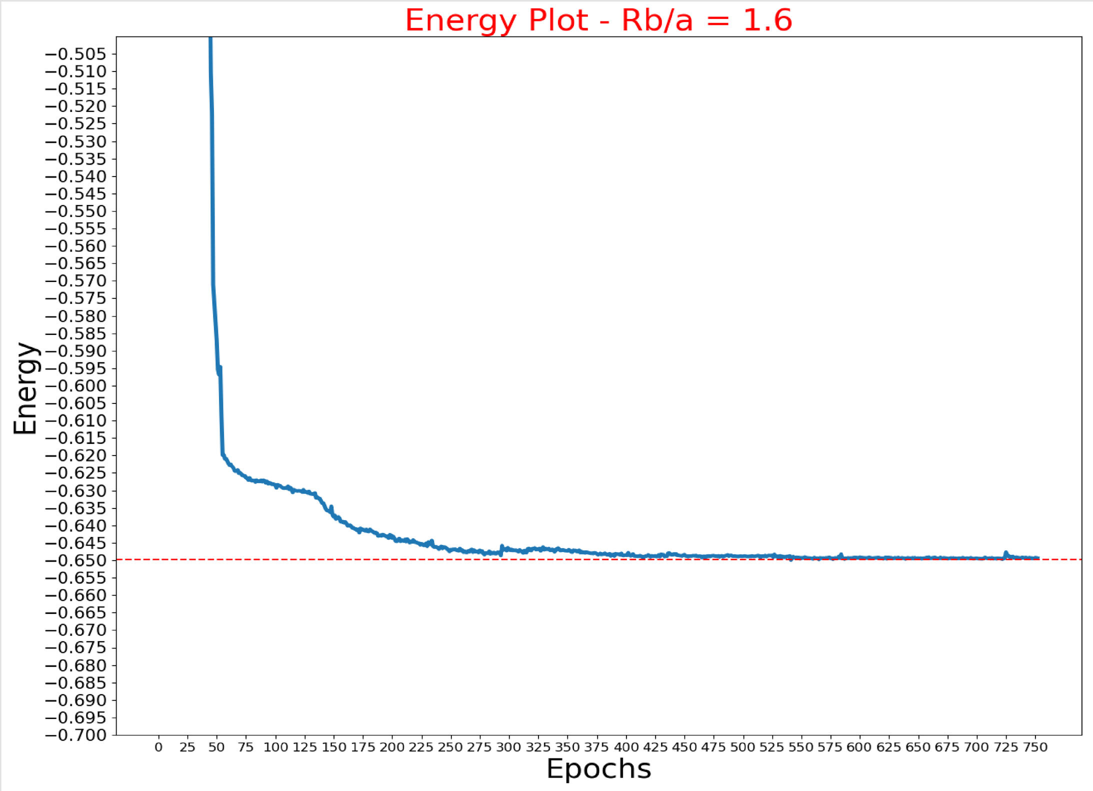


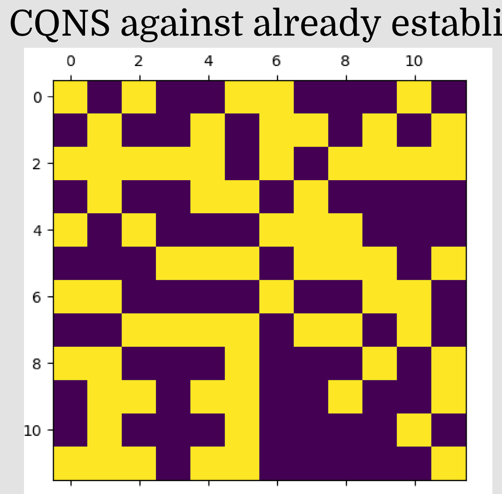
Fig 3: Convergence of CQNS on 12 X 12 lattice with R_b = 1.6

The results showed that the ground state energy converges at approximately y = - 0.6498.

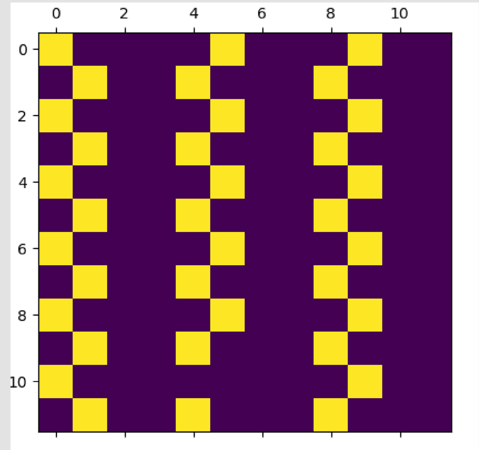
Lattice Ground State Phase

The next step was to observe the phases of the lattice at ground state. This was integral because it would prove the effectiveness of CQNS against already established results[2].

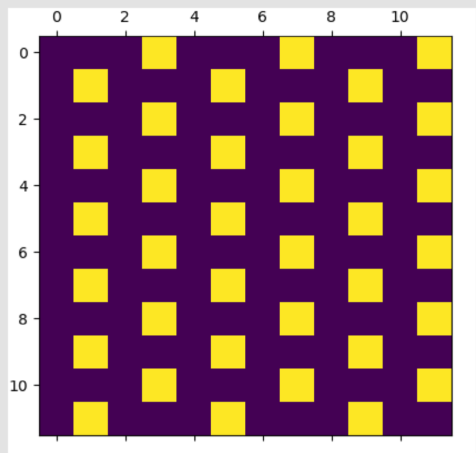
'Atom' in Rydberg state
'Atom' in ground state



Epoch 0: Random starting lattice constructed inside program to begin optimization



Epoch 18: Some patterning is seen in the lattices sampled by CQNS as it minimizes the energy



Epoch 627: As energy converges ground state phase appears in agreement with established results[2]

Further Research

Square Lattice – Comparisons of the ground state phases and energies within a square lattice with different values for the aforementioned variables would further cement the fidelity of CQNS.

Triangular Lattice – The triangular lattice is a more frustrated system with experimental data that CQNS can replicate. Further work is being done on this.

Kagome Lattice – the Kagome lattice has been linked with exotic behavior and new quantum materials; therefore, using CQNS to verify and build on the numerical data available is of interest.

Higher Dimensional Lattices – It has already been established that if CQNS can be applied to a 1D system it can be applied to a 2D system. Thus, it can be applied to higher dimensional system. No hard experimental or numerical data has been found on this topic which makes it an area of interest.

References

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