Rydberg Simulation to Quantum Scars

Avikar Periwal
Department of Physics, Stanford University, Stanford, CA 94305
(Dated: December 22, 2020)

Submitted as coursework for PH470, Stanford University, Spring 2020

Simulation of quantum systems with quantum mechanical objects has been a goal of physicists since Feynman. Quantum mechanical systems are inherently intractable in classical systems. A coherently controlled quantum simulator should then give us to insight into quantum mechanics by making measurements that we cannot easily compute. In this paper I will describe an experiment using neutral atoms to simulate a Hamiltonian, and show how a surprising lack of ergodic behavior motivated new interpretations of quantum mechanical theory.

I. INTRODUCTION

Simulations of quantum systems are difficult on classical systems. In a quantum lattice model, adding additional lattice sites increases the system size exponentially, rather than polynomially for a classical system. There are a variety of clever methods to simulate quantum systems on a classical computer, but they necessarily must make some assumption to decrease the effective size of the Hilbert space.

However, with enough control, it is possible to directly build quantum mechanical systems that can lead to new discoveries. Neutral atoms provide a pathway to generating large-scale tunable simulators. There are a variety of trapping techniques, and lasers can be tightly focused down to engineer a wide variety of interactions between different atoms.

The quantum simulator used energy levels of neutral atoms as their spin states. With clever trapping techniques, they were able to create a 1D array of spins, and study systems with short ranged interactions. In a quench experiment, with the initial state prepared as a low-energy state of one Hamiltonian, the group saw non-thermalizing dynamics, despite the system not having disorder, or obvious symmetries. This lead to a revival in the theory of scars[2], originally proposed in the 1980s, as an explanation for these non-thermalizing dynamics. Furthermore, while there are a variety of systems that do not thermalize, such as many-body localizing systems, or integrable Hamiltonians, it is not clear to what degree systems can be non-thermal. In this paper I will present experimental work from the Lukin group at Harvard on building a quantum system, and discuss how their results using a quantum simulator led to new insights in the form of quantum scars, which are only weakly non-thermal.

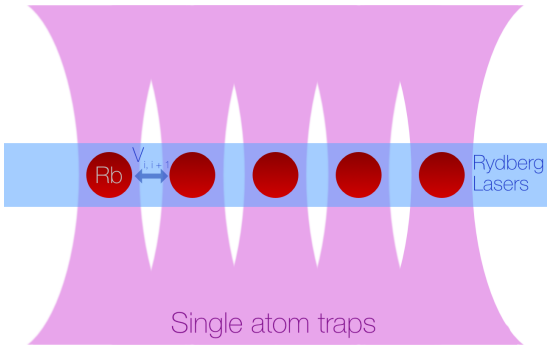

FIG. 1: Experimental apparatus schematic.

II. EXPERIMENT

In this experiment, the Harvard group begin with ^{87}Rb atoms in a magneto-optical trap, that are then loaded into optical tweezers[1]. Each tweezer has a waist of roughly 1 μm, and this small waist causes pairs of atoms to interact and form molecules. Molecules will no longer be trapped in the optical tweezers, and this leads to single atoms trapped in each tweezer, if the initial number of atoms was odd. Thus, after loading the atoms into the tweezers, each tweezer will have $\sim 1/2$ chance of having a single atom. By rearranging the traps with atoms, the Harvard group can reliably load single arrays of 51 atoms.

Ordinarily, neutral atoms do not have strong enough interactions to observe any dynamics on the time scale of trapping. However, if the atoms are placed in a state with very large principal quantum number n, then the larger size of the atom can be used to induce interactions between the atoms. These large n states are called Rydberg states and the interaction energy scales as $\sim n^{11}/r^6$.

The individual atoms are excited into the Rydberg state using a pair of focused lasers that couples to each atom equally, schematic shown in fig. 1. Each atom can

then be in either the ground state g, or the Rydberg state r. The driving laser has a coupling to each atom, Ω, and some detuning Δ from the actual transition. The coupling Ω switches the atom from g to r, while the detuning adds an effective energy cost for being in the Rydberg state. In addition, two atoms that are simultaneously excited into the Rydberg state will have an interaction. This leads to the Hamiltonian

$$H = \sum_i (\Omega(gr + rg)_i - \Delta n_i) + \sum_{i,j} V_{ij} n_i n_j, \quad (1)$$

where $n_i = r_i r_i$. We can identify $(gr + rg)_i = \sigma_i^x$.

V_{ij} scales with the spacing between individual tweezers. If the spacing is small enough, then $V_{i,j} > \Omega$ eventually. This is the so-called Rydberg blockade, and physically it means that an atom excited to the Rydberg state prevents neighboring atoms from being simultaneously in the Rydberg state. As interaction strength increases, the spacing between nearest excited atoms must increase.

The phases of the system can be probed via an adiabatic sweep. Using optical pumping, all atoms can be prepared initially in g. If $\Delta < 0$, then the ground state of this Hamiltonian remains in the state where all atoms are in g. Slowly sweeping the detuning of the laser field from negative to positive should transfer from the ground state to a Z_n ordered state. The Z_n ordered state is characterised by individual atoms appearing at the excited spacings every n atoms. The Z_3 state for example is a chain of $rggrggrgg\cdots$. The exact value of n is determined by the scaling of V_{ij} vs. Ω, and so by adjusting the spacing between tweezers different Z_k states can be realized.

The experiment then moves on to measure quench dynamics. From an initial Z_2 state ($rgrg\cdots/grgr\cdots$), prepared using the adiabatic sweep, the detuning Δ is suddenly set to 0, by suddenly changing the frequency of the Rydberg lasers to be on resonance. This results in a series of oscillations in the state, going from $rgrgrgrgr$ to $grgrgrgrg$ and back again. These oscillations are relatively long-lived, showing more than 6π of oscillation. Note that if $\Delta = 0$, the two decay timescales go as $1/\Omega$ and $1/V_{i-1,i}$. However, the oscillations are much longer lived than either of these timescales. In addition, the oscillation frequency is not the same as for a set of non-interacting atoms.

These dynamics can be seen directly for 9 spins. However, for larger system sizes, preparing a perfect Z_2 state is tricky. The adiabatic sweep might not be fully adiabatic, and in general there are detection and preparation errors that will scale geometrically in system size. In larger ensembles, defects in the preparation of the Z_2 state result in an average bulk without features. Random domain walls wash out the order observed in each state. However, as the small 9 qubit system oscillates between the two ordered states, there is a period of minimal order. This can be characterized by a large density of domain walls in any individual shot at a time in between the the two ordered extremes. Looking at the density of the domain walls as a function of time then shows the oscillations between the states, and can be used to characterize larger spin systems.

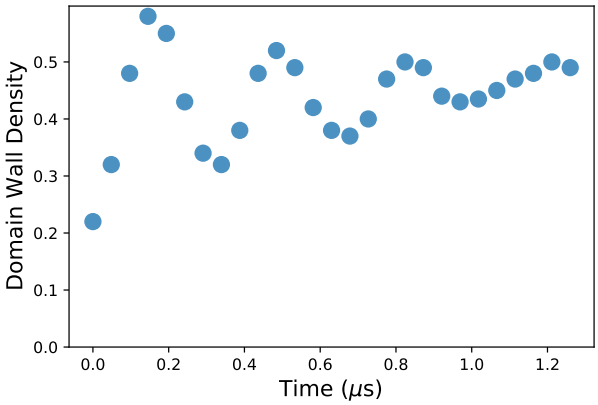

FIG. 2: Domain wall density for a 51 spin system shows the same 6π of oscillation seen in the 9 spin system. Redrawn from experimental results presented in fig. 6b. Source: A. Periwal

The modulation in domain wall density for a 51 spin system is shown in fig. 2, and has the same frequency as the 9 spin system.

This Hamiltonian seems to have no conserved quantities beyond the total energy, so these long-lived oscillations provide an exciting puzzle.

III. QUANTUM SCARS

In classical chaos, there exist periodic orbits even in classical systems. For example, a billiards ball bouncing around a table can have a stable orbit, if the initial conditions are correctly chosen. Indeed, there may be an infinite number of such orbits, but the total measure in phase space will be 0[2]. In the early 1980s, scientists began expanding this idea to quantum mechanics, notably Steven McDonald, Allan Kaufman, and Eric Heller[2,6]. These stable trajectories were termed "scars". Heller in particular showed that for a single particle there is a large overlap between these periodic orbits and some wave functions of the single particle.

The experiment described, however, involves a many body phenomena, but the idea put forward nearly 40 years ago provides valuable insights into understanding the experimental results. The theory results described here were published by Turner et. al. in 2018, but there have been a variety of different papers investigating scarred states and the PXP model.

Note that $n_i = (1 + \sigma_i^z)/2$. Working in the limit where $V = V_{i,i+1} > \Omega$ yields

$$H = \sum_i n_i n_{i+1} + \Omega/2V \sum_i \sigma_i^x. \quad (2)$$

The Rydberg blockade restricts the Hilbert space to remove nearest neighbor simultaneous excitations, and so defining the projection operator $P_i = gg$, the original Hamiltonian after the quench is expressed as the PXP model.

$$H = \sum_i P_{i-1}\sigma_i^x P_{i+1} \tag{3}$$

While individual defects were common in the preparation of the Z_2 state, in the theoretical analysis, the Rydberg blockade was kept as a hard constraint. The dimension of the Hilbert space, rather than being 2^L, becomes limited, since states with adjacent Rydberg excitations are never allowed. Adding an additional spin to a chain with open boundary conditions increases the dimension of the Hilbert space by the dimension of the Hilbert space with one fewer atom. Since the one atom case has a dimension of 2, this means that $D(L) = F_{L+2}$, where F denotes the Fibonacci sequence.

It is important to note that the PXP model has an inversion symmetry. In the experimental case, any inhomogeneity in the Rydberg beam will break these symmetries, but when doing numerics, these must be addressed.

As a preliminary check, the level spacing statistics of the PXP model are computed, and these are clearly non-Poissonian for a variety of system sizes, and so the Hamiltonian does not seem integrable.

Just as the experiment started from a Z_2 charge density wave, in these initial calculations, the Turner group starts with some initial Z_k density wave states, as well as a $g\cdots g$ state. The midpoint partition entanglement entropy for 4 distinct k values was calculated at different times. All the different initial states show different growth rates of entanglement entropy. Most interestingly, the entanglement entropy showed oscillations at the same frequency found in the experiment. The same frequency oscillations are additionally found in nearest neighbor correlation functions. However, this should perhaps not be so surprising. After all, simulating the Hamiltonian in question better lead to dynamics that line up with the experimental results.

This is consistent with the analysis done by the experimental team. They noted that the Z_2 state did not reach thermal equilibrium after a quench, while other states, like the $g\cdots g$ state, quickly reached the thermal value. This is sketched in fig. 3. While the two states have the same energy density, the Z_2 initial state, which is an infinite temperature state, shows non-vanishing oscillations around a non-thermal value. Since the initial state is what is driving the oscillations in the system, the next step in analysis is to look at how the initial state of the system interacts and compares with the PXP Hamiltonian.

The next calculation lead to the real insight in understanding the dynamics of the Rydberg simulator. The key idea seen is that any non-ergodic behavior is dependent on the initial state of the system, rather than just on the Hamiltonian. It then makes sense to look at the

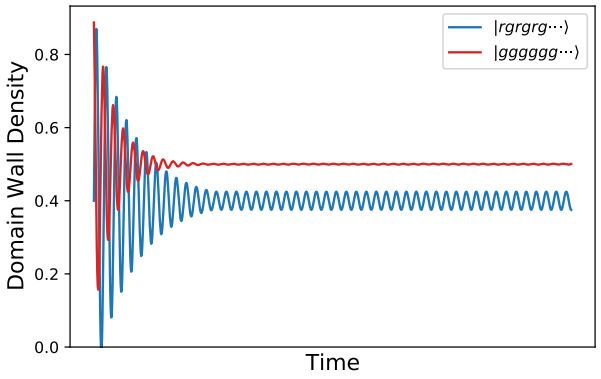

FIG. 3: A sketch of domain wall density as a function of time, based on fig. S10 from[1]. Blue curves show time evolution of the Z_2 state, while red curves show time evolution of the $g\cdots g$ state. The Z_2 state has long lived oscillations, especially in the constrained Hamiltonian. The state beginning with no Rydberg excitations quickly reaches the thermal expectation, and does not show the same oscillations.

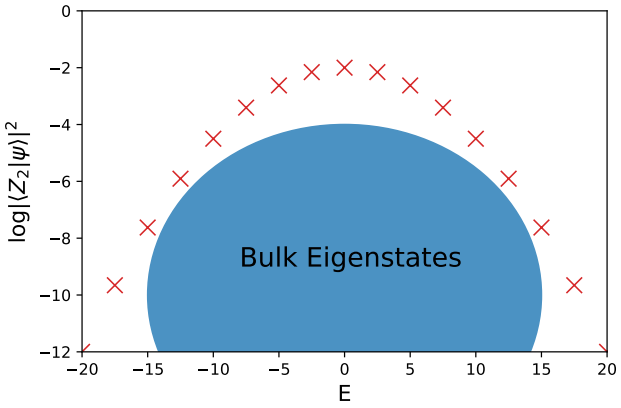

FIG. 4: Eigenstates plotted with respect to energy and overlap with Z_2 state. Red crosses show scarred states, which have strong overlap with the forward scattering approximation states. Figure adapted from fig. 3a from[7]. Soure: A. Periwal.

overlap between the Z_2 state and the eigenstates of the Hamiltonian. This is shown schematically in fig. 4. There is an obvious group of eigenstates that have an abnormally large overlap with the Z_2 state at a fixed, specific, energy. The energy spacing between these states is the same as the oscillation frequency observed in the dynamics, up to a factor of 2 for since the 0 qubit can have two possible states.

It is possible to characterize these states using a method called the "forward scattering approximation". To begin, the Hamming distance between two strings a and b is the number of characters in a that must be changed to turn a into b. Now, our Hamiltonian can be

decomposed. Earlier we noted that $\sigma_x = gr + rg$, and so we can decompose $H = H^+ + H^-$, with

$$H^+ = \sum_{i \text{ even}} P_{i-1} r_i g_i P_{i+1} + \sum_{i \text{ odd}} P_{i-1} g_i r_i P_{i+1}.$$

$H^+ Z_2$ gives a superposition of every state with a single spin flip, while H^- annihilates Z_2. Induction and a little more algebra extends this to say that H^+ increases the Hamming distance from the Z_2 state by 1, and H^- decreases the Hamming distance. These creation/annihilation operators define a ladder of states $n \propto H^n Z_2$. This ladder structure lets us write a Hamiltonian in this forward scattering basis which has only elements that are one off the main diagonal.

Since n has Hamming distance n from Z_2, this Hamiltonian naturally has only n eigenstates. Plotting the overlap of these n eigenstates with the Z_2 state yields the same band of abnormal overlap states. This is somewhat intuitive. We are looking at states that are derived by applying some operator repeatedly to the Z_2 state, so these states should not be too far away from Z_2. However, in a general thermal state, a small basis of order L states would not be able to approximate a generic eigenstate in a thermalizing Hamiltonian.

These special many-body eigenstates are scars, localized in on specific region of the Hamiltonian. Initializing a state in this basis, as done via the adiabatic sweep into the Z_2 state yields an initial state that stays within this localized region and exhibits non-thermalizing dynamics, even when the system is globally thermalizing. This is a new theory of ergodicity-breaking, that is distinct from localization or symmetry.

As the name suggests, the forward scattering approximations is not exact. It is not understood where these states come from in the full model, or when scars can be observed.

The Turner group demonstrates some amount of robustness to deviations in the Hamiltonian. Small perturbations of the Hamiltonian show some of the same oscillations. However, even small changes to the Hamiltonian show a dramatically faster timescale to thermalizaiton.

IV. OUTLOOK

The experimental and theory results explained here have lead to a variety of other work on the PXP model. For example, some recent work suggests that a deformation of the PXP model moves it closer to integrability, and the PXP Hamiltonian is close to an integrable point for some unknown parent Hamiltonian[4]. Further work has shown that some eigenstates of the PXP Hamiltonian at infinite temperature violate ETH, and that these states with some manipulations have strong overlap with the Z_2 state[5].

Without doubt, there is more to study in quantum scars, and other groups are finding evidence for the phenomenon in experimental systems[3]. These advances can hopefully continue to help our theoretical understanding of quantum many-body dynamics.

[1] Hannes Bernien, Sylvain Schwartz, Alexander Keesling, Harry Levine, Ahmed Omran, Hannes Pichler, Soonwon Choi, Alexander S Zibrov, Manuel Endres, Markus Greiner, et al. Probing many-body dynamics on a 51-atom quantum simulator. *Nature*, 551(7682):579–584, 2017.

[2] Eric J Heller. Bound-state eigenfunctions of classically chaotic hamiltonian systems: scars of periodic orbits. *Physical Review Letters*, 53(16):1515, 1984.

[3] Wil Kao, Kuan-Yu Li, Kuan-Yu Lin, Sarang Gopalakrishnan, and Benjamin L. Lev. Creating quantum many-body scars through topological pumping of a 1d dipolar gas, 2020.

[4] Vedika Khemani, Chris R Laumann, and Anushya Chandran. Signatures of integrability in the dynamics of rydberg-blockaded chains. *Physical Review B*, 99(16):161101, 2019.

[5] Cheng-Ju Lin and Olexei I Motrunich. Exact quantum many-body scar states in the rydberg-blockaded atom chain. *Physical review letters*, 122(17):173401, 2019.

[6] Steven W McDonald and Allan N Kaufman. Spectrum and eigenfunctions for a hamiltonian with stochastic trajectories. *Physical Review Letters*, 42(18):1189, 1979.

[7] Christopher J Turner, Alexios A Michailidis, Dmitry A Abanin, Maksym Serbyn, and Zlatko Papić. Weak ergodicity breaking from quantum many-body scars. *Nature Physics*, 14(7):745–749, 2018.