Information in the Quantum XY Spin Chain

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The quantum XY spin chain is a one-dimensional statistical mechanics model used to understand the behavior of materials through their microscopic quantum spins and their interactions with their nearest neighbors. This spin chain and related models exhibit uniquely quantum behavior in the low-temperature limit, particularly quantum phase transitions. In this project, the XY spin chain ground state is found using density matrix renormalization group methods, and information quantities relating to spin measurements can be measured. These methods can be extended to other quantum models, expanding upon results on information content and signatures of phase transitions in classical spin chains.

INTRODUCTION

Spin systems are useful in statistical mechanics for studying emergent behavior of systems composed of a large number of particles. Each such model consists of either classical or quantum 'spins', whose state can be determined by discrete (up and down) or continuous (angle from z-axis) parameters. They can vary in dimension, lattice structure, and interaction between particles. Nearest neighbor interactions are both computationally simple and exhibit interesting behavior, so they are common in spin models. One of the earliest spin models to be studied was the nearest-neighbor Ising model, which exhibits a phase transition between a ferromagnetic and a disordered phase in 2 and 3 dimensions. Generally spin models correspond to many physical systems, from simple ferromagnets to quantum spin liquids and other exotic states of matter [1].

Classical spin systems have been studied through the lens of information theory by treating states of the spin chain as strings of data and then finding thermodynamic entropies and correlations between spins along the chain [2]. In this analysis the entropy decomposition for the 1D Ising Model exhibits signatures of phase transitions, particularly in the peak of the bound information (corresponding to spatial correlations in the spin chain), which can clearly be seen in Figure 1. This analysis can also be used for a given classical spin chain to create causal state models (which can be either classical or quantum in nature) that reproduce the desired statistics of the spin chain [3].

The goal of this project is to extend the work done on information theoretic properties of classical spin systems (particularly the 1D Ising model) to quantum spin systems. This introduces a number of challenges not present in the case of classical spin systems relating to simulation and measurement. The first is that for a given state of the quantum spin chain, individual spins are not in a definite states (up or down) due to non-classical correlations. In the case of classical spin chains, each site can be updated individually until equilibrium is reached. However, this local operation is not allowed for quantum spin chains, and instead we must treat the state of the chain as a whole during simulation. Therefore we must use density matrix renormalization group (DMRG) methods, which are designed to work in the limit of zero temperature to find a ground state of the system. Further detail is given in the main body of this report, and efforts at measuring spin-spin correlations are described.

BACKGROUND

Classical Spin Chains

Classical spin systems such as the Ising Model and the XY Model are useful for studying magnetism and other material properties. In 1D these systems are referred to as spin chains. The Ising spin chain has been the subject of considerable interest, and its Hamiltonian is

$$H = J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{1}$$

where J is the interaction strength, the first sum is over nearest neighbors and represents the spin-spin interaction, h is the transverse field strength, and $\sigma = -1, +1$.

The classical XY model is also relevant and can be thought of as representing spins in a plane with a continuous angular degree of freedom. Its Hamiltonian is

$$H = J \sum_{<i,j>} \mathbf{s}_i \cdot \mathbf{s}_j - \sum_i \mathbf{h} \cdot \mathbf{s}_i = J \sum_{<i,j>} \cos(\theta_i - \theta_j) - h \sum_i \cos\theta_i \tag{2}$$

where θ_i represents the orientation of spin i with respect to the external field.

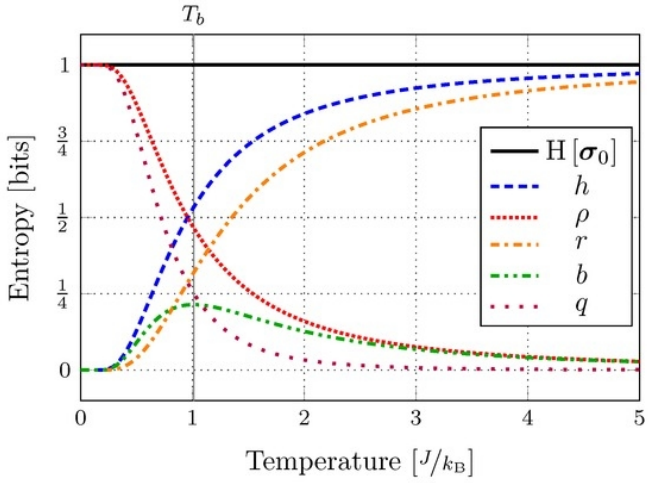

FIG. 1: The Entropy Decomposition for the 1D, nearest-neighbor, ferromagnetic spin-1/2 Ising model, from [2]

Information Quantities for Classical Spin Chains

Classical spin chains lend themselves naturally towards a computational mechanics interpretation. Spin configurations can be viewed as processes consisting of up spins (1) and down spins (0). The string of bits obtained by reading spin measurements left to right from a spin chain is a particular instance of the process, and the distribution over all these possible configurations is dependent on temperature. The form of this dependence is the Boltzmann distribution,

$$P(X_{-\infty:\infty}) \propto e^{\frac{-H}{k_B T}} \tag{3}$$

where $X_{-\infty:\infty}$ is the spin chain configuration, H is the Hamiltonian for the spin chain, and k_B is Boltzmann's constant. At low temperature the configuration is predictable since spins will almost always align. At high temperature the spin orientations are nearly random, since thermal effects outweigh the nearest-neighbor interactions. At intermediate temperatures the configurations are structured and contain local, spatial correlations. This is represented by the peak in the bound entropy in Figure 1 for the Ising spin chain.

The states of classical spin chains with nearest-neighbor interactions can also be represented by ϵ-machines, which consist of a set of causal states and transitions between them with certain probabilities. The ϵ-machine for the Ising spin chain is shown in Figure 2 where the transition probabilities, $(T_{00}, T_{01}, T_{10}, T_{11})$, are determined by the interaction strength and temperature. The two causal states correspond to the measurement most recently seen along the chain (either up or down).

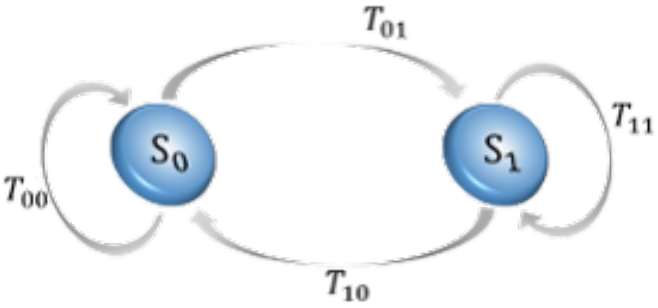

FIG. 2: The ϵ-machine for nearest-neighbor Ising spin chain, from [3]

Quantum Spin Chains

Quantum spin chains (in contrast with their classical counterparts) can only be described using quantum statistical mechanics. The state of the chain can be a complicated linear superposition of different states of the individual spins, and local spin measurements on a given state have probabilistic rather than deterministic outcomes. The states of the spin-1/2 chain exist in a Hilbert space of dimension 2^L where L is the length of the spin chain. Many different basis vectors of this Hilbert space can contribute to a given state of the chain.

Quantum Phase Transitions

Simulations of quantum systems are most successful when targeting the ground state of the system. As a result, studies of quantum spin chains cannot show signatures of phase transitions in the entropy decomposition when temperature is changed, as classical spin chains do. Luckily there is another class of phase transitions (called quantum phase transitions) which occur at zero temperature when some other parameter is varied, such as interaction strength, pressure, magnetic field strength or concentration of a dopant in a material [**?**]. Quantum ground states are generically non-trivial and exhibit interesting behavior due to non-classical spatial correlations, but the specific properties of the ground state vary with position in the phase space. One specific example of a quantum phase transition in the Transverse XY Model between a Mott Insulator phase and and superfluid phase is detailed below.

DYNAMICAL SYSTEM: THE QUANTUM XY MODEL

The system being simulated here is the spin-1/2 quantum XY spin chain with nearest-neighbor interactions. It is a simplification of the Heisenberg Model,

which has spin components oriented in 3D. The Heisenberg Hamiltonian is

$$H = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j = J \sum_{<i,j>} S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \quad (4)$$

where the sum is taken over nearest neighbors. The dot product of the neighboring spins represents the interaction between them. For $J < 0$, the model is ferromagnetic, and energy is minimized when the spins are aligned. For $J > 0$, the model is antiferromagnetic, and energy is minimized when spins are pointing in opposite directions. By constraining the spins to exist in only two dimensions we get the XY model, which has the Hamiltonian

$$H = J \sum_{<i,j>} S_i^x S_j^x + S_i^y S_j^y = \frac{J}{2} \sum_{<i,j>} S_i^+ S_j^+ + S_i^- S_j^- \quad (5)$$

where J^+ and J^- are the raising and lowering operators associated with the spins, and the second expression is obtained by performing a Jordan-Wigner transformation on the first expression [4].

The XY Model with Transverse field is also of interest because it is a slight variation on the above Hamiltonian that exhibits a quantum phase transition between a Mott Insulator Phase and a superfluid phase at T=0 [5]. Its Hamiltonian is

$$H = J \sum_{<i,j>} S_i^x S_j^x + S_i^y S_j^y - K \sum_i S_i^z \quad (6)$$

where K is the strength of the field oriented in the z-direction. This phase transition occurs at a critical is shown in Figure **??**. The Mott Insulator phase is an ordered phase where the individual spins are essentially localized, whereas the superfluid phase exhibits long-range order, and this distinction is expected to be reflected in information quantities for the ground states at various field strengths.

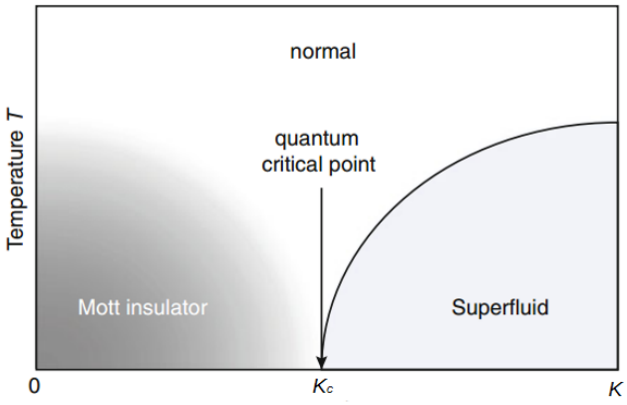

FIG. 3: Phase Diagram for the XY Model in a Transverse Field showing the quantum phase transition from a Mott Insulator to a superfluid, modified from [**?**]

METHODS

Density Matrix Renormalization Group

For classical spin chains sites can be updated individually, which means the computational cost scales with L. In contrast, simulating quantum spin chains requires updated the entire Hilbert space, so computation costs scale exponentially as 2^L. In order to find states of a quantum systems with a small Hilbert space, the traditional approach is to exactly diagonalize the Hamiltonian and observe the energy spectrum. However, for a spin chain of even moderate length the exponential growth of the Hilbert space makes this difficult. A group of computational techniques known as density matrix renormalization group (DMRG) methods can be successful when the computational cost becomes too great for exact diagonalization [6]. One drawback is that these methods are designed to find the ground states for quantum Hamiltonians rather than arbitrary, finite-temperature states. In classical systems T=0 states are often trivial, but quantum ground states exhibit a wider variety of interesting behavior, including quantum phase transitions.

DMRG methods truncate the size of the Hilbert space by ignoring the basis states which contribute little to the ground state. In general, DMRG algorithms start with a single spin and add neighboring spins until the Hilbert space grows above a maximum size that is set in advance (m). When adding a spin grows the Hilbert space to a size greater than m, the Hilbert space is truncated by diagonalizing the existing block of spins. The basis of the block is changed to the eigenbasis, and only the m greatest eigenvectors are retained. This procedure is repeated each time a spin is added to the chain until the desired system size is reached. For this project, the python code 'simple-dmrg' was modified to represent the quantum XY Hamiltonian.

Quantum Spin Measurements

One complication of using DMRG methods is that the basis in which the ground state is represented is changed at every step of the algorithm. Thus the final state of the system cannot be easily interpreted in terms of individual spin states. The energy of the system can easily be extracted from the final state with arbitrary basis states, but measuring any other observable of interest requires extra effort. The operators corresponding to spin measurements must be rotated into the new basis

each time the Hilbert space is truncated. Their transformation follows the equation

$$(S_i^z)_j = O_j((S_i^z)_{j-1} \otimes I_d)O_j^\dagger \tag{7}$$

where $(S_i^z)_{j-1}$ is the operator for the spin in the z-direction of site i measured in terms of the previous basis states, O_j is the matrix rotating into the new basis, and I_d is the identity matrix of dimension d, which is required so $(S_i^z)_j$ has the right dimension in the new basis. This operator is then truncated along with the state of the chain so that only the first m eigenvalues/eigenvectors are relevant.

Information Quantities for Quantum Spin Chains

By applying transformed spin operators to the each spin in the ground state of the XY spin chain from the DMRG algorithm, spin chain orientations that are equivalent to classical states can be obtained. Then computational mechanics techniques can be applied to these states to characterize the structure and information theoretic properties of the spin chain. However this approach of using local spin operators to measure individual spins and characterize the simpler, classical configurations is expected to destroy the entanglement between sites [7]. Some of this entanglement would be transferred into classical correlations, and the rest probably cannot be characterized by classical information measures. In that case, computational mechanics would not be able to capture the full behavior of the system, and its information content cannot be represented by an ϵ-machine or q-machine. This opens the door for the intriguing possibility of a more general quantum model which would be able to fully reproduce the information theoretic quantities of quantum spin chains.

RESULTS

In this project, the quantum XY spin chain has been successfully simulated so far and energy measurements have been fully made. These are shown in Figure 3. As the length of the spin chain is increased, the energy per site approaches the ground state energy, which is exactly known to be $\frac{-1}{\pi}$ [8]. The ground state energy for other quantum Hamiltonians is easy with existing code as well, including the XY Model with transverse field. Spin measurements are now possible by modifying the 'simple-dmrg' code to update spin operators at each step. At multiple points in this project, the focus has shifted because the initial approach was flawed. Additional complications such as the measurement of spin operators took more time than anticipated to complete, so a full analysis of classical spin configurations from sequentially measuring spins along the final spin chain state was not possible.

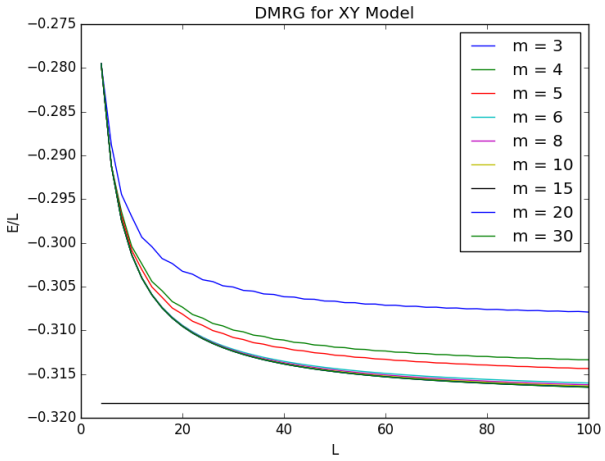

FIG. 4: The ground state energy from dmrg methods for the quantum XY spin chain for different spin chain lengths (L) and dmrg Hilbert space sizes(m), compared to the exact value (black line)

This is a focus of work in the near future and should be attainable. Another important qualification is that, since dmrg methods are designed for finding ground states, observing a phase transition in which temperature acted as a control parameter (as in the classical case) would not be possible. This required a shift towards quantum phase transitions with other control parameters, particularly the XY Model in a transverse field, in which field strength is the relevant parameter.

CONCLUSION

This aim and scope of this project has shifted repeatedly since it began. It became clear that some steps that are simple in the case of classical spin chains are non-trivial for quantum ones. In particular, the process of taking spin measurements using DMRG methods and the possibility of seeing quantum phase transitions at T = 0 were not anticipated. The quantum XY spin chain is still worth studying despite these extra challenges. With DMRG methods, we have successfully found ground states for the XY model and have the capacity to do so for various other quantum Hamiltonians. Measurement of individual spins (and other observables) is now possible for these spin chains. Furthermore a natural testing ground for these information properties presents itself in the form of quantum phase transitions, which require only slight modifications to our existing work.

There is much future work to do on this project. The most obvious extension of this work should be generating large batches of spin measurement data. With this the analysis done for classical spin chains can be recreated for

the quantum XY spin chain at T=0. It is possible that this will simply recreate the behavior of the classical XY spin chain because the quantum nature of the spin chain (i.e. the non-classical correlations between spins) will not be apparent in these classical information measures. In that case, intrinsically quantum information measures, such as bipartite entanglement between two regions of the chain, may capture the interesting behavior instead.

The ultimate goal of this research project, which should be obtainable with more time, is capturing quantum phase transitions through information quantities (either classical or quantum). This can be definitively answered using the XY-model with transverse field, which has a phase transition at T=0 for a certain field strength. Such a result would prove that uniquely quantum behavior is captured in these information quantities. Finally this work could lead to ϵ-machine and q-machine representations of quantum spin chains. It is also possible that there is no simple analogy to representations by either of those model classes. In a particular state of the chain, every spin can be entangled with every other spin, which suggests that a model of this chain might have to output quantum states upon measurement rather than classical bits. In that case the spin chain results could point to a more general generator/predictor for purely quantum systems.

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