Simulation of a quantum phase transition in one dimension

Adele Jackson, Australia, Jacob Laxer, Canada,
Mentor: Ori Alberton, PI: Prof. Ehud Altman
Department of Condensed Matter Physics

A phase transition is an abrupt qualitative change in the properties of a system when some external parameter is smoothly varied. Simulating a chain of particles with correlated spins under a magnetic field perpendicular to the orientation of the spins gives a phase transition when quantum effects are considered. Although there are an exponential number of possible states of the system, matrix decomposition was used to efficiently iteratively approximate the ground state of the system. Using this algorithm, a phase transition is demonstrated with a critical value when the strength of the magnetic field is equal to the force of correlation. As well as providing a simple example of a quantum phase transition, this system demonstrates entanglement between spins. Due to this, the algorithm used to study the spins can be applied to efficiently simulate the behaviour of a quantum system with a low degree of entanglement.

I. INTRODUCTION

Phase transitions are abrupt qualitative changes in the macroscopic properties of a system caused by smoothly changing some external parameter. They occur at some critical value of the parameter. Phase transitions are generally a product of the interaction of many particles, and cannot be predicted from the behaviour of one or two particles. One example would be water, where smoothly decreasing temperature from above to below the freezing point causes a qualitative change in the behaviour of the water as it freezes. Examples of phase transitions involving quantum mechanical effects are superconductors, where the electrons become aligned at temperatures below some critical temperature T_c, causing current to be passed through the material without any resistance.

We investigated a phase transition occurring in a one dimensional chain of sites, each with an associated spin, described by the Ising model in a transverse field. The spin of a particle is an intrinsic angular momentum, and is described in terms of orientation: for the particles in the Ising model, the possibilities are up or down, represented by $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. In this model, neighbouring spins are coupled in such a way that they prefer to be aligned parallel to each other, in the z direction. Additionally, there is a magnetic field of strength h in the x direction.

In this model, the energy of some configuration of spins is given by

$$E = -\sum \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x$$

where h is the strength of the magnetic field, i is the site number and σ_i^z is the spin at site i in the z direction (and similarly for σ_i^x). At zero temperature, the system prefers a state with minimal energy. When $h = 0$, the energy is minimised by having the spin at a site the same as that of its neighbour, so the spins are either all $|\uparrow\rangle$ or all $|\downarrow\rangle$. [1]

Due to quantum mechanical effects, a possible state of a spin is also it being in some superposition of up and down. A spin in the state $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$ has a probability proportional to $|\alpha|^2$ of being observed to have spin up, and proportional to $|\beta|^2$ of being observed to have spin down. Similarly, the system as a whole has a state that is a superposition of all its possible states. For example, a system can be in a state such that there are equal probabilities of all spins being measured as spin up, or all spins being measured as spin down, but no chance of a mixture of up and down. For two sites this would mean this system is in the state $\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$. [2]

To calculate the energy of some given combination of spins, we represent the spin $\alpha|\uparrow\rangle + \beta|\downarrow\rangle$ by the vector $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$, and measure the observed spin in some direction by applying the Paüli matrix operators:

$$\sigma^z_{\alpha|\uparrow\rangle+\beta|\downarrow\rangle} = \begin{pmatrix}\alpha & \beta\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

$$\sigma^x_{\alpha|\uparrow\rangle+\beta|\downarrow\rangle} = \begin{pmatrix}\alpha & \beta\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

We represent the state of the system in the basis of all possible combinations of the spins of the sites. For example, for two spins, a state of the system would be

$$\alpha_1|\uparrow\uparrow\rangle + \alpha_2|\uparrow\downarrow\rangle + \alpha_3|\downarrow\uparrow\rangle + \alpha_4|\downarrow\downarrow\rangle$$

This is expressed as the vector

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix}$$

For each value of h there is a Hamiltonian operator H, which is a matrix that, when applied to the vector representing the state of the system, gives the energy of the system. The ground state of the system is the normalised vector v with $Hv = \lambda_v v$ for some minimal constant λ_v, as λ_v is equal to the energy of the system.

As h becomes much larger than one, the ground state approaches $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ for all sites, meaning that there are no long-range correlations between sites, as the observed values appear completely random. However, at $h = 0$ there is perfect correlation between sites, as either all spins in the $|\uparrow\rangle$ state, and the other with all the spins in the $|\downarrow\rangle$ state. So there must be a qualitative change in the behaviour of the system at some point. [3]

The ground state of a system for some magnetic field strength h is the combination of states of the sites in the chain that has the lowest energy. In experimental conditions, a chain of spins would only be in this state when they are not excited – that is to say, at zero temperature. Thus, this system can only be accurately studied theoretically. We used numerical methods to analyse this system and look at the square of the average expectation value of the spins of the sites for a varying number of sites and strength of magnetic field. We expect to see a phase transition that is increasingly sharp with an increasing number of sites.

II. METHOD

To simulate a system of n sites, we first used exact diagonalization. To construct the Hamiltonian operator H to calculate the energy of a state in this basis (where I_i is the identity operator on site i), we have:

$$\begin{aligned} H &= \sum \sigma_i^z \sigma_{i+1}^z + \sum \sigma_i^x \\ &= \sigma_1^z \sigma_2^z I_3 \dots I_n + I_1 \sigma_2^z \sigma_3^z \dots I_n + \dots + I_1 \dots \sigma_{n-1}^z \sigma_n^z \\ &+ \sigma_1^x I_2 \dots I_n + I_1 \sigma_2^x \dots I_n + \dots + I_1 I_2 \dots \sigma_n^x \end{aligned}$$

Using this Hamiltonian, the energy of the state ψ is equal to $\langle\psi| H |\psi\rangle$. The ground state of the system is then the normalised eigenvector of the operator with the lowest eigenvalue. However, as there are 2^n possible combinations of states of sites, a state of the system requires 2^n numbers to express. For a system of even 300 sites, more numbers are needed to express the ground state than there are atoms in the universe.

To improve this time and memory requirement, note that interactions between spins are local. It will be reasonable to assume that, in the ground state, spins separated by a large distance will not be strongly entangled with one another, as the only direct interactions are between neighbouring sites. Because of this, we can express the ground state of the system using time and memory requirements that grow linearly with the number of sites and exponentially with the amount of entanglement. [4]

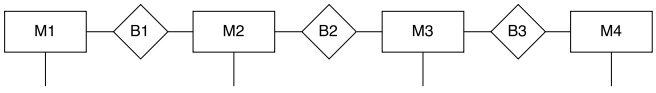

FIG. 1: Matrix product state for four sites

First we decomposed the state to a matrix product state (MPS), composed of n matrices $M_1, M_2, M_3, \dots M_n$ connected by $n-1$ bonds $B_1, B_2, B_3, \dots B_{n-1}$ (Figure 1). Each bond has two indices – to the matrices on either side of it – while each matrix bar the edge two has three: to the bonds on each side of it, and one external index, which is the index of the physical site.

Expressing the general state of the system as an MPS is done by repeatedly finding the singular value decomposition (SVD) of the matrix we needed to decompose. The singular value decomposition of a matrix M is the three matrices U, S and V such that $M = USV$ and S is a diagonal matrix. Doing calculations over the i^{th} bond is then equivalent to partitioning the sites at the i^{th} bond and operating on the two sets.

Truncating S to limit the number of entries (and then truncating U and V to discard the rows and columns the truncated matrix no longer needed) keeps its size from growing exponentially along the chain of matrices. Although spins across the chain can potentially all be entangled, causing the growth in time taken to compute the ground state

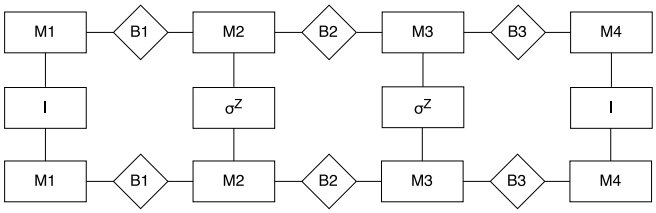

FIG. 2: MPS structure for the correlation between the second and third sites

to still be exponential, truncating the least significant correlations to keep only some fixed maximum number of them controls this.

To find the value of the product of some operators applied to this state, we contract the MPS with its conjugate transpose with the relevant operator for each site applied across that site. Figure 2 shows the structure that is contracted to find $\sigma_2^z\sigma_3^z$ for a four-site system. Figure 3 demonstrates the labels assigned to each of the indices as the individual matrices are multiplied together for applying σ^z to a four-site system. Continuing the process by multiplying the rest of the matrices onto the result would give the number that is the result of applying $I_1\sigma_2^z I_3 I_4$ to the state given in Figure 1.

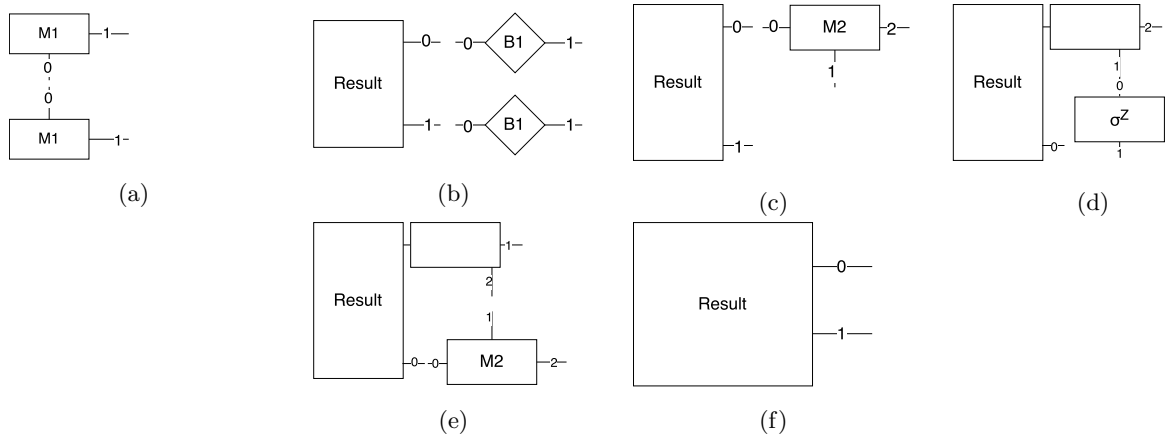

FIG. 3: The first six steps of finding the expected value of the spin in the z-direction of the second site using MPS

We can apply an operator across two sites i and $i+1$ by multiplying $B_{i-1}M_iB_iM_{i+1}B_{i+1}$ (where those exist), contracting this with the operator, and then separating this out again using SVD. Theory shows that taking some random initial state and, applying the operator O such that $\log O = \tau\left(\sigma_i^z\sigma_{i+1}^z + h\sigma_i^x I_{i+1}\right)$ for some small constant τ to each neighbouring pair of sites produces a better approximation to the ground state. The exponential of a matrix is calculated using Taylor polynomials. This is the basis of the Time Evolving Block Decimation algorithm (TEBD). [4]

TEBD consists of applying O to all the sites of the state for some t times. The result is a good approximation to the ground state, and is calculated in a time proportional to tm^2n (where t is the number of steps, m is the number of entries of S kept after truncation, and n is the number of sites). Taking a smaller τ improves the accuracy of the approximation, but only if t is also increased (as τ is comparable to a step size). We used values of $\tau = 0.5$ and $t = 500$.

After finding the ground state, contracting the matrix together with the σ^z operator across the i^{th} and j^{th} sites for each i and j and summing the results gives the expectation value of the square of the magnetisation $= \langle(\sum_i \sigma_i^z)^2\rangle$. Using this algorithm, we were able to find this for systems of up to 144 sites.

III. RESULTS

Using the exact diagonalization algorithm, we calculated the expected value of the average spin of each site for two, four, six and eight sites (Figure 4). As is seen in the figure, the expected average spin value drops faster with an increasing number of sites, as was theoretically predicted.

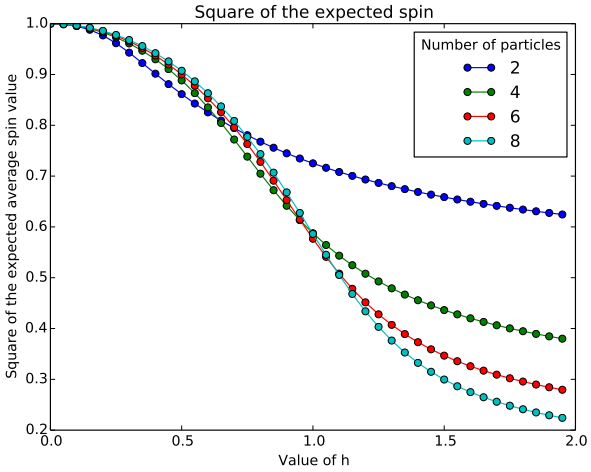

FIG. 4: Average spin value for two to eight sites

The expected value approaches zero with increasing magnetic field (denoted by h), indicating that for large h all spins are in the state that is a superposition of half spin up and half spin down. Additionally, Figure 4 shows that while for greater than two sites, the expected average spin value crosses at approximately $h = 1.0$, the curve for two sites has a substantially different shape. We hypothesise that this is due to the presence of only one bond, such that all the sites in the system have no bond on one side, causing edge effects. We were unable to produce a graph for more than eight sites using this method, as the time required for each point increased exponentially.

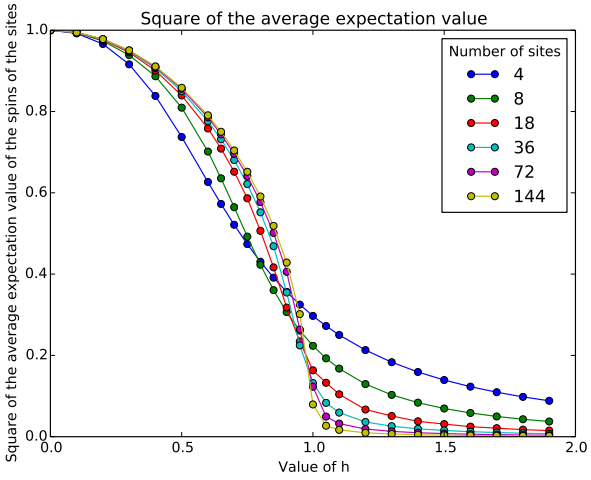

FIG. 5: Average spin for four to 144 sites

Using the TEBD algorithm, we then produced approximate graphs for higher values of the number of sites, up to 144 sites (Figure 5). Again, as predicted, the graph dropped progressively closer to zero with an increasing number of sites. With this higher number of sites, it can be seen that the graph starts to approach vertical as h approaches one from below, and horizontal for h greater than one, showing that one is the critical value of h if it is indeed a phase transition. Furthermore, theory predicts that, if this is an Ising phase transition, the square of the expectation value for a finite number of sites near the critical value of h is given by $\frac{1}{L}\left\langle\left(\sum_i \sigma_i^z\right)^2\right\rangle = L^{0.25} f\left(L(h-h_c)\right)$ where L is the number of sites, h_c is the critical value of h (in this case $h_c = 1$, and f is some unknown characteristic function. Thus, plotting $L(h-1)$ against $\frac{L^{0.25}}{L}\left\langle\left(\sum_i \sigma_i^z\right)^2\right\rangle$ should give the same graph for all L. Figure 6 shows this plot, and as expected, near we have the functions for all values of L approximating the same function. This demonstrates that the effect seen is indeed an Ising phase transition.

We used the TEBD algorithm to predict the average energy of the spins to test it, as energy can be analytically

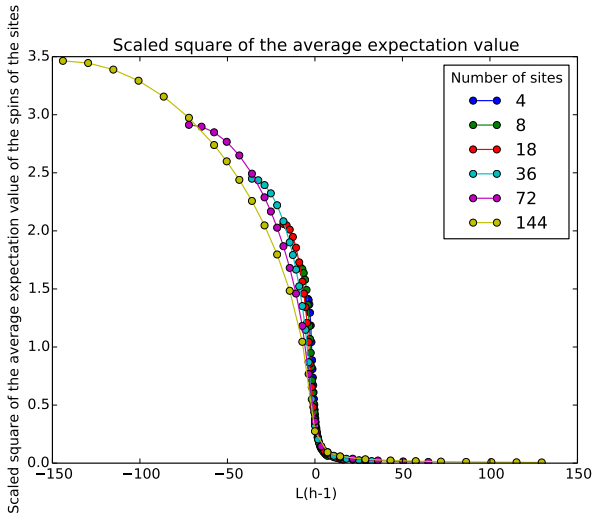

FIG. 6: Scaled expectation value

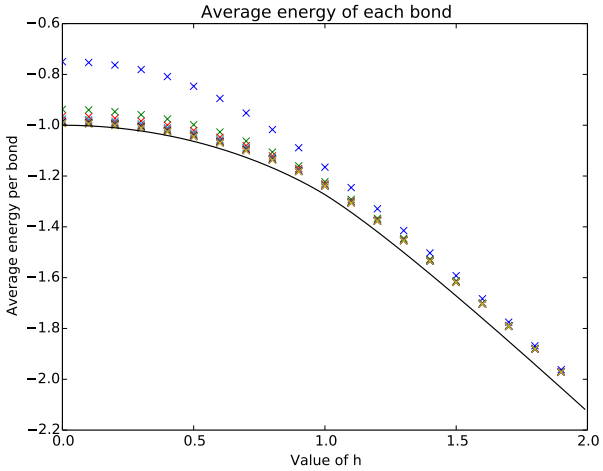

FIG. 7: Average energy for four to 144 sites

predicted for a system with an infinite number of sites. As seen in Figure 7, the predicted average energy using the matrix approximation approaches the exact energy. There is, however, a constant error. This is due to an approximation in the TEBD algorithm: it assumes that for matrices H_1 and H_2, $e^{\tau(H_1+H_2)} = e^{\tau H_1} e^{\tau H_2}$. There is an error incurred in this that is $O(\tau^2)$. Lowering the value of τ would increase the accuracy at the cost of taking more time to calculate values.

IV. DISCUSSION

Using the new algorithm, the main issue in time usage was in the calculation of the expected value. In theory, as contracting the state on itself without any operators always gives a result of 1, it should be possible to only contract the matrices between the two sites and the bonds next to them. While this would not improve the time complexity, it would substantially improve the constant in front of it.

V. CONCLUSION

Once magnetic field strength becomes equal to the strength of coupling between spins, a phase transition occurs in this one-dimensional Ising chain. This is one of the simplest known models in which a quantum phase transition occurs.

Further, the TEBD algorithm used to find it has applications to quantum systems where the degree of entanglement is low, as it uses resources linearly proportional to the number of sites, but exponentially proportional to the degree of entanglement. In situations such as this one, where there is entanglement primarily within a finite radius around each site, it is therefore very useful.

VI. ACKNOWLEDGMENTS

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