# Finding extreme eigenvalues of quantum spin chains

The physics explored in this project is the way in which the magnetization of a one dimensional Ising model in its ground state is destroyed by quantum fluctuations. The model is,

$$H = -J \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z + \lambda \sum_{i=1}^{L} \sigma_i^x \tag{1}$$

where $\sigma_i^z, \sigma_i^x$ are Pauli matrices. The strength of the quantum fluctuations is tuned by $\lambda$, while the ground state ferromagnetic order is produced by $J > 0$. The ratio $\lambda/J$ is the important parameter and we can study the problem as a function of chain length $L$ and this ratio. We consider spin half systems on chains of length $L$ with periodic boundary conditions.

The Hilbert space of this many body problem is of dimension $2^L$, so the many body problem is fully described by the $2^L \times 2^L$ Hamiltonian matrix. The objective is to construct this matrix and store it in sparse matrix form, and then find the ground state and first excited state of the Hamiltonian using sparse matrix algorithms.

The states of the system can be labelled by an integer $s$ which runs from 0 to $2^L - 1$. If we find the binary form of this integer and then change each zero in this binary form to $-1$, then each integer uniquely generates a spin configuration and we systematically run over the basis vectors of the Hilbert space. Using this ordering of the basis set we are ready to set up the Hamiltonian matrix. Since the matrix is sparse it is very inefficient to explore each matrix element $< s|\hat{S}|s' >$ as most of these are zero. Instead for each state $|s >$, we can apply the Hamiltonian $\hat{H}$ to generate a set of states that couple to $s$. This enables us to fill out each row of the Hamiltonian matrix in a systematic and efficient manner. It is useful to store the Hamiltonian matrix in the following way: Define two linear arrays, $values(NV)$ and $locations(NV)$ to store the finite values of the Hamiltonian and the columns at which these values lie. Define two more "pointer" arrays $start(L)$ and $number(L)$ to indicate the position in these arrays where the values and locations of the non-zero elements of the $i^{th}$ row start and end.

Now write a subroutine to take a matrix product using this matrix in sparse storage form. This is the rate limiting step of the algorithm. The simplest procedure to find the lowest eigenvalues of a large matrix is the iterative power method where we choose a random initial vector of length $2^L$ and simply act on it with the Hamiltonian. Other methods based on sparse matrix methods,

such as the Lancsos method are in general called Krylov subspace methods and form the basis of the area of sparse matrix linear algebra. If we only want the ground state the iterative power method projects out the state with the highest magnitude eigenvalue. We want the ground state and if the largest eigenvalue has magnitude greater than the ground state, we simply shift the Hamiltonian matrix by a value $-a_{shift}$ times the identity matrix and then use the iterative power method. Once the highest magnitude eigenvalue is found we simply add $a_{shift}$ to find the true ground state eigenvalue. The magnetization can be calculated from the ground state eigenvector and this can be plotted as a function of the parameter $\lambda/J$.

To find the first excited state and other higher eigenvalues the procedure is essentially the same, so if we want the first "m" lowest eigenvalues, we start with "m" initial vectors and make them orthonormal. Then we apply the matrix and again reorthogonalize them. This procedure is iterated until the eigenvalues of the $m \times m$ matrix of the "m" vectors converges to the lowest three eigenvalues. The energy difference between the lowest and next lowest eigenvalue is called the mass gap and shows an interesting behavior as a function of the ratio $\lambda/J$.

General background on the area, including connections to the Ising model in higher dimensions and lattice gauge theory is:

- J. Kogut, Rev. Mod. Phys. 51, 659713 (1979) "An introduction to lattice gauge theory and spin systems"

A paper where you can find values for the mass gap is:

- C. Hamer and M.N. Barber, J. Phys. A: Math. Gen. 14 241 (1981) "Finite-lattice methods in quantum Hamiltonian field theory. I. The Ising model"