

Project Proposal

Non-equilibrium dynamics and thermalisation in simple quantum systems

To understand and model the behaviour of a simplified quantum system as it thermalises. We will investigate the behaviour of a spin-1/2 system using a computer simulation. The Eigenstate thermalization hypothesis (ETH) suggests that for a system prepared in some initial state where the expectation value of an observable \hat{O} is far from that given by the microcanonical ensemble of this system, the expectation value of \hat{O} will ultimately evolve in time to its value predicted by a microcanonical ensemble, without the invocation of any random processes. We shall simulate non-equilibrium quantum systems and hope to demonstrate this process.

States

You can have a spin-1/2 system in the S_z basis, with up and down eigenstates going as

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

With eigenstates

$$up = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, down = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

IF you add another spin state, you gain the combined systems:

$$|\uparrow\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |\uparrow\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |\downarrow\uparrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |\downarrow\downarrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The combined S^{tot} is given by the operation of $S_{z1} + S_{z2}$ only on the correct part of the state - so S_{z1} sees the first spin, and S_{z2} the second.

$$S^{tot} |\uparrow\uparrow\rangle = (S_{z1} + S_{z2})(|\uparrow\rangle_1 + |\uparrow\rangle_2) = S_{z1} |\uparrow\rangle_1 + 0 + S_{z2} |\uparrow\rangle_2 + 0 = \frac{\hbar}{2} |\uparrow\rangle_1 + \frac{\hbar}{2} |\uparrow\rangle_2 = \hbar |\uparrow\uparrow\rangle$$

And the matrix form of the operator S^{tot} is given by

$$S^{tot} = \begin{bmatrix} \langle \uparrow\uparrow | S^{tot} | \uparrow\uparrow \rangle & \langle \uparrow\uparrow | S^{tot} | \uparrow\downarrow \rangle & \langle \uparrow\uparrow | S^{tot} | \downarrow\uparrow \rangle & \langle \uparrow\uparrow | S^{tot} | \downarrow\downarrow \rangle \\ \langle \uparrow\downarrow | S^{tot} | \uparrow\uparrow \rangle & \langle \uparrow\downarrow | S^{tot} | \uparrow\downarrow \rangle & \langle \uparrow\downarrow | S^{tot} | \downarrow\uparrow \rangle & \langle \uparrow\downarrow | S^{tot} | \downarrow\downarrow \rangle \\ \langle \downarrow\uparrow | S^{tot} | \uparrow\uparrow \rangle & \langle \downarrow\uparrow | S^{tot} | \uparrow\downarrow \rangle & \langle \downarrow\uparrow | S^{tot} | \downarrow\uparrow \rangle & \langle \downarrow\uparrow | S^{tot} | \downarrow\downarrow \rangle \\ \langle \downarrow\downarrow | S^{tot} | \uparrow\uparrow \rangle & \langle \downarrow\downarrow | S^{tot} | \uparrow\downarrow \rangle & \langle \downarrow\downarrow | S^{tot} | \downarrow\uparrow \rangle & \langle \downarrow\downarrow | S^{tot} | \downarrow\downarrow \rangle \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix}$$

This matrix can be found by a summation over the Kronecker products of the basis matrices and the Identity matrix.

```
ArrayFlatten[
  Outer[Times, PauliMatrix[3], IdentityMatrix[2]] +
  Outer[Times, IdentityMatrix[2], PauliMatrix[3]]
] // MatrixForm
```

The hamiltonian of this system can be formed using the Kronecker product of the individual basis elements. This is implemented in Mathematica as `Outer[Times, Sz, Sz]`, and a custom impl was used in C. This matrix is diagonal, and as such the eigenvalues are the diagonal elements and the eigenvectors are just unit vectors.

$$H^{tot} = S_z \otimes S_z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The Hamiltonian for a state measured in an inconsistent basis, for example $S_{z2} \otimes S_{y1}$, is not diagonal.

A good primer is <http://electron6.phys.utk.edu/qm1/modules/m10/twospin.htm>.