

Non-equilibrium dynamics and thermalisation in simple quantum systems

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Abstract

We aim 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) states 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 consisting of a several spin system coupled to a large bath and demonstrate this process.

The Eigenstate Thermalisation Hypothesis (ETH)

The time evolution of quantum systems is fully determined by the Schrodinger equation(Schrödinger 1926). Operationg on a known inital state, the future states of the system can be totally determined without any probabilistic quantaties emerging, even if attempting to mesure this state will in general involve a probability distribuion over mesuremnet results.

This property of complete deteminisim stands in contrast to the conventional way to determine the time evolution of a complex classical system. In this formalistim, states are probability distributions over syatems that are at each instant locally thermally equilbulirated, and the future state of the system can only be determined by the forms of it's probability distribution.

The Eigenstate Thermalisation Hypothesis attempts to bridge this gap by showing how highly non-equilibirum quantum states can evolve to resemble equilbulirated states(Srednicki 1994).

The density matrix and limiting our observations of a system

Derivation of the reduced density matrix for a system-bath state

Define the basis of system and bath in both the system and bath indexed states that are not a eigenbasis of the Hamiltonian and a singly indexed state of the eigenfunctions of H.

$$|\psi\rangle = \sum_{ij} C_{ij} |S_i B_j\rangle$$
$$|\psi\rangle = \sum_n C_n |n\rangle$$

Right multiply by $\langle S_i B_j|$, and obtain

$$C_{ij} = \sum_n C_n \langle S_i B_j | n \rangle$$

Using the result for a element of the reduced density matrix,

$$\hat{\rho}_{S_1, S_2}^{\text{reduced}} = \sum_n C_{1n} C_{2n}^*$$

And substituting the result for the separated indexed coefficients in terms of the basis coefficients,

$$\hat{\rho}_{S_1, S_2}^{\text{reduced}} = \sum_n \sum_{mm'} C_m \langle S_1 B_n | m \rangle C_{m'}^* \langle m' | S_2 B_n \rangle$$

And we can apply the time evolution operator to this element as we know the eigenenergies in the eigenfunction basis.

$$\hat{\rho}_{S_1, S_2}^{\text{reduced}} = \sum_n \sum_{mm'} \langle S_1 B_n | m \rangle \langle m' | S_2 B_n \rangle C_m C_{m'}^* e^{\frac{-i(E_m - E_{m'})t}{\hbar}}$$

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>.

To find S^2 , the total spin including interactions, you need to find $S_1 \cdot S_2$. S is defined in the full 4 element basis.

$$S_1 \cdot S_2 = S_{1x} \cdot S_{2x} + S_{1y} \cdot S_{2y} + S_{1z} \cdot S_{2z} = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The Eigensystem of this is given by

$$\begin{pmatrix} -\frac{1}{4}(3\hbar^2) & \frac{\hbar^2}{4} & \frac{\hbar^2}{4} & \frac{\hbar^2}{4} \\ \{0, -1, 1, 0\} & \{0, 0, 0, 1\} & \{0, 1, 1, 0\} & \{1, 0, 0, 0\} \end{pmatrix}$$

Calculated results

$$|\psi\rangle = |\uparrow\downarrow\rangle$$

$$\hat{\rho}^{\text{reduced}}(t) = \begin{pmatrix} \sin^2\left(\frac{t\hbar}{2}\right) & 0 \\ 0 & \cos^2\left(\frac{t\hbar}{2}\right) \end{pmatrix}$$

And this state oscillates between the up and down energy expectation values.

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$\hat{\rho}^{\text{reduced}}(t) = \begin{pmatrix} \frac{1}{4}(3 - \cos(t\hbar)) & \frac{1}{4}(\cos(t\hbar) + i \sin(t\hbar) + 1) \\ \frac{1}{4}(\cos(t\hbar) - i \sin(t\hbar) + 1) & \frac{1}{4}(\cos(t\hbar) + 1) \end{pmatrix}$$

And this state oscillates between the up and down energy expectation values.

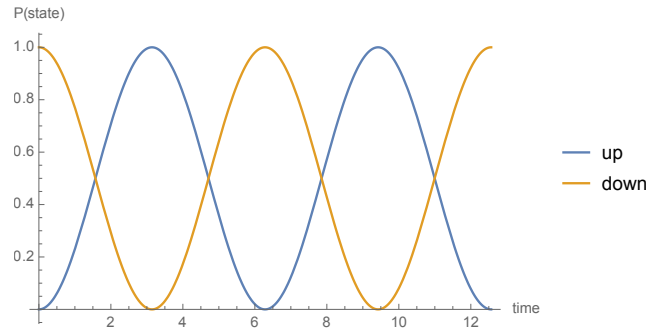


Figure 1: Time evolution of the system portion of the $|\uparrow\downarrow\rangle$ state

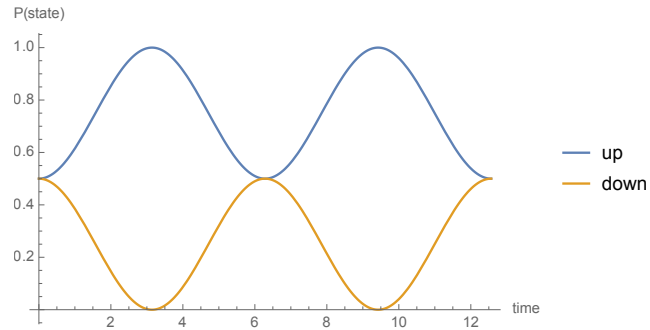


Figure 2: Time evolution of the system portion of the $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ state

Performing calculations in Mathematica

By extending the definition of the Hamiltonian to

```

NoSpins = 2;
NoStates = 2^NoSpins;
NoBasis = 2^(NoSpins - 1) - 1;
PauliPosN[n_, l_] :=
  Table[If[curr == n, \[HBar]/2 PauliMatrix[dim],
    IdentityMatrix[2]], {curr, 1}];
Sdimn[dim_, NSpins_] :=
  Apply[Dot,
    Table[Nest[ArrayFlatten,
      Apply[Outer, {Times}~Join~PauliPosN[pos, NSpins]], NSpins], {pos,
        NSpins}]];

H = ArrayFlatten[Sum[Sdimn[dim, NoSpins],
  {dim, {1, 2, 3}}]];
SeperatedStates[s_, b_] := Apply[
  Join, Apply[
    Outer, {Times}~Join~
      Table[{BitGet[b, n], Boole[BitGet[b, n] == 0]}, {n, 0,
        NoSpins - 2}]~Join~{{Boole[s == 1], Boole[s == 0]}}, {0,
        NoSpins - 2}];

CombinedStates = Table[Normalize[evec], {evec, Eigenvectors[H]};
CombinedE = Eigenvalues[H];
phi = 1/\[Sqrt]2 (SeperatedStates[1, 0] + SeperatedStates[0, 0]);
CombinedCoeffs = Table[Dot[phi, CombinedStates[[k]]], {k, NoStates}];
\[Rho][s1_, s2_] := ExpToTrig[!(
  \*UnderoverscriptBox[\(\[Sum]\), \((n = 0)\), \((NoBasis)\)] \(\
  \*UnderoverscriptBox[\(\[Sum]\), \((m = 1)\), \((Length[
    CombinedStates]\)] \(\
  \*UnderoverscriptBox[\(\[Sum]\), \((p = 1)\), \((Length[
    CombinedStates]\)] Dot[Conjugate[SeperatedStates[s1, n]],
    CombinedStates[\(\[\]\)\(\[m]\)\(\[\]\)] Dot[
      Conjugate[CombinedStates[\(\[\]\)\(\[p]\)\(\[\]\)]],
      SeperatedStates[s2,
        n]] CombinedCoeffs[\(\[\]\)\(\[m]\)\(\[\]\)] Conjugate[
        CombinedCoeffs[\(\[\]\)\(\[p]\)\(\[\]\)]
  \*SuperscriptBox[\(E\), \(\(-I\)\ \((CombinedE[\(\[\]\)\(\[m]\)\(\[\]\)] -
    CombinedE[\(\[\]\)\(\[p]\)\(\[\]\)]\) t/\[HBar]\)]\)\)\)\)
]
p = Simplify[
  ArrayFlatten[Table[Table[\[Rho][s1, s2], {s1, 0, 1}], {s2, 0, 1}]]];

```

Introduction to the Xeon Phi

References

Schrödinger, E. 1926. “An Undulatory Theory of the Mechanics of Atoms and Molecules.” *Physical Review* 28 (6). American Physical Society (APS): 1049–70. doi:10.1103/physrev.28.1049.

Srednicki, Mark. 1994. “Chaos and Quantum Thermalization.” *Phys. Rev. E* 50 (2). American Physical Society (APS): 888–901. doi:10.1103/physreve.50.888.