

# 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

In

## 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.

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

## Optimising the performance of the reduced density calculation.

We can define several relevant basis for this problem as the eigensystems for a selection of Hamiltonians, a completely separated basis where no interactions are considered, a system with the system fully connected except for the links connecting the subsystem we measure and the bath, and a fully connected system that we wish to probe.

The separated basis can be trivially defined as the hamiltonian is diagonal as the outer product of the constituent states. In bra-ket notation this is given by

$$|S_1 S_2 \dots S_n\rangle = |S_1\rangle |S_2\rangle \dots |S_n\rangle$$

And in the representation where a up-spin is given by  $(1, 0)^T$  and down by  $(0, 1)^T$ , this is a one-hot encoding (D. Harris and Harris 2012) of the state, in a vector of length  $2^n$  where  $n$  is the number of sites.

$$|S_1 S_2 \dots S_n\rangle = \begin{pmatrix} S_{1-up} \\ S_{1-down} \end{pmatrix} \otimes \begin{pmatrix} S_{2-up} \\ S_{2-down} \end{pmatrix} \dots \otimes \begin{pmatrix} S_{n-up} \\ S_{n-down} \end{pmatrix}$$

The representations of the states in the system-bath basis and fully combined basis cannot be defined without reference to the hamiltonian describing the system, and in general any system-bath state  $|SB\rangle$  or totally combined state  $|N\rangle$  will be formed as a linear combination of all of the separated basis states. We are always able to form the more complex basis as a function of the separated basis states as the separated basis is complete.

As this separated basis is easy to define, we will use it as the computational basis and all hamiltonians will be defined numerically in this basis. This leads to the more-connected systems having non-diagonal representations, due to the calculation procedure using the interaction terms in the separated basis.

We can't find operators that would allow us to represent both the energy of the states and the interaction terms that are diagonal in the same basis, so may as well use the clearest.

however in order to diagonalize them without diagonal operators it is required to calculate a concrete eigensystem and this is exactly the computational process needed to find representations in the separated basis, so we can take the separated basis as our only basis for concrete representations.

In order to directly calculate the reduced density matrix for the combined system, we calculate many expressions of the form

$$\sum_n \sum_m \langle S_1 B_n | m \rangle$$

We can interpret this as looking up the  $(S_1 B_n, m)$ th element of a matrix we call  $X$ .

We define  $X$  to be a lookup table for the overlaps between the fully separated states we wish to find the reduced density matrix in and the combined states.

$$X[SB, m] = \langle S_1 S_2 \dots S_n | m \rangle$$

If we form the matrices  $[|S_1 S_2 \dots S_n\rangle]$  and  $[|m\rangle]$ , where the square brackets indicate the matrix of eigenvectors. For example,

$$[|S_1 S_2 \dots S_n\rangle] = [|00\rangle, |01\rangle, \dots, |nn\rangle]$$

Using this, we can efficiently calculate the overlaps between all the states using a single matrix product.

$$X = [|S_1 S_2 \dots S_n\rangle] \cdot [|m\rangle]$$

As a conventional matrix product, this can be calculated efficiently. In order to compute the reduced density matrix, we lookup the multiplicative overlap values from this matrix.

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

This however still results in a very large number of nested loops in order to calculate the reduced density matrix. As an alternative, we return to the definition of the full density matrix and calculate it for the time dependant state, and take the partial trace directly.

$$\hat{\rho} = |\psi\rangle \langle \psi| = \sum_{mm'} C_m C_{m'}^* e^{\frac{-i(E_m - E_{m'})t}{\hbar}} |m\rangle \langle m'|$$

We define the partial trace as the trace over the bath states, with the states expanded using the identity operators for the system portion.

$$Tr_b(\hat{O}) = \sum_b (\mathbb{I}_{\text{system}} \otimes \langle b|) \hat{O} (|b\rangle \otimes \mathbb{I}_{\text{system}})$$

$$Tr_b(\hat{\rho}) = \sum_b \sum_{mm'} (\mathbb{I}_{\text{system}} \otimes \langle b|) |m\rangle \langle m'| (|b\rangle \otimes \mathbb{I}_{\text{system}}) C_m C_{m'}^* e^{\frac{-i(E_m - E_{m'})t}{\hbar}}$$

We can then calculate the reduced density matrix in the separated basis with

$$\rho_{S_1, S_2}^{\text{reduced}} = \langle S_1 | \text{Tr}_b(\hat{\rho}) | S_2 \rangle$$

$$\rho^{\text{reduced}} = [\text{SystemEigenvectors}]^\dagger \cdot \text{Tr}_b(\hat{\rho}) \cdot [\text{SystemEigenvectors}]$$

The advantage of this approach is each of the stages has at worst a 2-level nesting of summations. This indicates that this form of calculation (determining full density matrix, taking partial trace, and expressing in chosen basis) avoids needless recomputation of values relative to the fully nested calculation that has 6 levels of summation.

The disadvantage is as the time-dependance is factored into the full density matrix, we need to fully recalculate for each timestep we sample at. The system at  $T+dt$  can be calculated without knowledge of the system at  $T$ , so can be done in parallel.

TEST what is faster.

## 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  $S^{\text{tot}}$  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.

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

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 hamilton of this system can be formed using the Kronecker product of the individual basis elements. This is implimented 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 Hamiltonion for a state mesured in a inconsistant 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.

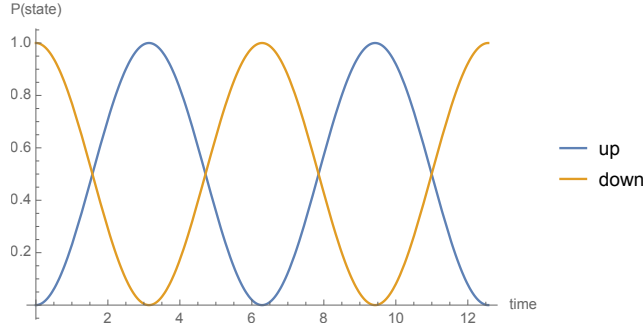


Figure 1: Time evolution of the system portion of the  $|\uparrow\downarrow\rangle$  state

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

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

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

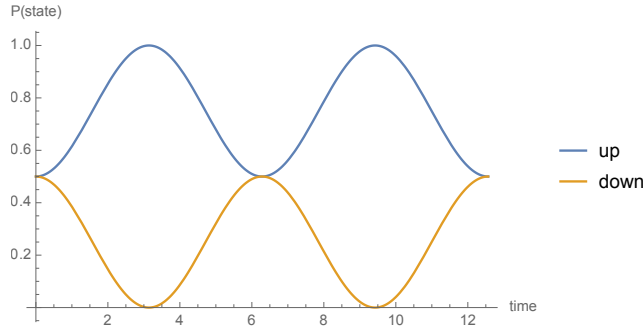


Figure 2: Time evolution of the system portion of the  $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\downarrow\rangle)$  state

## 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

Harris, David, and Sarah Harris. 2012. *Digital Design and Computer Architecture*. Elsevier.

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.