Notes on Entropy

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1 Entropy in Classical Physics

1.1 What is entropy?

There are many seemingly different answers to this question. Entropy is described as

1. A measure of our ignorance of a system,
2. A measure of the amount of information contained in a system,
3. A measure of the disorder of a system ,
4. A property of a thermodynamic system in thermal equilibrium at (absolute) temperature T, which increases by an infinitesimal quantity

   $$dS = \frac{đQ}{T}, \tag{1.1.1}$$

   when the total energy of the system increases by $đQ$.

Item 2 might appear to be contradictory. However, information theorists quantify information in terms of the information obtained by measuring the value of a certain quantity (a surprise factor). We will return to this later.

These seemingly diverse meanings of the word "entropy" are, in fact, related, in view of the fact that the precise (mathematical) definition of entropy – the 'Shannon entropy'– is common to all these, albeit with different applications (different physical quantities corresponding to the variables used in Shannon' definition of entropy.)

1.2 Microstates and Macrostates

Before we can elaborate on this we need to define (and explain) two quantities, which describe the state of a system.

Microstate
A microstate is labelled by the complete set of all quantities which describe the state of a system. In the case of a system consisting of N particles moving in three dimensions, these quantities are the position vectors $\mathbf{x}_i$ and the momentum vectors $\mathbf{p}_i$ where $i = 1 \cdots N$ runs over the N particles.

The space of all microstates is a 6^N dimensional, known as "phase-space", whose axes are the $3N$ components of each $\mathbf{x}_i$ and the $3N$ components of each $\mathbf{p}_i$. Although we are confining ourselves to classical physics for the moment, we "borrow" from Quantum Physics the fact that due to the uncertainty principle each microstate occupies a volume h^3 in phase-space (h being Plank's constant). This means that the quantities used to label a microstates are actually discrete.

For particles with non-zero spin (a concept also "borrowed" from Quantum Physics), the description of the state also requires specification of a component of the spin for each particle.

Macrostates

A macrostate is labelled by some subset of the variables that determine a particular microstate. These correspond to the quantities that an experimentalist can measure. Since this will be less or equal to the number of quantities which define the macrostate (usually much less) there will be several (usually many) microstates for each macrostate.

The entropy of a system is a function of the quantities that define a macrostate. We see immediately that this means that the entropy of a system can vary from one observer to another reflecting a difference in their ability to make measurements, and consequently to specify the values of the set of variables that label a given macrostate. So that entropy is very much subjective. The entropy used in thermodynamics refers to a particular way of labelling macrostates.

For the case of a system of spin-$\frac{1}{2}$ particles, a macrostate might be labelled by the total energy of the N particles, without knowing the energies of the individual particles. On the other hand, it could have more macroscopic variables, such as the number of particles in a particular volume of space, without knowing the exact positions of all the particles. The entropy in such cases would be different.

For the example of particles with a given spin, in the case of spin-$\frac{1}{2}$, we might know how many of the particles are spin-up, so that this would be specified in the macrostate, but have no knowledge of the spin orientations of the individual particles.

1.3 Shannon Entropy

Suppose the microstate of a system be labelled by the values of N quantities $X_i,\ (i = 1 \cdots N)$, (N might be infinite) Let $p(\{x\})$ be the probability that these values are x_i, then the Shannon entropy, H of the system is defined as

$$H \ = -\sum_{\{x\}} p(\{x)\} \log_2(p(\{x\})), \tag{1.3.1}$$

where the sum goes over all possible sets of values of $\{x\} \equiv x_1, x_2 \cdots x_N$.

The logarithm is taken to base 2 because in information theory $\log_2 N$ is the number of binary bits required to store a number between 0 and $N-1$. In thermodynamics the entropy (which we designate by S) is defined in terms of natural logarithms and furthermore there is an overall factor equal to the Boltzmann constant κ_B, i.e.

$$S \ = \ \kappa_B \ln 2\, H. \tag{1.3.2}$$

We see that the entropy (as defined by Shannon) depends on the probability distribution of the quantities x_i. This probability distribution is determined by what we know about the system. In particular, for a macrostate labelled by r quantities Y_a, $(a = 1 \cdots r)$, the probability distribution and hence the entropy is a function of the values y_a which label the macrostate.

As an example, take a collection of N coins which can either be heads-up or tails-up. There are a total of 2^N possible microstates specifying the state of each coin. Each microstate is a sequence of 0's and 1's, which form a number x consisting of N binary bits. In other words, each microstate corresponds to a number, x, (written inn binary) between 0 and $2^N - 1$. For true coins, the probability of the coin begin heads-up or tails-up is precisely $\frac{1}{2}$. There are 2^N possible these is equally likely, so that each sequence, x, occurs with a probability

$$p(x) \; = \; \frac{1}{2^N}$$

The Shannon entropy of a set of N true coins is then

$$H \; = \; N \log_2 2 \; = \; N.$$

The Shannon entropy is the number of binary bits required to specify a sequence.

For example, if we have 10 coins, three of the 2^N possible sequences could be

$$\begin{array}{ll} 0,0,1,0,1,1,1,0,0,0 & (1) \\ 0,1,1,0,1,0,1,0,0,0 & (2) \\ 0,0,1,0,1,1,1,0,1,0 & (3), \end{array}$$

where 1 represents heads-up and 0 represents tails-up. $p(\{x\})$ is the probability of obtaining a distribution $\{x\}$. If the macrostate is not specified, then the entropy of these 10 coins is 10.

Suppose the macrostate is defined by specifying the number of coins that are heads-up. For example, suppose we know that four of the coins are heads-up but we don't know which four. Then the distributions (1) and (2) shown above are allowed with some probability, but distribution (3), which has five coins with heads-up, is not allowed - its probability is zero. This will affect the determination of the entropy. In actual fact the entropy in such a case is lower than the case where we do not know how many coins are heads-up, reflecting the fact that for such a macrostate we have more knowledge (less ignorance) of the state of the system. Of the 2^{10} possible sequences of 10 coins only the 210 have a non-zero probability and so the Shannon entropy is reduced from 10 to $\log_2(210) = 7.7$.

Thus we see in general that the entropy of a system is a function of the values, y_a of the quantities that label the macrostate. The specification of the macrostate restricts the sum over the allowed microstates. The quantities, Y_a, which determine the macrostate are functions of all the quantities x_i which determine the microstate. Therefore, For a given macrostate, we can rewrite the Shannon entropy as

$$H = \sum_{\{x\}} \left\{ p(\{x\}) \log_2(p(\{x\}) \prod_{a=1}^{r} \delta_{(Y_a(\{x\})-y_a)} \right\}. \tag{1.3.3}$$

In other words, the sum over the microstates is restricted to those for which the quantities Y_a which label the macrostate take the values y_a.

In the above example of 10 coins, we just specify hoew many are heads-up and so $r = 1$. The sum over all *allowed* microstates goes over all 10-bit binary numbers which have exactly four bits set to 1 - i.e. the sum over all distributions of 10 heads or tails with the condition that four and only four of the coins are heads. out of the 1024 possible distributions of 10 coins)microstates) only 210 of then have four heads-up coins.

1.4 Principle of Maximum Entropy

What remains now is to determine the probability distribution. In order to do this we invoke the principle of maximum entropy, which asserts:

The probability distribution which best describes the current knowledge of a system is the distribution for which the Shannon entropy is maximal.

The probability, $p(\{x\})$ to obtain a set of quantities $\{x\}$ which describes a microstate, is the distribution of the different possible sets of quantities $\{x\}$ over a very large number, $\mathcal{N}$, copies (known as an 'ensemble') of the system under investigation, Strictly we should take the limit $\mathcal{N} \to \infty$, but we need it to be sufficiently large that the number of copies of the system, which are in the ste $\{x\}$ is $\mathcal{N}\, p(\{x\})$,

There are two possible ways to approach this.

1.4.1 Microcanonical ensembles

This is an ensemble of $\mathcal{N}$ systems. all in the same macrostate, i.e. all of these have the same values of the functions $Y_a(\{x`_i\})$, which label the macrostates, but they have different values of the microstate variables $\{x\}$, subject to the constraints

$$Y_a(\{x\} \ = \ y_a. \tag{1.4.1}$$

The Shannon entropy is given by

$$H \ = \ -\sum_{\{x\}'} p(\{x\}) \ln\left(p(\{x\})\right), \tag{1.4.2}$$

where $\sum_{\{x\}'}$ means sum over the sets if variables $\{x\}$ which are compatible with the constraints (1.4.1). For all the other sets of microstate variables, the probability is zero.

This is maximized subject to the constraint that the probability summed over all the permitted sets of variables $\{x\}$ is unity. This maximum is found by setting the function derivative of

$$H - \lambda \sum_{\{x\}'} p(\{x\})$$

to zero. λ is a Lagrange multiplier whose value is obtained from the requirement that the sum of all the probabilities is unity. This leads to the result that the probability takes the same value for *all* allowed sets of variables, i.e

$$p(\{x\}) \;=\; \frac{1}{\Omega(\{y\})}, \tag{1.4.3}$$

where

$$\Omega(\{y\}) \;\equiv\; \sum_{\{x\}} \prod_a \delta\left((Y_a(\{x\}) - y_a\right) \tag{1.4.4}$$

is the number of microstates compatible with the macrostate. The statement that in the absence of any further information about the system, the probabilities for all sets of microstate variables, compatible with a given macrostate, are equal, seems a reasonable assumption and is compatible with the maximisation of the Shannon entropy.

The entropy, which is a function of the values of Y_a that label the macrostate, is then given by

$$H(\{y\}) \;=\; \log_2\left(\Omega(\{y\})\right). \tag{1.4.5}$$

For example, for a set of N coins r of which are heads-up, the number of possible microstates is the number of ways of selecting r elements from a total of N elements, i.e.

$$\Omega(r) \;=\; \frac{N!}{(N-r)!r!},$$

and the Shannon entropy is

$$H(r) \;=\; \log_2(N!) - \log_2((N-r)!) - \log_2(r!)$$

if N and r are both very large, then we may use Stirling's approximation to obtain

$$H(r) \;\approx\; N\log_2 N - (N-r)\log_2(N-r) - r\log_2 r.$$

1.4.2 Canonical ensembles

A canonical ensemble is a (large) number, $\mathcal{N}$, of copies of copies of the system, which are not necessarily in the same macrostate, i.e. they do *not* have the same values of y_a for the variables Y_a, that label the macrostate but the average values of the y_a, averaged over the who ensemble are known. The probability distributions are functions of a set of variables μ_a, which bare conjugate to the variables Y_a and which encode the average values of y_a. In thermodynamics, one of the variables that labels the macrostates is the total energy, E, of all the particles in the system. The corresponding conjugate variable is β which is inverse to the (absolute) temperature

$$\beta \;=\frac{1}{\kappa_B T}.$$

This can be taken as the definition of temperature, and it is related to the average total energy $\overline{E}$. over the ensemble of systems.

For a general variable Y_a which labels a macrostate, its average value over the $\mathcal{N}$ systems in the ensemble is

$$\overline{y_a} = \frac{1}{\mathcal{N}} \sum_{\alpha=1}^{\mathcal{N}} y_a(\alpha), \tag{1.4.6}$$

where the sum is over all the systems in the ensemble and $y_a(\alpha)$ is the value of y_a in system α.

If the probability for a system to be in a microstate labelled by $\{x\}$ is $p(\{x\})$ then we define the "expectation value $\langle y_a \rangle$ to be

$$\langle y_a \rangle = \sum_{\{x\}} Y_a(\{x\}) p(\{x\}). \tag{1.4.7}$$

These two quantities coincide as the number of systems, $\mathcal{N}$, in the ensemble goes to in infinity

$$\lim_{\mathcal{N} \to \infty} \langle y_a \rangle = \overline{y_a}. \tag{1.4.8}$$

This is the proper definition of "probability".

At this point, it is more convenient to revert to natural logarithms and introduce a denominator factor of $\ln 2$ in the definition of Shannon entropy.

$$H = \frac{-1}{\ln 2} \sum_{\{x\}} \{p(\{x\}) \ln(p(\{x\}))\} \tag{1.4.9}$$

For canonical ensembles, the probability of a system being in a microstate $\{x\}$ is obtained by maximizing the Shannon entropy subject to the constraints

$$Y_a(\{x\}) = \langle y_a \rangle = \sum_{\{x\}} Y_a(\{x\}) p(\{x\}),$$

The conjugate variables μ_a act as Lagrange multipliers, so that the probability for a particular microstate is given by maximizing the quantity

$$\frac{-1}{\ln 2} \sum_{\{x\}} p(\{x\}) \left\{ \ln(p(\{x\}) + \sum_a \mu_a Y_a(\{x\}) \right\},$$

This leads to

$$p(\{x\}) = \frac{1}{Z(\{\mu_a\})} \exp\left\{ -\sum_a \mu_a Y_a(\{x\}) \right\} \tag{1.4.10}$$

where

$$Z(\{\mu_a\}) \equiv \sum_{\{x\}} \exp\left\{ -\sum_a \mu_a Y_a(\{x\}) \right\} \tag{1.4.11}$$

is called the "partition function". Its presence in the denominator in (1.4.10) guarantees that the sum of al;l probabilities is unity.

We note here that we may rewrite (1.4.11) in terms of a sum over the allowed values of y_a which label the macrostates as,

$$Z(\{\mu_a\}) \equiv \sum_{\{y\}} \Omega(\{y\}) \exp\left\{-\sum_a \mu_a y_a\right\}, \tag{1.4.12}$$

where Ω is defined in (1.4.4) and is is the "density of states", i.e. the number of microstates for which the paramteres that label the macrostate take the values y_a.

Once this partition function has been determined, the expectation value of the macrostate variables y_a are given by

$$\langle y_a\rangle(\{\mu_a\}) = \frac{1}{Z(\{\mu_a\})}\sum_{\{x\}} Y_a(\{x\}) \exp\left\{-\sum_a \mu_a Y_a(\{x\})\right\} = -\frac{\partial}{\partial\mu_a}\ln Z(\{\mu_a\}) \tag{1.4.13}$$

and the entropy (as a function of the conjugate variables μ_a is given by

$$H(\{\mu_a\}) = \frac{1}{\ln 2}\left\{\ln Z(\{\mu_a\}) + \sum_a \mu_a \langle y_a(\{\mu_a\})\rangle\right\} \tag{1.4.14}$$

Conversely, from the entropy determined using a microcanonical ensemble, as a function of the values of the macroscopic variables, y_a, we can obtain the values of the conjugate variables μ_a by partially differentiating (1.4.14) w.r.t. μ_b, making use of (1.4.13) to get

$$\ln 2\,\frac{\partial H}{\partial\mu_b} = \sum_a \mu_a \frac{\partial^2}{\partial\mu_a\partial\mu_b}\ln Z = \sum_a \mu_a \frac{\partial\langle y_a\rangle}{\partial\mu_b} \tag{1.4.15}$$

Now consider the conjugates μ_a to be functions of the average values of the macroscopic parameters, y_a, i.e $\mu_a(\langle y_b\rangle)$ and multiply both sides by $\partial\mu_b/\partial\langle y_c\rangle$, and contract over b

$$\ln 2 \sum_b \frac{\partial\mu_b}{\partial\langle y_c\rangle}\frac{\partial H}{\partial\mu_b} = \sum_{a,b} \mu_a \frac{\partial\langle y_a\rangle}{\partial\mu_b}\frac{\partial\mu_b}{\partial\langle y_c\rangle}.. \tag{1.4.16}$$

If we treat the Shannon entropy, H as a function of the average values of the macroscopic variable, y_a, then using the chain rule, the LHS of (1.4.16) becomes

$$\ln 2\,\frac{\partial H(\langle y_d\rangle\})}{\partial\langle y_a\rangle)}$$

and the RHS is

$$\sum_a \mu_a \frac{\partial\langle y_a\rangle}{\partial\langle y_c\rangle} = \sum_a \delta_{ac} = \mu_c$$

to obtain

$$\mu_c \;=\; \ln 2 \frac{\partial}{\partial y_c} H((\{y\}) \tag{1.4.17}$$

Moreover, we have a useful relation between the infinitesimal change, dH, in Shannon entropy due to an infinitesimal change, $d\mu_b$, of the conjugate variables, μ_b.

From the chain rule:

$$dH \;= \sum_a \frac{\partial H}{\partial \mu_a} d\mu_a$$

and

$$d\langle y_b\rangle > \;=\; \sum_a \frac{\partial \langle y_b\rangle}{\partial \mu_a} d\mu_a$$

Taking the partial derivative of (1.4.14),

$$\ln 2 \frac{\partial H}{\partial \mu_a} \;=\; \frac{\partial \ln Z}{\partial \mu_a} + \langle y_a\rangle + \sum_b \mu_b \frac{\partial \langle y_b\rangle}{\partial \mu_a}$$

Using (1.4.13) we see that the first two terms cancel and we are left with

$$dH \;=\; \frac{1}{\ln 2} \sum_a \mu_a d\langle y_a\rangle. \tag{1.4.18}$$

In thermodynamics for which $y_a = E$, and all the members of the ensemble occupy the same volume, the total energy of the system and $\mu_a = 1/T$, this is the familiar result

$$TdS \;\equiv\; \kappa_B T \ln 2\, dH \;=\; d\langle E\rangle.$$

We return to the example of the set of N coins. Introducing a variable, μ, conjugate to the number r of coins with heads-up, and accounting for the number of ways we can select r coins with heads-up out of a total of N coins, the partition function is

$$Z(\mu) \;=\; \sum_{r=0}^{N} \frac{N!}{(N-r)!r!} e^{-\mu r} \;=\; \left(1 + e^{-\mu}\right)^N$$

The expectation value of r is then

$$\langle r\rangle \;=\; -\frac{\partial}{\partial \mu} Z(\mu) \;=\; N \frac{e^{-\mu}}{(1 + e^{-\mu})}.$$

or

$$\mu \;=\; \ln \left(\frac{N - \langle r\rangle}{\langle r\rangle} \right)$$

and the entropy is

$$H(\mu) \;=\; \frac{N}{\ln 2} \left\{ \ln\left(1 + e^{-\mu}\right) + \frac{\mu\, e^{-\mu}}{1 + e^{-\mu}} \right\}.$$

Writing μ is terms of $\langle r\rangle$, we see that this gives he same expression as we obtained for the entropy in the limit of a large number, N of coins.

We note further that if we write H as a function of $\langle r\rangle$

$$H(\langle r\rangle \ = \frac{N}{\ln 2}\left(-(N-\langle r\rangle)\ln(N-\langle r\rangle)-\langle r\rangle\ln\langle r\rangle\right),$$

and differentiate w.r.t. $\langle r\rangle$ we recover

$$\mu \ = \ \ln 2\,\frac{\partial H(\langle r\rangle)}{\partial\langle r\rangle} \ = \ \ln\left(\frac{N-\langle r\rangle}{\langle r\rangle}\right)$$

The entropy of the set of coins has a maximum value, $H=N$, for $\mu=0$. For this value $\langle r\rangle = N/2$. This is what happens if we toss a true coin N times. This entropy is maximal because we have little knowledge of the coin. On the other hand for non-zero values of μ we would obtain average values for r which differ from $N/2$ ($\langle r\rangle < N/2$ for positive μ and $\langle r\rangle > N/2$ for negative μ. An experiment to measure the average number of times the coin lands on heads then gives us information about the nature of the coin and consequently reduces our ignorance of the coin. In the asymptotic limit $\mu \to \infty$ the coin will never land on heads ($\langle r\rangle = 0$) and in this case we have absolute knowledge of the nature of the coin and the entropy is zero.

This is demonstrated in Fig.1, in which the probability of a collection of 10 coins to have r with heads up (after being tossed), for the cases of a true coin and two fraudulent coins. The entropy is larger for the true coin than for the fraudulent coins.

We can check similarly that as $\mu \to \infty$, so that the coin *always* lands on tails the entropy also vanishes (this is seen by expanding the expression for entropy as a power series in $e^{-\mu}$).

For systems whose macrostates depend on the values of several parameters canonical ensembles are actually a hybrid of canonical and microcanonical ensembles, in which some of the variables defining the macrostate are taken to be the same in the different copies of the system comprising the ensemble, whereas others are different and only their average value can be deduced. For example in thermodynamics a "canonical ensemble" is taken to mean an ensemble of systems for which the total energies differ but the number of particles and (in the case of a gas) the volume occupied are the same for all the systems in the ensemble. In this case there is only one conjugate variable, β from which one can deduce the average value of the total energy - this is known as the "internal energy", U of the ensemble (the word 'internal' means that we discount any collective energy of all th systems in the ensemble – they are assumed to be at rest relative to each other and relative to the observer.)

Ensembles for which the numbers of particles differ between members of the ensemble are called "grand canonical ensembles" and the variable conjugate to the number of particles is called the "thermodynamic potential".

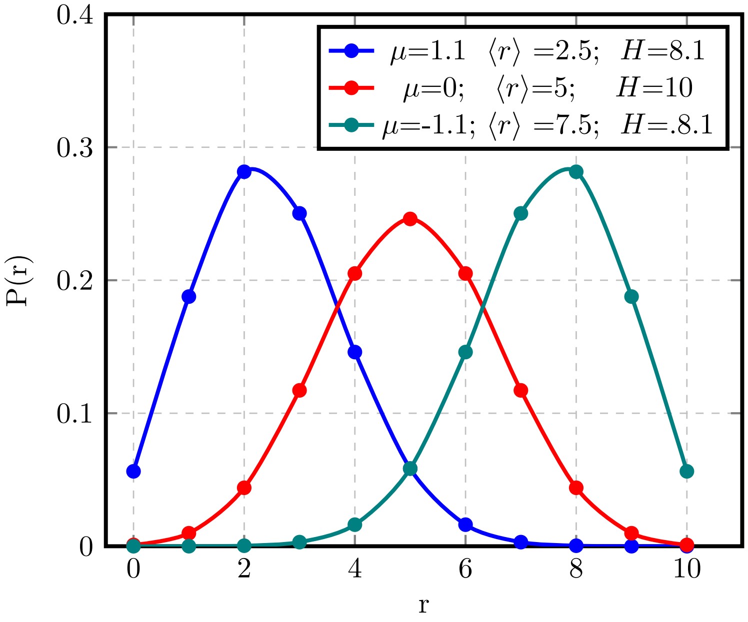


Figure 1: Probabilities of a system of 10 coins having r coins with heads up. For the true coin (red) the average number is 5, as expected and this system of coins has the largest entropy. The blue and green curves correspond to fraudulent coins for which heads occurs more often (green) or less often blue) than expected.

1.5 Loaded Roulette Wheel

A proper roulette wheel has the same probability for the boule to land on any number x between $x = 0$ and $x = 36$. In other words the probability, $p[(x)$ to land on x is given by

$$p(x) \;=\; \frac{1}{37}$$

The average value for x is 18 and the Shannon entropy is

$$H \;=\; -\sum_{x=0}^{36} \frac{1}{37} \log_2 \left(\frac{1}{37} \right) \;=\; \log_2(37)$$

The house makes a profit because it only pays out 35 to 1.

However, if the wheel has a small bias, parametrized by μ, then the probability of the boule to land on x is

$$p(x) \;=\; \frac{e^{-x\mu}}{\sum_{x'=0}^{36} e^{-x'\mu}} \;=\; \frac{(1 - e^{-37\mu})\, e^{-x\mu}}{(1 - e^{-\mu})}$$

The average value (expectation value) of x is

$$\langle x \rangle \;=\; \frac{e^{-\mu}}{(1 - e^{-\mu})} - 37 \frac{e^{-37\mu}}{(1 - e^{-37\mu})},$$

and the entropy is

$$H \;=\; \log_2\left(1-e^{-37\mu}\right) - \mu\frac{e^{-37\mu}}{\left(1-e^{-37\mu}\right)} - \;\log_2\left(1-e^{-\mu}\right) + \mu\frac{e^{-\mu}}{\left(1-e^{-\mu}\right)}$$

This has a maximum for $\mu = 0$. For non-zero values of μ we have the knowledge that the average value of x differs from its value for a true roulette wheel. The reduced entropy is a reflection of this extra knowledge.

If $\mu > 0.0016$ then the probability of the boule landing on zero exceed 1/36 so that betting on it will eventually beat the house. The average value of x is reduced to 17.8 and the entropy reduced to $\log_2 36.99$ (a very tiny difference but nevertheless significant).

For an even more crooked roulette wheel, let's go to Rick's "Cafe Americain" in Casablanca. Rick has information about his wheel that he would not have if the wheel were not fixed – when he nods to the Croupier the boule lands on 22.

Suppose Rick had been a bit subtler and had fixed the wheel so that the boule had an enhanced chance of landing in 22. Such a wheel would have a probability to land on x equal to

$$p(x) \;=\; \frac{1}{Z(\mu)}\exp\{-\mu\,(x-22)^2\} \tag{1.5.1}$$

with

$$Z(\mu) \;=\; \sum_{x=0}^{36}\exp\{-\mu\,(x-22)^2\} \tag{1.5.2}$$

This is a distribution in which both the average value of x and the average value of x^2 are known.

The probability to land on a particular number x is plotted for three values of μ. We see that all of these distributions are peaked at $x = 22$, but as μ becomes larger, the peaks become sharper.

This means that as μ increases the width of the peak, which is a measure of the RMS deviation, decreases, indicating an increase in information about the roulette wheel and consequently a decrease in its entropy. This is shown in Fig.3.

1.6 Information and Communication

The answer to a question, for which the answer is either is either "yes" or "no" requires one bot of information. The bit is st" (i.e. takes the value 1) if the answer is "yes" and unset (value 0) if the answer is "no". *A priori* we have no reason to assume that one answer os more likely than another and so the probability of either answer is $\frac{1}{2}$ and the entropy of a bit of information is

$$h \;=\; -\sum_{i=0,1} p_i\log_2(p_i) \;=\; \log_2(2) \;=1.$$

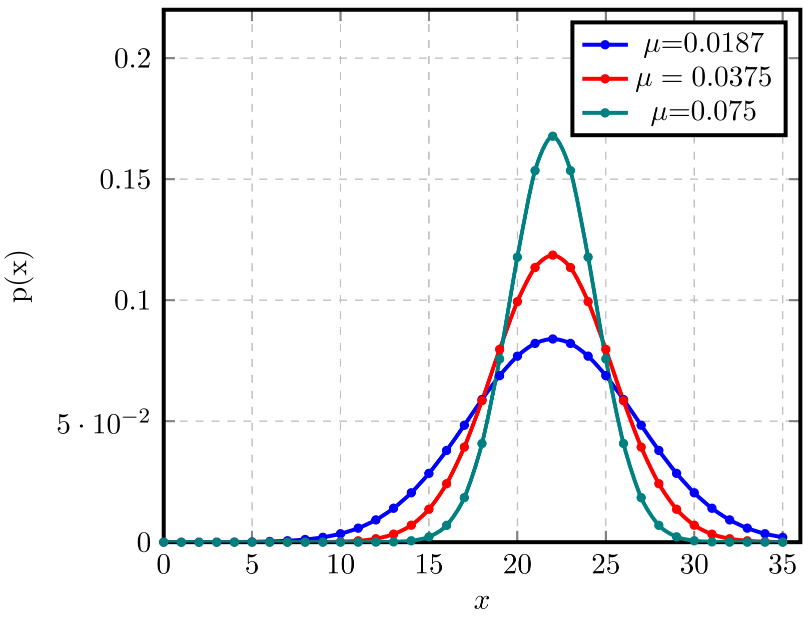


Figure 2: Probability distributions with average value $\langle x \rangle = 22$ form different values of Lagrange multiplier μ

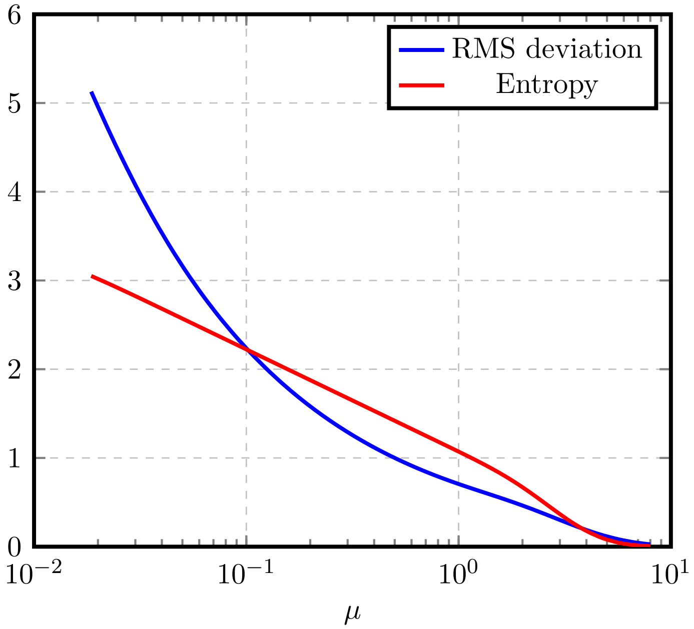


Figure 3: RMS deviation and entropy plotted against μ

A message (this might be a short message, or an entire book or entire encyclopaedia) is usually stored on a computer in ASCII, which requires ne byte per symbol. If we assume that a computer byte has an equal probability to be in any of its 256 states, the entropy of a message consisting of N symbols would be $8N$

This is very wasteful as only a small fraction of the 256 possible states of byte (8 bits) is actually used. The information contained in the message could be communicated using only (26) capital letters and a space to separate words, and a few punctuation marks (including a space to separate words)- so we would only need 32 different states and the message can be communicated using "bytes" of 5-bits - for which the entropy of an N symbol message would be $5N$.

However, we have assumed that each symbol occurs in a message with equal probability. In such a case the total number, Ω, of different message, which we could send would be

$$\Omega \ = \ 32^N,$$

giving us a Shannon entropy

$$H \ = \ \log_2 \Omega \ = \ 5N$$

.

This is certainly not the case. For a text in English the letter 'E' occurs with a frequency of 12%, whereas 'Z' occurs with a frequency of 0.07%. The most common symbol is the space which occurs with a frequency of about 18%. Information theory can be used to encode all the symbols unambiguously in such a way that the most frequently used are encoded with the smallest number of symbols, enabling the message to be communicated as efficiently as possible - i.e. using the smallest number of bits.

The entropy of the message is now more complicated. For each symbol, the Shannon entropy is

$$h \ = \ \sum_{i=0}^{31} p_i \log_2 \left(\frac{1}{p_1} \right),$$

where p_i is is probability frequency of a symbol being i. $\log_2(1/p_o)$ is called the "surprise" factor - the less frequent the occurrence of a symbol the greater the surprise at finding it!. Using the frequencies of symbols found in several long English language texts, the entropy of a message of N symbols is reduced from

In the case of information contained in a message, there is little to gain by introducing a conjugate variable μ_i for each symbol i, since we know the probability distribution by studying a large number of texts (interestingly the entropy per symbol varies very little whether the sample used to obtain the probabilities is the complete works of Shakespeare or the King James bible.

So far, we have assumed that the probability of a symbol being a letter i is independent of the symbol which precedes or follows. This is not the case. A further economizing on the number of bits required to communicate a message by noticing that for any given language some sequences of letters are more frequent than others. In English, for example, we don't use diphthongs very often so that a vowel is more likely to be followed by a consonant and the letters 'S', 'C', 'T' and 'P' are often followed by 'H'. A reduction in the entropy per symbol of a message can be obtained by considering the frequency of pairs of symbols. We do not go into such details here, but this forms an important part of information theory.

1.7 Conditional Entropy

Consider a system for which the macroscopic states are labelled by the values of two quantities Y and Z.

Let $p(y, z)$ be the probability that these labels take the values y and z respectively.

The Shannon entropy is then

$$H(Y, Z) \ = -\sum_{y,z} p(y, z) \log_2(p(y, z,). \tag{1.7.1}$$

If the probabilities to find the system in the state y and z are totally uncorrelated then

$$p(y, z) = p(y)p(z)$$

and the entropy is

$$H(Y, Z) \ = -\sum_{y} p(y) \sum_{z} p(z) \log_2(p_z) - \sum_{z} p(z) \sum_{y} p(y) \log_2(p_y) \ = \ H(Y) + H(Z)$$

The joint entropy is simply the sum of the entropies for the cases where the macrostate is labelled by either Y or Z.

However, if the probabilities are correlated, so that the probability of Z taking the value z depends on the value of Y as a result of soime interaction between the quantities Y and Z, then we need to use Bayes theorem, which tells us that the probability of finding $Y = y$ and $Z = z$ is

$$p(y, z) \ = \ p(y|z)p(z),$$

where $p(y|z)$ is the probability to find $Y = y$ given that $Z = z$.

The essence of Bayes theorem is the fact that we could equally have written

$$p(y, z) \ = \ p(z|y)p(y),$$

and equating the two gives a relation between the two probabilities $p(y)$ and $p(z)$ given the two conditional probabilities $p(y|z)$ and $p(z|y)$ (the probability of finding $Z = z$, given a value of y).

The Shannon entropy is now

$$H(x, y) \ = \ \sum_{y,z} p(z)p(y|z) \left(\log_2(p(y|z) + \log_2(p_z)\right). \tag{1.7.2}$$

This differs from $H(Z) + H(Y)$ unless $p(y|z) = p(y)$, i.e. there is no correlation.

The difference between $H(Y, Z)$ and $H(Y) + H(Z)$ is called the "mutual information", $I(Y, Z)$, where

$$I(Y, Z) = H(Y) + H(Z) - H(Y, Z) \tag{1.7.3}$$

If the quantities Y and Z are completely correlated then

$$p(y, z) = p(y)\delta_{yz}$$

and the Shannon entropy

$$H(Y, Z) \; = \; H(Y) \; = \; H(Z)$$

reflecting the fact that the macrostate is completely determined by specifying the value of *either* Y *or* Z.

For situations between the two extremes (partial correlation) we have a "degree of disorder", which is quantified by the "equivocation" or "entropy of disorder.

$$H(Y|Z) \; \equiv \; H(Y, Z) - H(Z). \tag{1.7.4}$$

This takes the values $H(Y)$ if the quantities are totally uncorrelated (maximum disorder) and zero if they are totally correlated (maximum disorder).

1.7.1 How untidy is my office?

As an example, we can try to quantify the untidiness of our office. Imagine a bookcase with N slots each of which can hold one book. The slots are labelled y which takes values from 0 to $N - 1$ from left to right. We also have N books which are labelled z taking values from 0 to $N - 1$ in some order - this could be alphabetical order of author or book-size. At this point we note the subjectivity of entropy since the observer can stipulate which subset of all the quantities labelling a microstate, are actually used to label the macrostate.

Now of we select at random a book from one of the slots, the probability that the slot is slot i is $p(y) = 1/N$. If the books are arranged in a totally untidy way the probability of the book being book j is also $p(z) = 1/N$ irrespective of the value of i (no correlation).

In this case the Shannon entropy is

$$H(Y, Z) \; - \sum_{x,y=0}^{N-1} \frac{1}{N^2)} \log_2 \left(\frac{1}{N^2} \right) \; = \; 2 \log_2 N.$$

The Shannon entropy of either the slots or the book is $\log_2 N$ and so we have an entropy of disorder

$$H(Y|Z) \; = \; \log_2 N.$$

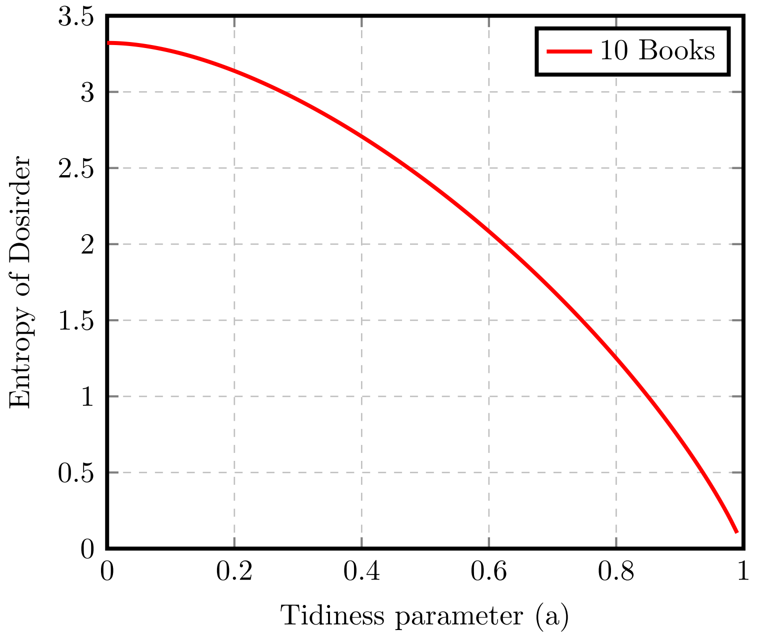


Figure 4: Entropy of disorder (equivocation entropy) for a bookshelf of 10 books as a function of tidiness parameter

On the other hand, if the book are exactly in their correct place then the probabilities are totally correlated and

$$p(y,z) \;=\; \frac{\delta_{yz}}{N}$$

The Shannon entropy is

$$H(Y,Z) \;=\; -\sum_{y,z=0}^{(N-1)} \frac{\delta_{yz}}{N}\log_2\left(\frac{1}{N}\right) \;=\; \log_2 N,$$

and the entropy of disorder is zero.

Between these two extremes we could have partially correlated probability distribution for which

$$p(y,z) = a\delta_{yz} + \frac{(1-a)}{N},$$

where the parameter a measures the degree of correlation and takes values between 0 and 1. Using $p(z) = 1/N$ this gives us the joint probability

$$p(y,z) \;=\; \frac{a}{N}\delta y,z + \frac{(1-a)}{N^2}$$

and inserting this into the expression for the Shannon entropy we find

$$H(Y,Z) \;=\; -\left(a+\frac{(1-a)}{N}\right)\log_2\left(a+\frac{(1-a)}{N}\right)-\frac{(1-a)N(N-1)}{N^2}\log_2\left(\frac{(1-a)}{N^2}\right)$$

and an entropy of correlation

$$H(Y|Z) \;=\; H(Y,Z)-\log_2(N),$$

which is plotted against the parameter a in Fig.4 for the case $N=10$.

1.8 Irreversible Processes.

The principle of maximum entropy, which tells us that the most probable distribution of microstates for a given macrostate is that which maximizes the entropy tells us what the entropy of a system is when it is in equilibrium.

For an interacting system, the interactions will give rise transitions between the microstates. Most interactions are invariant under time reversal, which means that the probability of a transition from a microstate $\{x\}$ to a microstate $\{x_i'\}$ is the same as the probability of a transition from microstate $\{x_i'\}$ to a microstate $\{xi\}$.

However, if $p(\{x'\}) \;<\; p(\{x\})$ the for an ensemble of a large number of copies of the system, there will be more transitions from $\{x_i'\}$ to $\{xi\}$ than from $\{x\}$ to $\{xi'\}$. The transitions will cause th system to fluctuate around a distribution with the largest probability, A state with the largest probability is then the equilibrium state and the interactions will only effect fluctuations around this equilibrium.

In other words, the entropy of a system in equilibrium for a given macrostate, is the maximum entropy that the system can have for that given macrostate.

The minimum entropy that a system can have is zero, corresponding to the state in which all of the microstate labels $\{x\}$ are known.

It is possible to prepare a state which is not in equilibrium – the entropy of the system will be less than its maximum value and will increase as the system makes transitions to its equilibrium state.

The fact that the system in a non-equilibrium state has to be "prepared" is the essence of the resolution of the apparent contradiction between the statement that entropy never decreases and the fact that the interactions between elements of a system are (to a very good approximation) invariant under time reversal.

If we make a video of a (french) billiard table (no pockets) showing billiard balls colliding against each other and bouncing off the cushions, and run it backwards, we would not see anything surprising. This is because the dynamics of the collisions between the balls or between the balls and the cushions is time reversal invariant. On the other hand, if we film a break in snooker in which a white ball crashes into a set of red balls arranged in a triangular configuration, after which the red balls move off in various different directions, then this movie would look very odd when run backwards. This is because the transition from an orderly state in which the red balls form a triangle has a lower entropy than the configuration in which the red balls are moving off in different directions. The initial state in which the red balls are organized is *not* an equilibrium state. The break is an irreversible process in which the entropy increases. After a few shots into the game, an approximate equilibrium state has been achieved and from then on running a movie backwards would not seem so strange – the transitions between different configurations of the balls (different microstates) are transitions between different microstates with maximum entropy. It is important to note that to create the initial, non-equilibrium state, some work had to be done on the system (by the match umpire) in order to arrange the red balls in the triangle for the start of the frame. The entropy of the engine that generated this work was increased, since energy had to be drawn form a hot reservoir, some of which is converted into work and the remaining energy is dissipated into a lower temperature reservoir. In the process of creating the initial state, entropy is transferred from the set of red balls to the engine (e.g. the umpire) - the total entropy of the balls plus the engine does not decrease.

We return yet again to the example of a set of N coins. We supposed that these coins interact with some external potential which causes a coin to flip with probability λ per unit time. Since the interaction is invariant under time reversal the probability of flipping from heads to tails is the same as the probability to flip form tails to heads.

Suppose that at some time t there are $r(t)$ coins with heads up and $N - r(t)$ with tails up. After a small interval, δt of time we have (averaged over an ensemble of a large number of copies of the N coins)

$$r(t + \delta t) \;=\; r(t) + \lambda \delta_t \left(N - r(t) - r(t)\right),$$

reflecting the fact that on average of the $N - r(t)$ coins with tails up, a fraction $lambba \delta t$ of them will flip to heads-up, but also an equal fraction of the $r(t)$ coins with heads-up will flip back to tails-up.

In the limit $\delta t \;\to\; 0$, this gives us a time-evolution differential equation

$$\frac{dr(t)}{dt} \;=\; \lambda \left(N - r(t)\right).$$

Supposing that at $t = 0$ we had the completely ordered state in which all coins were tails-up ($r(0) = 0$), the solution is

$$r(t) \;=\; \frac{N}{2}\left(1 - e^{-2\lambda t}\right).$$

Note that as $t \;\to \infty$, the system reaches its equilibrium state in which half of the coins are heads-up - this is the macrostate with the largest number of microstates and therefore the equilibrium value.

The Shannon entropy at time t is then

$$H(t) \;=\; \log_2\left(\frac{N!}{(N - r(t)!)r(t)!}\right) \;\approx\; N \log_2\left(\frac{2}{(1 + e^{-2\lambda t})}\right) + \frac{N}{2}\left(1 - e^{-2\lambda t}\right)\log_2\left(\frac{(1 + e^{-2\lambda t}}{1 - e^{-2\lambda t}}\right).$$

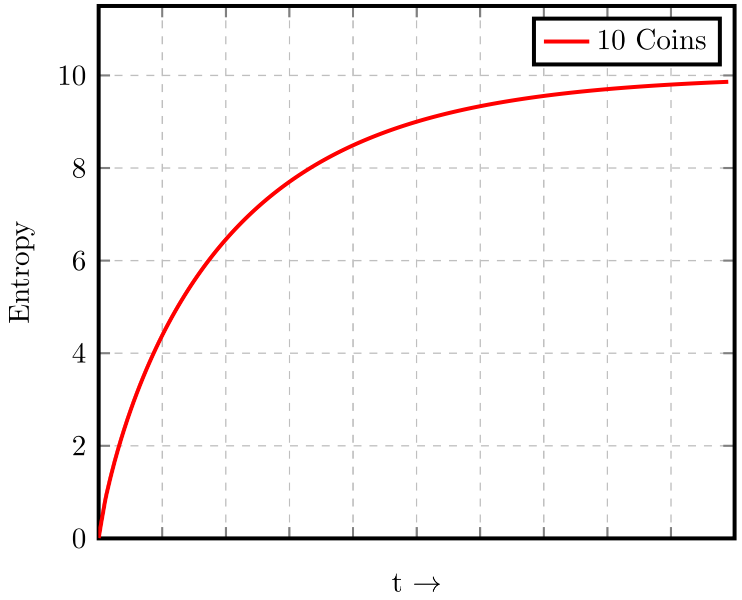


Figure 5: Time dependence of entropy of 10 coins, with initial state for whioch all coins a re tails-up.

This is zero for $t = 0$ where we have a completely ordered state and increases monotonically to its equilibrium (maximum) value of N as $t \rightarrow \infty$. *The entropy never decreases.* For the case of 10 coins, the time dependence of the Shannon entropy is shown in Fig.5.

1.9 Phase-Space and Louiville's Theorem

For a system consisting of N spinless particles the microstate can be labelled by specifying the position three-dimensional vector, $\mathbf{x}_i$, and three dimensional momentum vector $\mathbf{p}_i$ for each of the N-particles. A microstate may therefore be represented as a point in a $6N$ dimensional state whose axes are the components of $\mathbf{x}_i$ and $\mathbf{p}_i$. Such a hyperspace is called "phase-space".

In classical mechanics, a microstate can be a point anywhere in phase space and so there are a continuously infinite number of possible microstates. A sum over microstates then becomes an integral over all phase space

$$\sum_{\{x\}} \rightarrow \prod_{i=0}^{N-1} d^3\mathbf{p}_i \prod_{j=0}^{N-1} d^3\mathbf{x}_j,$$

and the probability is replaced by a probability density, $\rho\left(\{\mathbf{p}_i\}, \{\mathbf{x}_j\}\right)$, where

$$\rho\left(\{\mathbf{p}_i\}, \{\mathbf{x}_j\}\right) \prod_{i=0}^{N-1} d^3\mathbf{p}_i \prod_{j=0}^{N-1} d^3\mathbf{x}_j$$

is the probability to find the system within a given infinitesimal volume of phase space.

A volume element in phase-space has dimensions and so the probability density also has dimensions. This makes it awkward to take its logarithm for the purpose of calculating the entropy. We therefore "borrow", from quantum physics the idea that due to Heisenberg's uncertainty principle a point in phase-space is replaced by a cell of dimension h^{3N}. The probability density, multiplied by h^{3N} and interpreted as a probability to find the system in a particular cell and the integral over phase-space is again a sum over all such cells. For classical systems this usually makes no difference as the phase-space integrals can be approximated by discrete sums.

If we know exactly the point occupied by the system, then we know everything about the system and its Shannon entropy is zero. On the other hand, if we only know the probability density, then the Shannon entropy is given by

$$H \;=\; -\int \prod_{i=0}^{N-1} d^3\mathbf{p}_i \prod_{j=0}^{N-1} d^3\mathbf{x}_j \, \rho\left(\{\mathbf{p}_i\},\{\mathbf{x}_j\}\right)\, \log_2\left(h^{3N}\rho\left(\{\mathbf{p}_i\},\{\mathbf{x}_j\}\right)\right) \tag{1.9.1}$$

For a macrostate at equilibrium (maximum entropy), the probability density is constant over the region of phase-space which is compatible with the labelling of the macrostate, and zero outside this region. In this case the Shannon entropy becomes

$$H(\{y_a\}) \;=\; \log_2 \Omega\left(\prod_a Y_a(\{\mathbf{p}_i\},\{\mathbf{x}_j\}) = y_a\right),$$

where $\Omega\left(\prod_a Y_a(\{\mathbf{p}_i\},\{\mathbf{x}_j\}) = y_a\right)$ is the volume of the region of phase space for which the quantities which define a macrostate take the values, y_a, which label the macrostate.

A classical system whose behaviour is determined by a Hamiltonian (i.e. no dissipative forces), sweeps out a well-defined path in phase-space. Hamilton's equations can be solved (in principle) such that if the phase-space point $\{\mathbf{p}_i\},\{\mathbf{x}_j\}$ is known at time $t=0$, one can predict, the phase-space point, $\{\mathbf{p}'_i\},\{\mathbf{x}'_j\}$, which the system will occupy at time t. Conversely if we know the microstate of the system is time t, we can use the (time reversed) Hamilton's equations to determine the initial microstate at time $t=0$. Furthermore, even if we do not know the the initial microstate, but we know the probability density then classical mechanics allows us to determine the probability density at a later times t.

In particular, we can use Hamiltonian mechanics to derive Louiville's theorem, which tells us that if the probability density at time $t=0$ occupies a certain volume, Γ in configuration space, then as the system, evolves, the region occupied by the non-zero probability density can change shape, but its volume remains unchanged.

As a simple example consider a free particle moving in one dimension. The phase-space is shown in Fig.6. At time $t=0$ the particle is known to be between x_0 and x_1 and with momentum between p_0 and p_1. The region of phase-space with non-zero probability density is a rectangle, shown on the left in Fig.6. At a later time the increase in position is larger for the larger momentum than for the lower momentum. The allowed range of x is still $(x_1 - x_0)$,

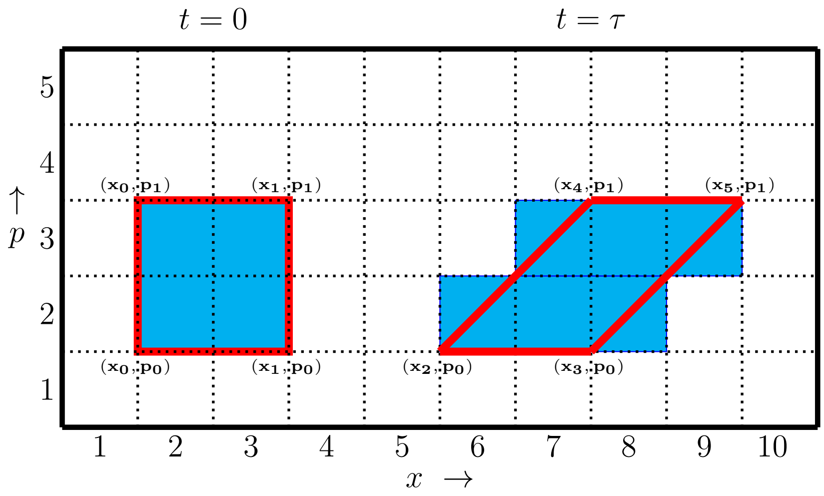


Figure 6: Phase-space diagram for particle moving in one dimension. At $t = 0$ the has a non-zero probability density for position x between x_0 and x_1, and momentum p between p_0 and p_1. The red lines are the boundaries of the "volume" occupied by the particle. The volume is the same in the $t = 0$ and $t = \tau$ states. The pale blue cells are the course-grained cells which are occupied by the phase-space of the particle. This volume is larger at $t = \tau$ than at $t = 0$

and the momentum (for a free particle) does not change, so that it is still between p_0 and p_1. The phase space region with non-zero probability density is now a parallelogram (shown on the right in Fig.6). This region is a different shape from the original region, but the area is the same as the are of the original rectangle, as required by Louiville's theorem.

This then appears to forbid the increase in entropy of a system as it reaches equilibrium. This apparent paradox is resolved if we introduce "coarse graining". We account for the fact that we cannot pin down the exact phase-space position with total precision. but only up to a certain resolution. This means that we granulate phase-space by introducing finite volume cells into the phase-space and rather than pin-point the exact point in phase-space of a given microstate, we can only specify into which of these cells it falls. Returning to the case of a single particle moving in one dimension, this is shown by the grid in Fig.6. The blue cells are the ones that are partially or totally occupied. We see that the number of blue cells for the initial distribution is four, whereas for distribution at time t, there are six blue cells. This means that although occupied volume the exact phase-space remains unchanged, the occupied volume of the granulated phase-space has indeed increased, leading to an increase in entropy.

The course-grained probability density is the probability density averaged over a particular course-graining cell. The grouping of many microstates into a single course-grained cell is equivalent to defining a macrostate. The coarse grained probability density is

$$\rho_{cg}(\{y\}) \ = \ \int \prod_{i=0}^{N-1} d^3\mathbf{x}_i \, d^3\mathbf{p}_i \prod_a \delta\left(Y_a\left(\{\mathbf{x}_i\}, \{\mathbf{p}_j\}\right) - y_a\right)$$

The entropy of a macrostate is the logarithm of the volume of phase-space in that particular course-graining cell. If the system is not initially in an equilibrium state then this volume can grow as it evolves in time, increasing the entropy until equilibrium is achieved.

1.10 Thermodynamics

So far we have considered entropy in statistics and information theory. The definition of entropy as used inn thermodynamics is (almost) the same as the definition of the Shannon entropy, where the macrostate is determined by specifying

1. The internal energy, U of the system. This is the sum of the energies of the particles on the system, but does *not* include the bulk kinetic energy of the system due to the motion of the centre-of-mass of the system or the bulk potential energy due to the positon of the centre-of-mass in a force field.
2. The volume in which the system is confined (this is usually only important in the case of gases.)
3. The number of particles, N, in the system.

Other properties, such as the total spin component in a given direction, may also be specified.

A further difference between the definition of entropy used in thermodynamics and the Shannon entropy is that the logarithms are taken to be natural logarithms and the thermodynamic entropy carries an overall factor of the Boltzmann constant, κ_B. The Shannon entropy is in units of bits (this is more convenient for information theory and computation) whereas thermodynamic entropy has units of joules per degree Kelvin (J/K). Thus the relation between Shannon entropy H, and thermodynamic entropy, S is

$$S = \kappa_B \ln 2 \, H.$$

There are several different types of ensembles used in thermodynamics.

1. **Microcanonical Ensemble:** This is a large number of copies of the thermodynamic system all of which have the same internal energy, volume and number of particles.
2. **Canonical Ensemble:** This is a large number of copies of the system confined to the same volume and with the same number of particles, but different internal energies. The average internal energy is deduced from the conjugate variable, $\beta \equiv 1/(\kappa_B T)$. This serves as a definition of temperature.
3. **Grand Canonical Ensemble:** This is an ensemble of copies of the system which not only have different energies but also different numbers of particles. The variable conjugate to the particle number multiplied by $\kappa_B T$) is called the "chemical potential" .

4. **Gibbs Ensemble.** This is an ensemble of copies of the system with the same number of particles, but different energies and also different volumes. The variable conjugate to volume is βP where P is the pressure.

The Boltzmann definition of entropy uses the quantity Ω which is the number of microstates for a given macrostate, specified by total internal energy, U, number of particles, N and volume V.

$$\Omega(U, V, N) \;=\; \sum_{\{x\}} \delta(U(\{x\}) - U)\delta(V(\{x\}) - V)\delta(UN\{x\}) - N).$$

The Boltzmann definition of entropy, S,, used in thermodynamics is

$$S(U, V, N) \;=\; \kappa_B \ln \Omega(U, V, N) \tag{1.10.1}$$

It coincides with the Shannon definition of entropy (up to a constant factor $\kappa_B \ln 2$ under the assumption that all microstates contributing to a given macrostate occur with equal probability.

Very often, we require the entropy as a function of temperature rather than internal energy. This can be obtained using the relation between temperature and internal energy

$$\frac{1}{T} \;=\; \frac{\partial S(U, V, N)}{\partial U}, \tag{1.10.2}$$

which is the inverse of the expression for the average value of U for a canonical ensemble, obtained by partial differentiation of the partition function. (1.10.2) can be inverted to find U as as function of T and inserted into (1.10.1) to obtain the entropy as a function of temperature. However, such an expression for entropy is usually more easily obtained by working directly with a canonical ensemble and calculating the partition function.

1.10.1 Example 1: Ensemble of spin-$\frac{1}{2}$ particles

Consider an ensemble of N spin-$\frac{1}{2}$ particles with magnetic moment μ in a uniform magnetic field, B, in the z-direction. Neglect the mutual interactions between the spinning particles.

The microstates are labelled by $s_z^{(1)}, s_z^{(2)} \cdots s_z^{(N)}$ where each s_z can take the values $\pm\frac{1}{2}$ The energy corresponding to a given microstate is

$$E_{n_+} \;=\; \mu B J_z,$$

where

$$J_z \;= \sum_{a=1}^{N} s_z^{(a)} \;=\; \frac{1}{2}\left(2n_+ - N\right),$$

n_+ boing the number of spin-up particles. Thus fixing the value of n_+ specifies the macrostate. It is most convenient to use the canonical ensemble.

The partition function may therefore be written

$$Z(\beta) \;=\; \sum_{n_+=0}^{N} {}^{N}C_{n+}\, e^{-\beta\mu B n_+}\, e^{\beta\mu B N/2} \qquad (1.10.3)$$

where

$${}^{N}C_{n+} \;=\; \frac{N!}{(N-n_+)!n_+!}$$

is the number of ways of selecting n_+ spins from a total of N. This is a binomial coefficient and so terms may be summed using the binomial theorem to yield

$$Z(\beta) \;=\; 2^N \cosh\left(\frac{1}{2}\beta\mu B\right)^N \qquad (1.10.4)$$

The internal, energy is then

$$U \;=\; -\frac{\partial}{\partial\beta}\ln Z(\beta) \;=\; -\frac{1}{2}N\mu B\tanh\left(\frac{1}{2}\beta\mu B\right), \qquad (1.10.5)$$

Here U strictly means the value of the total energy of the spins, averaged over all the copies of the system in the canonical ensemble. Previously this was denoted by $\langle U\rangle$. Here and henceforth we drop the $\langle\ \rangle$ The entropy (as a function of temperature) is given by

$$S(T) \;=\; \kappa_B\ln(Z) + \frac{1}{T}U \;=\; \kappa_B N\Bigg[\ln 2 + \ln\Bigg(\cosh\Bigg)\frac{\mu B}{2\kappa_B T}\Bigg)\Bigg) - \frac{\mu B}{2\kappa_B T}\tanh\left(\frac{\mu B}{2\kappa_B T}\right)\Bigg]\Bigg) \qquad (1.10.6)$$

Note that when the applied magnetic field is zero the entropy is simply $N\kappa_B\ln 2$ which is the logarithm of the number of possible microstates for the N spin-$\frac{1}{2}$ particles (times κ_B), but if a magnetic field is applied one knows the average value of J_z for an ensemble of such systems and the entropy decreases.

We could have arrived at (1.10.5) and (1.10.6) starting with a microcanonical ensemble of systems of N spins, all of which have a total energy $U = \mu B(N - 2n_+)$. The entropy is

$$\begin{aligned} S(U) \;&=\; \kappa_B\ln\Omega(n_+) \;=\; \kappa_B\ln\left(\frac{N!}{(N-n_+)!n_+!}\right) \\ &\approx\; \kappa_B\left(N\ln N - (N-n_+)\ln(N-n_+) - n_+\ln(n_+)\right) \\ &=\; N\ln\left(\frac{2N}{N+2U/(\mu B)}\right) - \frac{1}{2}\left(N - \frac{2U}{\mu B}\right)\ln\left(\frac{N+2U/(\mu B)}{N-2U/(\mu B)}\right) \qquad (1.10.7) \end{aligned}$$

Differentiating w.r.t U we obtain an expression for the temperature T

$$\frac{1}{T} \;=\; \frac{\partial S(U)}{\partial U} \;=\; -\frac{\kappa_B}{\mu B}\ln\left(\frac{N+2U/(\mu B)}{N-2U/(\mu B)}\right).$$

This is the inverse of (1.10.5), and inserting (1.10.5) into (1.10.7) we recover (1.10.6).

1.10.2 Example 2: Perfect Gases - Sackur tetrode Formula

The entropy of a perfect gas was first calculated independently by Otto Sackur and Hugo Tetrode on 1911. They used a microcanonical ensemble, but it is much easier if we consider a canonical ensemble of identical mono-atomic particles of mass m in thermal equilibrium at inverse temperature β. Thw paricles are at position $\mathbf{x}_i$ with momentum $\mathbf{p}_i$, $i = 1 \cdots N$.

The partition function is

$$Z(\beta, V, N) \;=\; \frac{1}{N!} \int \frac{1}{h^N} \prod_{i=1}^{N} d^3\mathbf{x}_i \prod_{i=1}^{N} d^3\mathbf{p}_i \exp\left(-\beta E(\{\mathbf{x}_i\}, \{\mathbf{p}_i\})\right)$$

The factor $1/N!$ accounts for the fact that it is impossible to distinguish between microstates which are related by the interchange of identical particles. This is again "borrowed" from quantum physics, but do *not* at this stage account for the symmetry or antisymmetry of wavefunctions under interchange of identical particles.

For non-interacting particles the total (internal) energy is the sum of the energies, ϵ_i of each particle

$$E \;=\; \sum_i \epsilon_i,$$

so that the partition function factorizes

Thus we have

$$Z(\beta, V, N) \;=\; \frac{1}{N!} \left[\frac{1}{h^3} \int d^3\mathbf{x} d^3\mathbf{p} \exp\{-\beta\epsilon(\mathbf{x}, \mathbf{p})\} \right]^N \tag{1.10.8}$$

For a free particle of mass m, the (non-relativistic) energy is given by

$$\epsilon(\mathbf{x}, \mathbf{p}) \;=\; \frac{p^2}{2m}$$

This is independent of $\mathbf{x}$ and so the integral over $d^3\mathbf{x}$ list simply generates a factor of V - the volume into which the particle is confined.

This leads to (setting $h = 2\pi\hbar$)

$$\begin{aligned} Z(\beta, V, N) &= \frac{1}{N!} \left[\frac{V}{(2\pi\hbar)^3} \int d^2\mathbf{p} \exp\{-\beta \frac{p^2}{2m}\} \right]^N \\ &= \frac{1}{N!} \left[\frac{V}{(2\pi\hbar)^3} \int dp 4\pi p^2 \exp\{-\beta \frac{p^2}{2m}\} \right]^N \\ &= \frac{1}{N!} \left[V \left(\frac{m}{2\pi^2\hbar^2\beta} \right)^{3/2} \right]^N \qquad (1.10.9) \end{aligned}$$

The partition function for an ensemble of N such (identical) molecules is

$$Z(\beta, V, N) \;=\; \frac{1}{N!} V^N \left(\frac{m}{2\pi^2\hbar^2\beta}\right)^{3N/2} \tag{1.10.10}$$

The internal total energy, $U =$, of the ensemble is given by

$$U \;=\; -\frac{\partial}{\partial\beta}\ln Z \;=\; \frac{3N}{2}\kappa_B T \tag{1.10.11}$$

(equipartition of energy)

The entropy is

$$S(T, V, N) \;=\; -\kappa_B \ln N! + \kappa_B N \left(\ln V + \frac{3}{2}\ln\left(\frac{m\kappa_B T}{2\pi^2\hbar^2}\right) + \frac{3}{2}\right) \tag{1.10.12}$$

For large N we can use Stirling's approximation and write

$$\ln N! \;\approx\; N\left(\ln N - 1\right),$$

so that finally we get

$$S(T, V, N) \;=\; N\kappa_B \left(\ln\left(\frac{V}{N}\right) + \frac{3}{2}\ln\left(\frac{m}{2\pi^2\hbar^2\beta}\right) + \frac{5}{2}\right) \tag{1.10.13}$$

Since the volume V is extensive, i.e. proportional to N, we see that the entropy is also extensive. However, this would *not* have been the case if we had forgotten the prefactor of $1/N!$ in the expression for the partition function of the ensemble.

1.10.3 Pressure

In the case of a gas, the partition function is a function of temperature, volume and number of particles. The entropy is given by

$$S \;=\; \kappa_B \ln Z + \frac{U}{T} \tag{1.10.14}$$

Taking the deriviate of this we have

$$dS \;=\; \kappa_B d(\ln Z) + \frac{dU}{T} - \frac{U}{T^2}dT \tag{1.10.15}$$

Since Z is a function of both temperature, T, and volume, V we have

$$d(\ln Z) \;=\; \frac{\partial \ln Z}{\partial T}_{V} dT + \frac{\partial \ln Z}{\partial V}_{|T} dV \tag{1.10.16}$$

From the expression for U we have

$$\frac{\partial \ln Z}{\partial T} dT \; = \; \frac{U}{\kappa_B T^2}.$$

Define the quantity "pressure" P as

$$P \; = \; \kappa_B T \frac{\partial \ln Z}{\partial V}_{|T} \tag{1.10.17}$$

and inserting into (1.10.15) and (1.10.16) we have

$$TdS \; = \; dU + PdV \tag{1.10.18}$$

Note that for a partition function for a perfect gas given by (1.10.10), we recvoer the perfect gas equation of state

$$P \; = \; \frac{N\kappa_B T}{V}.$$

If we compare this with the expression from the first law of thermodynamics for $đQ$ a small quantity of heat introduced to a system

$$đQ \; = \; dU + dW,$$

we see that this is consistent with (1.10.18) if we identify P as mechanical pressure such that

$$dW \; = \; PdV \tag{1.10.19}$$

and leads to the second law of thermodynamics

$$đQ \; = \; TdS \tag{1.10.20}$$

In thermodynamics, we define the Helmloltz free energy, F as

$$F(T, V, N) \; \equiv \; -\kappa_B T \ln Z(T, V, N) \tag{1.10.21}$$

so that (1.10.14) can be rewritten as

$$F \; = \; U - TS. \tag{1.10.22}$$

1.10.4 Gibbs Ensemble

Alternatively, we could use a Gibbs ensemble of systems that have different volumes (but the same number of particles) with an average value determined by the conjugate variable $P/(\kappa_B T)$. For a given phase-space point, the volume occupied by the gas is s function of the positions $\mathbf{x}_i$ of the N particles in the system - it is the maximum volume of a tetrahedron formed from four of the particle positions:

$$V(\{\mathbf{x}_i\}) \;=\; \max_{i,j,k,l}\left((\mathbf{x}_i - \mathbf{x}_j)\cdot(\mathbf{x}_i - \mathbf{x}_j)\wedge(\mathbf{x}_i - \mathbf{x}_l)\right).$$

The partition function is then a function of pressure and temperature

$$Z_G(P,T) \;=\; \frac{1}{h^{3N}}\int\prod_{i=0}^{N-1} d^3\mathbf{x}_i \prod_{j=0}^{N-1} d^3\mathbf{p}_i \exp\left(-\beta(E(\{\mathbf{x}_i\},\{\mathbf{p})_I\}) + PV(\{\mathbf{x}_i\})\right),$$

where the subscript G indicates that the partition function is calculated in the Gibbs ensemble and is a function of P and T.

The entropy is given by

$$S \;=\; \left(\kappa_B \ln Z_G + \frac{U}{T} + \frac{PV}{T}\right),$$

where U means the average internal energy of the ensemble given by

$$U \;=\; \kappa_B T^2 \frac{\partial Z_G}{\partial T} \tag{1.10.23}$$

and V is the average volume given by

$$V \;=\; -\kappa_B T \frac{\partial Z_G}{\partial P}. \tag{1.10.24}$$

Using the chain rule

$$dS \;=\; \frac{\partial Z_G}{\partial T} dT + \frac{\partial Z_G}{\partial P} dP,$$

and the definitions of and U and V given by (1.10.23) and (1.10.24), we recover (1.10.18).

The Gibbs free energy, G is defined as

$$G(T,P,.N) \;=\; \kappa_B \ln Z_G \;=\; U + PV - TS. \tag{1.10.25}$$

1.11 Identical Particles

Accounting for the indistinguishability of identical particles as by dividing the partition function by $N!$, as in (1.10.8) is not quite correct. It is more properly accounted for by labelling the microstates in terms of "Fock-space" states $(n_0, n_1, n_2 \cdots)$ where n_i is the number of particles which occupy a single particle state labelled by i - this could be the point in one-particle (6-dimensional) phase space for a single particle supplemented with a label associated with the particle's spin state.

It is simpler to consider a grand canonical ensemble, in which the total number of particles differs form one copy of the system to another, but possesses an average value $\langle N\rangle$ determined by the dependence of the grand partition function $\mathcal{Z}$, on a conjugate variable $\beta\mu$, where μ is called the 'chemical potential".

The grand partition function can be written as

$$\mathcal{Z}(\beta, V, \mu) \;=\; \prod_i \sum_{n_i} \exp\left(\beta(\mu - E_i)n_i\right) \tag{1.11.26}$$

There are two types of identical particles

- **Bosons:** These are particles with integer spin and any number of particles can exist in a given state. For such particles

  $$\sum_{n_i=0}^{\infty} \exp\left(\beta(\mu - E_i)n_i\right) \;=\; \frac{1}{(1-\exp\left(\beta(\mu - E_i)\right))},$$

  so that

  $$\mathcal{Z}(\beta, V, \mu) \;=\; \prod_i \frac{1}{(1-\exp\left(\beta(\mu - E_i)\right))}. \tag{1.11.27}$$

- **Fermions** These are particles with half-odd integer spin, for which n_i can only take the values 0 or 1 so that

  $$\sum_{n_i=0}^{1} \exp\left(\beta(\mu - E_i)n_i\right) \;=\; \left(1+\exp\left(\beta(\mu - E_i)\right)\right),$$

  so that

  $$\mathcal{Z}(\beta, V, \mu) \;=\; \prod_i \left(1+\exp\left(\beta(\mu - E_i)\right)\right). \tag{1.11.28}$$

Let us consider a grand canonical ensemble of systems of free spin-0 bosons of mass m, confined to a volume V at temperature $T = (\kappa\beta)^{-1}$, and a chemical potential mu.

It is difficult to calculate the produce over all allowed states and so we take the (natural) logarithm and calculate the sum over allowed states.

$$\ln \mathcal{Z}(\beta, V, \mu) \;= -\sum_i \ln\left(1-\exp\left(\beta(\mu - E_i)\right)\right)$$

The sum over all allowed states maybe approximated by an integral over phase space divided by the phase-space volume h^3 of each state. It turns out that this approximation excludes the ground state whose energy is zero, so that this term has to be added in by hand, yielding

$$\ln \mathcal{Z}(\beta, V, \mu) \;=\; -\frac{1}{h^3}\int d^3\mathbf{x}\, d^2\mathbf{p} \ln\left(1-\exp\left(\beta(\mu - p^2/2m)\right)\right) + \ln\left(1-e^{\beta\mu}\right)$$

The integral over $\mathbf{x}$ yields the volume V and the integral over the angular parts of the momentum yields a factor of 4π, so that we may write

$$\ln \mathcal{Z}(V, \beta, z) \;=\; \frac{2\pi V}{h^3}\left(\frac{2m}{\beta}\right)^{3/2}\int_0^\infty dy\, y^{1/2}\, \ln\left(1 - ze^{-y}\right) + \ln\left(1 - z\right)$$

where we have changed variable to

$$y \;=\; \beta\frac{p^2}{2m}$$

and introduced the "fugacity"

$$z \;\equiv\; e^{\beta\mu}$$

The integral over y can be performed in terms of a polylogarithm function $\mathrm{L_{i5/2}}(z)$, so that we end up with the result

$$\ln \mathcal{Z}(V, \beta, z) \;=\; \frac{V}{h^3}\left(\frac{2\pi m}{\beta}\right)^{3/2}\mathrm{Li}_{5/2}(z) + \ln\left(1 - z\right) \qquad (1.11.29)$$

For the case of fermions, we get a similar result with $\mathrm{Li}_{5/2}(z)$ replaced by $-\mathrm{Li}_{5/2}(-z)$.

The pressure P is given by

$$P \;=\; \frac{1}{\beta}\frac{\partial}{\partial V}\ln \mathcal{Z} \;=\; \frac{1}{\beta V}\ln \mathcal{Z}, \qquad (1.11.30)$$

The internal energy, U (we mean the average value but drop the $\langle\rangle$) is given by

$$U \;=\; -\frac{\partial \ln \mathcal{Z}}{\partial \beta}_{|z,V} \;=\; \frac{3}{2\beta}\ln \mathcal{Z} \qquad (1.11.31)$$

The number of particles N is given by

$$N \;=\; \frac{1}{\beta}\frac{\partial \ln \mathcal{Z}}{\partial \mu}_{|\beta,V} = z\frac{\partial}{\partial z}\ln \mathcal{Z} \;=\; \frac{V}{h^3}\left(\frac{2\pi m}{\beta}\right)^{3/2}\mathrm{Li}_{3/2}(z) + \frac{z}{(1 - z)} \qquad (1.11.32)$$

and the entropy is given by (using $\ln z = \beta\mu$)

$$S \;=\; \kappa_B \ln \mathcal{Z} + \frac{U}{T} - \frac{\mu N}{T} \qquad (1.11.33)$$

1.11.1 Entropy of Mixing

Consider two different boxes of gas, each of volume V and each containing N (spin-0) molecules. The boxes are placed side by side and they share a common wall, as shown on the left of Fig,7. The

Figure 7: The mixing of two gases when the wall separating them is removed. This produces an increase in the entropy

The partition function is

$$Z(\beta, V.N) \;=\; \frac{1}{N!}V^N\left(\frac{m_1}{2\pi^2\hbar^2\beta}\right)^{3N/2}\frac{1}{N!}V^N\left(\frac{m_2}{2\pi^2\hbar^2\beta}\right)^{3N/2} \tag{1.11.34}$$

The total entropy is

$$S \;=\; S_1 + S_2 \;=\; 2N\kappa_B\left(\ln\left(\frac{V}{N}\right) + \frac{3}{2}\ln\left(\frac{\overline{m}}{2\pi^2\hbar^2\beta}\right) + \frac{5}{2}\right) \tag{1.11.35}$$

($\overline{m}$ is the geometric mean of the molecular masses of the two gasses).

If the connecting wall is removed, the two gases mix as shown on the right of Fig.7. Each gas is now contained in a volume of $2V$ and so the entropy increases by

$$\Delta S_{mix.} \;=\; 2N\kappa_B \ln 2. \tag{1.11.36}$$

The unmixed gas contains the information that *all* the molecules of gas 1 are on the left whereas *all* the molecules of gas 2 are on the right. When the gases mix, this information is lost and so the entropy goes up.

The entropy of mixing is the application in thermodynamics of the entropy of disorder.

But what happens if the two gases are identical as shown in Fig,8. In this case there is no change of state of the gas – there is no loss of information loss and therefore there should be no increase in entropy. This is the Gibbs paradox.

The resolution of the "paradox" lies in the prefactor $1/N!$ for the partition function of N identical particles.

The partition function for the two boxes of (identical gas) is

$$Z_< \;=\; \left(\frac{1}{N!}V^N\left(\frac{m_1}{2\pi^2\hbar^2\beta}\right)^{3N/2}\right)^2 \tag{1.11.37}$$

The partition function for $2N$ molecules on a volume $2V$ is

$$Z_> \;=\; \frac{1}{(2N)!}(2V)^{2N}\left(\frac{m_1}{2\pi^2\hbar^2\beta}\right)^{3N} \tag{1.11.38}$$

Figure 8:

Using Stirling's formula we find that for large N

$$(2N)! \;\approx\; 2^{2N}(N!)^2,$$

so that these two partition functions and consequently the two entropies are identical – there is no entropy of mixing

1.11.2 Irreversibility in Thermodynamics

If you drop an egg on the floor it smashes to pieces and yoke runs over the floor. we would not expect the interactions between the small pieces of egg to reconstruct themselves into a whole egg.

The egg is initially in a metastable state -stable under small disturbances, but a state which is highly ordered in which he molecules of the yoke are confined to a fixed volume and the crystals of egg-shell are arranged in a particular way - so the entropy the whole egg is low.

When the eggs is sufficiently disturbed by coming into contact with the floor, the initial metastable equilibrium is destroyed and egg then makes a transition between its low entropy state and one of the many high entropy states.

The hen that prepared the egg had to do a lot of work to create such an ordered object. The ordered egg stores this work as potential energy.

The process is irreversible in that the egg will not *spontaneously* reconstruct itself in the course of the interactions between the molecules of broken egg or their interaction with the environment. the statement that entropy increases is a statistical statement, and should strictly be replaced to the statement that the probability that entropy will decrease is negligibly small. There are far more states with large entropy than states with low entropy and so even though the interactions of the bits of the egg with each other or with the environment can effect transition to any final state, it is far more likely that the final state will also be a disordered state.

The entropy of a localized system (or a "subsystem" can be reduced, creating more "order", but this requires work (as experienced by anybody who has mopped up a broken egg in order to make the kitchen tidier). If the subsystem is in thermal equilibrium with a heat bath a temperature T_0, then the work done is dissipated into heat bath. The Second Law of Thermodynamics tells us that in order to generate the work we need to take energy from a best bath at a higher temperature, T_1, so that the increase in entropy due to energy transferred from a higher temperature heat bath to a lower temperature heat bath exceeds the decrease in entropy of the subsystem whose “order” has been increased.

The mixing of two gases when the connecting wall is removed can be reversed, as we shall see on the next section. When this happens the entropy of mixing is lost – the entropy of the gas goes down. However, in order to do this we need to do some work on the gas, which is transformed into energy. Since the gas is held in equilibrium with a thermal bath at constant temperature, the energy from the work done is transmitted to the thermal bath, thereby increasing the entropy of the bath. The total entropy of the gas plus the thermal bath cannot decrease, but it can be transferred from one to the other.

1.12 What Do We Get from the Sun

Ask the average person what we get from the sun and you will probably get the answer “energy”. Inform them that (almost) *all* of the energy we receive from the sun is radiated back into the atmosphere (and from there to outer space) and they are likely to be both surprised and confused.

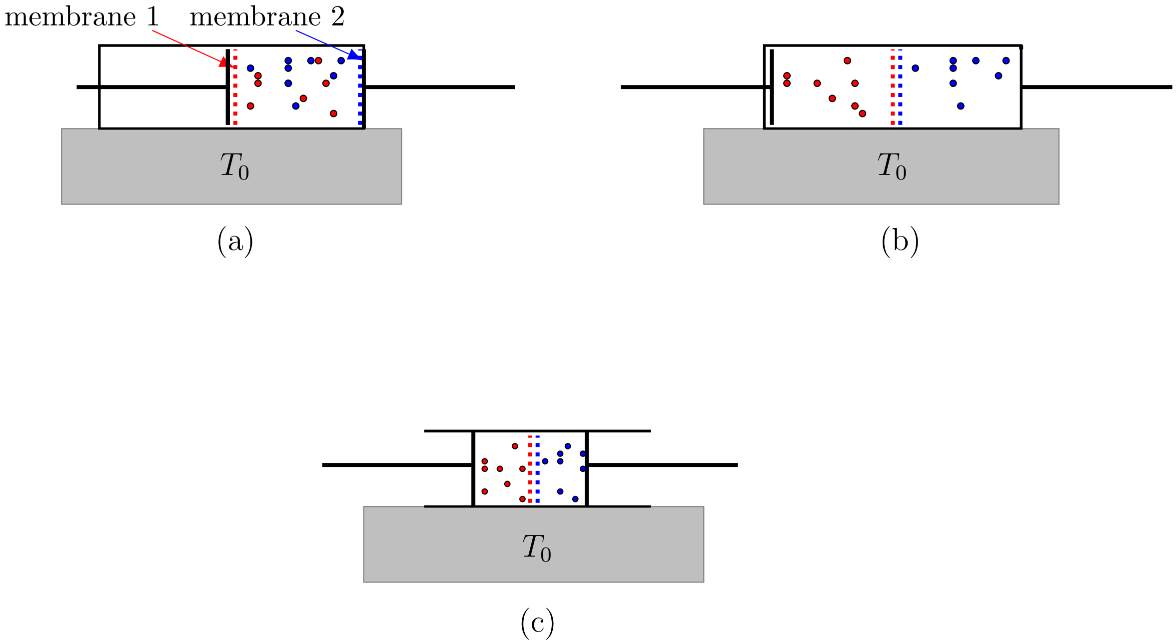
Radiation arrives on Earth from the sun at a rate of about 3×10^{17} watts. It arrives as blackbody radiation at a temperature of 6000 K (equivalent to $8 \times 10^{-20}\,J$), the temperature of the surface of the sun, and radiates it at the temperature of the Earth – 300K (equivalent to $4 \times 10^{-21} J$.. The entropy of the re-radiated energy (inversely proportional to the temperature) is much larger than the entropy of the incoming radiation. Entropy is “expelled” into the atmosphere at a rate of around 10^{38} bits per second.

The second law of thermodynamics tells us that the total entropy of the Universe cannot increase, but it *can* be exchanged between different parts. This means that the (Shannon) entropy on Earth can be decreased and this enables the creation of information or order.

Most of the order takes the form of converting a random distribution of different molecules into proteins and hence the creation of life forms. Living creatures then contribute further to this order.

- Plants grow
- Birds build nests (and lay highly ordered eggs in them)
- Beavers build dams
- Homo Sapiens builds the Taj Mahal and paints the Mona Lisa.

As a less ambitious example of using sunlight to create order, we consider a method for separating a mixture of two perfect gases thereby lowering the entropy by removing the entropy of mixing. This requires doing some work, ΔW, on the gas. The work is supplied



(a) (b) (c)

Figure 9: Thought experiment which uses work (in the last step) to separate two mixed gases and remove the entropy of mixing. The molecules of gas 1 are represented by red dots and gas 2 by blue dots. The semi-permeable membrane 1 which allows gas 1 molecules to pass is represented by a red dashed line and the semi-permeable membrane 2 which allows gas 2 molecules to pass is represented by a blue dashed line.

by taking energy ΔE from the sum at the sun's surface temperature T_1 and radiating the balance $\Delta E - \Delta W$ into the atmosphere at the temperature of the Earth, T_0.

The "setup" is shown in Fig.9. At the initial stage, (a), the mixture of gases consisting of N molecules of each gas, is confined to a volume V in the right-hand side of a cylinder, between two pistons. There is a semi-permeable membrane (membrane 1 – shown as a red dotted line) at the left wall of the cylinder, which allows gas 1 (red) to pass but not gas 2 (blue). At the right wall there is another semi-permeable membrane (membrane 2 – shown as a blue dotted line) which allows gas 2 (blue) to pass through but not gas 1 (red). This second membrane is connected to the piston on the left (not shown) so that as the piston is withdrawn, membrane 2 moves with it so that the volume between the left piston and membrane 2 remains equal to V. The entire apparatus is kept at constant temperature, T_0 by keeping it in thermal equilibrium with a heat bath.

In stage (b) the left piston and membrane 2 are withdrawn until membrane 1 and membrane 2 are in contact (the combination of he two membranes constitutes a hard wall between the two gases). All of gas 1 is to the left of the membranes and all of gas 2 is on the right. There is no change of entropy in this process, since both gases still occupy a volume V (and are held st the same temperature. Furthermore no work is done since the work done by gas 1 on the left piston is exactly balanced by the work done on gas 1 by membrane 2, There is no flow of energy to or from the thermal bath.

In the final step, (c) the left piston is decoupled from membrane 2 and both pistons are pushed in so that the volume of each compartment is reduced to $V/2$. We now have the original volume of gas but the two gases are separated. The entropy of the two gasses has decreased by

$$\Delta S_{mix.} \;=\; 2N \ln 2, \tag{1.12.1}$$

since the gases now occupy half of their original volume. Work, ΔW, is needed to compress the gas

$$\Delta W \;=\; -\int_V^{V/2} P(V) dV. \tag{1.12.2}$$

For a perfect gas

$$P \;=\; \frac{2N\,\kappa_B T_0}{V},$$

so that

$$\Delta W \;=\; 2N\kappa_B T_0 \ln 2 \tag{1.12.3}$$

This is converted into internal energy of the gas and immediately expelled into the thermal bath in order to maintain the temperature of the gas.

In order to produce the necessary work energy ΔE must be extracted from the sun at temperature T_1 and energy $\Delta E - \Delta W$ is expelled into the cold reservoir (atmosphere) at temperature T_0.

According to the second law of thermodynamics

$$\Delta E \;\geq\; \frac{T_1 \Delta W}{(T_1 - T_0)} \;=\; \frac{T_1}{T_0} \Delta S_{mix.} \tag{1.12.4}$$

Ultimately all of this energy is expelled into the atmosphere at temperature T_0, so that the entropy of the atmosphere increases by

$$\Delta S_{atm.} = \Delta E \left(\frac{1}{T_0} - \frac{1}{T_1} \right) \geq \Delta S_{mix.}. \tag{1.12.5}$$

We see that whereas the entropy of the system *can* be reduced by performing work on it – thereby creating order, it is necessary to extract energy from the sun at high temperature and expel into into the atmosphere at low temperature, thereby increasing the entropy of the atmosphere by more than the decrease in entropy required to order the system.

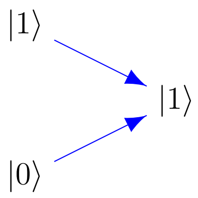
1.13 Landauer's Principle

So far, entropy of information and thermodynamic entropy have been treated as separate entities, albeit determined by the same equation relating entropy to the probabilities of a system being in a certain microstate (up to an overall constant of $\kappa_B \ln 2$). However, in 1961 Landauer showed these were really the same. Information has to be stored somewhere physical, such as a computer, a notebook or a brain. Landauer showed that in order to erase a bit of information from a device at equilibrium with a heat bath at temperature T required the input of at least a quantity of energy

$$đQ = \kappa_B T \ln 2.,$$

so that the thermodynamic entropy of the heat bath increases by at least $\kappa_B \ln 2$. In other words, the process of erasing information converts information entropy into thermodynamic entropy.

A computer straight from the factory has no information in its memory. All the bits are set to $|0\rangle$ – the probability of each bit being 0 is unity – and the entropy is zero. If we store one bit of information in the computer – whether a certain proposition is true or false the Shannon entropy of one bit is increases to 1. *A priori*, the proposition is as likely to be true or false, but we do not know which. In order to erase that information, we require act on that bit with a process for which the final state of the bit is $|0\rangle$ irrespective of whether it was initially in the state $|0\rangle$ or $|1\rangle$.



This is clearly not a reversible process. Classical interactions are deterministic and so if we start with a bit in the state $|0\rangle$ and subject it to any interaction we know with certainty

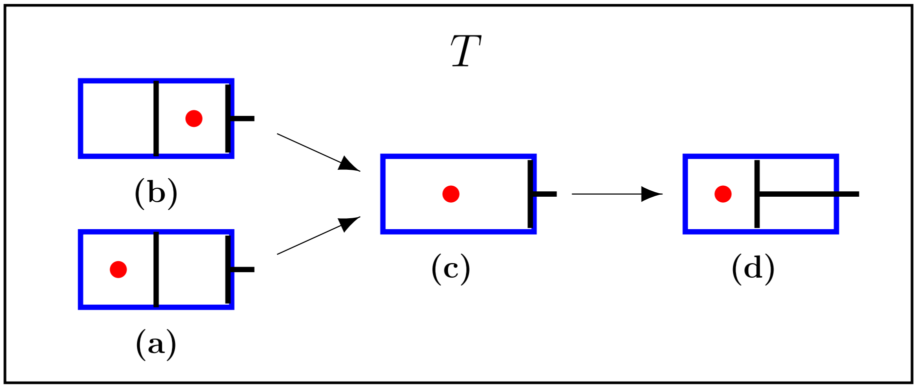


Figure 10: Erasure of a single bit of memory. Initial state is either $|0\rangle$, (a), or $|1\rangle$, (b), The barrier is removed, (c), so that the molecule occupies the entire volume, irrespective of which state it was initially. The piston is then pushed in to compress the volume occupied by the gas to its original volume. The heat generated by the work done is dissipated into the heat bath, thereby increasing its entropy by $\kappa_B \ln 2$.

if it will end up in the state $|0\rangle$ or $|1\rangle$. The entropy of any physical system which undergoes an irreversible process increases.

An example of how such an erasure of information could occur can be seen from a bit of information which consists of a molecule of a perfect gas in a box with two compartments - the molecule in the left compartment means the bit is in state $|0\rangle$ and the right compartment means the bit is in state $|1\rangle$. The erasure takes place in two stages. In the first stage the barrier between the two compartments is removed. The molecule is then free to move throughout the box. A piston is then used from the right side and the "gas" is compressed into the left hal f. It is then in the state $|0\rangle$ regardless of whether it was initially in the left or the right compartment. The work, W, done on the gas during that compression is

$$W \; = \; -\int_{V}^{V/2} P(V')dV'.$$

For one molecule of an ideal gas at temperature T

$$P(V) \; = \; \frac{\kappa_B T}{V},$$

so the work done is

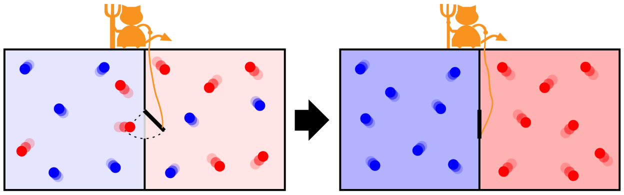
$$W \; = \; \kappa_B T \ln 2.$$

Since the gas is held at constant temperature, the energy equivalent of this work is dissipated into the heat bath, increasing its entropy by

$$\Delta S \; = \; \kappa_B \ln 2.$$

The general principle expounded by Landauer in 1961 has been disputed (i.e. can we find a way of erasing information which requires less energy?). However,in 2012, an experiment was carried out by Berut et. al. which confirmed the Landauer principle.

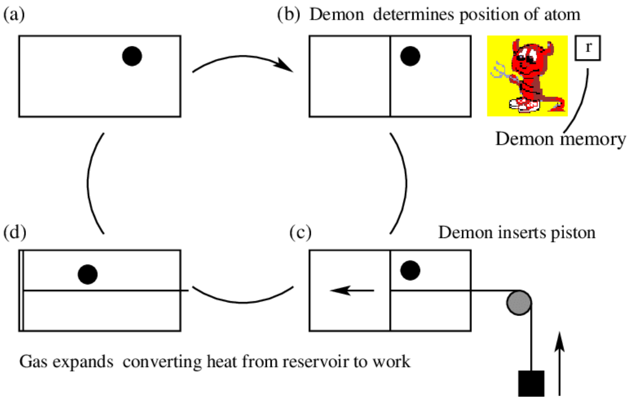
1.13.1 Maxwell's Demon



Landauer's principle has been used by Bennet to debunk the apparent paradox of Maxwell's demon. The demon proposed by Maxwell operates a trap door between two compartments of a gas. He is able to measure the velocity of each molecule which approaches the trap-door and opens it only if the molecule from the left has above the average kinetic energy of the gas molecules or the molecule from the right has less than the average kinetic energy.

In this way the right-hand compartment becomes hotter as the average kinetic energy of the molecules on the right increases. Conversely, the left-hand compartment becomes cooler as the average kinetic energy of the molecules on the left decreases. This clearly violates the Second Law of Thermodynamics.

1.13.2 Szilard's Demon



A simplification was proposed by Szilard who considered an "engine" consisting of a single molecule which is either in the left half of a box or in the right half. The demon observes the molecule and then inserts a piston in the empty compartment and pushes it until the volume of the box is halved. This can be done without expenditure of work, since the part of the box through which the piston moves is empty. The box is in equilibrium with a heat bath at temperature T. The single molecule "gas" can now push against the piston until the original volume of the box is recovered. In doing this, the "gas" does work

$$W = \kappa_B T \ln 2.$$

The energy required for this work is extracted from the heat bath, but no energy is expelled into another heat bath. Heat has been extracted from the (only) heat bath and converted into work. The demon can once again observe the compartment which contains the molecule and repeat the process indefinitely, taking heat from a thermal bath and converting it all into work thereby violating Clausius' statement the Second Law of Thermodynamics.

The resolution of this apparent paradox lies in the fact that the engine and the demon must be taken together. For the union of the engine *and* the demon, the process described above is *not* a complete cycle. Information on which compartment initially contained the molecule is stored in the demon's memory. The cycle is only completed if this memory is erased. According to the Landauer principle the energy required to erase each bit of memory is greater or equal to the work done by the engine alone, and the heat dissipated into the heat bath is at least as great as the heat which is converted into work by the engine alone.

1.14 Black Holes

The relationship between information entropy and thermodynamic entropy enabled Bekenstein to estimate the entropy of a black hole. (We restrict ourselves here to not rotating black holes with zero electric charge.)

A particle can contain several properties and therefore several bits of information. The minimum information that it can contain is the single bit which stores the (binary) answer to the question "does the particle exist".

If the particle is outside a black hole then a measurement can be performed to answer this question. However, when the particle falls into a black hole this bit of information is lost. More precisely, the information is converted into an increase

$$\Delta S \;=\; \kappa_B \ln 2, \tag{1.14.1}$$

in the thermodynamic entropy of the black hole.

The largest particle that can fall into a black hole is a particle whose radius R is equal to the radius of the horizon. This is the Schwarzschild radius, R_S, and is related to the mass, M, of the black hole by

$$R_s \;=\; 2\frac{GM}{c^2}. \tag{1.14.2}$$

From the Uncertainty Principle the minimum mass, ΔM of a particle that can be dropped into a black hole of radius R_S is one for which the Compton wavelength is smaller than the radius of the block hole horizon.

$$\Delta M \;>\; \frac{\hbar}{R_s c}. \tag{1.14.3}$$

The addition of such a mass to the black hole increases its radius by

$$\Delta R_S \;=\; 2\frac{G\Delta M}{c^2}. \tag{1.14.4}$$

A more careful derivation using the dynamics of general relativity generates a correction of a factor of $\frac{1}{2}$.

The increase in the area of the horizon of the black hole is

$$\Delta A \;=\; 8\pi R_S \Delta R_S. \tag{1.14.5}$$

From (1.14.3) and (1.14.4) (corrected by $\frac{1}{2}$) we obtain the inequality for the increase in area of the black hole

$$\Delta A \;>\; 8\pi l_P^2, \tag{1.14.6}$$

where $l_P = \sqrt{\hbar G/c^3}$ is the Planck length. The minimum value of ΔA is the increase in the area of the black-hole horizon when a particle containing a single bit of information falls into the black hole. In other words it is the increase in the area of the black-hole horizon when one bit of information is erased, generating a change in thermodynamic entropy, ΔS, given by (1.14.1). We see, therfore, that the entropy S_{bh} of a black hole is proportional to the area, A, of the holizon and is given by

$$S_{bh} \;=\; \frac{\ln 2\, \kappa_B c^3}{8\pi\hbar G} A \tag{1.14.7}$$

The entropy of a black hole of mass M is (using (1.14.2))

$$S_{bh} \;=\; \frac{2\ln 2\, \kappa_B G}{\hbar c^3} M^2 \tag{1.14.8}$$

This allows us to define a black-hole temperature

$$T_{bh} \;=\; \left(\frac{1}{c^2}\frac{\partial S_{bh}}{\partial M}\right)^{1} \;=\; \frac{\hbar c^3}{4\ln 2\, G\, \kappa_B M} \tag{1.14.9}$$

For non-rotating, uncharged, black holes, their macrostate is defined entirely by their mass (energy). More generally, a black hole can possess angular momentum and electric charge, but these are the only observables and therefore completely define the macrostate. The entropy of the black hole is the logarithm of the number of possible microstates for the material which make up a black hole of a given mass, angular momentum and electric charge.

1.14.1 Geroch's Perpetual Motion Machine:

In 1971, Robert Geroch devised a perpetual motion machine using a black hole. A cavity was filled with blackbody radiation,energy E from a heart bath at temperature T. The cavity is then lowered to the horizon of a black hole, at which point the energy, as measured by the distant observer, vanishes. A quantity of work $W = E$ can be extracted during this process. The cavity deposits a fraction. ϵ, of its proper energy (energy observed by am observer who os co-moving with the cavity) and the cavity is raised to its original position. In this process work $(1-\epsilon)E$ has to be done on the cavity and this is less than the work extracted during the its downward journey. The energy of the remaining radiation in the cavity $(1-\epsilon E$ is then returned to the heat bath. The net effect is the extraction of a quantity of energy ϵE from the heat bath, which is equal to the net work done. This violates Kelvin's statement of the Second Law of Thermodynamics.

Beckenstein pointed out that for a spherical cavity of radius b, if a point on the surface is in contact with the horizon of the back hole, the remainder of the cavity is outside the black hole and so the energy (as measured by the distant observer) is not completely zero, but has energy

$$E_{min} \;=\; \frac{1}{2}\frac{E\,b}{R_S},$$

where R_S is the radius of the black-hole horizon. The net work done by the engine is then

$$W \;=\; \epsilon E\left(1-\frac{b}{2R_S}\right),$$

whereas the net heat extracted from the heat bath is $\epsilon\, E$, so the efficiency of the engine reduced from unity to

$$\eta \;=\; \left(1-\frac{b}{2R_S}\right).$$

In order to fill a cavity with black-body radiation, the radius of the cavity has to be larger than than the characteristic wavelength of blackbody radiation at temperature T.

$$b \;>\; \xi\frac{\hbar\pi c}{2\kappa_B T},$$

where ξ is a constant of order unity, so that the efficiency of the engine is

$$\eta \;<\; 1-\xi\frac{\hbar\pi c^3}{4G\,\kappa_B M}\frac{1}{T}.$$

Setting ξ to $\pi/4\ln 2$ (Beckenstein's argument involved order of magnitude estimates), this may be written

$$\eta \;<\; 1-\frac{T_{bh}}{T}$$

where we have used (1.14.9). This is exactly the limit on the efficiency imposed by the Second Law of Thermodynamics for an engine working between a heat bath of temperature T and a heat bath with the temperature of the black hole.

A more rigorous derivation of the entropy, from examination of Quantum Field Theory in a Schwarzschild metric, of a black hole by Hawking yields the result

$$S_{bh} \;=\; \frac{\kappa_B c^3}{4\hbar G}A. \tag{1.14.10}$$

2 Entropy in Quantum Physics

2.1 Quantum Superposition

A quantum system is in a quantum state $|\Psi\rangle$, which is generally a superpositon basis vectors in a Hilbert space $\mathcal{H}_X$

$$|\Psi\rangle \ = \ \sum_{\{x\}} C_{\{x\}} |\{x\}\rangle. \tag{2.1.1}$$

here $\{x\}$ are a set of eigenvalues of a complete set of commmuting operators $\hat{X}_i, \ (i = i \cdots N)$, which label a microstate.

The square modulus of the coefficients, $\left|C_{\{x\}}\right|^2$ are the probabilities that a simulataneous measurement of the quantities X_i will yield the set of eigenvalues $\{x\}$. The conservation of probabilities then tells us that

$$\sum_{\{x\}} \left|C_{\{x\}}\right|^2 \ = \ 1 \tag{2.1.2}$$

The basis vectors of the Hilbert space are orthonormal

$$\langle\{x\}|\{x'\}\rangle \ = \ \delta_{\{x\}\{x'\}} \ \equiv \ \prod_{i=1}^{N} \delta_{x_i x'_i} \tag{2.1.3}$$

2.2 Density Matrix

The density matrix, ρ, associated with the state $|\Psi\rangle$ is

$$\rho \ = \ |\Psi\rangle\langle\Psi| \ = \ \sum_{\{x\},\{x'\}} C_{\{x\}} C^*_{\{x'\}} |\{x\}\rangle\langle\{x'\}| \tag{2.2.1}$$

The diagonal elements of the density matrix are the probabilities that a measurement of X_i will yield $\{x\}$.

The density matrix is idempotent, i.e.

$$\begin{aligned}
\rho \cdot \rho \ &= \ \sum_{\{x\},\{x'\}\{x''\}\{x'''\}} C_{\{x\}} C^*_{\{x'\}} C_{\{x''\}} C^*_{\{x'''\}} |\{x\}\rangle\langle\{x'\}|\{x''\}\rangle\langle\{x'''\}| \\
&= \ \sum_{\{x\}\{x'\}} C_{\{x\}} C^*_{\{x'\}} \sum_{\{x\}\{x''\}} C_{\{x''\}} C^*_{\{x''\}} |\{x\}\rangle\langle\{x'\}| \quad \text{(using (2.1.3)} \\
&= \ \sum_{\{x\}\{x'\}} C_{\{x\}} C^*_{\{x'\}} |\{x\}\rangle\langle\{x'\}| \ \text{ (using (2.1.2)} \\
&= \ \rho.
\end{aligned} \tag{2.2.2}$$

This can be shown using the orthonormality relation (2.1.3) and the conservation of probabilities (2.1.2).

Furthermore, since the diagonal elements are probabilities, the conservation of probabilities tells us that

$$\mathrm{Tr}\,\rho \ = 1 \tag{2.2.3}$$

A matrix which is idempotent and whose trace is unity can only have one non-zero eigenvalue whose value is unity.

2.3 Von Neumann Entropy

The entropy of a qunatum system was define by von Neumann to be

$$H_{vN} \ = \ -\mathrm{Tr}\left(\rho \log_2 \rho\right). \tag{2.3.1}$$

This is independent of the choice of basis vectors of the Hilbert space and therefore can be calculated in the system of basis vectors for which the density matrix is diagonal. In this basis the eigenvalues are zero except for one of them which is unity. From this we conclude that the von Neumann entropy of a pure quantum state is zero.

This makes sense if we interpret entropy as a measure of what we do not know about a system. If the quantum state of a system is known, then we know everything that we can know about that system with restrictions imposed by Quantum Physics.

2.4 Quantum Macrostates and Microstates

Whereas the complete set, $\{x\}$, of eigenvalues of the operators X_i determine a given microstate, a macrostate is determined by a (usually small) subset of these, namely by the eigenvalues of a subset of operators $\hat{Y}_a(\hat{X}_i)$.

The Hilbert space of the system is partitioned into the Hilbert space, $\mathcal{H}_Y$, of the "body" and a Hilbert space $\mathcal{H}_Z$ of the "environment" (usually assumed to have a much larger dimension than the Hilbert space of the body, which label the macrostates). The environment is space of operators $\hat{Z}_b(\hat{X}_i)$, which are orthogonal to the operators of the Hilbert space $\mathcal{H}_Y$ in the sense that

$$\begin{aligned}\sum_i \frac{\partial Y_a}{\partial X_i}\frac{\partial Z_b}{\partial X_i} \ &= \ 0 \\ \mathcal{H}_x \ &= \ \mathcal{H}_Y \otimes \mathcal{H}_Z.\end{aligned}$$

Example:
A system of N spin-$\frac{1}{2}$ particles, for which the microstates are labelled by the eigenvalues of the z-component of spin of each particle,

$$\hat{X}_i \ = \hat{s}_z^{(i)},$$

but where the macrostates are labelled by the total z-component of spin

$$\hat{Y} \equiv \hat{J}_Z = \sum_{i=1}^{N} \hat{s}_z^{(i)}$$

The orthogonal operators Z_b may be written

$$\hat{Z}_b = \sum_{j=1}^{(N-b)} \hat{s}_Z^{(j)} - \frac{(N-b)}{N}\hat{Y},$$

(any independent set of linear sums of these operators can also be used.

The quantum state $|\Psi\rangle$ is now written as a sum over the products of the eigenvectors of the operators $\hat{Y}_a$ and $\hat{Z}_b$, namely

$$|\Psi\rangle = \sum_{\{y\}\{z\}} C_{\{y\}}^{\{z\}} |\{y\}\rangle \otimes |\{z\}\rangle, \tag{2.4.1}$$

where $|\{y\}\rangle$ and $|\{z\}\rangle$ are basis vectors in Hilbert space $\mathcal{H}_Y$ and $\mathcal{H}_Z$ respectively.

2.5 Entanglement

In some cases, these quantum states are said to be factorizable. This occurs if the coefficients take the form

$$C_{\{y\}}^{\{z\}} = U_{\{y_0\}}^{\{y\}} V_{\{z_0\}}^{\{yz\}} \tag{2.5.1}$$

where U and V are unitary matrices in Hilbert spaces $\mathcal{H}_Y$ and $\mathcal{H}_Z$ respectively. In this case the quantum state may be written as a single (outer) product of a state in Hilbert space $\mathcal{H}_Y$ and a state in Hilbert space $\mathcal{H}_Z$:

$$|\Psi\rangle = |\{y_0\}\rangle \otimes |\{z_0\}\rangle. \tag{2.5.2}$$

If the composition (2.5.1) is *not* possible then the state is said to "entangled" and cannot be transformed by unitary transformations within the Hilbert spaces into a single product.

Example:
Two spin-$\frac{1}{2}$ particles - $|0\rangle$ is the $s_z = -\frac{1}{2}$ state and $|1\rangle$ $s_z = +\frac{1}{2}$ state.

The state

$$|\Psi\rangle = \frac{1}{2}\left(|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right)$$

can be written as

$$|\Psi\rangle = \left(\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)\right) \otimes \left(\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)\right),$$

and we can write this as

$$|\Psi\rangle = |1\rangle' \otimes |1\rangle',$$

where

$$\begin{pmatrix} |1\rangle' \\ |0\rangle' \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} |1\rangle \\ |0\rangle \end{pmatrix}$$

The state is therefore a factorizable state.

On the other hand, the state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle\right)$$

cannot be factorized in this manner. It is an entangled state.

2.6 Schmidt Decompostion

The general expansion of an entangled state (2.4.1) involves a sum over both the Hilbert spaces $\mathcal{H}_Y$ and $\mathcal{H}_Z$. However, the Schmidt decomposition allows this to be written in the form of a single sum

$$|\Psi\rangle = \sum_\alpha \sqrt{p_\alpha} |\{y_\alpha\}\rangle \otimes |\{z_\alpha\}\rangle, , \tag{2.6.1}$$

where $|\{y_\alpha\}\rangle$ and $|\{z_\alpha\}\rangle$ are unique vectors in the Hilbert spaces $\mathcal{H}_Y$ and $\mathcal{H}_Z$ respectively, for each value of α in the (single) sum.

We do not prove this statement, demonstrate for the case of finite dimensional Hilbert spaces

$$\dim\{\mathcal{H}_Y\} = M, \quad \dim\{\mathcal{H}_Z\} = N, \quad (M \, < \, N),$$

how to determine the coefficients $\sqrt{p_\alpha}$.

The state-vectors $|\{y_\alpha\}\rangle$ and $|\{z_\alpha\}\rangle$ are related to the basis vectors of $\mathcal{H}_Y$ and $\mathcal{H}_Z$ by unitary matrices:

$$|\{y_\alpha\}\rangle = U_{\{y_\alpha\{}^{\{y\}} |\{y\}\rangle \tag{2.6.2}$$

and

$$|\{z_\alpha\}\rangle = V_{\{z_\alpha\}}^{\{z\}} |\{z\}\rangle \tag{2.6.3}$$

We write the coefficients in the form of a rectangle $M \times N$ matrix $C_{\{y\}}^{\{z\}}$. Inserting (2.6.2) and (2.6.3) into (2.6.1) and comparing with (2.4.1), we see that the matrix C may be written

$$C = U^\dagger \sqrt{P} V \tag{2.6.4}$$

where $\sqrt{P}$ is a rectangular $M \times N$ matrix with diagonal values

$$\sqrt{P}_\alpha^{\ \beta} = \sqrt{p_\alpha}\delta_{\alpha\beta}, \ (\beta \, \leq \, M),$$

Similarly, taking the Hermitian conjugate of (2.6.4),

$$C^\dagger = V^\dagger (\sqrt{P})^\dagger U.$$

This means that U is the unitary matrix that diagonalizes $C\,C^\dagger$ and V is the unitary matrix that diagonalizes $C^\dagger\,C$. The non zero eigenvalues of either of these diagonalized matrices are $\left(\sqrt{p_\alpha}\right)^2 \;=\; p_\alpha$ $(\alpha = 1\cdots M)$.

Example: Let the dimension of Hilbert space $\mathcal{H}_Y$ be 2 (the body) and the dimension of the Hilbert space $\mathcal{H}_Z$ be 3 (the environment). In particle physics, an example of this would be the hadrons $\Sigma^\pm$, Σ^0 which have spin-$\frac{1}{2}$. The state of the Σ can be described in terms of the third component of spin which can take values $\pm\frac{1}{2}$ and the third component of isospin, which can take the values $1, 0, -1$. A general entangled state can bt written

$$|\Psi\rangle \;=\; \sum_{I_3, s_z} C_{s_z, I_3} |I_3\rangle \otimes |s_z\rangle$$

The rectangular matrix $\mathbf{C}$ is

$$\mathbf{C} \;=\; \begin{pmatrix} C_{+,1} & C_{-,1} \\ C_{+,0} & C_{-,0} \\ C_{+,-1} & C_{-0,-1} \end{pmatrix}$$

We assume these coefficients are all real - they can be rendered real by an appropriate $U(1)$ transformation for each state Choose angles $\omega, \psi, \theta, \phi$ such that

$$C_{+,1} \;=\; \cos\omega\cos\psi\cos\phi\cos\theta - \sin\omega\sin\psi\sin\phi \tag{2.6.5}$$

$$C_{-,1} \;=\; \cos\omega\sin\psi\cos\phi\cos\theta - \sin\omega\cos\psi\sin\phi \tag{2.6.6}$$

$$C_{+,0} \;=\; -\cos\omega\cos\psi\sin\phi\cos\theta - \sin\omega\sin\psi\cos\phi \tag{2.6.7}$$

$$C_{-,0} \;=\; \cos\omega\sin\psi\sin\phi\cos\theta - \sin\omega\cos\psi\cos\phi \tag{2.6.8}$$

$$C_{+,-1} \;=\; -\cos\omega\cos\psi\sin\theta \tag{2.6.9}$$

$$C_{-,-1} \;=\; \cos\omega\sin\psi\sin\theta \tag{2.6.10}$$

U is the rotation matrix

$$U \;=\; \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix}$$

and V is the rotation matrix

$$V \;=\; \begin{pmatrix} \cos\theta\cos\phi & -\cos\theta\sin\phi & -\sin\theta \\ \sin\phi & \cos\phi & 0 \\ \cos\theta\sin\phi & -\sin\theta\sin\phi & \cos\theta \end{pmatrix}$$

The Schmidt decomposed state is now written

$$|\Psi\rangle \;=\; \sum_{\tilde{I}_3, \tilde{s}_z} \sqrt{\mathbf{P}}_{\tilde{s}_z}^{\tilde{I}_3} |\tilde{I}_3\rangle |\tilde{s_z}\rangle$$

where the matrix $\sqrt{\mathbf{P}}$ is

$$\sqrt{\mathbf{P}} \;=\; \begin{pmatrix} \cos\omega & 0 \\ 0 & \sin\omega \\ 0 & 0 \end{pmatrix}$$

2.7 Reduced Density Matrix

The reduced density matrix is constructed by tracing over all possible values of the environment variables $\{z\}$

$$(\tilde{\rho}_Y)_{\{y\}}^{\{y'\}} \;=\; \sum_{\{z\}} C_{\{y\}}^{\{z\}} C^{\dagger\,\{y'\}}_{\{z\}} |\{y\}\rangle\langle\{y\prime\}| \tag{2.7.1}$$

If we rotate the Hilbert space for the body, $\mathcal{H}_Y$ using the unitary transformation of the Schmidt decomposition, then the reduced density matrix is diagonal

$$\tilde{\rho}_Y \;=\; \sum_{\alpha} p_\alpha |\{y_\alpha\}\rangle\langle\{y_\alpha\}| \tag{2.7.2}$$

This is the density matrix for a state which is *not* a pure quantum state, but an ensemble of systems in different macrostates states with a probability p_α to be in in the state $|\{y_\alpha\}\rangle$.

The density matrix for such a "mixed state" is no longer idempotent, but has eigenvalues p_α, with the only restriction imposed by the conservation of probability

$$\sum_{\alpha} p_\alpha \;=1$$

The von Neumann entropy

$$H_{vN} \;=\; -\mathrm{Tr}\left(\tilde{\rho}_Y \log_2 \tilde{\rho}_Y\right) \;= \sum_{p_\alpha} p_\alpha \log_2 p_\alpha \tag{2.7.3}$$

is now non-zero unless the state of the system is factorizable, in which case all the p_α vanish except one, which is then unity.

The above example of the spin-$\frac{1}{2}$ particle, with isospin one. the third component is to be an environment variable, i.e. we define the macrostate in terms of the z-component of spin irrespective of the electric charge of the particle. The reduced density matrix (in the Schmidt decomposition) is then

$$\tilde{\rho} \;=\; \left(\begin{array}{cc} \cos^2\omega & 0 \\ 0 & \sin^2\omega \end{array} \right).$$

and the von Neumann entropy is

$$H_{vN} \;=\; -\cos^2\omega \log_2(\cos^2\omega) - \sin^2\omega \log_2(\sin^2\omega)$$

This is zero if ω is a multiple of $\pi/2$ for which values the state is factorizable into the product of a spin state and an isospin state. The maximum entanglement occurs for $\omega = \pi/4$, for which the von Neumann entropy is 1.

We can also construct a reduced density matrix by tracing over the variables of the body to obtain

$$\tilde{\rho}_Z \; = \sum_{\{y\}} C^{\dagger\{y\}}_{\{z\}} C^{\{z'\}}_{\{y\}} |\{z\}\rangle\langle\{z'\}|$$

In the bases of the Schmidt decomposition, we may write this as

$$\tilde{\rho}_Z \; = \sum_{\alpha} p_\alpha |\{z_\alpha\}\rangle\langle\{z_\alpha\}|$$

The non-zero eigenvalues of the reduced density matrix $\tilde{\rho}_Z$ are the same as the eigenvalues of $\tilde{\rho}_Y$, so that they both lead to the same von Neumann entropy. This symmetry between the reduced density matrices when tracing over the body or the environment leads to the apparent paradox in the Schroedinger cat (thought) experiment.

2.8 Entropy of Entanglement

The von Neumann entropy can therefore be taken as a measurement of entanglement. The principle of maximum entropy is then equivalent to the statement that the most probable mixed state is one for which the entanglement is maximal.

If there is no information about the system, then maximum possible value of the entropy occurs when the eigenvalues of the reduced density matrix are all equal (taking the value $1/N$ where N is the dimensionality of the reduced density matrix). For a maximally entangled state the eigenvalues of the reduced density matrix are all equal.

An irreversible process is one in which an initial state is either factorizable or only entangled with some subset of the environment states. For example, in a Joule expansion experiment in which the gas is confined by a barrier to the left hand half of a box, the gas must be in a microstate in which the wavefunction of each gas molecule is in some superposition of the subset of wavefunction for a particle in a box, which only have support in the left-hand half of the box. For any set of variables for the gas which label the macrostates, the entanglement is only between the "body" states and the states of the environment, which are non-zero only in the left-hand part of the box. Once the barrier is removed, interactions (collisions) between the gas molecules will eventually lead to entanglement will *all* of the environment states and the von Neumann entropy increases.

2.8.1 Example: Two Coupled Harmonic Oscillators

We consider two uncoupled coupled harmonic oscillators with unit mass. The "body" is oscillator 1 and the environment is oscillator 2.

If the oscillators are uncoupled, the Hamiltonian is

$$\mathrm{H} \; = \; \frac{1}{2}\left(p_1^2 + p_2^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2\right) \tag{2.8.1}$$

with energy eigenfunctions

$$\Psi_{m_1 m_2}(x_1, x_2) \; = \; \psi^{\omega_1}_{m_1}(x_1)\psi^{\omega_2}_{m_2}(x_2), \tag{2.8.2}$$

where $\psi^{\omega}_{m}(x)$ are the energy eigenfunction for an oscillator with frequency ω, and energy eigenvalues

$$E_{m_1,m_2} \; = \; \left(m_1 + \frac{1}{2}\right)\omega_1 + \left(m_2 + \frac{1}{2}\right)\omega_2 \tag{2.8.3}$$

The uncoupled system is not entangled. If the system is in the state with quantum numbers m_1, m_2,The density matrix in configuration space -an

$$\rho^{x'_1 x'_2}_{x_1 x_2} \; = \; \psi^{\omega_1}(x_1)\psi^{\omega_1}_{m_1}(x'_1)\psi^{\omega_2}_{m_2}(x_2)\psi^{\omega_2}_{m_2}(x'_2) \tag{2.8.4}$$

The reduced density matrix is obtained by multiplying by $\delta(x_2 - x'_2$ and integrating over x_2 and x'_2. Using the normalization properties of the wavefunctions, this gives

$$\tilde{\rho}^{x'_1}_{x_1} \; = \; \psi^{\omega_1}(x_1)\psi^{\omega_1}_{m_1}(x'_1). \tag{2.8.5}$$

This is an idempotent matrix and therefore the von Neumann

If we add a coupling term $2\omega^2_{12}x_1x_2$ to the Hamiltonian, it becomes

$$\mathrm{H} \; = \; \frac{1}{2}\left(p_1^2 + p_2^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_{12}^2 x_1 x_2\right) \tag{2.8.6}$$

This may be written as

$$\mathrm{H} \; = \; \frac{1}{2}\left(p_+^2 + p_-^2 + \omega_+^2 x_+^2 + \omega_-^2 x_-^2\right), \tag{2.8.7}$$

where

$$\begin{aligned} x_+ \; &= \; \cos\alpha x_1 + \sin\alpha x_2 \\ x_- \; &= \; \cos\alpha x_2 - \sin\alpha x_1 \\ \left(\omega_+^2 + \omega_-^2\right) \; &= \; \left(\omega_1^2 + \omega_2^2\right) \\ \left(\omega_+^2 - \omega_-^2\right)\cos 2\alpha \; &= \; \left(\omega_1^2 - \omega_2^2\right) \\ \left(\omega_+^2 - \omega_-^2\right)\sin 2\alpha \; &= \; \omega_{12}^2 \end{aligned}$$

The eigenvalues of the Hamiltonian are

$$E_{n_1,n_2} \; = \; \left(n_1 + \frac{1}{2}\right)\omega_+ + \left(n_2 + \frac{1}{2}\right)\omega_- \tag{2.8.8}$$

The corresponding wavefunctions are

$$\Psi_{n_1,n_2}(x_+, x_-) \; = \; \psi^{(\omega_+)}_{n_1}(x_+)\cdot\psi^{(\omega_-)}_{n_2}(x_-) \tag{2.8.9}$$

Written in terms of the original coordinates x_1, x_2, this is

$$\tilde{\Psi}_{n_1,n_2}(x_1,x_2) \;=\; \psi^{(\omega_+)}_{n_1}\left(\cos\alpha\, x_1+\sin\alpha\, x_2\right)\cdot\psi^{(\omega_-)}_{n_2}\left(-\sin\alpha\, x_1+\cos\alpha\, x_2\right),. \tag{2.8.10}$$

We can expand these energy eigenfunctions in term of the eigenfunctions for the uncoupled system

$$\tilde{\Psi}_{n_1,n_2}(x_1,x_2) \;=\; \sum_{m_1m_2} A^{n_1n_2}_{m_1m_2}\Psi_{m_1m_2}(x_1,x_2) \tag{2.8.11}$$

From the orthonormality of the wavefunctions

$$\begin{aligned} A^{n_1n_2}_{m_1m_2} \;&=\; \int dx_1dx_2\psi^{*\omega_1}_{m_1}(x_1)\psi^{*(\omega_2)}_{m_2}(x_2)\left(\psi^{\omega+}_{n_1}\right)\left(\cos\alpha\, x_1+\sin\alpha\, x_2\right) \\ &\quad\times\left(\psi^{\omega_-}_{n_2}\right)\left(-\sin\alpha\, x_1+\cos\alpha\, x_2\right) \end{aligned} \tag{2.8.12}$$

In the limit of no coupling we have

$$A^{n_1n_2}_{m_1m_2} \;=\; \delta_{n_1m_1}\delta_{n_2m_2}$$

For a given pair of values, m_1, m_2, of the decoupled system the density matrix is

$$\rho_{n_1n_2}^{\;\;n_1'n_2'} \;=\; A^{n_1n_2}_{m_1m_2}\left(A^{n_1'n_2'}_{m_1m_2}\right)^* \tag{2.8.13}$$

The reduced density matrix is constructed by tracing over n_2, n_2'

$$\tilde{\rho}_{n_1}^{\;\;n_1'} \;=\; \sum n_2 A^{n_1n_2}_{m_1m_2}\left(A^{n_1'n_2'}_{m_1m_2}\right)^* \tag{2.8.14}$$

For zero coupling, this reduced density matrix contains only one non-zero diagonal element (equal to unity). But for non-zero coupling the reduced density matrix has eigenvalues $\lambda^{(m_1m_2)}_n$ and the non-zero von Neumann entropy id the entropy of entanglement:

$$H_{ent} \;=\; -\sum_n \lambda^{(m_1m_2)}_n \log_2\left(\lambda^{(m_1m_2)}_n\right) \tag{2.8.15}$$

For $m_1, m_2 \gg 1$ the reduce density matrix will only have non-negligible support in the region $n_1 \sim m_2$, $n_1 \sim m_2$ so that it should be possible to diagonalize it numerically. For small interactions ($\omega_{12}^2 \ll \omega_1^2, \omega_2^2$), the integrals required to construct the non-negligible matrix elements can be performed numerically after a suitable change of variable of integration.

2.9 Von Neumann vs. Shannon Entropy.

For a given partition of the Hilbert space into two factors $\mathcal{H}_Y$ and $\mathcal{H}_Z$, the von Neumann entropy of a particular entangled state is uniquely defined. The same is *not* true of the Shannon entropy which, in general is larger than the von Neumann entropy.

The Shannon entropy (denoted by $H_{Sh.}$), is defined as

$$H_{Sh.} \;=\; \sum_i p_i \ln p_i, \tag{2.9.1}$$

where p_i the probability of finding the system in a given microstate i. However, this is not uniquely defined as a unitary transformation of the microstates

$$|i\rangle \;\to\; |i'\rangle \;\equiv\; \sum_j U_{i'j}|j\rangle$$

will generally lead to different probabilities $p_{i'}$.

On the other hand, the von Neumann entropy

$$H_{vN} \;=\; \sum_a \tilde{\lambda}_a \,\ln \tilde{\lambda}_a, \tag{2.9.2}$$

where $\tilde{\lambda}_a$ are the eigenvalues of the reduced density matrix, $\tilde{\rho}_A$. These are invariant under a unitary transformation of the basis states. In the representation of the Schmidt decomposition, the reduced density matrix is diagonal, so that the eigenvalues *are* the diagonal elements of the density matrix and for that choice of basis vectors, the Shannon and von Neumann entropies are equal.

Example 1: We consider a three dimensional Hilbert space $\mathcal{H}_X$ for the body and a two dimensional Hilbert space $\mathcal{H}_Z$ for the environment. The system might be a pion in one of three charge states and the environment could ve a spin-$\frac{1}{2}$ particle. The system is entangled via a measuring apparatus which generated a magnetic field in the positive z-direction if the pion is charged, forcing the spin-$\frac{1}{2}$ into the $s_z = +\frac{1}{2}$ state (denoted by $|+\rangle$), and in the negative z-direction (denoted by $|-\rangle$)if the pion is uncharged, forcing the spin-$\frac{1}{2}$ into the $s_z = -\frac{1}{2}$ state, The general entangled state may be written

$$|\Psi\rangle \;=\; \cos\theta|0\rangle\otimes|-\rangle + \sin\theta\cos\phi|1\rangle\otimes|+\rangle + \sin\theta\sin\phi|-1\rangle\otimes|+\rangle$$

The selection imposed by the measuring apparatus sets the coefficients of $|0\rangle|+\rangle$ and $|\pm1\rangle|-\rangle$ to zero.

The reduced density matrix is

$$\tilde{\rho}_A \;=\; \begin{pmatrix} \sin^2\theta\cos^2\phi & \sin^2\theta\sin\phi\cos\phi & 0 \\ \sin^2\theta\sin\phi\cos\phi & \sin^2\theta\sin^2\phi & 0 \\ 0 & 0 & \cos^2\theta \end{pmatrix}, \tag{2.9.3}$$

giving a von Neumann entropy

$$H_{vN} \;=\; -\cos^2\theta\log_2\left(\cos^2\theta\right) - \sin^2\theta\log_2\left(\sin^2\theta\right) \tag{2.9.4}$$

However, for the Shannon entropy we note that the probabilities for the three charge states are

$$p_{+1} = \sin^2\theta\cos^2\phi,\;\; p_0 = \cos^2\theta,\;\; p_{-1} = \sin^2\theta\sin^2\phi,$$

yielding a Shannon entropy

$$\begin{aligned} H_{Sh.} \;&-\; -\cos^2\theta\log_2\left(\cos^2\theta\right) - \sin^2\theta\cos^2\phi\log_2\left(\sin^2\theta\cos^2\phi\right) - \sin^2\theta\sin^2\phi\log_2\left(\sin^2\theta\sin^2\phi\right) \\ &=\; H_{vN} - \sin^2\theta\left(\cos^2\phi\log_2\left(\cos^2\phi\right) + \sin^2\phi\ln\left(\sin^2\phi\right)\right) \qquad (2.9.5) \end{aligned}$$

Since $\cos^2\phi ln\left(\cos^2\phi\right)$ and $\cos^2\phi ln\left(\cos^2\phi\right)$ are both negative semi-definite We see that

$$H_{Sh.} \geq H_{vN},$$

with the equality only applying if ϕ is a multiple of $\pi/2$.

Example 2: We consider three spin-$\frac{1}{2}$ particles and the Hilbert space of the system to be the eigenstates of

$$J_Z \;\equiv\; \sum_{i=1}^{3} s_z^{(i)}$$

and we represent the environment Hilbert space in terms of the simultaneous eigenstates of the independent operators

$$\begin{aligned} J_2 &\equiv 2s_z^{(2)} - s_z^{(1)} - s_z^{(3)} \\ J_3 &\equiv s_z^{(1)} - s_z^{(3)} \end{aligned}$$

There are eight possible microstates corresponding to the two possible values of s_z for each particle. there are 4 possible macrostates corresponding to the 4 possible values of J_z

A maximally entangled superposition of the eight possible spin states

$$|\Psi\rangle \;=\; \frac{1}{\sqrt{8}}\left(|\uparrow\uparrow\uparrow\rangle, +|\uparrow\uparrow\downarrow\rangle, +|\uparrow\downarrow\uparrow\rangle, +|\downarrow\uparrow\uparrow\rangle, +|\uparrow\downarrow\downarrow\rangle, +|\downarrow\uparrow\downarrow\rangle, +|\downarrow\downarrow\uparrow\rangle, +|\downarrow\downarrow\downarrow\rangle\right). \tag{2.9.6}$$

This can be written in terms of the eigenstates of J_Z, J_2, J_3 as

$$\begin{aligned} |\Psi\rangle \;=\; & \frac{1}{\sqrt{8}}\left(\left|\frac{3}{2}\right\rangle_Y \otimes |0,0\rangle_Z + \left|\frac{1}{2}\right\rangle_Y \otimes |1,1\rangle_Z + \left|\frac{1}{2}\right\rangle_Y \otimes |-2,0\rangle_Z + \left|\frac{1}{2}\right\rangle_Y \otimes |1,-1\rangle_Z + \right. \\ & \left. \left|-\frac{1}{2}\right\rangle_Y \otimes |-1,1\rangle_Z + \left|-\frac{1}{2}\right\rangle_Y \otimes |2,0\rangle_Z + \left|-\frac{1}{2}\right\rangle_Y \otimes |-1,-1\rangle_Z + \left|-\frac{3}{2}\right\rangle_Y \otimes |0,0\rangle_Z\right) \qquad (2.9.7) \end{aligned}$$

The reduced density matrix is

$$\tilde{\rho}_Y = \frac{1}{8}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \qquad (2.9.8)$$

with eigenvalues

$$p_\alpha = 0, \frac{1}{4}, \frac{3}{8}, \frac{3}{8},$$

so that the von Neumann entropy is

$$H_{vN} = 3 - \frac{3}{4}\ln 3 - \frac{1}{4}\ln 2. \qquad (2.9.9)$$

On the other hand the numbers of states with $J_z = 3/2, 1/2, -1/2, -3/2$ is $1, 3, 3, 1$ respectively, so that the probabilities, p_{J_Z} of the system being in a state with a given value of J_Z are

$$p_{3/2} = \frac{1}{8},\ p_{1/2} = \frac{3}{8},\ p_{-1/2} = \frac{3}{8},\ p_{-3/2} = \frac{1}{8},$$

leading to a Shannon entropy

$$H_{Sh.} = 3 - \frac{3}{4}\log_2 3, \qquad (2.9.10)$$

which exceeds the von Neumann entropy by $\frac{1}{4}\ln 2$.

Note that there are only two non-zero off-diagonal elements of the reduced matrix element which occur when all the spins are in the same direction. This persists for ensembles of larger numbers of spins. For N spin-$\frac{1}{2}$ particles, only the $J_Z = N/2$ and $J_Z = -N/2$ are both entangled with the same environment state $|0, 0, \cdots 0\rangle$. For large ensembles the difference between the von Neumann entropy and Shannon entropy becomes negligible.

Example 3: Again we take three spin-$\frac{1}{2}$ particles, but in this case, we assume that we are interested (i.e. can measure) not only total J_Z but also the eigenvalue of $J_3 \equiv s_z^{(1)} - s_z^{(3)}$. The 12 basis vectors of $\mathcal{H}_Y$ are now labelled by the two eigenvalues of J_Z and J_3 and the 5 basis vectors of the environment, $\mathcal{H}_Z$ are labelled by the eigenvalues of $J_2 \equiv \left(2s_z^{(2)} - s_z^{(1)} - s_z^{(3)}\right)$.

A maximally entangled state is now written

$$|\Psi\rangle = \frac{1}{\sqrt{8}}\left(\left|\frac{3}{2}, 0\right\rangle_A |0\rangle_B + \left|\frac{1}{2}, 1\right\rangle_A |1\rangle_B + \left|\frac{1}{2}, 0\right\rangle_A |-2\rangle_B + \left|\frac{1}{2}, -1\right\rangle_A |1\rangle_B + \right.$$
$$\left. \left|-\frac{1}{2}, 1\right\rangle_A |-1\rangle_B + \left|-\frac{1}{2}, 0\right\rangle_A |2\rangle_B + \left|-\frac{1}{2}, -1\right\rangle_A |-1\rangle_B + \left|-\frac{3}{2}, 0\right\rangle_A |0\rangle_B\right) \qquad (2.9.11)$$

The reduced density matrix is 12×12 matrix whose eigenvalues are

$$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{8}, \frac{1}{8}, 0, 0, 0, 0, 0, 0, 0$$

This gives a von Neumann entropy

$$H_{vN} \; = \; \frac{9}{4}.$$

This differs from the previous case. Note that the entropy for the case where the system is described by two variables is actually larger than the entropy in which it is described by only one variable. On the other hand, the dimension of the environment $\mathcal{H}_Z$ is smaller. The von Neumann entropy is the same whether the trace is taken over $\mathcal{H}_A$ or $\mathcal{H}_B$ – the non-zero eigenvalues of the reduced density matrices $\tilde{\rho}_Y$ and $\tilde{\rho}_Z$ are the same.

In this case there is always only one microstate for each macrostate (eigenstate of $\mathcal{H}_A$) so that the Shannon entropy is simply

$$H_{Sh.} \; = \; 3,$$

which again is larger than the von Neumann entropy.

In general, the Shannon entropy will be larger than the von Neumann entropy unless the reduced density matrix is diagonal in the basis used to label the states for the Shannon entropy. In that case the diagonal elements of the reduced matrix elements are the eigenvalues of the reduced density matrix and are also the sums of the probabilities of all the microstates which form a given macrostate. The Shannon entropy and von Neumann entropies coincide in that case.

A striking example of this is an ensemble of N non-interacting spin-$\frac{1}{2}$ particles. Let us take the basis for the microstates to be the components of the spin of the particles along the z-axis. If the macrostate is defined in terms of the total spin along the z-axis, the reduced density matrix is diagonal with the i^{th} elements equal to the probabilities for the ensemble to have a total spin $(N-i)/2$ in the z direction and the von Neumann and Shannon entropies are both equal to

$$H \; = \; \log_2\left({}^N C_i\right).$$

On the other hand, if we take as the basis for the microstates the components of microstates to be the components of the spins along the x-axis, then the von Neumann entropy is unchanged, since the reduced matrix element in the new basis is simply a unitary transformation of the original reduced density matrix and its eigenvalues are unchanged. But we know that if the component of spin in the x-direction is known then there is an equal probability that the component of the spin in the z-direction being $+\frac{1}{2}$ or $-\frac{1}{2}$. The Shannon entropy in this case is N, which is larger than the von Neumann entropy (except in the case $i = N/2$).

2.10 Measurement

Measurement is an irreversible process. A body (the object whose macrostate properties are to be determined by measurements) is brought into contact with an environment) the measuring apparatus) in which a way that they form an entangled state - a sum of products of the body state in certain state and the apparatus in a corresponding state which registers (some of) the properties of the body.

The state of the system before measurement can be written

$$|\Psi\rangle_< \ = \ \sum_{\{y\}} a_[\{y\}|\{y\}\rangle \otimes \ \sum_{\{z\}} b_[\{z\}|\{z\}\rangle.$$

This is a factorizable state - there is no entanglement and the von Neumann entropy is zero.

After the measurement we have an entangled state, which may be written in the bases Schmidt decomposition

$$|\Psi\rangle_> \ = \ \sum_{\alpha} \sqrt{p_\alpha}|\{y_\alpha\}\rangle \otimes |\{z_\alpha\}\rangle,$$

Meaning that there is a probability p_α that the body is in the macrostate labelled by $\{y_\alpha\}$.

The measurement is not complete until the density matrix has been reduced to the reduced density matrix by tracing over the variables $\{z\}$. This reduced density matrix has a positive von Neumann entropy - indicating that an irreversible process has taken place.

There is *no* unitary transformation which performs this task – under unitary transformations an idempotent density matrix remains idempotent. Quantum physics does *not* perform the task of constructing the reduced density matrix and needs to be supplemented in order to describe the process of measurement. The formation of the reduced density matrix is equivalent to the notion of "wavefunction collapse".

2.10.1 Revisiting Schoedinger's cat

In this example the system is the cat and the environment is a spin-$\frac{1}{2}$ particle is a superposition state

$$\cos\theta|\uparrow\rangle + \sin\theta|\downarrow\rangle,$$

where again for simplicity I assume that the coefficients are real.

The cat "paradox" appears because usually we consider the body to be much smaller than the environment so we would naturally take the cat to be the environment - i.e. we treat the cat as a measuring device, but here we consider the cat to be the body and the spin-$\frac{1}{2}$ particle is the envirpnment..

A live cat is in a state

$$|\text{live}\rangle = \sum_{n_\uparrow} a_{n_\uparrow}|n_\uparrow\rangle,$$

where $n_\uparrow$ labels the quantum numbers of all states describing a live cat. A dead cat is in a state

$$|\mathrm{dead}\rangle = \sum_{n_\downarrow} b_{n_\downarrow}|n_\downarrow\rangle,$$

where $n_\downarrow$ labels the quantum numbers of all states describing a dead cat.

Initially the cat is alive and so the initial state of the system is in a separable state

$$|\Psi_i\rangle \;=\; \left(\sum_{n_\uparrow} a_{n_\uparrow}|n_\uparrow\rangle\right) \otimes \left(\cos\theta|\uparrow\rangle + \sin\theta|\downarrow\rangle, \right). \tag{2.10.1}$$

The cat has has zero entropy as the state is separable

The interaction between the cat and the environment effects transitions

$$\begin{aligned}
|n_\uparrow\rangle \otimes |\uparrow\rangle &\longrightarrow \sum_{m_\uparrow} U^{(1)\,m_\uparrow}_{n_\uparrow}|m_\uparrow\rangle \otimes |\uparrow\rangle \\
|n_\downarrow\rangle \otimes |\uparrow\rangle &\longrightarrow \sum_{m_\uparrow} U^{(2)\,m_\uparrow}_{n_\downarrow}|m_\uparrow\rangle \otimes |\uparrow\rangle \\
|n_\downarrow\rangle \otimes |\downarrow\rangle &\longrightarrow \sum_{m_\downarrow} U^{(3)\,m_\downarrow}_{n_\downarrow}|m_\downarrow\rangle \otimes |\downarrow\rangle \\
|n_\uparrow\rangle \otimes |\downarrow\rangle &\longrightarrow \sum_{m_\downarrow} U^{(4)\,m_\downarrow}_{n_\uparrow}|m_\downarrow\rangle \otimes |\downarrow\rangle
\end{aligned} \tag{2.10.2}$$

$U^{(1)}, \cdots U^{(4)}$ are unitary matrices.

After this interaction he system (the cat plus the spin-$\frac{1}{2}$ particle) is in an entangled state is

$$|\Psi_f\rangle \;=\; \cos\theta \sum_{n_\uparrow, m_\uparrow} a_{n_\uparrow} U^{(1)\,m_\uparrow}_{n_\uparrow}|m_\uparrow\rangle \otimes |\uparrow\rangle + \sin\theta \sum_{n_\uparrow, m_\downarrow} a_{n_\uparrow} U^{(4)\,m_\downarrow}_{n_\uparrow}|m_\downarrow\rangle \otimes |\downarrow\rangle \tag{2.10.3}$$

Now if we construct the density matrix trace over the states of the spin-$\frac{1}{2}$ particle (environment), we find that the reduced density matrix for the cat is block-diagonal

$$\rho_{\mathrm{cat}} \;=\; \begin{pmatrix} \cos^2\theta\rho_{\mathrm{alive}} & 0 \\ 0 & \sin^2\theta\rho_{\mathrm{dead}} \end{pmatrix} \tag{2.10.4}$$

where the density sub-matrices are is

$$\begin{aligned}
(\rho_{\mathrm{alive}})^{m}_{m'} &= \sum_{n,n'} a_n a^*_{n'} U^{(1)\,m}_{n} U^{(1)\dagger\,m'}_{n'} \\
(\rho_{\mathrm{dead}})^{m}_{m'} &= \sum_{n,n'} a_n a^*_{n'} U^{(4)\,m}_{n} U^{(4)\dagger\,m'}_{n'}
\end{aligned}$$

These sub-matrices can be diagonalized and each has one eigenvalues equal to unity, so the von Neumann entropy is

$$H_{vN} \;=\; -\left(\cos^2\theta\log_2\left(\cos^2\theta\right)+\sin^2\theta\log_2\left(\sin^2\theta\right)\right) \tag{2.10.5}$$

and $\cos^2\theta$, $\sin^2\theta$ are the classical probabilities to find the cat alive or dead. Note that the for the maximally entangled state $\theta=\pi/4$ and the entropy of the cat is 1.

This is certainly an over-simplification because the cat is probably not initially in pure state, but is already part of an entangled state - i.e. the density matrix for the cat has many eigenvalues as a result of previous interactions with a larger environment.

2.11 More Examples

2.11.1 Two spin-$\frac{1}{2}$ particles

The four possible states are $|\uparrow\uparrow\rangle$, $|\downarrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\downarrow\rangle$.

It is convenient to write the most general superposition of these four states in the form

$$\begin{aligned}|\Psi\rangle \;=\; \frac{1}{\sqrt{1+e^{-\mu}}}\Big(& \left(\cos\alpha\cos\beta-\sin\alpha\sin\beta e^{-\mu/2}\right)|\uparrow\uparrow\rangle\\ &+\left(\cos\alpha\sin\beta+\sin\alpha\cos\beta e^{-\mu/2}\right)|\uparrow\downarrow\rangle\\ &+\left(\sin\alpha\cos\beta+\cos\alpha\sin\beta e^{-\mu/2}\right)|\downarrow\uparrow\rangle\\ &+\left(\sin\alpha\sin\beta-\cos\alpha\cos\beta e^{-\mu/2}\right)|\downarrow\downarrow\rangle\Big)\end{aligned} \tag{2.11.1}$$

The sum of the squares of the coefficients is unity and for convenience the phases have been set to zero.

In the limit $\mu\to\pm\infty$, this superposition is an unentangled state and can be written

$$|\Psi\rangle \;=\; (\cos\alpha|\uparrow\rangle+\sin\alpha|\downarrow\rangle)\otimes(\cos\beta|\uparrow\rangle+\sin\beta|\downarrow\rangle) \tag{2.11.2}$$

For any finite μ, we have an entangled state. The reduced density, $\tilde{\rho}_{(1)}$ matrix, generated by tracing over the spin state of the second spin-$\frac{1}{2}$ is

$$\tilde{\rho}_{(1)} \;=\; \frac{1}{(1+e^{-\mu})}\begin{pmatrix}\cos^2\alpha+\sin^2\alpha\, e^{-\mu} & \cos\alpha\sin\alpha\,(1-e^{-\mu})\\ \cos\alpha\sin\alpha\,(1-e^{-\mu}) & \sin^2\alpha+\cos^2\alpha\, e^{-\mu}\end{pmatrix} \tag{2.11.3}$$

The fact that the angle β drops out of the expression for the reduced density matrix is a consequence of the Schmidt decomposition theorem.

The eigenvalues of the reduced density matrix are

$$\lambda_1 \;=\; \frac{1}{(1+e^{-\mu})}, \quad \lambda_2 \;=\; \frac{e^{-\mu}}{(1+e^{-\mu})}, \tag{2.11.4}$$

For a canonical ensemble, these are the probabilities that particle 1 has z-component of spin $-\frac{1}{2}$ and $+\frac{1}{2}$ respectively. μ is the conjugate variable to $s_z^{(1)}$.

The von Neumann entropy, which is a function of μ is

$$H_{vN}(\mu) \;=\; \log_2(1+e^{-\mu}) - \frac{\mu}{(1+e^{\mu})\ln 2}. \tag{2.11.5}$$

This takes its maximum value of $\ln 2$, when $\mu = 0$ for which the superposition (2.11.1) is maximally entangled. For infinite μ the entropy is zero – the component spin of particle 1 in the z-direction, $s_z^{(1)}$, is *definitely* $\pm\frac{1}{2}$. For finite μ the entanglement is maximal subject to the condition

$$\langle s_z^{(1)} \rangle \;==\; \mathrm{Tr}\left(\hat{s}_z^{(1)}\tilde{\rho}_{(1)}\right) \;=\frac{1}{2}\tanh(\mu/2).$$

In this case the expectation of $s_z^{(1)}$ is the only macrostate variable and so its expectation value determined the degree entanglement. A quantity such as the square total spin, S^2 which could be used to describe the original entangled state, is lost when the reduced density matrix is constructed because the operator $\hat{S}^2$ acts on the Hilbert space of *both* spin-$\frac{1}{2}$ particles.

2.11.2 Heisenberg Ferromagnet

This is an ensemble of N spin-$\frac{1}{2}$ particles with nearest neighbour interactions.

The states of this system can be labelled by eigenvalues of the total J_z operator, which counts how many spins, n_+ are "up"

$$J_z \;=\; n_+ - \frac{N}{2}$$

This is an "integrable system"" so that there are a total of N mutually commuting operators, i.e. $(N-1)$ operators that commute with J_z. One of these is the operator

$$J^2 \;=\; \left|\sum_i \mathbf{s}_i\right|^2,$$

with eigenvalues $J(J+1)$. J takes values in integer steps between 0 to $N/2$ for even N and between $\frac{1}{2}$ to $N/2$ for odd N. We call the remaining $N-3$ operators (classified by Bethe) $Q_3 \cdots Q_N$ and they have eigenvalues $q_3 \cdots q_N$.

Thus a pure state can be labelled

$$\left|J_z, J^2, q_3 \cdots q_n\right\rangle$$

We will define the macrostates as states which are labelled only by J_z – the sum of the z-components of the individual spins. The reduced density matrix, $\tilde{\rho}$, is then constructed by tracing over the eigenvalues J and $q_3 \cdots q_N$.

$$\tilde{\rho}_{J_z J_z'} \;=\; |J_z, J, q_3 \cdots q_n\rangle\langle J_z', J', q_3' \cdots q_n'] \; \delta_{JJ'}\delta_{q_3 q_3'} \cdots \delta_{q_n q_n'} \tag{2.11.6}$$

The von Neumann entropy determined from this reduced matrix element coincides with the Shannon entropy provided the pure quantum state is maximally entangled, meaning that it is a superposition of states equal coefficients for all states with a given value of J_z.

The reduced density matrix can be diagonalized and the eigenvalues are the probabilities of finding the state with a particular value of J_z. In that case the entropy is the logarithm of the umber of ways that the N spins can be configured so that $N/2 + J_z$ are spn-up and the rest spin-0down, i.e the number of ways of selecting $N.2 + J_z$ from N,

$$H \;=\; \log_2\left(\frac{N!}{(N/2 - J_z)!\,(N/2 + J_z)}\right) \;\approx\; N\log_2\left(\frac{2N}{\sqrt{N^2 - 4J_z^2}}\right) - J_z\log_2\left(\frac{N - 2J_Z}{N + 2J_z}\right)$$

2.11.3 Two equal frequency coupled Harmonic Oscillators

We can get a little further analytically if we consider two coupled harmonic oscillators of the same mass 9taken to be unity) and the same frequency

The Hamiltonian may then be written

$$\mathrm{H} \;=\; \frac{1}{2}\left\{p_1^2 + p_2^2 + \left(\omega_+^2 + \omega_-^2\right)\left(x_1^2 + x_2^2\right) + \left(\omega_+^2 - \omega_-^2\right)2x_1x_2\right\} \tag{2.11.7}$$

$$\text{Let } x_+ \equiv \frac{(x_1 + x_2)}{\sqrt{2}}, \quad x_- \equiv \frac{(x_1 - x_2)}{\sqrt{2}},$$

This gives us two uncoupled harmonic oscillators with Hamiltonian

$$H \;=\; \frac{1}{2}\left\{p_+^2 + p_-^2 + \omega_+^2 x_+^2 + \omega_-^2 x_-^2\right\} \tag{2.11.8}$$

Ground State:
The ground state wavefunction is

$$\Psi_0(x_+, x_-) \;=\; \frac{1}{\sqrt{\pi}}\left(\omega_+\omega_-\right)^{1/4}\exp\left\{-\omega_+ x_+^2 - \omega_-^2 x^{‘2}_-\right\} \tag{2.11.9}$$

In terms of x_1, x_2

$$\Psi_0(x_1, x_2) \;=\; \frac{1}{\sqrt{\pi}}\left(\omega_+\omega_-\right)^{1/4}\exp\left\{-\left(\frac{\omega_+ + \omega_-}{2}\right)\left(\frac{x_1^2 + x_2^2}{2}\right) - \left(\frac{\omega_+ - \omega_-}{2}\right)x_1x_2\right\} \tag{2.11.10}$$

We find the reduced density matrix for oscillator 1 by tracing over the coordinate x_2. This leads to the entanglement of the two oscillators and yields the reduced density matrix

$$\begin{aligned}\hat{\rho}(x_1, x_1') &= \frac{1}{\pi}\sqrt{\omega_+\omega_-}\exp\left\{-\left(\frac{\omega_+ + \omega_-}{2}\right)\left(\frac{x_1^2 + {x_1'}^2}{2}\right)\right\} \\ &\times \int_{-\infty}^{\infty} dx_2 \exp\left\{-\left(\frac{\omega_+ + \omega_-}{2}\right)x_2^2 + \left(\frac{\omega_+ - \omega_-}{2}\right)x_2\,(x_1 + x_1')\right\} \\ &= \frac{1}{\sqrt{\pi}}\sqrt{(\gamma - \beta)}\exp\left\{-\gamma\left(\frac{x_1^2 + x_1'^2}{2}\right) + \beta x_1 x_1'\right\}, \qquad (2.11.11)\end{aligned}$$

where

$$\gamma - \beta \;=\; \frac{2\omega_+\omega_-}{(\omega_+ + \omega_-)}, \quad \beta = \frac{1}{4}\frac{(\omega_+ - \omega_-)^2}{(\omega_+ + \omega_-)} \qquad (2.11.12)$$

Eigenfunctions and eigenvalues of reduced density matrix
First we show that $\exp(-\alpha x^2/2)$ is an eigenfunction for a particular value of α and calculate the corresponding eigenvalue.

$$\int_{-\infty}^{\infty} dx_1'\sqrt{\frac{\gamma - \beta}{\pi}}\exp\left\{-\gamma\left(\frac{x_1^2 + x_1'^2}{2}\right) + \beta x_1 x_1'\right\}\exp\left\{-\alpha x_1'^2/2\right\} \;=\; \sqrt{\frac{2\,(\gamma - \beta)}{\gamma + \alpha}}\exp\left\{\left[\frac{\beta^2}{(\gamma + \alpha)} - \gamma\right]x_1^2/2\right\}. \qquad (2.11.13)$$

$\exp\{-\alpha x^2/2\}$ is an eigenfunction if

$$\exp\left\{\left[\frac{\beta^2}{(\gamma + \alpha)} - \gamma\right]\frac{x_1^2}{2}\right\} \;=\; \exp\left\{-\alpha\frac{x_1^2}{2}\right\},$$

which is true provided

$$\frac{\beta^2}{\alpha + \gamma} \;=\; \gamma - \alpha,$$

i.e.

$$\alpha^2 = \gamma^2 - \beta^2 \;=\; (\gamma - \beta)(\gamma + \beta). \qquad (2.11.14)$$

From (2.11.12) we have

$$\gamma + \beta \;=\; \frac{4\omega_+\omega_- + (\omega_+ - \omega_-)^2}{2(\omega_+ + \omega_-)} \;=\; \frac{1}{2}(\omega_+ - \omega_-), \qquad (2.11.15)$$

so that

$$\alpha \;=\; \sqrt{\omega_+\omega_-} \qquad (2.11.16)$$

The (lowest) eigenvalue, λ_0, is given by

$$\begin{aligned}\lambda_0 &= \sqrt{\frac{2\,(\gamma-\beta)}{\gamma+\alpha}} = \frac{\sqrt{2(\gamma-\beta)(\gamma+\alpha)}}{\gamma+\alpha} = \frac{\sqrt{2\gamma^2-2\beta\gamma-2\alpha\beta+2\alpha\gamma}}{\gamma+\alpha} \\ &= \frac{\sqrt{\gamma^2+\alpha^2+\beta^2-2\beta\gamma-2\alpha\beta+2\alpha\gamma}}{\gamma+\alpha} = \frac{\alpha+\gamma-\beta}{\alpha+\gamma} = (1-\xi), \qquad (2.11.17)\end{aligned}$$

where, using (2.11.14),

$$\xi \equiv \frac{\beta}{\alpha+\gamma} = \frac{\gamma-\alpha}{\beta}. \qquad (2.11.18)$$

$$\begin{aligned}\gamma+\alpha &= \frac{8\omega_+\omega_- + \omega_+^2 + \omega_-^2 - 2\omega_+\omega_- + 4\sqrt{\omega_+^3\omega_-} + 4\sqrt{\omega_+\omega_-^3}}{4(\omega_+ + \omega_-)} \\ &= \frac{\left(\sqrt{\omega_+}+\sqrt{\omega_-}\right)^4}{4(\omega_+ + \omega_-)}, \qquad (2.11.19)\end{aligned}$$

and we can write

$$\beta = \frac{\left(\sqrt{\omega_+}+\sqrt{\omega_-}\right)^2\left(\sqrt{\omega_+}-\sqrt{\omega_-}\right)^2}{4(\omega_+ + \omega_-)} \qquad (2.11.20)$$

so that

$$\xi = \left(\frac{\sqrt{\omega_+}-\sqrt{\omega_-}}{\sqrt{\omega_+}+\sqrt{\omega_-}}\right)^2. \qquad (2.11.21)$$

We may also write ξ as

$$\xi = \frac{\beta'}{1-\sqrt{1-\beta'^2}}, \qquad (2.11.22)$$

where $\beta' \equiv \beta/\gamma$.

Excited States:

Mehler's formula realtes a Gaussian integrand with two variables into a sum of products of Hermite polynomials:

$$\frac{1}{\sqrt{1-\xi^2}}\exp\left\{-\frac{\xi^2\,(z^2+w^2)}{(1-\xi^2)} + \frac{2\xi zw}{(1-\xi^2)}\right\} = \sum_{n=0}^{\infty}\frac{\xi^n}{2^n n!}H_n(z)H_n(w),) \qquad (2.11.23)$$

where $H_n(x)$ are Hermite polynomials of x.

From (2.11.18),

$$\begin{aligned}\left(1-\xi^2\right) &= 1-\frac{\beta^2}{(\gamma+\alpha)^2} \\ &= \frac{(\gamma+\alpha-\beta)(\gamma+\alpha+\beta)}{(\alpha+\gamma)^2} = \frac{(\gamma^2+\alpha^2-\beta^2-2\alpha\gamma)}{(\alpha+\gamma)^2} \\ &= \frac{2\,(\alpha^2+\alpha\gamma)}{(\alpha+\gamma)^2} = \frac{2\alpha}{(\alpha+\gamma)} \qquad (2.11.24)\end{aligned}$$

$$\xi \;=\; \frac{\gamma - \sqrt{\gamma^2 - \beta^2}}{\beta} \tag{2.11.25}$$

$$\alpha \;=\; \sqrt{\gamma^2 - \beta^2} \tag{2.11.26}$$

Using (2.11.23), setting

$$z \equiv \sqrt{\alpha} x_1, \quad w \equiv \sqrt{\alpha} x_1',$$

we have

$$\begin{aligned}
\hat{\rho}(x_1, x_1') \;&=\; \sqrt{\gamma - \beta} \exp\left\{-\gamma \left(x_1^2 + x_1'^2\right)/2 + \beta x_1 x_1'\right\} \\
&=\; \frac{(1-\xi)}{\sqrt{2}} \sqrt{(\alpha+\gamma)(1-\xi^2)} \sum_{n=0}^{\infty} \frac{\xi^2}{2^n n!} H_n(\sqrt{\alpha} x_1) H_n(\sqrt{\alpha} x_1') \exp\left\{-\frac{\alpha}{2}\left(x_1^2 + x_2'^2\right)\right\} \\
&=\; (1-\xi)\sqrt{\alpha} \sum_{n=0}^{\infty} \frac{\xi^2}{2^n n!} H_n(\sqrt{\alpha} x_1) H_n(\sqrt{\alpha} x_1') \exp\left\{-\frac{\alpha}{2}\left(x_1^2 + x_2'^2\right)\right\} \qquad (2.11.27)
\end{aligned}$$

Using the orthonormality relation of Hermite polynomials

$$\int_{-\infty}^{\infty} dx H_n\left(\sqrt{\alpha} x\right) H_m\left(\sqrt{\alpha} x\right) \exp\left\{-\alpha x^2\right\} \;=\; \frac{1}{\sqrt{\alpha}} 2^n n! \delta_{mn},$$

we see that

$$f_n(x) \;\equiv H_n\left(\sqrt{\alpha} x\right) \exp\{-\alpha x^2/2\} \tag{2.11.28}$$

are eigenfunctions of the reduced density matrix with eigenvalues

$$\lambda_n \;=\; (1-\xi)\xi^n. \tag{2.11.29}$$

(Note that the sum of all the eigenvalues is one, as expected – the eigenvalues are the probabilities to find the first harmonic oscillator in the state $|n\rangle$.).

The entropy of entanglement is therefore

$$\begin{aligned}
H_{ent.} \;&=\; -\sum_{n=0}^{\infty} \lambda_n \log_2(\lambda_n) \;=\; -\left(\log_2(1-\xi) + \sum_{n=0}^{\infty} n\xi^n \log_2(\xi)\right) \\
&=\; -\left(\log_2(1-\xi) + \frac{\xi}{(1-\xi)} \log_2(\xi)\right) \qquad (2.11.30)
\end{aligned}$$

Fock Space Approach:

The ground state is $|0\rangle_+ \otimes |0\rangle_-$ and obeys the relations

$$\begin{aligned}
a_+\left(|0\rangle_+ \otimes |0\rangle_-\right) \;&\equiv\; \sqrt{\frac{1}{2}}\left(\sqrt{\omega_+}\, x_+ + i\frac{p_+}{\sqrt{\omega_+}}\right)\left(|0\rangle_+ \otimes |0\rangle_-\right) \;=\; 0 \\
a_-|0\rangle_+ \otimes |0\rangle_- \;&\equiv\; |0\rangle_+ \otimes \sqrt{\frac{1}{2}}\left(\sqrt{\omega_-}\, x_- + i\frac{p_-}{\sqrt{\omega_-}}\right)|0\rangle_- \;=\; 0 \qquad (2.11.31)
\end{aligned}$$

Consider the operator

$$\hat{A}_1 \;\equiv\; \frac{1}{\sqrt{1-\xi}}\left(a_1+\sqrt{\xi}a_2^\dagger\right) \;=\; \frac{1}{2\left(\omega_+\omega_-\right)^{1/4}}\left(\left(\sqrt{\omega_+}+\sqrt{\omega_-}\right)a_1+\left(\sqrt{\omega_+}-\sqrt{\omega_-}\right)a_2^\dagger\right) \tag{2.11.32}$$

where

$$a_{1(2)} \;\equiv\; \frac{1}{\sqrt{2}}\left(\left(\omega_+\omega_-\right)^{1/4}x_{1(2)}+i\frac{p_{1(2)}}{\left(\omega_+\omega_-\right)^{1/4}}\right) \tag{2.11.33}$$

In terms of coordinates x_+, x_-, and momenta p_+, p_-

$$\hat{A}_1 \;=\frac{1}{2}\left(\sqrt{\omega_+}\,x_++\sqrt{\omega_-}\,x_-+\frac{i}{\sqrt{\omega_+}}p_++\frac{i}{\sqrt{\omega_+}}p_-\right) \;=\; \frac{1}{\sqrt{2}}\left(a_++a_-\right) \tag{2.11.34}$$

Similarly

$$\hat{A}_2 \;\equiv\; \frac{1}{\sqrt{1-\xi}}\left(a_2+\sqrt{\xi}a_1^\dagger\right) \;=\; \frac{1}{\sqrt{2}}\left(a_+-a_-\right) \tag{2.11.35}$$

Both of these operators annihilate the ground state $|0\rangle_+|0\rangle_-$. From (2.11.32) and (2.11.21) we therefore have

$$a_1\left(|0\rangle_+\otimes|0\rangle_-\right) \;=\; -\sqrt{\xi}a_2^\dagger\left(|0\rangle_+|0\rangle_-\right) \tag{2.11.36}$$

and from (2.11.34) we therefore have

$$a_2\left(|0\rangle_+\otimes|0\rangle_-\right) \;=\; -\sqrt{\xi}a_1^\dagger\left(|0\rangle_+\otimes|0\rangle_-\right) \tag{2.11.37}$$

We can expand the ground-state vector in the Hilbert space $\mathcal{H}_+\otimes\mathcal{H}_-$, i.e $|0\rangle_+|0\rangle_-$ in terms of basis vectors in the Hilbert-space $\mathcal{H}_1\otimes\mathcal{H}_2$, i.e. $|n\rangle_1\otimes|m\rangle_2$

$$|0\rangle_+\otimes|0\rangle_- \;=\; \sum_{n,m}C_{nm}|n\rangle_1\otimes|m\rangle_2 \tag{2.11.38}$$

We may assume that the coefficients C_{nm} are real.

The reduced matrix density matrix formed by tracong over the Hilbert space $\mathcal{H}_2$ is then given by

$$\hat{\rho}_{nn'} \;=\; \sum_{m=0}^{\infty}C_{nm}C_{n'm} \tag{2.11.39}$$

Using the raising and lowering operator relations, (2.11.36) gives

$$\sum_{n,m}C_{n,m}\sqrt{n-1}|n-1\rangle_1|m\rangle_2 \;=\; -\sqrt{\xi}\sum_{n,m}C_{n,m}\sqrt{m+1}|n\rangle_1|m+1\rangle_2 \tag{2.11.40}$$

Making the shifts $n\to(n-1),\ m\to(m+1)$, this may be rewritten

$$C_{nm} \;=\; -\sqrt{\xi}\sqrt{\frac{m}{n}}C_{(n-1)(m-1)} \tag{2.11.41}$$

Similarly (2.11.37) leads to

$$C_{nm} \;=\; -\sqrt{\xi}\sqrt{\frac{n}{m}}C_{(n-1)(m-1)} \tag{2.11.42}$$

(2.11.41) and (2.11.42) are consistent provided

$$C_{nm} \;=\; \sqrt{(1-\xi)}\,(-\xi)^{n/2}\,\delta_{mn} \tag{2.11.43}$$

where the prefactor $\sqrt{1-\xi}$ has been chosen to satisfy the normalization condition

$$\sum_{mn} C_{nm}^2 \;=\; 1.$$

The reduced density matrix is therefore

$$\hat{\rho}_{nn'} \;=\; (1-\xi)\xi^n\delta_{nn'} \tag{2.11.44}$$

with eigenvalues given by (2.11.29), (calculated using the wavefunction representation).

We can now rewrite the ground state in the form

$$|0\rangle_+ \otimes |0\rangle_- \;=\; \sqrt{1-\xi}\,\exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}|0\rangle_1 \otimes |0\rangle_2 \tag{2.11.45}$$

Excited States:

Consider the excited state, $|1,0\rangle$, defined by

$$|1,0\rangle \;\equiv \hat{A}_1^\dagger|0\rangle_+ \otimes |0\rangle_- \tag{2.11.46}$$

where the raising operator $A_1^\dagger$ is the conjugate of the lowering operator, $\hat{A}_1$, defined in (2.11.32).

Using (the conjugate of) (2.11.32) and (2.11.45), we have

$$\begin{aligned} |1,0\rangle \;&=\; \left(a_1^\dagger + \sqrt{\xi}a_2\right)\exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}(|0\rangle_1 \otimes |0\rangle_2) \\ &=\; \left(a_1^\dagger + \sqrt{\xi}\left[a_2, \exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}\right]\right)(|0\rangle_1 \otimes |0\rangle_2)\,, \end{aligned} \tag{2.11.47}$$

where we have used $a_2\,(|0\rangle_1 \otimes |0\rangle_2) = 0$.

$$\left[a_2, \exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}\right] \;=\; -\sqrt{\xi}\,\exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}a_1^\dagger \tag{2.11.48}$$

so that

$$\hat{A}_1|0,0\rangle \;=\; \sqrt{1-\xi}\,\exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}a_1^\dagger\,(|0\rangle_1 \otimes |0\rangle_2) \tag{2.11.49}$$

Applying this raising operator n times se have

$$\begin{aligned}|n,0\rangle &\equiv \frac{1}{\sqrt{n!}}\hat{A}_1^n|0,0\rangle = \frac{1}{\sqrt{n!}}\sqrt{(1-\xi)}^{(n+1)}\exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}\left(a_1^\dagger\right)^n(|0\rangle_1\otimes|0\rangle_2)\\ &= (\sqrt{1-\xi})^{(n+1)}\exp\left\{-\sqrt{\xi}a_1^\dagger a_2^\dagger\right\}(|n\rangle_1\otimes|0\rangle_2)\,. \end{aligned}\tag{2.11.50}$$

The prefactor $1/\sqrt{n!}$ is required to ensure that $|n,0\rangle$ is properly normalized. Expanding the exponential we have

$$|n,0\rangle = (\sqrt{1-\xi})^{(n+1)}\sum_j\sqrt{\frac{(n+j)!}{n!j!}}\left(-\sqrt{\xi}\right)^j(|(n+j)\rangle_1\otimes|j\rangle_2)\,,\tag{2.11.51}$$

so that

$$\langle n,0|n,0\rangle = (1-\xi)^{(n+1)}\sum_j\frac{(n+j)!}{n!j!}\xi^j = 1\tag{2.11.52}$$

Here we have used

$$\sum_j\frac{(n+j)!}{n!j!}\xi^j = (1-\xi)^{(-n-1)}.\tag{2.11.53}$$

We will also need its derivative w.r.t. $\ln\xi$,

$$\sum_j\frac{(n+j)!}{n!(j-1)!}\xi^j = (n+1)\xi(1-\xi)^{(-n-2)}.\tag{2.11.54}$$

We note that these states form a complete set and can be taken as a definition of excited states but they are *not* eigenstates of the Hamiltonian, except for the ground state.

The density matrix for a system in the state $|n,0\rangle$ can be written in terms of the basis vectors in the Hilbert space $\mathcal{H}_1\otimes\mathcal{H}_2$ is

$$\rho\equiv|n,0\rangle\langle n,0| = (1-\xi)^{(n+1)}\sum_{j,k}\sqrt{\frac{(n+j)!(n'+k)!}{(n!)^2j!k!}}(-\sqrt{\xi})^{(j+k)}|(n+j)\rangle_1\langle(n+k)|\otimes|j\rangle_2\langle k|\tag{2.11.55}$$

The reduced density matrix for oscillator one is obtained by tracing over the Hilbert space $\mathcal{H}_2$, i.e. we replace $|j\rangle_2\langle|k|$ by δ_{jk} to obtain a diagonal reduced density matrix

$$\hat{\rho}_{(n+j),(n+j')} = (1-\xi)^{(n+1)}\frac{(n+j)!}{n!j!}\xi^j\delta_{jj'}\tag{2.11.56}$$

The entanglement entropy is therefore

$$H_{ent.} = -(1-\xi)^{(n+1)}\sum_j\frac{(n+j)!}{n!j!}\xi^j\log_2\left((1-\xi)^{(n+1)}\frac{(n+j)!}{n!j!}\xi^j\right)\tag{2.11.57}$$

Using (2.11.53) and (2.11.54) this may be rewritten

$$
\begin{aligned}
H_{ent,} \;&=\; -\Bigg[(n+1)\left(\log_2(1-\xi)+\frac{\xi\log_2\xi}{(1-\xi)}\right) \\
&\qquad +(1-\xi)^{(n+1)}\sum_j \xi^j\frac{(n+j)!}{n!j!}\log_2\left(\frac{(n+j)!}{n!j!}\right)\Bigg] \qquad (2.11.58)
\end{aligned}
$$

2.11.4 N Coupled Oscillators

We consider N coupled harmonic oscillators and form the reduced density matrix by tracing over the coordinates of oscillators $(n+1)\cdots N$.

$$
\mathrm{H} \;=\; \sum_{\alpha=1}^{N}\left[\frac{1}{2}P_\alpha^2+\frac{1}{2}\sum_\beta X_\alpha\left(\mathbf{\Omega}\cdot\mathbf{\Omega}\right)_{\alpha\beta}X_\beta\right] \qquad (2.11.59)
$$

We define the macrostate to be labelled by vectors in the Hilbert space of oscillators $1\cdots n$ and the environment to be the Hilbert space of oscillators $(n+1)\cdots N$. We therefore write

$$
\mathbf{X} = \left(y_1\cdot y_n, z_1\cdots z_{(N-n)}\right),
$$

and the $N\times N$ matrix

$$
\mathbf{\Omega} \;=\; \begin{pmatrix}\mathbf{\Omega}_A & \mathbf{\Omega}_C \\ \mathbf{\Omega}_C^T & \mathbf{\Omega}_B\end{pmatrix},
$$

where $\mathbf{\Omega}_A$ is an $n\times n$ matrix, $\mathbf{\Omega}_C$ is an $(N-n)\times(N-n)$ matrix, and $\mathbf{\Omega}_B$ is a rectangular $(N-n)\times n$ matrix.

The ground-state wavefunction is

$$
\Psi_0(\mathbf{X}) \;=\; \left(\det\left(\frac{\mathbf{\Omega}}{\pi}\right)\right)^{1/4}\exp\left\{-\frac{1}{2}\mathbf{X}\cdot\mathbf{\Omega}\cdot\mathbf{X}\right\}, \qquad (2.11.60)
$$

where

$$
\mathbf{X}\cdot\mathbf{\Omega}\cdot\mathbf{X} \;=\; \mathbf{y}\cdot\mathbf{\Omega}_A\cdot\mathbf{y}+\mathbf{z}\cdot\mathbf{\Omega}_C\cdot\mathbf{z}+\mathbf{y}\cdot\mathbf{\Omega}_B\cdot\mathbf{z}+\mathbf{z}\cdot\mathbf{\Omega}_B^T\cdot\mathbf{y} \qquad (2.11.61)
$$

$$
\mathbf{\Omega}\cdot\mathbf{\Omega} \;=\; \begin{pmatrix}\mathbf{\Omega}_A\cdot\mathbf{\Omega}_A+\mathbf{\Omega}_B\cdot\mathbf{\Omega}_B^T & \mathbf{\Omega}_A\cdot\mathbf{\Omega}_B+\mathbf{\Omega}_B\cdot\mathbf{\Omega}_C \\ \mathbf{\Omega}_B^T\cdot\mathbf{\Omega}_A+\mathbf{\Omega}_C\cdot\mathbf{\Omega}_B^T & \mathbf{\Omega}_C\cdot\mathbf{\Omega}_C+\mathbf{\Omega}_B^T\cdot\mathbf{\Omega}_B\end{pmatrix} \qquad (2.11.62)
$$

The reduced density matrix is obtained by tracing over the coordinates $\mathbf{z}, \mathbf{z}'$

$$\begin{aligned}\hat{\rho}(\mathbf{y}, \mathbf{y}') &= \left(\det\left(\frac{\mathbf{\Omega}}{\pi}\right)\right)^{1/2} \int d^{(N-n)}\mathbf{z} \\ &\qquad \exp\left\{-\frac{1}{2}\left(\mathbf{y}\cdot\mathbf{\Omega}_A\cdot\mathbf{y} + \mathbf{z}\cdot\mathbf{\Omega}_C\cdot\mathbf{z} + \mathbf{y}\cdot\mathbf{\Omega}_B\cdot\mathbf{z} + \mathbf{y}\cdot\mathbf{\Omega}_B^T\cdot\mathbf{x}\right)\right\} \\ &= \mathcal{N}\exp\left\{-\frac{1}{2}\left(\mathbf{x}\cdot\mathbf{\Gamma}\cdot\mathbf{x} + \mathbf{x}'\cdot\mathbf{\Gamma}\cdot\mathbf{x}'\right) + \mathbf{x}\cdot\mathbf{\Delta}\cdot\mathbf{x}'\right\}, \qquad (2.11.63)\end{aligned}$$

where

$$\mathbf{\Delta} \equiv \frac{1}{2}\mathbf{\Omega}_B\cdot\mathbf{\Omega}_C^{-1}\cdot\mathbf{\Omega}_B^T \qquad (2.11.64)$$

and

$$\mathbf{\Gamma} = \mathbf{\Omega}_A - \mathbf{\Delta}. \qquad (2.11.65)$$

The prefactor $\mathcal{N}$ is not specified but is chosen to ensure conservation of probability, i.e.

$$\int d^n\mathbf{x}\,\hat{\rho}(\mathbf{x}, \mathbf{x}) = 1.$$

We now change variables

$$\mathbf{y} = \rightarrow \mathbf{w} \equiv \mathbf{U}\cdot\mathbf{\Gamma_D}^{-1/2}\cdot\mathbf{y},$$

where $\mathbf{\Gamma_D}$ is the diagonalized matrix $\mathbf{V}\cdot\mathbf{\Gamma}\cdot\mathbf{V}^T$,

$$\left(\mathbf{\Gamma_D}\right)_a^{\ b} = \gamma_a\delta_{ab},$$

and $\mathbf{U}$ is the orthogonal matrix that diagonalizes the matrix $\mathbf{\Gamma_D}^{-1/2}\cdot\mathbf{\Delta}\cdot\mathbf{\Gamma_D}^{-1/2}$,, i.e.

$$\left(\mathbf{U}\cdot\mathbf{\Gamma_D}^{-1/2}\cdot\mathbf{\Delta}\cdot\mathbf{\Gamma_D}^{-1/2}\cdot\mathbf{U}^T\right)_a^{\ b} = \beta_a\delta_{ab}$$

The reduced density matrix in terms of the new variables $\mathbf{w}$, $\mathbf{w}'$ is

$$\hat{\rho}(\mathbf{w}, \mathbf{w}') = \prod_{a=1}^{n}\sqrt{\frac{1-\beta_a}{\pi}}\exp\left\{-\frac{1}{2}\left(w_a^2 + w_a'^2 + \beta_a w_a w_a'\right)\right\}. \qquad (2.11.66)$$

Again the normalization constant is appropriately chosen to ensure that the trace of the reduced density matrix is unity.

This reduced density matrix is the product of n reduced density matrices for a "body" oscillator coupled to a n environment oscillator whose individual eigenvalues are given by (2.11.29).

$$\lambda_a = (1-\xi_a)\,\xi_a^{j_a}, \quad \text{where } \xi_a \equiv \frac{\beta_a}{1+\sqrt{1-\beta_a^2}} \qquad (2.11.67)$$

(see (2.11.250, (2.11.26)).

The eigenvalues of the reduced density matrix (2.11.66) are labelled by n integers. j_a, $(a = 1 \cdots n)$:

$$\lambda_{j_1 \cdots j_n} \; = \; \prod_{a=1}^{n} (1-\xi_a)\; \xi_a^{j_a}, \qquad \text{where} \;\; \xi_a \equiv \; \frac{\beta_a}{1+\sqrt{1-\beta_a^2}} \tag{2.11.68}$$

The entanglement entropy

$$\begin{aligned} H_{ent.} \; &= \; -\sum_{j_1 \cdots j_n} \lambda_{j_1 \cdots j_n} \log_2 \left(\lambda_{j_1 \cdots j_n}\right) \\ &= \; -\sum_{a=1}^{n} \prod_{k \neq a} \left(\sum_j (1-\xi_k))\xi_k^j \right) \sum_l (1-\xi_a)\, \xi_a^l \log_2 \left((1-\xi_a)\, \xi_a^l\right) \end{aligned} \tag{2.11.69}$$

Using

$$\sum_j (1-\xi)\xi^j \; = \; 1,$$

and

$$\sum_j (1-\xi)\xi^j \ln\left(\xi^j\right) \; = \; \frac{\xi}{(1-\xi)} \ln \xi$$

we arrive at

$$H_{ent.} = \sum_{a=1}^{n} H_{ent.}^{a}, \tag{2.11.70}$$

where

$$H_{ent.}^{a} \; = \; -\left(\log_2 (1-\xi_a) + \frac{\xi_a}{(1-\xi_a)} \log_2 \xi_a \right) \tag{2.11.71}$$

We consider the particular case where $N = 2$, $n = 1$, but unlike the above example the frequencies without the interaction term are unequal.

Write

$$\mathbf{\Omega} \cdot \mathbf{\Omega} = \begin{pmatrix} A & B \\ B & C \end{pmatrix}.$$

The square root matrix, $\mathbf{\Omega}$, has the form

$$\mathbf{\Omega} \; \equiv \; \begin{pmatrix} \omega_A & \omega_B \\ \omega_B & \omega_C \end{pmatrix} \tag{2.11.72}$$

where

$$
\begin{aligned}
\omega_A &= \frac{A \pm \sqrt{AC - B^2}}{\sqrt{D}} \\
\omega_B &= \frac{B}{\sqrt{D}} \\
\omega_C &= \frac{C \pm \sqrt{AC - B^2}}{\sqrt{D}}, \qquad \text{with } D = A + C \pm 2\sqrt{AC - B^2}
\end{aligned}
\tag{2.11.73}
$$

For $B \ll A, C$ these become (to leading order in B and with positive values for both diagonal elements)

$$
\begin{aligned}
\omega_A &\approx \sqrt{A} \\
\omega_B &\approx \frac{B}{\sqrt{A} + \sqrt{C}} \\
\omega_C &\approx \sqrt{C}
\end{aligned}
\tag{2.11.74}
$$

In this case we have

$$\Delta = \frac{\omega_B^2}{2\omega_C} \tag{2.11.75}$$

$$\Gamma = \frac{2\omega_A\,\omega_C - \omega_B^2}{2\omega_C} \tag{2.11.76}$$

$$\beta = \frac{\Delta}{\Gamma} = \frac{\omega_B^2}{(2\omega_A\omega_C - \omega_B^2)} \tag{2.11.77}$$

$$\xi = \frac{\omega_B^2}{\left(\sqrt{\omega_A\,\omega_C} + \sqrt{\omega_A\,\omega_C - \omega_B^2}\right)^2} \tag{2.11.78}$$

We note that in the approximation

$$\omega_B \ll \omega_A, \omega_C$$

$$\xi \approx \frac{\omega_B^2}{4\,\omega_A\,\omega_C} \tag{2.11.79}$$

2.11.5 Free Massless Scalar Field

$$\mathrm{H} = \int d^3\mathbf{r}\frac{1}{2}\left(\pi(\mathbf{r}^2) + (\boldsymbol{\nabla}\phi(\mathbf{r})^2\right) \tag{2.11.80}$$

We work in spherical polar coordinates, $(r, \theta\phi)$, since we will be seeking the reduced density matrix obtained by tracing over the field coordinates inside a sphere of a given radius, R.

$$d^3\mathbf{r} \ = r^2 \sin\theta d\theta d\phi dr$$

and expand the field $\phi(\mathbf{r})$ and conjugate momentum $\pi(\mathbf{r})$ in spherical harmonics.

$$r\phi(\mathbf{r}) \ = \ \sum_{l,m} \phi_{lm}(r) Y_{lm}(\theta, \pi) \tag{2.11.81}$$

$$r\pi(\mathbf{r}) \ = \ \sum_{l,m} \pi_{lm}(r) Y_{lm}(\theta, \phi). \tag{2.11.82}$$

The Hamiltonian becomes

$$\mathrm{H} \ = \ \sum_{l,m} \mathrm{H}_{lm}, \tag{2.11.83}$$

where

$$\mathrm{H}_{lm} \ = \ \frac{1}{2}\int dr \left(\pi_{lm}(r)^2 + r^2 \left(\frac{d}{dr}\frac{\phi_{lm}(r)}{r} \right)^2 + \frac{l(l+1)}{r^2}\phi_{lm}(r)^2 \right) \tag{2.11.84}$$

The entanglement entropy obtained by tracing out the field values for $r < R$ is the sum of the entropies of each partial wave component. Moreover, the azimuthal symmetry tells us that for each value of l the sum over the magnetic quantum number, m, just introduces a factor of $(2l+1)$ and so we may write

$$H_{ent.}(R) \ = \ \sum_l (2l+1) H^l_{ent.}(R) \tag{2.11.85}$$

where $H^l_{ent.}(R)$ is the entropy of a system whose Hamiltonian is H_{lm} (for any m between $\pm l$.)

Next we discretize the radial direction r in steps of δ, so that $r = j\delta$ and the entanglement radius $R = \left(n + \frac{1}{2}\right)\delta$. The field only has support on concentric spheres whose radial separation is δ. In this way we introduce an ultraviolet cut-off, $1/\delta$. We can introduce an infrared cut-off by imposing a maximum value, of N for the index j, i.e. we confine the system to a sphere of radius $R_{max.} = N\delta$.

Transforming:

$$\begin{aligned} \int dr \ &\rightarrow \ \delta \sum_{j=1}^{N}, \\ \phi_{lm}(r) \ &\rightarrow \ \phi_j, \\ \pi_{lm} \ &\rightarrow \ \pi_j/\delta, \\ r\frac{d}{dr}\frac{\phi_{lm}(r)}{r} \ &\rightarrow \ \frac{1}{\delta}\left(j + \frac{1}{2}\right)\left(\frac{\phi_{j+1}}{j+1} - \frac{\phi_j}{(j)}\right). \end{aligned} \tag{2.11.86}$$

ϕ_k and π_j obey the commutation relation

$$[\pi_j, \phi_k] \; = \; -i\delta_{jk} \tag{2.11.87}$$

The Hamiltonian for partial wave l for this discretized field, (set of coordinates) ϕ_j is then

$$\mathrm{H}l\left(\{\pi_j\},\{\phi_j\}\right) \; = \; \frac{1}{2\delta}\sum_{j=1}^{N}\left(\pi_j^2 + \left(j+\frac{1}{2}\right)^2\left(\frac{\phi_j}{j} - \frac{\phi_{j+1}}{(j+1)}\right)^2 + \frac{l(l+1)}{j^2}\phi_j^2\right) \tag{2.11.88}$$

.

This is the Hamiltonian of (2.11.59) with the square frequency

$$\begin{aligned}(\mathbf{\Omega}\cdot\mathbf{\Omega})_{jk} \; = \; & \left(\left(j+\frac{1}{2}\right)^2 + l(l+1)\frac{1}{j^2}\right)\delta_{jk} - \left(j+\frac{1}{2}\right)^2\frac{1}{j(j+1)}\delta_{k(j+1)} \\ & - \left(j-\frac{1}{2}\right)^2\frac{1}{j(j-1)}\delta_{k(j-1)}\end{aligned} \tag{2.11.89}$$

The reduced density matrix is obtained by tracing over $\phi_j, \; j = 1\cdots n$.

There are only nearest neighbour interactions. Nevertheless, in general, there will be entanglement between the first ϕ_j outside the sphere of radius R. ϕ_{n+1} and all of the coordinates $\phi_j, \; j = 1\cdots n$). The entanglement entropy has to be calculated using the method for N coupled oscillators, with the matrix $\mathbf{\Omega}$ obtained by finding the square root of $\mathbf{\Omega}\cdot\mathbf{\Omega}$ given by (2.11.89).

However, if the angular momentum, l, is sufficiently large ($l \gg N$), the entanglement between ϕ_n and $\phi_{(n+1)}$ is of order $1/l^2$ (the diagonal terms in $\mathbf{\Omega}\cdot\mathbf{\Omega}$ dominate the off-diagonal terms by $\mathcal{O}(l^2)$) and so, to leading order in $1/l^2$, we need only consider the entanglement between ϕ_n and $\phi_{(n+1)}$, the entanglement between ϕ_j and $\phi_{(n+1)}$ $(j < n)$) being higher order in $1/l^2$.

Furthermore the $n, (n+1)$ sub-matrix of $\mathbf{\Omega}$ may be written

$$\begin{pmatrix} \omega_A & \omega_B \\ \omega_B & \omega_C \end{pmatrix}$$

where, to leading order in $1/l^2$

$$\omega_A \; \approx \; \frac{\sqrt{l(l+1)}}{n} \tag{2.11.90}$$

$$\omega_B \; \approx \; \frac{\left(n+\frac{1}{2}\right)}{2\sqrt{l(l+1)}} \tag{2.11.91}$$

$$\omega_C \; \approx \; \frac{\sqrt{l(l+1)}}{(n+1)} \tag{2.11.92}$$

Then using (2.11.79)

$$\xi_n \;\approx \frac{\omega_B^2}{4\,\omega_a\,\omega_C} \;\approx\; \frac{\left(n+\frac{1}{2}\right)^2 n(n+1)}{16l(l+1)} \tag{2.11.93}$$

$$H_{ent}^{l,n} \;=\; -\left(\log_2(1-\xi_n) + \frac{\xi_n \log_2 \xi_n}{(1-\xi_n)}\right) \;\approx\; -\xi_n\,(\log_2 \xi_n - 1) \tag{2.11.94}$$

(since $\xi_n \ll 1$).

This contribution to the total entanglement entropy seems to grow as n^4. so that for large radius R, it increases as R^4. This is *not* the dominant contribution to the total entanglement entropy, but has been calculated in order to demonstrate that the sum over angular momentum l is convergent. The dominant contribution comes from smaller angular momentum and has to be calculated numerically. Numerical calculations yield an entanglement entropy that grows as n^2 – in other words the entanglement entropy is proportional to the surface area of the sphere as is the case for the Beckenstein entropy of a black hole.