

Entropy and information

Entropy is one of the most fundamental concepts in science. It is so fundamental that you probably have heard it in everyday conversations at some point in your life. In this lecture, we will learn the quantitative definition of entropy, quantitative definition of "amount of information", find the connection between entropy and information, and apply it to physical and biological systems. This seems like a lot but as with the other topics in physics that we studied so far, if you keep in mind that all these seemingly many different things are governed by just a few principles, then you will be okay.

Quantifying information

Consider a coin. It has two sides: Head and tail. You throw the coin in the air. When it lands on the ground, it will land on either its tail or its head. Let's say that you throw the coin N times and write down the sequence of results. Say you write "0" for "head" and "1" for "tail". Then after throwing the coin N times, you might get the following sequence of events:

00100110111011011...101 (sequence of N **binary digits**)

You can think of this sequence of binary digits as a "message". After all, computers use binary digits. Each digit is called a **bit**. Looking at above sequence of bits, can you *predict* what the next digit would be if you flip the coin one more time? (i.e., can you guess whether you'll get a 0 or a 1?). If you got a sequence like

1111111...111 (sequence of N binary digits)

then you might predict that if you flip the coin one more time, you'll get another "1". You'd suspect that the coin is engineered so that it prefers to land on a tail ("1"). But if you throw the coin N times and obtain the following sequence

00100110111011011...1001 (sequence of N binary digits)

then you cannot predict whether you'll get a "1" or a "0" at the next ($N+1$ st) flip. You would say that getting a "0" is equally likely as getting a "1" at the next flip of the coin. Intuitively this is because the **amount of disorder** in the above sequence is fairly high. *As seen in this example, the amount of disorder in the sequence "measures" how predictable a message is* (here the message is the string of N bits). The higher the amount of disorder in a message, the more difficult it is for you to predict the next digit in the message.

We want to make this intuitive notion into a mathematical rigorous quantity. Let's propose a *definition of the amount of information in a message*, which may or may not be generated by flipping coins. We allow for non-binary messages. That is, in a string of N digits, we allow each digit to have one of M possible characters. In the coin flip example above, we had a binary bit ($M=2$). But other values for M are also possible. For example, suppose you are rolling a 6-sided dice. Then $M=6$. For the English language, $M=26$. Note that a string of N alphabet characters may not necessarily mean anything. For example, we

can have a message with length 5, such as afbcd. But this message doesn't mean anything in English. But it's okay. We don't ask whether the message has a meaning. The message can be anything, including non-sense.

Suppose we have N events (e.g., event = coin flip). Each event can have one of M possible outcomes. Suppose that each one of the M outcomes has an equal chance of occurring. Let's propose the following as a definition of the *amount of information (I) in a string of N digits* and see if it's a sensible definition:

$$I = \log_2 M^N$$

Note that this is the number of binary digits (bits) required to represent a message of length N . We can rewrite above as

$$I = N \cdot \log_2 M$$

We did not derive above equation. We are simply proposing this as our definition of the amount of information in a message. Is this a good definition? Is it sensible? Before addressing these questions, let's first rewrite above equation. Note that

$$\log_2 M = (\log_2 e) \ln(M)$$

where "ln" is the natural logarithm (log base e). To see this, note that if $M=e^x$, then $(\log_2 e) \ln(M)$ becomes $x(\log_2 e)$, which in turn is equal to $\log_2 e^x$, which is indeed equal to $\log_2 M$. Furthermore, we note that $(\log_2 e) = 1/\ln(2)$, where "ln" is \log_e . Thus we can rewrite I as

$$I = NK(\ln M)$$

where $K=1/\ln(2)$. Note that in the example of N binary digits (i.e., the N coin flips), we have

$$I = N$$

which is just the total number of digits in the sequence. I is just the total number of bits (0 or 1) that is necessary to transmit all possible messages of length N , with each digit encoded by one of M possible characters. This is in fact what our computers do. More precisely, suppose you have a black box. You cannot see through it. You don't know exactly what is inside it. The only thing you know about the box is that inside it is a message of length N and that it is written in a language with M characters (e.g., $M=26$ for English). Say you want to store this message in your computer that uses binary digits (i.e., 0 or 1). How many bits should you reserve in your computer to store this message? The answer is I . Suppose inside the blackbox, you have a message of length 4 and you're told that it is written in binary digits (0s and 1s). But you don't know any more than that. Our definition of I says that we need 4 bits reserved in our computer to store this message. Now, suppose you open the box and see that the message is 0001. Once you *know* this by *opening the black box*, then in fact you can say

"Well, the three 0's in front of the '1' are unimportant. The computer only needs to know the '1'. So I only need to store the '1' in the computer and throw out the '0', just like when I write the number 810, I do not need to write 0000810. So actually, I don't need all those extra bits to store the '1'".

But this is only because you opened the box. The main point is that if you were *uncertain* of what the message inside the box actually is, then you need to have those "place holders" in your computer as sort of a "back up" for all possible messages with length N in the box.

Why is the logarithm in our definition of amount of information I ? The answer is that we want information to be *additive*. That is, we want to define the amount of information so that if we have two messages, one with length N_1 that is written in a language that has M_1 characters, and another message with length N_2 that is written in a language that has M_2 characters, then we want the total amount of information of the two messages written next to each other be I_1+I_2 , where I_1 is the amount of information of the 1st message and I_2 is the amount of information of the 2nd message. This turns out to be true due to the logarithm in our definition. Let's check this. First note that

$$I_1 = N_1 K (\ln M_1)$$

and

$$I_2 = N_2 K (\ln M_2)$$

Now if we write the two messages side-by-side, then the total length of the message is N_1+N_2 and the total possible number of messages is

$$M_1^{N_1} M_2^{N_2}$$

Thus according to our definition of amount of information I , the total information of the two messages combined is

$$\begin{aligned} I &= K \ln(M_1^{N_1} M_2^{N_2}) \\ &= K \ln(M_1^{N_1}) + K \ln(M_2^{N_2}) \\ &= N_1 K \ln(M_1) + N_2 K \ln(M_2) \\ &= I_1 + I_2 \end{aligned}$$

Thus indeed, the logarithm in our definition of information quantity enables information from two messages to be *additive*. This matches our intuitive notion of what we think information content should be.

Let's note another property. If you do not know exactly what the message will be, but are only told that it has length N with each position having one of M possible characters, then the I as defined above tells you how many bits you need in order to represent every one of the possible M^N messages. Having that many bits (I bits) ensures that you have enough bits

to cover the exact one message that you end up getting from your black box. But suppose $M=1$ and $N=10$. This means that the message is 10 letters long, each letter of the message must be of one particular alphabet because $M=1$. In this case, you know exactly what the message will be. It will be

1111111111 (ten "1"s).

Here we have $I = NK(\ln M) = 10K(\ln 1) = 0$. This means that because you know for certain what the message will come out of a machine, you have zero uncertainty in the content of the message.

So the higher the amount of information I is, the more *uncertain* you're about what message is contained inside the black box. Unlike the term "information" that we use in everyday conversations, the mathematical definition of information says that the more amount of information I you have, the more uncertain you're about the message that you're about to receive (or uncover by opening the box). This means that there is *more disorder* in the message inside the box.

Quantifying entropy

Suppose we have a box of volume V . It has N gas particles inside it. The total energy of all the particles combined is E . Let's suppose that the box is closed off from the rest of the world. This means that no particles can enter or exit the box. So there will always be N particles inside the box. Also, we assume that no heat or other types of energy can enter or exit the box. Thus the total energy of the box is E at all times. We say that this kind of system is a **closed system**. We also call such a system an **isolated system**.

What can we say about such a box of particles? Well, at any given moment in time, each gas particle has some position and some velocity. Different particles will have different positions and likely different velocities. These particles are diffusing around, perhaps moving chaotically inside the box. Some particles will collide with each other, some will collide with the walls of the box, and so on. In summary, trying to keep track of each individual particle inside the box, especially when N is a large number, is a hopelessly complex task. In fact, at a typical room temperature and pressure, there are about 10^{22} gas particles in a 1-liter box. That is a *huge* number of particles. It is practically impossible to measure the position and velocity of every one of the 10^{22} gas particles in a box at a given instant in time, and then apply Newton's laws to each particle to determine how every one of those 10^{22} gas particles will move. So we have two choices. One is to just give up and focus on a system with a few (two or three) objects, like a block sliding down an inclined plane (two objects). The other option is to find a different conceptual framework to understand a system with many particles.

The second option is the one that scientists have taken. Let's turn to our box of N particles again. Again, assume that N is a large number. We clearly cannot say exactly where and how fast each of the N particles are moving inside the box at any given moment in time. But if we *could* measure the position and velocity of every particle inside the box at a given moment in time, that detailed state of the system of N particles is called the **microstate of the system**. Over time, the microstate of the box of particles will change at a mind-boggling rate because every collision between any two particles causes a change in those two particles' positions and velocities (and thus changing the microstate, which is defined by the values of positions and velocities of every one of the N particles). So over time, many collisions between many particles will occur. This means that over time, we get a *random* sequence of microstates. It's randomly varying over time because there are chaotic and randomly moving and colliding particles inside the box. So we cannot predict the exact sequence of microstates over time. But we can predict *how many* microstates the box of particles can potentially have (notice that this situation is similar to the situation of our black box containing an unknown message).

Let Ω represent the total number of microstates that the box can be in. Here Ω is the Greek letter "Omega" (as a capital letter, the small case form is ω , which is also called "omega" and was used to represent an angular velocity). Entropy is defined as the amount of information in a physical system. Here a physical system can be a black box that contains gas particles instead of an unknown message. Say we have N particles inside the box instead of a message of length N . From our discussion of the amount of information I in the previous section, we know that the information content of a physical system is $I = K \cdot \ln(\Omega)$, where $K = 1/\ln 2$. Now note that for a typical physical system like a box of gas, Ω must be a very large number because there must be a huge number of microstates that the particles can be in. In fact, $\ln(\Omega)$ is typically much larger than the Avogadro number, 6.02×10^{23} . As humans, we cannot understand such large numbers. So the convention is to multiply I by a small number to compensate for the typically astronomical values of $\ln(\Omega)$. Historically, this constant is related to the average thermal energy of a particle. That number is k_B/K , where k_B is called the **Boltzmann constant**. It's value is 1.38×10^{-23} Joule/Kelvin. So it is a constant that has units of energy / temperature. Note that it is a very small number. So multiplying $I = K \ln(\Omega)$ by this small number k_B/K should give us a more manageable and humanly-understandable number. The result is called the entropy of the system: $S = \frac{k_B}{K} K \ln(\Omega)$. We multiply by k_B/K instead of just k_B for historical reasons. Thus the entropy is defined as

$$S = k_B \ln(\Omega)$$

This is the famous entropy formula. You might have seen it before. Now you also know where it comes from and why it is defined in this way. $\ln(\Omega)$ is a dimensionless number so S has the same dimension as the Boltzmann constant, energy / temperature. But note that at the end of the day, S is measuring the information content (disorder or the unpredictability) of a physical system such as a box of gas particles. The important quantity is the $\ln(\Omega)$, not the Boltzmann constant.

Let's make this idea concrete by calculating it for a concrete system. We will consider a box of gas particles. We call it an "ideal gas".

Example 1. Ideal gas of one particle inside a box with a fixed energy E

What is the number of states that a box of gas particles can be in?

To simplify our task, consider a box of volume V that contains just one particle. The particle has a kinetic energy. It has no potential energy (we ignore the gravitational energy of the particle). Say E is the kinetic energy. At a given time, the particle has a position (x, y, z) and velocity \vec{v} . So we have

$$E = \frac{1}{2}mv^2$$

The total number of positions inside the box is

$$\Omega_{\text{positions}} = \frac{V}{a}$$

where a is a small cubic volume ("pixel" of space, if you will). a can be the volume of the particle. Then above equation is just counting how many "pixels" of space can fit inside the box's volume V (i.e., the total number of positions that the particle can be in). At any position, the particle can move with velocity \vec{v} . At each point, it can move in any direction. What is the total number of possible velocity vectors? As long as the length of the vector \vec{v} satisfies this equation

$$E = \frac{1}{2}mv^2$$

it is allowed. That is, any velocity vector that satisfies $|\vec{v}| = \sqrt{2E/m}$ is an allowed velocity vector of the particle. Note that a velocity vector can be written as $\vec{v} = (v_x, v_y, v_z)$, a vector in 3-dimensions. Such a vector lives in a "velocity space" rather than the more familiar "position space" that we usually call (x, y, z) . Any vector in this velocity space whose arrowhead (tip) ends on the surface of a sphere of radius $\sqrt{2E/m}$ is an allowed velocity vector of the particle. Note that velocity vectors that point in all possible directions form this spherical surface. The surface area of the sphere A is

$$A = 4\pi \frac{2E}{m}$$

Note that A has dimension of speed squared (e.g., $(\text{km}/\text{hr})^2$). This makes sense because that would be the area in the velocity space. In position space, the area would have dimension of length squared (e.g., km^2). Just like we divided the volume V by the volume of the particle ' a ' to get a dimensionless number, we need to divide A by a constant that has dimension of speed squared in order to convert A into a dimensionless number, namely the number of velocities that the particle can have. It's not important to know exactly what this constant is. It comes from quantum mechanics. What is important is that you know why we need it (i.e., the number of allowed velocities must be a dimensionless number). We will call this constant n_a .

So the total number of states that the particle inside the box can have is

$$\Omega = \frac{A}{n_a} \Omega_{\text{positions}}$$

So the entropy is:

$$S = k_B \ln \left(\frac{A}{n_a} \Omega_{\text{positions}} \right) = k_B \ln \left(\frac{4\pi}{n_a} \frac{2E}{m} \right) + k_B \ln(V/a)$$

This is the famous entropy formula for a gas of one particle. It tells us that if you increase the box's volume V , then the entropy increases. Above formula for entropy also says that the entropy increases if you increase energy. To get the rate of change of entropy with respect to energy, we can take the derivative of S with respect to energy:

$$\frac{dS}{dE} = \frac{k_B}{E}$$

This is a simple looking equation. Just rearranging some terms, we can rewrite above as

$$E = k_B \left(\frac{dS}{dE} \right)^{-1}$$

The term $\left(\frac{dS}{dE} \right)^{-1}$ on the right hand side of above equation has units of Kelvin, which is a unit of temperature. We use T to represent this:

$$T = \left(\frac{dS}{dE} \right)^{-1}$$

T is called the **temperature** of the system. This is how we *define* the temperature. The important point is not whether you measure the temperature in Kelvins (the *SI* unit of conventional temperature) or in degrees Celsius. Rather, the important point is *what temperature actually means*. It's a rate of change that we found above. A high temperature means that if you change the energy of the gas particle, its entropy does not change much. In this case, dS/dE is small, so T is large. A low temperature means that if you change energy of the gas particle, its entropy changes by a lot. In this case, dS/dE is large, so T is

small. So temperature relates how the number of states that system (here a box of one gas particle) can have with its energy. Furthermore, if we now substitute T into the above equation, we get

$$E = k_B T$$

So the temperature also measures the energy of the system. And it should, because we saw above that the fundamental temperature actually has units of energy. The only reason we measure it in Kelvins (or in degree Celsius, which is $273\text{K} + x$ (in C) = T), is because of the Boltzmann constant (again, nothing special, just a number so we can talk about temperature in Kelvins instead of energy in everyday language).

Example 2. Ideal gas of N particles in a box of volume V and fixed energy E .

Suppose now we have N particles inside a box. The total energy of all the particles combined is E . The box has volume V . What is the entropy of the box of gas particles? Here we have a constraint. The total energy of all the N particles in the box is E . That is,

$$E = \sum_{i=1}^N \frac{mv_i^2}{2}$$

Here v_i is the speed of the particle number i . In terms of the i -th particle's velocity $\vec{v}_i = (v_{i1}, v_{i2}, v_{i3})$, we can write the i -th particle's speed as

$$\begin{aligned} v_i &= |\vec{v}_i| \\ &= \sqrt{v_{i1}^2 + v_{i2}^2 + v_{i3}^2} \end{aligned}$$

so we have

$$\frac{mv_i^2}{2} = \sum_{j=1}^3 \frac{mv_{ij}^2}{2}$$

and thus

$$E = \sum_{i=1}^N \sum_{j=1}^3 \frac{mv_{ij}^2}{2}$$

Since the mass m is the same for every particle and the $1/2$ also appears in every term in the sum, we can factor them outside the summation, and then rearrange the terms to get

$$\frac{2E}{m} = \sum_{i=1}^N \sum_{j=1}^3 v_{ij}^2$$

Note that if we have $N=1$, we get back the situation in the previous example: The box of just one particle with energy E . Now we would like to repeat the kind of "area" calculation that we did for the case of one particle in the previous example. There we found that the velocity vector of the particle, defined by its three components, v_x , v_y , and v_z , had to have a length

equal to $\sqrt{2E/m}$ but could point in any direction in the 3-dimensional space as long as it had this length. This meant that the tip of the vector (the arrowhead) had to lie on a surface of a sphere with radius $\sqrt{2E/m}$. The total number of such vectors was the surface area of the sphere. Now returning to our example here with N particles, the challenge is interpreting above equation in a similar way (i.e., in terms of a sphere). Except now, in the sum in the equation above, we have 3 terms for each i , and there are N values for i . So we have a total of $3N$ terms in the sum. Suppose you have a vector with p components like this:

$$\vec{x} = (x_1, x_2, \dots, x_{p-1}, x_p)$$

What is the length of this vector? Well we know that when $p=2$, we have a 2-dimensional space (i.e., a plane). There the vector would have length

$$|\vec{x}| = \sqrt{x_1^2 + x_2^2}$$

And when $p=3$, we have a 3-dimensional space. There the vector would have length

$$|\vec{x}| = \sqrt{x_1^2 + x_2^2 + x_3^2}$$

Now, what happens when $p=4$? Can you guess what the length of the vector is in a 4-dimensional space? The answer is

$$|\vec{x}| = \sqrt{x_1^2 + x_2^2 + x_3^2 + x_4^2}$$

And in p -dimensions in general, the length of the vector is

$$|\vec{x}| = \sqrt{x_1^2 + x_2^2 + x_3^2 + \dots + x_{p-1}^2 + x_p^2}$$

For $p > 3$, it is tough to visualize what a p -dimensional space would look like. It is safe to say that no one really knows how to visualize space that has more than 3-dimensions. Even (almost) none of the mathematicians can visualize these higher dimensions! But we can imagine that just as there are 2 perpendicular axes in 2-dimensions of space (i.e., x-axis, and y-axis), and 3 perpendicular axes in 3-dimensions of space (i.e., x-axis, y-axis, and z-axis), a p -dimensional space would consist of p perpendicular axes. Above formula for length comes from the fact that in p -dimensional space, there are p perpendicular axes (it's a generalization of Pythagorean theorem in p -dimensions).

Going back to our original problem of computing the entropy of N particles in a box, we can now see that right-hand side of the formula we derived above:

$$\frac{2E}{m} = \sum_{i=1}^N \sum_{j=1}^3 v_{ij}^2$$

is representing the square of the length of a vector with $3N$ components. It is the length of a vector in $3N$ -dimensions of space (i.e., $p=3N$ in above discussion). So above equation is describing a vector that can point in any direction in a $3N$ -dimensions of space, but with a fixed length equal to $\sqrt{2E/m}$. Such a vector sweeps out a surface of a sphere in $3N$ -

dimensional space. The surface will have dimension of $3N-1$. Now what is an area of a sphere in $3N$ dimensions?

In a 2-dimensional space (i.e., a plane), the equation

$$C^2 = x_1^2 + x_2^2$$

describes a circle of radius C (also called a 2-dimensional sphere of radius C). A vector $\vec{x} = (x_1, x_2)$ that satisfies above equation is a vector with length C that points in any direction in 2-dimensional space. That is, any vector whose tip (arrowhead) lies on the outline (boundary) of the circle. The circle has circumference (length) equal to $2\pi C$. We also say that the 2-dimensional sphere has boundary area equal to $2\pi C$.

In a 3-dimensional space, the equation

$$C^2 = x_1^2 + x_2^2 + x_3^2$$

describes a sphere of radius C (also called a 3-dimensional sphere of radius C). A vector $\vec{x} = (x_1, x_2, x_3)$ that satisfies above equation is a vector with length C that points in any direction in a 3-dimensional space. That is, any vector whose tip (arrowhead) lies on the surface (boundary) of the sphere. The sphere has surface area equal to $4\pi C^2$. We also say that the 3-dimensional sphere has boundary area equal to $4\pi C^2$.

In a p -dimensional space, the equation

$$C^2 = x_1^2 + x_2^2 + x_3^2 + \dots + x_{p-1}^2 + x_p^2$$

describes a p -dimensional sphere of radius C . A vector $\vec{x} = (x_1, x_2, x_3, \dots, x_{p-1}, x_p)$ that satisfies above equation is a vector with length C that points in any direction in a p -dimensional space. That is, any vector whose tip (arrowhead) lies on the surface (boundary) of the p -dimensional sphere. We want to know the boundary area of this p -dimensional sphere. By dimensional analysis and by looking at the pattern from 2-dimensional sphere (circle, *boundary area* = $2\pi C$) and 3-dimensional sphere (ordinarily called just a "sphere", *boundary area* = $4\pi C^2$), can you guess what the boundary area of a p -dimensional sphere is? The answer is that the boundary area of a p -dimensional sphere is ρC^{p-1} , where ρ is just some number (like the 2π in the 2-dimensional sphere and the 4π in the 4-dimensional sphere). For us the exact value for the constant ρ is unimportant. The important point is that the boundary area of the p -dimensional sphere depends on the radius as C^{p-1} .

Going back to our original problem, remember that we had

$$\frac{2E}{m} = \sum_{i=1}^N \sum_{j=1}^3 v_{ij}^2$$

So based on our discussion above, this equation is telling us that we're interested in all vectors in $3N$ -dimensional space whose length is $\sqrt{2E/m}$ and whose tip (arrow head) ends

on a $3N$ -dimensional sphere of radius $\sqrt{2E/m}$. The area of the boundary of this $3N$ -dimensional sphere is

$$A = \rho \left(\frac{2E}{m} \right)^{\frac{3N-1}{2}}$$

Again, ρ is just some number that is not important for us. Then the total number of velocities that the system can have is

$$\Omega_{velocity} = \frac{A}{n_a}$$

where n_a is the area of the smallest pixel in $3N$ -dimensional space that you can have (it's a constant that we need to multiply A to get a dimensionless number $\Omega_{velocity}$). Then the total number of states is

$$\Omega = \Omega_{positions} \times \Omega_{velocity}$$

Plugging in the results for $\Omega_{positions}$ and $\Omega_{velocity}$, we have

$$\Omega = \left(\frac{V}{a} \right)^N \frac{\rho}{n_a} \left(\frac{2E}{m} \right)^{\frac{3N-1}{2}}$$

So the entropy of the box of N particles is

$$S = k_B \ln \left(\left(\frac{V}{a} \right)^N \frac{\rho}{n_a} \left(\frac{2E}{m} \right)^{\frac{3N-1}{2}} \right) = k_B N \ln(V) + \frac{3N-1}{2} k_B \ln \left(\frac{2E}{m} \right) + k_B \ln(\text{constant})$$

And taking the derivative of S with respect to energy, we get

$$\frac{dS}{dE} = k_B \frac{3N-1}{2E}$$

This is a simple looking equation. Just rearranging some terms, we can rewrite above as

$$E = \frac{3N-1}{2} k_B \left(\frac{dS}{dE} \right)^{-1}$$

And as we noted in the previous example with one particle in a box, we have

$$T = \left(\frac{dS}{dE} \right)^{-1}$$

thus we can rewrite above equation as

$$E = \frac{3N-1}{2} k_B T$$

We can make an approximation here. Above is an exact result for N particles. Typically we deal with very large number of particles (so N is very large). For example, we can have an Avogadro number of particles (i.e., $N = 6.02 \times 10^{23}$). Then $N-1$ is approximately equal to N . So we can write above equation in a simpler looking form as

$$E = \frac{3N}{2} k_B T$$

Example 3. Relating temperature with molecular motion (N particles in a box with volume V)

Here we will relate the temperature T in above equation with molecular motion of particles (this is the notion of T that you are perhaps more familiar with). The calculations that we will do in this example are also explained in Section 17.1 of your book.

First, let's calculate the force that one particle exerts on the walls of the box. The box contains N particles. But we will assume that each particle acts independently of each other. So if we know the average force that one particle exerts on the wall, then we just need to multiply it by N to get the average of the total force that all N particles exert on the wall of the box. Let's say that each molecule has mass m . Each molecule moves inside the box, hits the walls of the box, then bounces off it. Let's just focus on one particle now. Each time this particle hits a wall, there is an exchange of some momentum between the wall and the particle (it's a collision between two bodies, like the collision problems that we studied several weeks ago). To simplify our analysis, let's suppose that the particle is moving with speed v_x and that it is moving parallel to one edge of the box (i.e., it is moving along the x -axis). Each side of the box has length L . After the particle collides with the wall and bounces off the wall, the particle's linear momentum changes from mv_x to $-mv_x$ (we're assuming elastic collision here, so momentum conservation says that this has to be the case). This means that the particle transfers momentum $2mv_x$ to the wall (and the wall transfers momentum $-2mv_x$ to the particle during the collision). This way the total momentum of the system (system = box + particle) remains unchanged after the collision. This should be the case due to conservation of momentum. This collision occurs every time that the molecule makes a round trip (from left end of the wall to the right end of the wall, then back and forth). This round trip takes a time $\Delta t = 2L/v_x$. So the momentum transfer per unit time is

$$\begin{aligned}\frac{\Delta \vec{p}}{\Delta t} &= \frac{2mv_x}{\Delta t} \\ &= \frac{2m(v_x)^2}{2L} \\ &= \frac{m(v_x)^2}{L}\end{aligned}$$

But we know that rate of change of momentum with respect to time is force by definition (i.e. $\vec{F} = d\vec{p}/dt$). Thus, what we calculated above is actually the force that the particle colliding with the wall exerts on the wall. We assumed above that the particle has a fixed speed v_x . But in reality, the particle's speed can vary. But for multiple collisions with the wall, the average force (momentum transfer / time) that the wall experiences is

$$\left\langle \frac{\Delta \vec{p}}{\Delta t} \right\rangle = \left\langle \frac{m(v_x)^2}{L} \right\rangle$$

$$= \frac{m\langle(v_x)^2\rangle}{L}$$

where $\langle \dots \rangle$ represents average of "...". Now note that there are actually N particles inside the box. We assume that each particle acts independently of each other.

$$\left\langle \frac{\Delta \vec{p}}{\Delta t} \right\rangle = N \frac{m\langle(v_x)^2\rangle}{L}$$

We denote $F_x = \left\langle \frac{\Delta \vec{p}}{\Delta t} \right\rangle$. Then **pressure** p is defined as the force per area of the wall. If V is the volume of the box, then $V=AL$, where A is the surface area of one of the walls of the cubic box. Then we have

$$p = N \frac{m\langle(v_x)^2\rangle}{V}$$

Note that there's nothing special about the x-direction. In fact, we can see that

$$\langle(v_x)^2\rangle = \langle(v_y)^2\rangle = \langle(v_z)^2\rangle$$

and

$$\begin{aligned} \langle v^2 \rangle &= \langle(v_x)^2\rangle + \langle(v_y)^2\rangle + \langle(v_z)^2\rangle \\ &= 3\langle(v_x)^2\rangle \end{aligned}$$

Thus above equation can be rewritten as

$$p = N \frac{m\langle v^2 \rangle}{3V}$$

Rearranging the terms, we get

$$3pV = Nm\langle v^2 \rangle$$

Now,

$$Nm\langle v^2 \rangle = 2E$$

Thus we have

$$\frac{3pV}{2} = E$$

In the previous example, we derived

$$E = \frac{3N}{2}k_B T$$

And so we can rewrite this as

$$\frac{3pV}{2} = \frac{3N}{2}k_B T$$

This becomes

$$pV = Nk_B T$$

This is called the "**ideal gas law**". In examples 2 and 3, we have thus derived the famous ideal gas law that you have often been told without derivation.

Example 4. Expressing the entropy of ideal gas of N particles in terms of temperature

In Example 2, we found

$$S = k_B N \ln(V) + \frac{3N}{2} k_B \ln\left(\frac{2E}{m}\right) + k_B \ln(\text{constant})$$

Here we are using the approximation $3N - 1 \approx 3N$ (assuming that N is large). Now, since

$$E = \frac{3}{2} N k_B T$$

we have

$$S(T, V) = N k_B \ln(V) + \frac{3N}{2} k_B \ln\left(\frac{3N k_B T}{m}\right) + k_B \ln(\text{constant})$$

Thus we see that if you increase the temperature, then the entropy increases as well. This is usually why we say that increasing the temperature tends to increase the amount of "disorder" of the system.