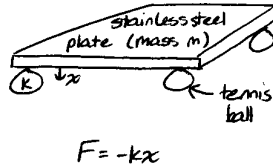
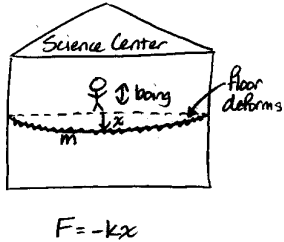
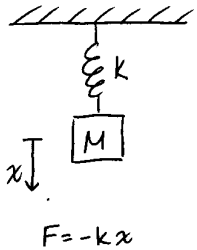


Feb 8, 2005 : Simple Harmonic Oscillator

①

Anything can be modeled (to 1st order) as a mass + spring
= "simple harmonic oscillator"



Equation of motion: $F = ma = m\ddot{x} = -kx$

$$m \frac{d^2x}{dt^2} = -kx$$

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x$$

2nd order differential equation

→ look at it and solve: $x = x_0 \cos(\omega_0 t)$
where $\omega_0 = \sqrt{\frac{k}{m}}$

Check the sol'n: $\frac{d^2x}{dt^2} = \frac{d}{dt}(-x_0 \sin(\omega_0 t) \cdot \omega_0)$

$$= -x_0 \cos(\omega_0 t) \cdot \omega_0^2$$

$$= -\frac{k}{m} x_0 \cos(\omega_0 t) = -\frac{k}{m} x \quad \checkmark$$

An SHO always exhibits sinusoidal motion.

OK, let's make things a little more complicated: add damping

- no such thing as perpetual motion
- spring will always stop bouncing eventually
- because when you set the spring in motion, energy sloshes back and forth between kinetic & potential, but slowly leaks out into heat, noise, etc.

②

The damping force always opposes the motion, and in fact the faster the motion, the larger the damping (think wind in your face when riding a bicycle).

So we can write: $F_{\text{damp}} = -\gamma \dot{x}$
damping coeff. velocity

Now we have:

$$F_{\text{tot}} = m\ddot{x} = F_{\text{spring}} + F_{\text{damp}}$$

$$= -kx - \gamma \dot{x}$$

$$m\ddot{x} + \gamma \dot{x} + kx = 0 \Rightarrow \ddot{x} + \frac{\gamma}{m} \dot{x} + \frac{k}{m} x = 0$$

another 2nd order differential eqn but we can't just use cos any more b/c derivative of cos is sine

Instead, we do a mathematical trick, and say $x = x_0 e^{i\omega t}$

[reminder: $e^{i\omega t} = \cos(\omega t) + i\sin(\omega t)$

(can prove it to yourself by Taylor-expanding both sides)]

Now the real motion of the mass is $\text{Re}(x) = \text{Re}(x_0 e^{i\omega t})$

As before, we plug in our "ansatz" = guessed sol'n

$$x = x_0 e^{i\omega t}; \quad \dot{x} = i\omega x_0 e^{i\omega t}; \quad \ddot{x} = -\omega^2 x_0 e^{i\omega t}$$

$$-\omega^2 x_0 e^{i\omega t} + \frac{\gamma}{m} i\omega x_0 e^{i\omega t} + \omega_0^2 x_0 e^{i\omega t} = 0$$

Both the real and imaginary parts of the left side must separately be zero.

$$x_0 e^{i\omega t} \underbrace{(-\omega^2 + \frac{\gamma}{m} i\omega + \omega_0^2)}_{\substack{\text{exponential} \\ \text{can't be} \\ \text{zero}}} = 0$$

So either $x_0 = 0$ (i.e. no amplitude of motion!) or

$$-\omega^2 + \frac{\gamma}{m} i\omega + \omega_0^2 = 0$$

Solving these separately gives: $\begin{cases} \text{Re: } \omega^2 = \omega_0^2 \\ \text{Im: } \omega = 0 \end{cases}$ Ack! contradiction!

③

So where did we make a false assumption?

Ans: we assumed α is real!

Lets see what happens if we let α be imaginary: $\alpha = a + bi$

$$-(a+bi)^2 + \frac{\gamma}{m}i(a+bi) + \omega_0^2 = 0$$

$$\begin{cases} \text{Re: } -a^2 + b^2 - b\frac{\gamma}{m} + \omega_0^2 = 0 \\ \text{Im: } -2ab + a\frac{\gamma}{m} = 0 \end{cases}$$

$$\Rightarrow b = \frac{\gamma}{2m}$$

$$-a^2 + \frac{\gamma^2}{4m^2} - \frac{\gamma^2}{2m^2} + \omega_0^2 = 0$$

$$a^2 = \omega_0^2 - \frac{\gamma^2}{4m^2}$$

$$\Rightarrow \alpha = \sqrt{\omega_0^2 - \frac{\gamma^2}{4m^2}} + \frac{\gamma}{2m}i$$

$$\Rightarrow x = x_0 e^{\underbrace{i\sqrt{\omega_0^2 - \frac{\gamma^2}{4m^2}}t}_{\substack{\text{oscillating part} \\ \text{slightly slower} \\ \text{than natural freq.} \\ \text{b/c of damping}}} } e^{\underbrace{-\frac{\gamma}{2m}t}_{\substack{\text{decaying} \\ \text{exponential}}}}$$

Check our math: if $\gamma=0$, does this reduce back to the simple solution $x = x_0 e^{i\omega_0 t}$? yes

OK, now suppose we drive this thing:

$$F_{\text{drive}} = f_0 \cos(\omega t)$$

↑ drive frequency
not necessarily same as
natural frequency = $\omega_0 = \sqrt{\frac{k}{m}}$

BUT drive frequency must be real!
(otherwise the drive itself would be decaying in time,
and we do want to assume a constant drive)

$$F_{\text{tot}} = F_{\text{spring}} + F_{\text{damp}} + F_{\text{drive}} = ma$$

$$-kx - \gamma \dot{x} + f_0 \cos(\omega t) = m\ddot{x}$$

$$\ddot{x} + \frac{\gamma}{m}\dot{x} + \frac{k}{m}x = \frac{f_0}{m} \cos(\omega t)$$

We still need to do our mathematical trick w/ imaginary numbers: ④

Let $x = x_0 e^{i\alpha t}$ and furthermore, $F_{\text{drive}} = f_0 e^{i\omega t}$

Substitute in the "ansatz":

$$-x_0 \alpha^2 e^{i\alpha t} + i\alpha \frac{\gamma}{m} x_0 e^{i\alpha t} + \frac{k}{m} x_0 e^{i\alpha t} = \frac{f_0}{m} e^{i\omega t}$$

$$(-\alpha^2 + i\alpha \frac{\gamma}{m} + \frac{k}{m}) x_0 e^{i\alpha t} = \frac{f_0}{m} e^{i\omega t}$$

Now we do another trick: we collect all the time-dependence on one side of the equation

$$\underbrace{(-\alpha^2 + i\alpha \frac{\gamma}{m} + \frac{k}{m}) x_0 m}_{\text{there's no time dependence here}} \frac{1}{f_0} = \frac{e^{i\omega t}}{e^{i\alpha t}} = e^{i(\omega-\alpha)t}$$

there's no time dependence here

\Rightarrow the right side must be time-independent too!

$e^{i(\omega-\alpha)t}$ has no time dependence \Rightarrow exponent must be zero

$$\Rightarrow \omega = \alpha$$

So when we drive the system, it always responds at driven frequency.

We're left with:

$$(-\omega^2 + i\omega \frac{\gamma}{m} + \omega_0^2) x_0 = \frac{f_0}{m}$$

Solving real & imaginary separately gives:

$$\begin{cases} \text{Re: } (-\omega^2 + \omega_0^2) x_0 = \frac{f_0}{m} \\ \text{Im: } \omega \frac{\gamma}{m} x_0 = 0 \end{cases}$$

Ack! motion is zero!

So where did we make a false assumption?

Ans: we assumed x_0 is real!

Lets see what happens if we let x_0 be imaginary: $x_0 \rightarrow x_0 e^{-i\theta}$

$$(-\omega^2 + i\omega \frac{\gamma}{m} + \omega_0^2) x_0 e^{-i\theta} = \frac{f_0}{m}$$

↑ $\cos\theta - i\sin\theta$

$$\begin{cases} \text{Re: } -\omega^2 \cos\theta + \omega \frac{\gamma}{m} \sin\theta + \omega_0^2 \cos\theta = \frac{f_0}{x_0 m} \\ \text{Im: } \omega^2 \sin\theta + \omega \frac{\gamma}{m} \cos\theta - \omega_0^2 \sin\theta = 0 \end{cases}$$

$$\tan \theta = \frac{\sin \theta}{\cos \theta} = \frac{-\omega \frac{Y}{m}}{\omega^2 - \omega_0^2}$$

If we drive it slower than resonance ($\omega < \omega_0 = \sqrt{\frac{k}{m}}$) then

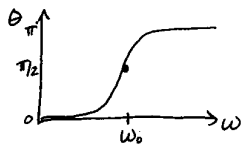
$$\tan \theta > 0 \Rightarrow 0 < \theta < \frac{\pi}{2}$$

If we drive it above resonance ($\omega > \omega_0 = \sqrt{\frac{k}{m}}$) then

$$\tan \theta < 0 \Rightarrow \frac{\pi}{2} < \theta < \pi$$

The motion is $x = x_0 e^{-i\theta} e^{i\omega t} = x_0 e^{i(\omega t - \theta)}$

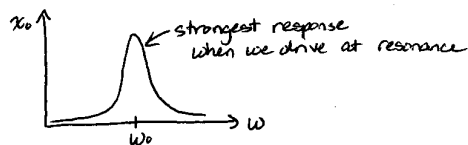
\Rightarrow the motion lags the drive by a phase θ



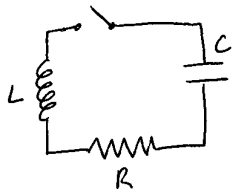
Plug θ back into the Re equation:

$$\tan \theta = \frac{\omega \frac{Y}{m}}{\omega_0^2 - \omega^2} \Rightarrow \sin \theta = \frac{\omega \frac{Y}{m}}{\sqrt{(\omega_0^2 - \omega^2)^2 + (\omega \frac{Y}{m})^2}}; \quad \cos \theta = \frac{\omega_0^2 - \omega^2}{\sqrt{(\omega_0^2 - \omega^2)^2 + (\omega \frac{Y}{m})^2}}$$

$$\Rightarrow x_0 = \frac{f_0/m}{\sqrt{(\omega^2 - \omega_0^2)^2 + (\omega \frac{Y}{m})^2}}$$



Analogy to electronics:



R: resistor, like damping: $V = IR$

C: capacitor, like spring: $V = \frac{q}{C}$

L: inductor, like mass: $V = L \frac{dI}{dt}$

note: $I = \dot{q}$

$$\Rightarrow V_{tot} = L\ddot{q} + R\dot{q} + \frac{1}{C}q = 0$$

Feb 15, 2005: Fourier transforms

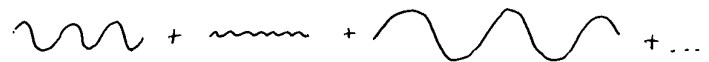
What's a Fourier transform?

2 ways to represent noise:

① time sequence of noise:

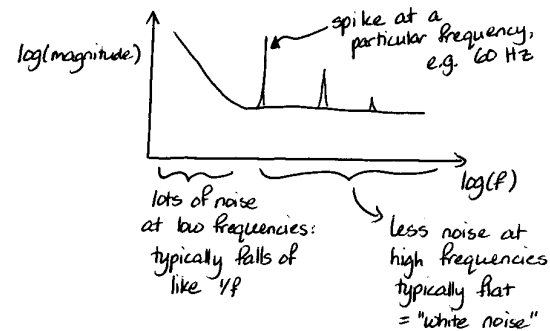


② or break it down into frequency components:



Every time trace can be uniquely represented as a sum of sinusoidal functions.

A typical frequency spectrum of noise looks like this:



Mathematically, the Fourier transform between time & frequency is:

$$\tilde{G}(f) = \int_{-\infty}^{\infty} g(t) e^{i2\pi ft} dt \quad [\text{Fourier transform}]$$

$$g(t) = \int_{-\infty}^{\infty} \tilde{G}(f) e^{-i2\pi ft} df \quad [\text{inverse Fourier transform}]$$

But in the real world, we measure a finite set of discrete data points, not a continuum.

Suppose we have N consecutive sampled values

$$h_k = h(t_k), \text{ where } t_k = k \cdot \Delta t \text{ for } k=0, 1, 2, \dots, N-1$$

(suppose N is even - actually usually $N=2^n$)

With N #'s of input, we can't get more than N frequencies of output information

(remember: if you have 2 eqns, you can't solve for 3 variables)

So we'll get info at the following freq's:

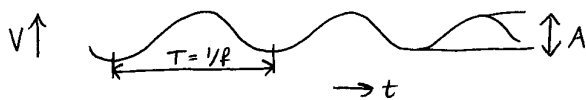
$$f_n = \frac{n}{N \Delta t}, \text{ where } n = -\frac{N}{2}, \dots, 0, \dots, \frac{N}{2}$$

We need to turn our integral into a sum:

$$\begin{aligned} \tilde{H}(f_n) &= \int_{-\infty}^{\infty} h(t) e^{2\pi i f_n t} dt \approx \sum_{k=0}^{N-1} h_k e^{2\pi i f_n t_k} \Delta t \\ &= \Delta t \sum_{k=0}^{N-1} h_k e^{2\pi i k n / N} \end{aligned}$$

Define: $H_n \equiv \sum_{k=0}^{N-1} h_k e^{2\pi i k n / N}$

Example What if we have a sine wave at frequency 60 Hz



Suppose we sample it for 2 sec at 180 Hz ($\Delta t = \frac{1}{180}$ s)

we have 360 data pts, so we should expect to get info about frequencies from $-\frac{N}{2} \left(\frac{1}{N \Delta t}\right) = -90$ Hz to $+90$ Hz

and we expect it to give us A at 60 Hz and zero elsewhere.

(2)

Let's test the formula:

$$H_n = \sum_{k=0}^{N-1} h_k e^{2\pi i k n / N}$$

$$h_k = h(t_k) = h(k \Delta t) = A \cos(2\pi \cdot 60 \text{ Hz} \cdot k \Delta t) = A \cos\left(\frac{2\pi}{3} k\right)$$

$$H_n = \sum_{k=0}^{359} A \cos\left(\frac{2\pi}{3} k\right) e^{2\pi i k n / 360}$$

$$= \sum_{k=0}^{359} \frac{A}{2} (e^{i \frac{2\pi}{3} k} + e^{-i \frac{2\pi}{3} k}) e^{2\pi i k n / 360}$$

$$= \frac{A}{2} \sum_{k=0}^{359} \left\{ \left[e^{2\pi i \left(\frac{n}{360} + \frac{1}{3}\right) k} \right] + \left[e^{2\pi i \left(\frac{n}{360} - \frac{1}{3}\right) k} \right] \right\}$$

$$= \frac{A}{2} \left\{ \frac{1 - \left[e^{2\pi i \left(\frac{n}{360} + \frac{1}{3}\right) 360} \right]}{1 - e^{2\pi i \left(\frac{n}{360} + \frac{1}{3}\right)}} + \frac{1 - \left[e^{2\pi i \left(\frac{n}{360} - \frac{1}{3}\right) 360} \right]}{1 - e^{2\pi i \left(\frac{n}{360} - \frac{1}{3}\right)}} \right\}$$

$$= \frac{A}{2} \left\{ \frac{1 - e^{2\pi i (n+120)}}{1 - e^{2\pi i \left(\frac{n}{360} + \frac{1}{3}\right)}} + \frac{1 - e^{2\pi i (n-120)}}{1 - e^{2\pi i \left(\frac{n}{360} - \frac{1}{3}\right)}} \right\}$$

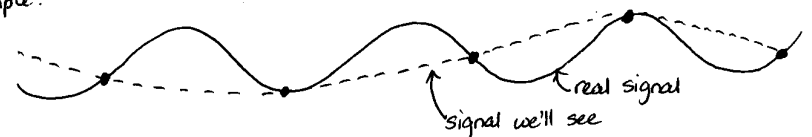
The numerators clearly vanish for all n , so the only values of n for which the whole expression H_n doesn't vanish are values for which the denominators also vanish.

$$\Rightarrow n = 240 \text{ and } 120$$

$$H_n = \begin{cases} A/2, & n = 120 \Rightarrow f_n = 60 \text{ Hz} \\ A/2, & n = 240 \Rightarrow f_n = -60 \text{ Hz} \\ 0, & n \neq 120, 240 \end{cases}$$

Q: what happens if we don't sample enough?

Example:



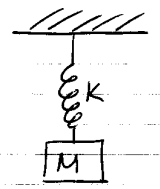
we can't tell the difference btwn 2 frequencies

\rightsquigarrow aliasing (Nyquist frequency)

(3)

①

Back to previous day's discussion with masses + springs:

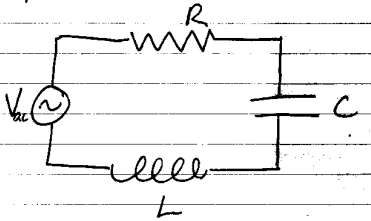


$$F_{tot} = ma = F_{spring} + F_{damp} + F_{drive}$$

$$m\ddot{x} = -kx - \gamma\dot{x} + f_0 \cos(\omega t)$$

$$m\ddot{x} + \gamma\dot{x} + kx = f_0 \cos(\omega t)$$

Compare to electronic circuit:



$$V_{ac} = V_R + V_C + V_L \quad (\text{Kirchoff's rule: voltages around a loop must sum to zero})$$

Again we need to solve for motion of something but what is that some thing?

Answer: we want the current flowing, and current is motion of charge, so we are solving for $I = \dot{q}$, and we draw the analogy:

$$q \leftrightarrow x$$

$$V_{ac} \leftrightarrow V_0 \cos(\omega t) \text{ is like driving force } f_0 \cos(\omega t)$$

②

R's and C's : (and L's ...)

3 basic components of electronic circuits : R, C, L

resistor R: resistance is measured in ohms (Ω)

In fact this Ohm guy even has a law named after him:

Ohm's law: $V = IR$
 voltage \uparrow current \uparrow resistance \leftarrow

If you put a voltage V across a resistor R , the current I will flow.

e.g. if $R = 1 \text{ k}\Omega$ (1000 Ω) and you put a voltage 10 V across, then a current $I = V/R = (10V)/(1000\Omega) = 0.01A$ or 10 mA will flow

As the current flows, energy is lost into heating the resistor, producing light, etc (what's the resistance of a light bulb?)

$$\text{power} = IV = I^2 R = V^2 / R$$

typically = 100 W, and we know wall is 110V

$$\Rightarrow 100W = \frac{(110V)^2}{R} \Rightarrow R = \sim 100\Omega$$

$$\Rightarrow I = \sim 1 \text{ Amp}$$

Note: typical household circuit breaker is 20 Amps (microwave is ~ 8 Amps)

OK, so $V_R = IR = \dot{q}R$

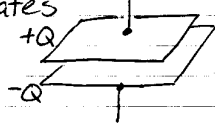
so by the analogy, R is like damping, makes sense b/c we know energy is lost into heat, etc

$$R \leftrightarrow \gamma$$

③

Capacitors: what are they?

2 conductors which store a difference in charge
Most often they are parallel plates



the more voltage you put across these plates, the more charge they will store

capacitance is defined as the ratio of the charge to the voltage: $C = \frac{q}{V}$

$$\Rightarrow V_C = \frac{q}{C}$$

so by analogy, C is like a spring
makes sense b/c if we draw this circuit:



then the charges will want to spring back to an equilibrium position, i.e. no charge on capacitor; the more charge we put, the more they will want to spring back

$$F_{\text{spring}} = -kx$$

$$V_C = \frac{q}{C}$$

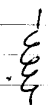
$$k \longleftrightarrow \frac{1}{C}$$

Inductors: what are they?

honestly they're not used much any more in real circuits b/c IC's have taken over

↑
integrated circuits

but, just to complete the analogy:



inductor is a coil of wire;
current flowing through a coil produces a magnetic field

④

If you try to change the current, that would result in a change in the field. But magnetic fields don't like to change. Instead, by Lenz' law, the changing B-field will induce a current to oppose the change. So an inductor puts "inertia" = "resistance to change" into the circuit.

$L \longleftrightarrow m$
resistance to change = inertia in a circuit inertial mass

$$V_L = L \frac{dI}{dt} = L \frac{dq}{dt} = L \dot{q}$$

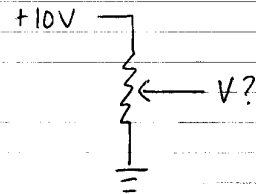
↑ ↑
resistance to change how fast the change is happening

Put it all together:

$$m\ddot{x} + \gamma\dot{x} + kx = f_0 \cos(\omega t)$$

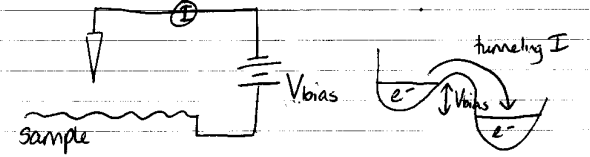
$$L\ddot{q} + R\dot{q} + \frac{1}{C}q = V_0 \cos(\omega t)$$

OK, simple R circuits:

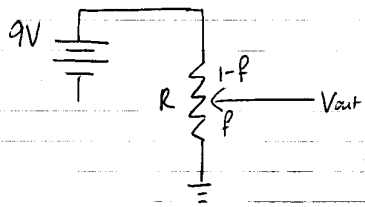


variable resistor = "potentiometer"
turn a screw, change the place on the resistor where V_{out} is connected
→ change V_{out}

Suppose we want a variable bias voltage for our STM
(remember:



⑤ So we might take a 9V battery and a "pot":



looks like V_{out} depends only on the fractional position of pointer:

$$V_{out} = f V_{in}$$

doesn't depend on R

But suppose $R = 1 \Omega$
 $\Rightarrow I = 9 \text{ Amps!}$

2 problems:

① $P = IV = 81 \text{ W}$

most resistors are only designed for $\frac{1}{4}$ Watt so the resistor will burn up!

② the battery has a finite amount of energy stored in it

e.g. 1.5V battery typically has $\sim 10 \text{ kJoules}$

9V battery typically has $\sim 20 \text{ kJoules}$

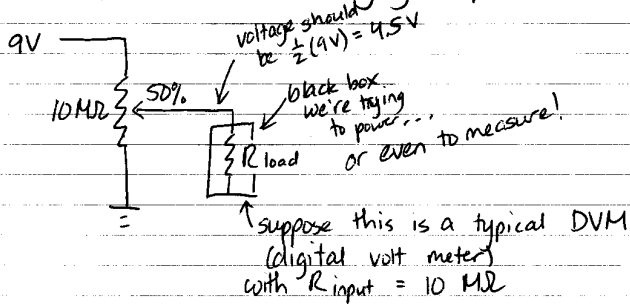
so with 1Ω resistance, we'll run down the battery in a short time:

$$\text{power} = \frac{\text{energy}}{\text{time}} \Rightarrow t = \frac{E}{P} = \frac{20 \text{ kJ}}{81 \text{ W}} = 4 \text{ min}$$

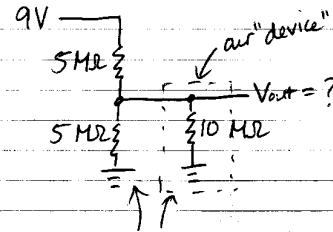
not good, we need STM to run for $> 4 \text{ min!}$

Solution: make R bigger
 the bigger the better?

well, it depends what we're trying to power...



⑥ Redraw this:



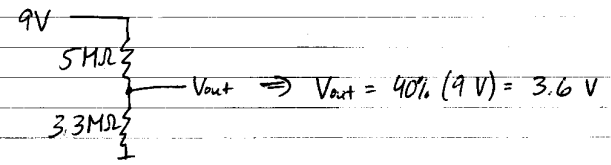
but here we have 2 R 's in parallel

R 's in parallel: add the reciprocals

$$R_{tot} = \left(\frac{1}{R_1} + \frac{1}{R_2} \right)^{-1} = \left(\frac{1}{5 \text{ M}\Omega} + \frac{1}{10 \text{ M}\Omega} \right)^{-1} = 3.3 \text{ M}\Omega$$

(Makes sense, we would expect it to be less than either R individually b/c now current has 2 places to flow, or a "wider river" w/ less R)

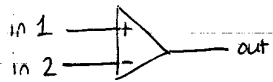
So now our voltage divider has:



Problem: "input resistance" of "load" is too low or "output resistance" of "source" is too high...

\leadsto lesson on op-amps

⑦ What does an op-amp do?



most simply, it has an open loop gain G and the output is $G \times (in\ 1 - in\ 2)$

typically G is something like 20,000

but practically speaking, these things are usually supplied by $\pm 15\text{ V}$ power supplies

that means that no matter how hard they try, they can't put out more than $\pm 15\text{ V}$ on the output actually, they "rail" somewhat below $\pm 15\text{ V}$

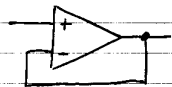
So, suppose we can have 10V out, what kind of input would be needed to give that?

$$V_{diff} = (in\ 1 - in\ 2) = \frac{V_{out}}{20,000} = \frac{10\text{ V}}{20,000} = 0.5\text{ mV}$$

But 0.5 mV is easily just noise picked up from the room as the two leads to the op-amp function as an antenna.

So, open loop, this op-amp is going to "rail" constantly.

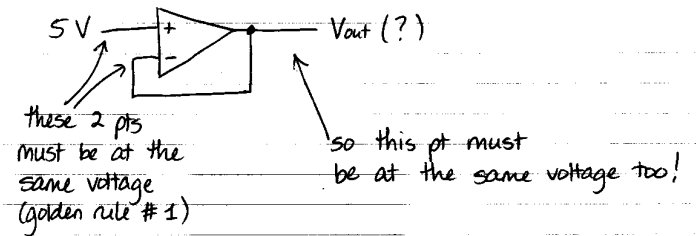
So we need to do some "feedback"



Once we have feedback, the op-amp obeys the 2 golden rules:

- ① the voltage difference between in 1 and in 2 is zero
- ② the inputs draw no current

⑧ So what happens now:



\Rightarrow output is 5V

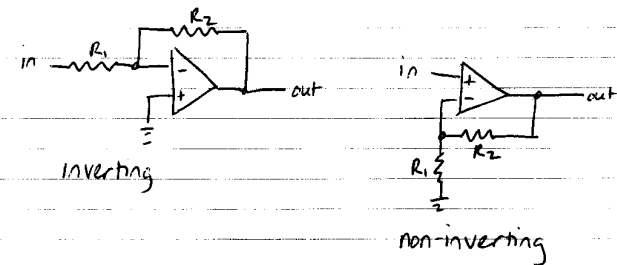
So why did we bother?

b/c what is the input resistance of this device?

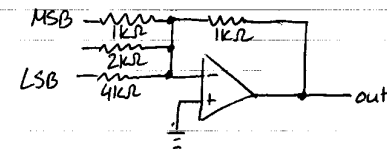
Well, golden rule #2 says it draws no current and if it draws no current, then input resistance is infinite \rightarrow never have this problem w/ too small "load" pulling the voltage down

This circuit is called a follower.

What about this:

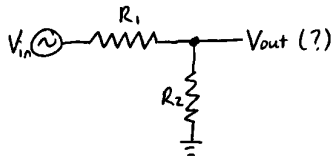


Or a simple digital to analog converter:



A follow-up on RC circuits and the difference between "resistance" and "impedance":

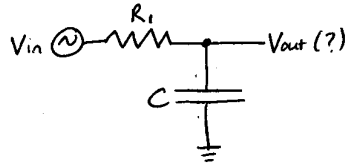
We know how to solve for the voltage out of a voltage divider, but what about an RC filter?



We know how to solve:

$$V_{out} = \frac{R_2}{R_1 + R_2} V_{in}$$

(frequency independent)



Add up the voltages:

$$V_0 \cos(\omega t) = IR_1 + \frac{Q}{C}$$

$$= R_1 \dot{Q} + \frac{1}{C} Q$$

We use our trick: $Q = q_0 e^{i\omega t}$

but remember driven SHO's always go at the driving frequency, so $\alpha = \omega$

And we also replace $V_0 \cos(\omega t) \rightarrow V_0 e^{i\omega t}$

$$\Rightarrow V_0 e^{i\omega t} = R_1 i\omega q_0 e^{i\omega t} + \frac{1}{C} q_0 e^{i\omega t}$$

$$V_0 = (i\omega R_1 + \frac{1}{C}) q_0$$

$$q_0 = \frac{V_0}{i\omega R_1 + \frac{1}{C}}$$

$$\Rightarrow V_{out} = \frac{q_0 e^{i\omega t}}{C} = \frac{\frac{1}{C}}{i\omega R_1 + \frac{1}{C}} V_0 e^{i\omega t}$$

Massage this to look like the $R_1 R_2$ circuit:

$$V_{out} = \frac{\frac{1}{i\omega C}}{R_1 + \frac{1}{i\omega C}} V_{in}$$

It looks like $\frac{1}{i\omega C}$ is a "generalized resistance" of the capacitor.

We call this the "impedance" = $Z = \frac{1}{i\omega C}$

Note that resistance is frequency independent, but impedance depends on frequency!

Feb 22, 2005 Density of States

We can't cover all of quantum mechanics, but let's start with a single formula, and call it an "axiom" and derive from that starting point - it turns out we can get pretty far.

$$\text{De Broglie formula: } p = \frac{h}{\lambda}$$

\uparrow momentum \uparrow wavelength
Planck's constant = 6.6×10^{-34} J·s

De Broglie relates wavelength (λ) to momentum (p).

Remember momentum is mass \times velocity: $p = mv$

Let's calculate λ for a tennis ball:

$$m \approx 100 \text{ g}$$

$$v \approx 100 \text{ mph (Venus Williams serve)}$$

$$100 \text{ mph} \cdot \frac{1 \text{ hr}}{3600 \text{ s}} \cdot \frac{1.609 \text{ km}}{1 \text{ mile}} \cdot \frac{1000 \text{ m}}{1 \text{ km}} \approx 50 \text{ m/s}$$

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{(6.6 \times 10^{-34} \text{ J}\cdot\text{s})}{(0.1 \text{ kg})(50 \text{ m/s})} \approx 1.2 \times 10^{-34} \text{ m}$$

too small to measure by any technique!

OK, move on to electrons

electrons are waves & particles

Can we describe an electron by both its position (x) and momentum (p)?

NO! violates the uncertainty principle!

$$(\text{uncertainty in } x)(\text{uncertainty in } p) > \frac{\hbar}{2}$$

Instead, we need to describe an e^- with a "wave function" $\Psi(x, t)$

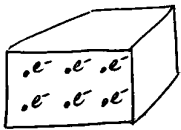
At a given time t , e^- has a probability to be at pt x of $|\Psi|^2$

More accurately: e^- has a probability to be btwn x and $x+dx$ of $|\Psi(x, t)|^2 dx$

Note: probabilities must add up to 1:

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$$

Now suppose we have a chunk of metal (e.g. sodium = Na) ②

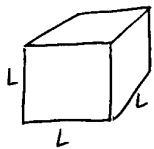


Each Na has closed shell + one extra e^-

These e^- are free to go anywhere in the metal

→ they are totally detached from the Na nucleus!

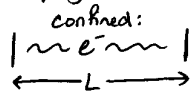
In fact, for the moment, we can just ignore the Na nuclei and treat the e^- as if it's in a box:



(call it a cube of side L for simplicity)

So this e^- is a wave which has to live in this box.

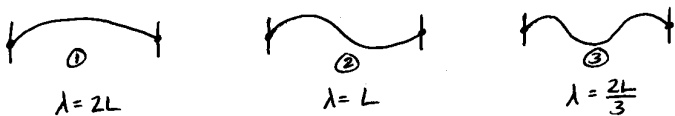
Let's simplify even further and look at only one dimension:



e^- can't get out of the box
(i.e. electrons aren't randomly flying out of the material - that would leave it charged)

So the probability to find the e^- at the very edge of the box must be zero.

How can we fit e^- waves into box w/ edges = zero?



① $\lambda = 2L$

② $\lambda = L$

③ $\lambda = \frac{2L}{3}$

and so on... $\lambda_n = \frac{2L}{n}$

$n = \#$ of "mode"

$\psi_1 = \sin(2\pi \frac{x}{2L})$

$\psi_2 = \sin(2\pi \frac{x}{L})$

$\psi_3 = \sin(2\pi \frac{x}{2L/3})$

It turns out to be convenient to define a "wavenumber" k in terms of the wavelength λ : $k \equiv \frac{2\pi}{\lambda}$ ③

Now we can write:

$\psi_1 = \sin(k_1 x)$

$\psi_2 = \sin(k_2 x)$

$\psi_3 = \sin(k_3 x)$

$k_1 = \frac{\pi}{L}$

$k_2 = \frac{2\pi}{L}$

$k_3 = \frac{3\pi}{L}$

Apparently $k_n = \frac{n\pi}{L}$.

Now for each "mode" we can ask:

what's the energy of the "mode"?

what's the momentum of the "mode"?

You can see intuitively that $E_3 > E_2 > E_1$

(e.g. think about shaking a slinky by one end: you'd have to shake faster to get the shorter wavelengths; or think about other kinds of waves you know: microwaves which have wavelengths around the excitation modes of water molecules which is how they cook your food, are higher energy than radio waves which you know from the size of the antenna must be $\sim 1m$)

More quantitatively, you know $E = \frac{1}{2}mv^2$

but we can write momentum = $p = mv$

and manipulate: $E = \frac{1}{2}mv^2 = \frac{1}{2}(mv) \left(\frac{mv}{m}\right) = \frac{p^2}{2m}$

Now we use deBroglie's formula: $p = \frac{h}{\lambda}$

$\Rightarrow E = \frac{h^2}{2m} \left(\frac{1}{\lambda}\right)^2$ sure enough, lower wavelength = higher energy

We can write the energy & momentum in terms of k :

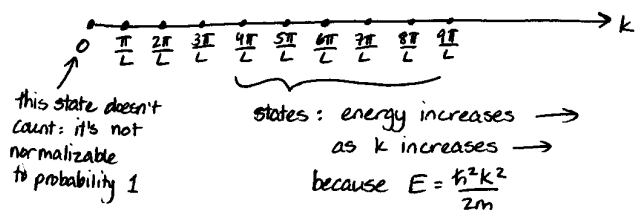
$p_n = \frac{h}{\lambda_n} = \frac{h}{2\pi} \frac{2\pi}{\lambda_n} = \hbar k_n$ where $\hbar \equiv \frac{h}{2\pi} = 1.05 \times 10^{-34} \text{ J}\cdot\text{s}$

$E_n = \frac{h^2}{2m} \left(\frac{1}{\lambda_n}\right)^2 = \frac{(h/2\pi)^2}{2m} \left(\frac{2\pi}{\lambda_n}\right)^2 = \frac{\hbar^2 k_n^2}{2m}$

$p = \hbar k$

$E = \frac{\hbar^2 k^2}{2m}$

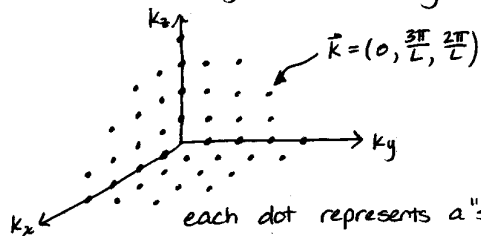
Sure enough, long wavelength (small k) states have less energy.^④
 Let's plot these states on a k -axis (momentum axis) instead of x -axis:



In physics, every system likes to go to its lowest energy state: e.g. a ball will roll to the bottom of the hill.

So as we put electrons into this system, they will go into the lowest k states first.

Now remember our system is actually 3-dimensional:



we talk about "wavevector" \vec{k} instead of "wavenumber" k

each dot represents a "state" or "mode"
 We could think of a state as occupying a little cube in k -space:

$$\left(\frac{\pi}{L}\right)^3$$

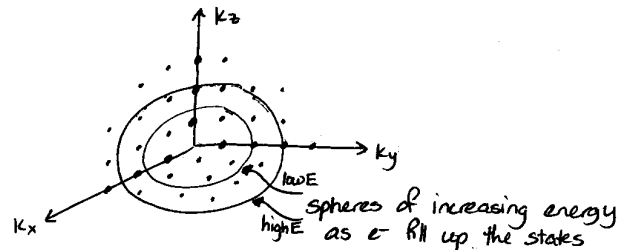
Now e^- are fermions, and because of the Pauli exclusion principle, they cannot sit in the same state.

So for each little cube in k -space we can put only 2 electrons:
 spin up \uparrow and spin down \downarrow

$$\frac{2}{(\pi/L)^3}$$

So the "density of states" in k -space is the # of states per unit volume in k -space, $\rho(k) = \frac{2}{(\pi/L)^3}$

As we put electrons into the material, they will start to fill up k -space with this density, starting at the origin (lowest energy)^⑤



So filling up the states from lowest energy is like blowing up a balloon in k -space! (Note that the way we defined our system, k must be positive, so we're actually only filling $1/8$ of a sphere.)

So what's the largest k we'll ever get to?

First we need to know how many electrons there are.

OK, suppose we have a $(1 \text{ cm})^3$ chunk of Na

$$\text{density} = 0.97 \text{ g/cm}^3$$

$$\text{atomic mass} = 23 \text{ g/mol}$$

$$N = \#e^- = (1 \text{ cm}^3 \text{ Na}) \times \frac{0.97 \text{ g}}{1 \text{ cm}^3} \times \frac{1 \text{ mol}}{23 \text{ g}} \times \frac{6 \times 10^{23} e^-}{1 \text{ mol}} \approx 2.5 \times 10^{22} e^-$$

These e^- fill out to radius k_{max} :

$$\underbrace{\frac{1}{8} \cdot \frac{4}{3} \pi k_{\text{max}}^3}_{\text{volume in } k\text{-space}} \cdot \underbrace{\frac{2}{(\pi/L)^3}}_{\text{density of states in } k\text{-space}} = N$$

$$\Rightarrow k_{\text{max}} = \left(3\pi^2 \frac{N}{L^3}\right)^{1/3}$$

\uparrow note that it doesn't depend on the size of our chunk of Na after all! it just depends on the density $N/L^3 = 0.97 \text{ g/cm}^3$ which is an intrinsic property of sodium

$\Rightarrow k_{\text{max}}$ is an intrinsic property of Na, and in fact we give it a special name "k-Fermi" = k_F

$$E_{\max} = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e} \left(3\pi^2 \frac{N}{L^3}\right)^{2/3} = \text{"Fermi energy"} = E_F$$

= energy of highest energy electron

$$\text{For Na: } \frac{(1.05 \times 10^{-34} \text{ J}\cdot\text{s})^2}{2(9.11 \times 10^{-31} \text{ kg})} \left(3\pi^2 \frac{2.5 \times 10^{22}}{(0.01 \text{ m})^3}\right)^{2/3} \approx 0.5 \times 10^{-18} \text{ J}$$

That doesn't sound like a lot of energy, but remember, it's per single electron! If this is the max energy, then the avg energy is roughly half that (actually slightly more) so the total energy for 10^{23} electrons is HUGE!

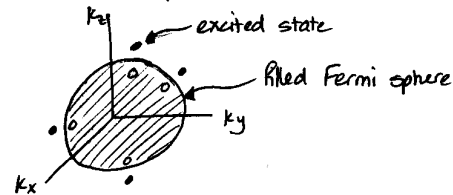
[The point is that since fermions are so unfriendly, they force each other to absurdly high energies. Notice that the energy increases with the density: if you compress the material you force the energy even higher. A point of interest is that neutron stars follow much the same physics: neutrons are fermions and they are packed together very densely at very high energies in neutron stars. The neutron star is prevented from collapsing to a black hole due to this outward pressure from the fermions not wanting to be compressed.]

Another way we can look at this energy is to convert it to a temperature. We can convert btwn energy & temperature using Boltzmann's constant $k_B = 1.4 \times 10^{-23} \text{ J/K}$ (we'll explain a little more about k_B next time)

$$E_F = k_B T_F \Rightarrow T_F = \frac{0.5 \times 10^{-18} \text{ J}}{1.4 \times 10^{-23} \text{ J/K}} \approx 30,000 \text{ K}$$

i.e. T_F is very hot (metal will melt before approaching T_F) this means most e^- are indeed in the ground state, i.e. lowest energy states at smallest k . Only when we approach T_F will an appreciable # of e^- be excited above k_{\max}

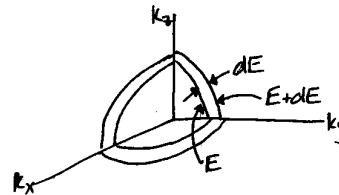
We often draw a picture like this:



OK, we got a little bit side-tracked. The goal is to calculate the density of states: $\rho(\epsilon) = \# e^- \text{ per energy}$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} (\text{distance from origin in } k\text{-space})^2$$

So spherical shells have equal energy



$\rho(\epsilon)d\epsilon = \# \text{ of states in this shell}$

[Note: I've been using ϵ and E interchangeably]

$$N = \frac{1}{8} \frac{4}{3} \pi k^3 \cdot \frac{2}{(\pi/L)^3} = \frac{1}{3\pi^2} L^3 k^3$$

$$dN = \frac{1}{\pi^2} L^3 k^2 dk$$

$$E = \frac{\hbar^2 k^2}{2m}$$

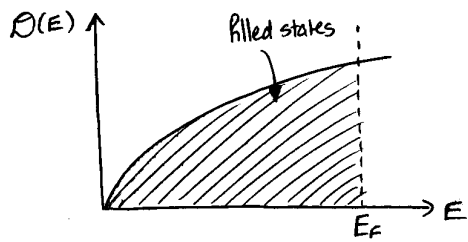
$$dE = \frac{\hbar^2}{m} k dk$$

$$\Rightarrow \rho(\epsilon) = \frac{\# \text{ states}}{\text{energy range}} = \frac{dN}{dE} = \frac{\frac{1}{\pi^2} L^3 k^2 dk}{\frac{\hbar^2}{m} k dk} = \frac{mL^3}{\pi^2 \hbar^2} k$$

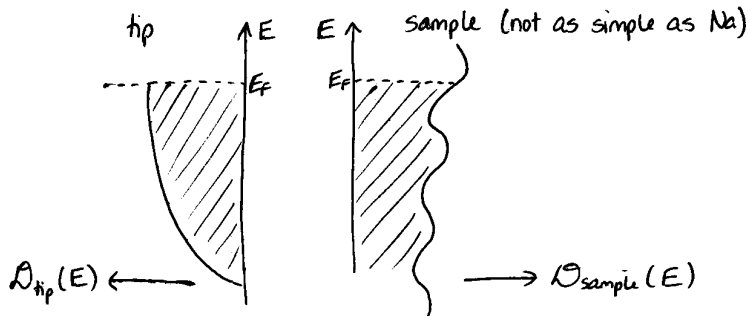
$$= \frac{mL^3}{\pi^2 \hbar^2} \sqrt{\frac{2mE}{\hbar^2}} = \frac{\sqrt{2m} mL^3}{\pi^2 \hbar^3} \sqrt{E}$$

So density of states in 3-dim goes like the square root of energy

⑧

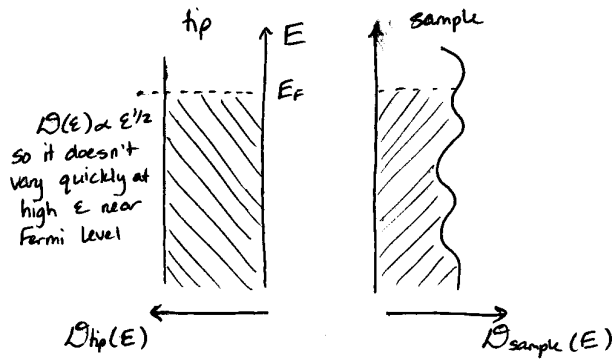


Typically in STM we see this diagram turned sideways:



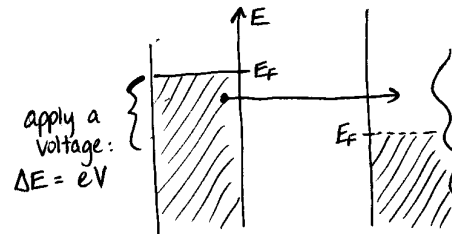
If tip and sample are electrically connected, their Fermi levels will be at the same energy (like 2 bowls of water connected by a tube: water levels will be equal even if the bowls have different depths & their bottoms are at different heights).

Typically also with STM we only probe the energies near the Fermi level so we throw away the bottom of the diagram:



⑨

Now if we put a voltage b/w tip and sample, we raise one Fermi level with respect to the other:



electrons tunnel:
tunneling current is proportional to (# filled states on left) x (# empty states on right)

→ STM measures the density of states $D(E)$

Question: back to the tennis ball, how do we reconcile the very small wavelength of the macroscopic tennis ball ($\lambda \approx 1.2 \times 10^{-34}$ m) with the wavelengths of the individual particles (electrons, etc) which make up the tennis ball? ①

Answer: still thinking about this, but here's the best guess so far.

A wavefunction is related to probability of finding a particle in a specific location:

$$\text{probability to find } e^{-} \text{ b/w } x \text{ and } x+dx = |\psi(x)|^2 dx$$

So how do we write a multi-particle wavefunction?

Well, what does a multiparticle wavefunction mean?

$$|\psi(x_1, x_2, t)|^2 \text{ probability to find particle \# 1 at } x_1 \text{ and particle \# 2 at } x_2$$

But probabilities multiply, so we can break it down:

$$\psi(x_1, x_2) = \psi_1(x_1) \psi_2(x_2)$$

So for the whole tennis ball, we'd have:

$$\psi_{\text{tennis ball}} = \psi_1(x_1) \psi_2(x_2) \dots \psi_N(x_N) \text{ where } N \approx 10^{23}$$

So it's clearly impossible to write down all 10^{23} factors in the wavefunction, or all 10^{23} coordinates.

One useful coordinate is the center-of-mass coordinate:

$$\vec{R} = (\vec{x}_1 + \vec{x}_2 + \vec{x}_3 + \dots + \vec{x}_N) / N$$

How can we write the wavelength in terms of the wavefunction?

Going back to our particle-in-a-box wavefunctions, we had

$$\psi_n(x_n) = \sin(k_n x_n)$$

We can also take note of the fact that the only physical meaning of the wavefunction is as a probability: $|\psi|^2$ ②

Since the probability involves the magnitude, ψ can be imaginary. In fact any multiplier of type $e^{i\theta}$ doesn't change the physical meaning of the wavefunction, so we can write $|\psi|^2 = |\psi e^{i\theta}|^2 = |\psi|^2 |e^{i\theta}|^2$

Furthermore, we can rewrite our sinusoidal wavefunctions in a more convenient form:

$$\psi_n(x_n) = e^{ik_n x_n}$$

$$\text{Now, notice that } \frac{d}{dx} \psi_n(x) = ik_n e^{ik_n x} = ik_n \psi_n(x) = \frac{2\pi i}{\lambda_n} \psi_n(x)$$

So we can get to the wavelength by taking the derivative of the wavefunction (this can be proved more rigorously)

For the whole tennis ball, the derivative we care about should be with respect to the center of mass coordinate:

$$\frac{d}{dR} = \frac{\partial x_1}{\partial R} \frac{d}{dx_1} + \frac{\partial x_2}{\partial R} \frac{d}{dx_2} + \dots + \frac{\partial x_N}{\partial R} \frac{d}{dx_N}$$

$$\psi(x_1, x_2, \dots, x_N) = e^{ik_1 x_1} e^{ik_2 x_2} \dots e^{ik_N x_N}$$

$$\frac{d\psi}{dR} = \{N(ik_1) + N(ik_2) + \dots + N(ik_N)\} \psi \approx N \sum_{j=1}^N k_j \psi$$

$$\text{So presumably } \frac{2\pi}{\lambda_{\text{tot}}} = k_{\text{tot}} \approx N \sum_{j=1}^N k_j = N \sum_{j=1}^N \frac{2\pi}{\lambda_j}$$

$$\Rightarrow \frac{1}{\lambda_{\text{tot}}} \approx N \sum_{j=1}^N \frac{1}{\lambda_j}$$

Each of these $\lambda_j \approx 1 \text{ \AA}$ (order of magnitude wavelength for electrons in materials)

this all looks pretty good except for that extra factor of N

$$\frac{1}{10^{-34} \text{ m}} \stackrel{?}{\approx} N \cdot N \frac{1}{1 \text{ \AA}} \text{ works out well except for that extra } N \dots ???$$

March 1, 2005 Fermi function (& what is temperature, really?) ①

$g = \#$ of accessible states of a system

All of our arguments from here on will be based on the assumption that quantum states are either accessible or inaccessible, and a system is equally likely to be in any accessible state

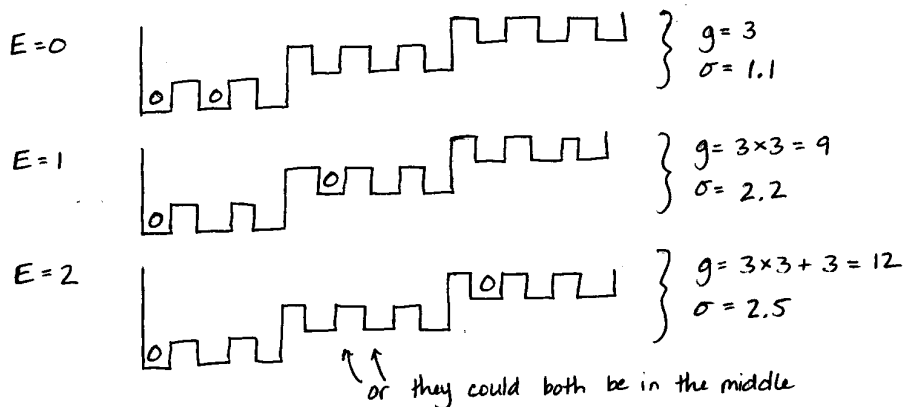
entropy = $\sigma = \ln g$

[We define entropy as a \ln b/c usually g is so large.]

One simple example is an electron (in zero B-field)

can be in state \uparrow or state \downarrow , i.e. $g = 2$ and $\sigma = \log(2)$

Another simple example is balls in holes:



Now suppose we have 2 systems in contact and energy can flow between them. Suppose they have energies: $U_1 = 0$ and $U_2 = 2$ (Note: often to avoid confusion we use U to represent energy instead of E)

We know the total energy is conserved: $U_{tot} = U_1 + U_2 = 2$

Total # of states = (# states in system 1) \times (# states in system 2)

$$g_{tot} = g_1 g_2 \Rightarrow \sigma_{tot} = \sigma_1 + \sigma_2$$

entropies add, b/c we used the logarithm

You know from experience that energy will flow until the temperatures are equal in the two systems!

When $U_1 = 0$ and $U_2 = 2$, we have ②

$$g_{tot} = 3 \times 12 = 36$$

When $U_1 = 1$ and $U_2 = 1$, we have

$$g_{tot} = 9 \times 9 = 81$$

When $U_1 = 2$ and $U_2 = 0$, we have

$$g_{tot} = 12 \times 3 = 36$$

So the total # of accessible states is $36 + 81 + 36 = 153$

And the probability that $U_1 = U_2 = 1$ is $\frac{81}{153}$ slightly more than half

So we see that the system will probably end up with $U_1 = U_2 = 1$

How can we quantify this?

We expect the system to end up in the most likely configuration, i.e. the configuration with the largest number of states, i.e. the configuration that maximizes the entropy.

$$\Rightarrow \text{maximize } \sigma_{tot}(U_1, U_2) = \sigma_1(U_1) + \sigma_2(U_2)$$

At the maximum, $d\sigma_{tot} = 0$ (derivative vanishes at extrema)

Also, by conservation of energy, if one system loses energy, the other system must gain the same amount of energy: $dU_1 = -dU_2$

$$d\sigma_{tot} = \frac{d\sigma_1}{dU_1} dU_1 + \frac{d\sigma_2}{dU_2} dU_2 = 0$$

$$\Rightarrow \frac{d\sigma_1}{dU_1} (-dU_2) + \frac{d\sigma_2}{dU_2} dU_2 = 0$$

$$\Rightarrow \frac{d\sigma}{dU_1} = \frac{d\sigma}{dU_2}$$

In other words, energy flows until the quantity $\frac{d\sigma}{dU}$ is equal in both systems.

We know the final temperature will be the same in both systems so temperature must be a function of $\frac{d\sigma}{dU}$

What if we just let $T = c \frac{d\sigma}{dU}$?

↑ some constant

That would be a problem b/c it would mean that energy would flow from the low temperature system to the high temperature system!

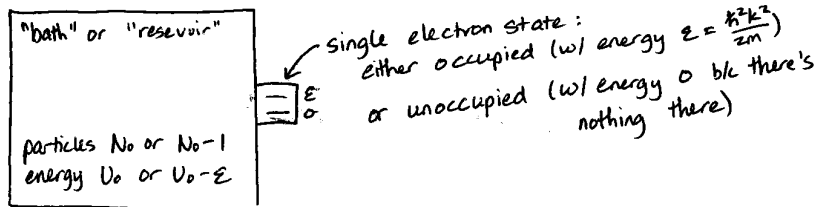
So instead we let $\frac{1}{T} = c \frac{d\sigma}{dU}$

and guess what! c turns out to be that Boltzmann constant

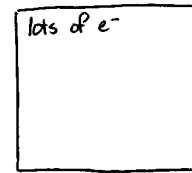
$$\frac{1}{k_B T} = \frac{d\sigma}{dU} \quad \text{where } k_B = 1.4 \times 10^{-23} \text{ J/K}$$

OK, now we're going to derive the "Boltzmann factor" which tells us the probability that a particular state is occupied. Last time when we calculated the density of states, we assumed that all the low energy states (inside the sphere of k_F) were occupied and all the higher energy states (outside k_F) were empty. But at finite temperature (i.e. $T > 0$) that's not strictly true. A small number of e^- will be excited, so a small number of states with $k < k_F$ will be empty and a small (equal) number of states with $k > k_F$ will be full. We need to calculate the probability b/c this will influence the tunneling current slightly.

Typically the way these arguments go, we focus on a single state and lump all the other states together into a "reservoir" or "bath" whose energy (of many e^-) is large compared to the single e^-



$U_{tot} = U_0 = \text{total energy is conserved}; N_0 = \text{total \# particles conserved}$



maybe a single e^-

case 1: 0 and 0 $\Rightarrow g = 1 \Rightarrow \sigma = 0$

case 2: 1 and $E \Rightarrow g = 1 \Rightarrow \sigma = 0$

case 1: N_0 and $U_0 \Rightarrow g(N_0, U_0) \Rightarrow \sigma(N_0, U_0)$

case 2: N_0-1 and $U_0-E \Rightarrow g(N_0-1, U_0-E) \Rightarrow \sigma(N_0-1, U_0-E)$

Total entropy: $\sigma_{tot} = \sigma_{bath} + \sigma_i = \sigma_{bath}$

The probability of finding the e^- in the separate state is:

$$P = \frac{(\# \text{ of states of bath if } e^- \text{ is in separate state})}{(\# \text{ of states of bath if } e^- \text{ is in separate state}) + (\# \text{ of states of bath if } e^- \text{ is in the bath})}$$

$$P = \frac{g(N_0-1, U_0-E)}{g(N_0-1, U_0-E) + g(N_0, U_0)} = \frac{\exp(\sigma(N_0-1, U_0-E))}{\exp(\sigma(N_0-1, U_0-E)) + \exp(\sigma(N_0, U_0))}$$

Since $N_0 \gg 1$ and $U_0 \gg E$, we can Taylor-expand σ about N_0 and U_0

$$\sigma(N_0-1, U_0-E) \approx \sigma(N_0, U_0) - E \frac{d\sigma}{dU} \Big|_{U_0} - \frac{1}{k_B T} \frac{d\sigma}{dN} \Big|_{N_0}$$

We haven't derived this, but it turns out this is $-E_F/k_B T$

[See Kittel & Kroemer, "Thermal Physics" chapter 5 for derivation]

$$\sigma(N_0-1, U_0-E) \approx \sigma(N_0, U_0) - \frac{E}{k_B T} + \frac{E_F}{k_B T}$$

$$g(N_0-1, U_0-E) = \exp(\sigma(N_0-1, U_0-E)) \approx \exp(\sigma(N_0, U_0)) \exp\left(\frac{E_F - E}{k_B T}\right)$$

$$P = \frac{e^{\sigma(N_0, U_0)} e^{(E_F - E)/k_B T}}{e^{\sigma(N_0, U_0)} e^{(E_F - E)/k_B T} + e^{\sigma(N_0, U_0)}} = \frac{e^{(E_F - E)/k_B T}}{e^{(E_F - E)/k_B T} + 1} = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

this is the Fermi function!

⑤

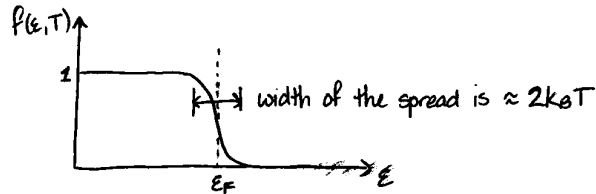
This is the probability that a state of energy ϵ is occupied:

often written $f(\epsilon, T) = \frac{1}{1 + e^{(\epsilon - \epsilon_F)/k_B T}}$

For $\epsilon \ll \epsilon_F$, the exponential in the denominator is negligible, so $f(\epsilon, T) \approx 1$. In other words, for $\epsilon \ll \epsilon_F$ all states are full, as we expect.

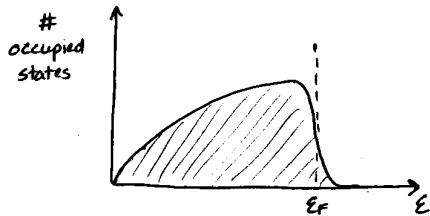
For $\epsilon \gg \epsilon_F$, the exponential in the denominator blows up, so $f(\epsilon, T) \approx 0$. In other words, for $\epsilon \gg \epsilon_F$ all states are empty, as we expect.

For $\epsilon \approx \epsilon_F$, $f(\epsilon, T)$ takes some value between 1 and 0:



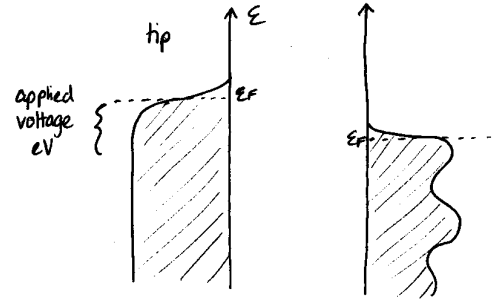
So, in the last discussion about tunneling, we ignored temperature effects. Now we take them into account:

The actual # of occupied states is the product of the # of available states times the probability that they're occupied:
 $\mathcal{D}(\epsilon) f(\epsilon, T)$



⑥

Now a look back at the tunneling diagram:



So our measurement of the density of states has a built-in inaccuracy due to temperature:

$2k_B T$ spread for tip + $2k_B T$ spread for sample

$$4k_B T = 4(1.4 \times 10^{-23} \text{ J/K})(300 \text{ K}) = 1.7 \times 10^{-20} \text{ J}$$

↑ room temp

$$= 0.105 \text{ eV}$$

[Remember: eV = "electron-Volt" - another unit of energy
 $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$]

So we'll have density of states smearing on order 100 meV