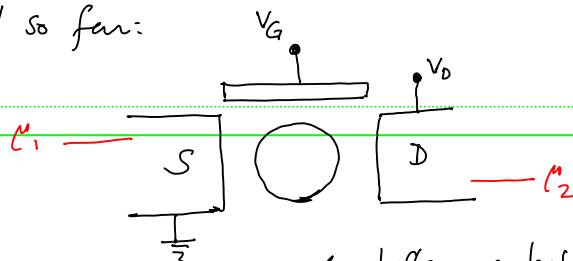


what we have learned so far:

Session 5

Note Title

9/15/2008

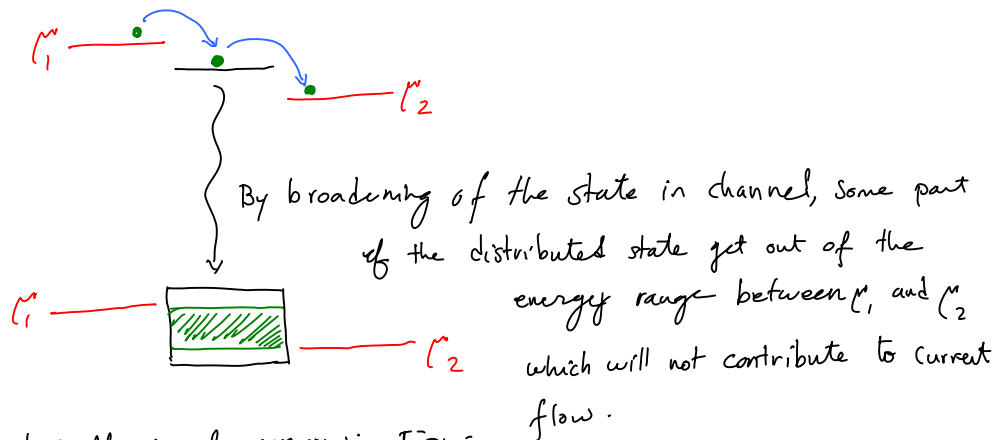


Current flows only if  $\mu_1 \neq \mu_2$ . The cause of difference between  $\mu_1$  &  $\mu_2$  is the applied voltage.

$$I = -\frac{2e}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$

$$N = \frac{\gamma_1 N_1 + \gamma_2 N_2}{\gamma_1 + \gamma_2} = \frac{2\gamma_1 f_1 + 2\gamma_2 f_2}{\gamma_1 + \gamma_2}$$

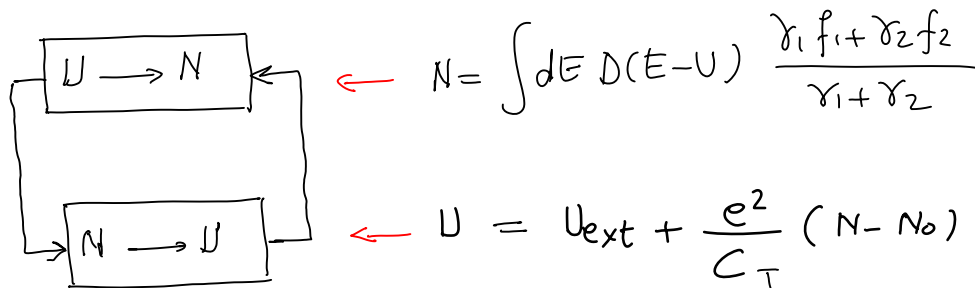
We also learned that we need to take into account the broadening, which happens due to coupling of channel states & source or drain. This sets a limit on the current. Why?



We then learned about small signal approximation:

$$I = v \frac{2e^2}{\hbar} \int dE D(E) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \left(-\frac{\partial f}{\partial E}\right)$$

If the bias is large, we have to consider the shift of the levels due to voltage & change in the number of electrons:



$$I = -\frac{e}{\hbar} \int dE D(E-U) \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$

## Coulomb Blockade

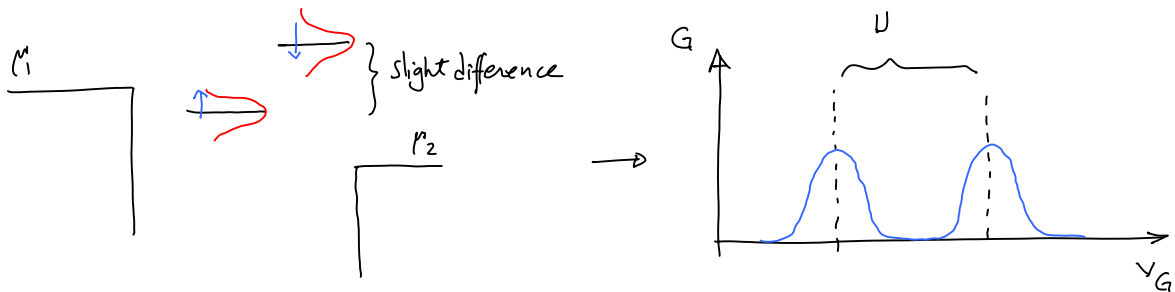
Sometimes in experiments, we observe two peaks rather than a single peak.

The peak's width is  $\gamma + k_B T$  (Coulomb blockade)

This occurs when  $U \gg k_B T + \gamma$

Reason: there are two energy levels corresponding to spin up and spin down.

When the first level is filled, the second level shifts up as it feels the potential due to the filled level.



This is called Coulomb blockade.

For small devices  $U = \frac{e^2}{C_T}$  can be very large as  $C_T$

becomes very small  $\Rightarrow$  the condition  $U \gg k_B T + \gamma$

under which Coulomb blockade happens is satisfied.

For example,  $C_T$  can be as small as  $10^{-6}$  PF:

$$\frac{e^2}{C_T} = \frac{1.6 \times 10^{-19}}{10^{-18}} = 160 \text{ meV}$$

Let's summarize what we have learned:

$$(A) \quad N = 2 \int dE D(E - U_{scf}) \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}$$

$$(B) \quad U_{scf} = U_{ext} + \frac{e^2}{C_T} (N - N_0)$$

$$(C) \quad I = V \frac{2e^2}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \int dE D(E - U_{scf}) (f_1 - f_2)$$

## How can we calculate the potential in the channel?

Solve the poisson's equation:

- ① first assume there is no change in the number of electrons in the channel and solve the Laplace equation:

$$\vec{\nabla} \cdot (\epsilon_r \vec{\nabla} V) = 0 \quad \text{if } \epsilon_r \text{ is constant} \rightarrow \nabla^2 V = 0$$

call this potential  $U_L$  (or  $U_{ext}$  as before.)

- ② When there is a change in the number of electrons in the channel, we have to solve poisson equation:

$$\vec{\nabla} \cdot (\epsilon_r \vec{\nabla} V) = - \frac{\Delta \rho}{\epsilon_0} \rightarrow V = \frac{e^2}{C_T} \Delta N$$

this is an additional potential to the laplace potential, which is due to the change in the number of electrons:

$$U = U_L + \underbrace{\frac{e^2}{C_T}}_{\text{Single electron charging energy}} \Delta N$$

Single electron charging energy due to the addition of one electron to the channel.

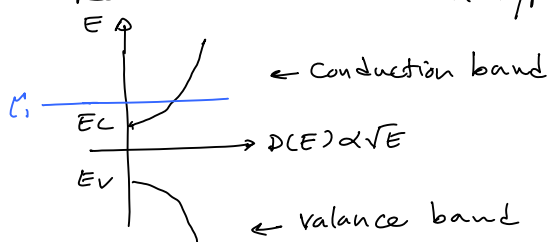
If  $\frac{e^2}{C_T} \gg \gamma \& k_B T \Rightarrow$  we enter a new transport regime which is **Coulomb blockade** regime.

## How can we apply this method to a bigger device?

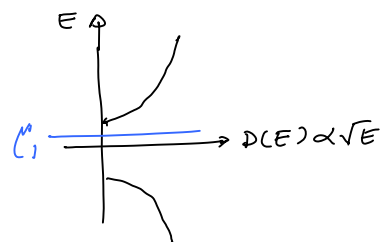
Bigger device has lots of levels  $\rightarrow$  each level in gate is broadened  $\rightarrow$  use density of states which is the sum of all broadened states.

example:

Let's consider an n-type transistor

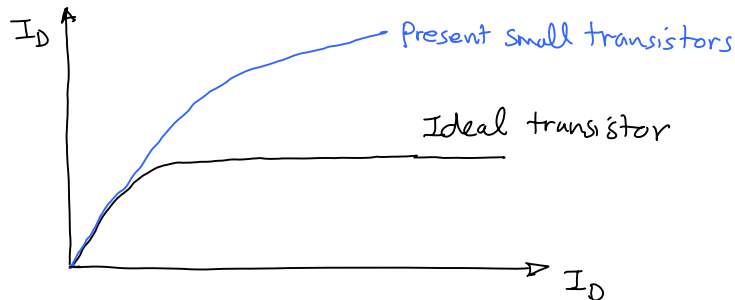


apply a negative voltage  $\rightarrow$



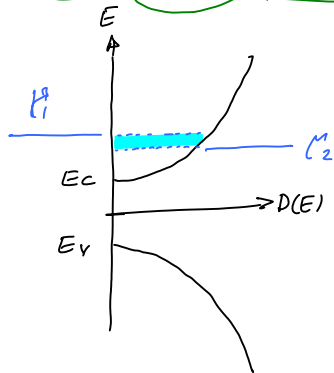
$\mu_1$  enters a region that there is no state so it doesn't conduct and the transistor is off.

How does the current voltage characteristic look like and how does it change with the gate voltage?

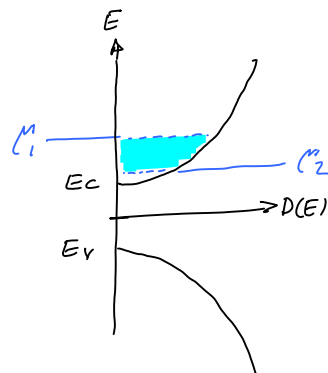


In a good transistor, the current  $I_D$  saturates - Why?

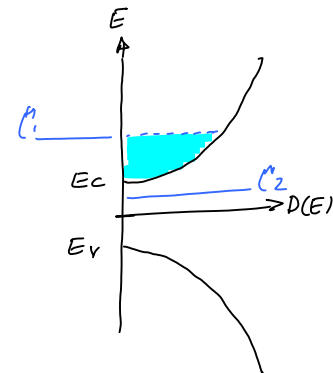
Let's look at the band diagram once again:



increase  $+V_D$   
 $\longrightarrow$



number of states between  $\mu_1$  &  $\mu_2$  increases  $\Rightarrow I_D$  increases



number of states between  $\mu_1$  &  $\mu_2$  doesn't change  $\Rightarrow I_D$  saturates

So why  $I_D$  doesn't saturate in small transistors?

The answer is that because the gate voltage also changes when the drain voltage is changed. By applying a positive voltage to the drain, the channel potential is lowered to some extent.

This will increase the numbers of states between  $\mu_1$  &  $\mu_2$ , which results in a higher conduction & current. So the current doesn't saturate.

In a good transistor, channel potential remains constant no matter what potential is applied to the drain. How can we do this in practice? we keep the gate very close to the channel (thin gate oxide) so that it is the gate voltage that determines the channel potential not the drain's.

What is the relation between the conductance of the device and the device length and width?

Ohm's law: as the device becomes longer, conductance becomes smaller, and as it becomes wider, conductance increases.  $G \propto \frac{W}{L}$

What if we use the theory that we have learned?  
Will the conductance change in a same manner?

We will see that  $G$  has similar dependency to  $W$ , but for dependency to  $L$ , we need further work.

Let's explain:

We know: More states  $\Rightarrow$  more current

Larger devices have obviously more number of states.

for example,

for a 2D solid: Number of states  $\propto$  Area:  $D \propto WL$

3D solid: # of states  $\propto$  Volume:  $D \propto AL$  ( $A$  is area)

So can we say  $G \propto D \propto AL$ ?

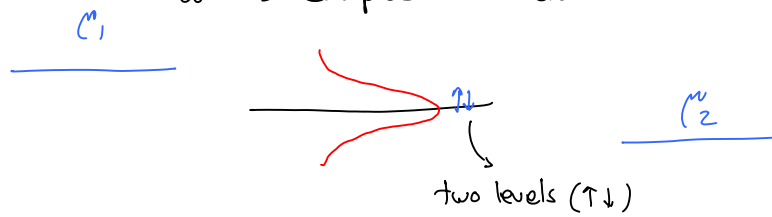
But that obviously contradicts Ohm's law ( $G \propto \frac{W}{L}$ ).

The answer is hidden in  $\gamma$ . As you make the device bigger,

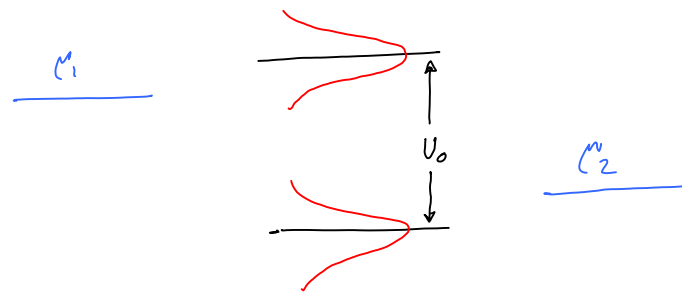
$\gamma$  decreases as  $1/L$ . Why?



broadened level in channel  
as it is coupled to contacts



when we apply bias, due to CB the levels are separated:



What lets us to treat the problem in a simple manner is that an electron in the channel feels some average potential due to its surroundings which is  $U$ . This method of doing things is called **mean field theory** and it's the bases of our understanding of current flow and all electronic properties.

The real big multi-electron problem is virtually insolvable.

There are many parameters involved that we cannot solve it exactly. So our job is to learn how to make approximations.

To validate our approximation we have to compare it with experimental results. The better match, the better the theory.

Now, we will stop talking about current for a few sessions.

Instead, we spend this time on energy levels in a given device.

These levels are eigenvalues of the Hamiltonian in the Schrodinger equation.

## Concepts:

In a multi-level conductor with  $n$  energy levels, we need  $n \times n$  matrices to describe the single level analogues:

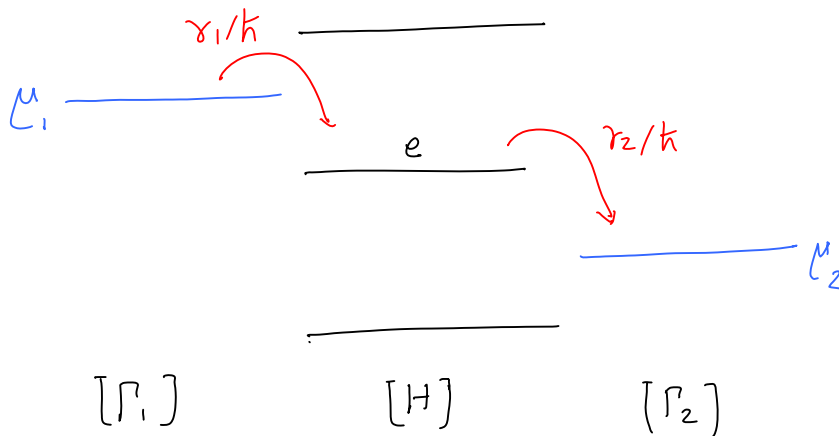
$$\mathcal{E} \longrightarrow [H] \quad n \times n \text{ Hamiltonian matrix}$$

$$\gamma_{1,2} \longrightarrow [\Gamma_{1,2}(E)] \quad \text{Broadening matrix}$$

$$2\pi D(E) \longrightarrow [A(E)] \quad \text{Spectral function}$$

$$U_{\text{scf}} \longrightarrow [U_{\text{scf}}] \quad \text{Self-consistent potential matrix}$$

$$N \longrightarrow [\rho] \quad \text{Density matrix}$$



Let's see how to write the Hamiltonian. We start from the simplest case that is Hydrogen atom. For anything more complicated than the H-atom, we cannot use analytical methods! Often to get the Hamiltonian for a given system, we must use numerical methods (e.g. finite difference method).

So, where does Hamiltonian come from?

Schrödinger equation!



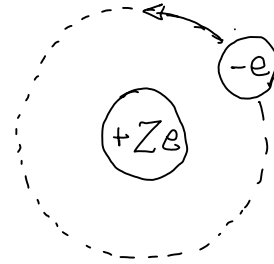
The Schrödinger equation:

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + U(\vec{r}) \Psi(\vec{r}, t)$$

For a single electron atom:

classically  $\frac{ze^2}{4\pi\epsilon_0 r^2} = \frac{mv^2}{r}$

$$\rightarrow v^2 = \frac{ze^2}{4\pi\epsilon_0 mr}$$



An electron energy is given as:  $E = \text{Potential} + \text{kinetic}$

$$E = -\frac{ze^2}{4\pi\epsilon_0 r} + \frac{1}{2}mv^2 = \frac{-ze^2}{4\pi\epsilon_0 r} + \frac{1}{2}m \left( \frac{ze^2}{4\pi\epsilon_0 mr} \right)$$

$$= -\frac{ze^2}{8\pi\epsilon_0 r}$$

- But this is WRONG! because energy must be discrete. (r is continuous).
- The electron is under continual centripetal acceleration and so must radiate EM waves, eventually collapsing into the nucleus.

How do we get around this?

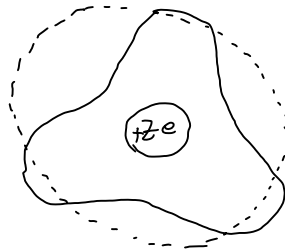
de-Broglie suggested that we endow the electron with wave like properties to get discrete energies.

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

Using this concept, circumference of a Hydrogen-like atom must be an integer multiple of  $\lambda$  such that:

$$2\pi r = n\lambda = n \frac{h}{mv}$$

So with a wave like character, only certain radii are allowed.



Surprisingly, this gives the correct energy levels in Hydrogen atom as in experiment.

de Broglie:  $2\pi r = n \frac{h}{mv}$   
 classical:  $v^2 = \frac{Ze^2}{4\pi\epsilon_0 mr}$

$$r_n = \left(\frac{n^2}{Z}\right) a_0 \quad \text{where } a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2}$$

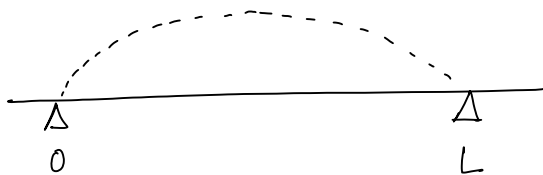
Substitute in  $E = -\frac{Ze^2}{8\pi\epsilon_0 r} \Rightarrow E_n = -\frac{Z^2}{n^2} E_0$  where  $E_0 = \frac{e^2}{8\pi\epsilon_0 a_0}$

This heuristic insight was put on a solid basis by the Schrodinger

Equation:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + U\psi$$

How does the Schrodinger equation lead to discrete energy levels? let's consider a vibrating string:



The general 1D wave equation is:

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$

$v$ : speed

$$u = Ae^{ikx - i\omega t}$$

Substitute  $\Rightarrow -\omega^2 Ae^{ikx - i\omega t} = v^2 (-k^2) Ae^{ikx - i\omega t} \Rightarrow \omega = vk$

when we clamp the two ends, we have a standing wave that is a superposition of  $+k$  and  $-k$  waves:

$$u = A (e^{ikx} + e^{-ikx}) e^{-i\omega t} = A \sin kx e^{-i\omega t}$$

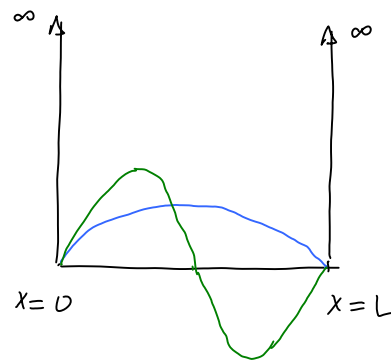
$$u(x=0)=0 \vee u(x=L)=0 \Rightarrow \sin kL = 0 \Rightarrow k = \frac{n\pi}{L}$$

$$\Rightarrow \omega = vk = \frac{n\pi v}{L}$$

Quantum analogue of a 1D vibrating string is a particle in a box (or infinite quantum well)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad 0 < x < L$$

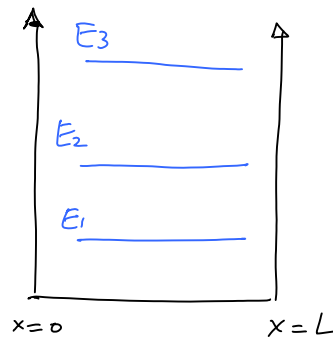
$$\psi(x,t) = e^{\pm ikx} e^{-iEt/\hbar} \quad E = \frac{\hbar^2 k^2}{2m} = \hbar\omega$$



$$\psi(x=0) = \psi(x=L) = 0$$

$$\rightarrow \psi(x,t) = A \sin kx e^{-i\omega t} \quad ; \quad k = \frac{n\pi}{L} \quad n=1, 2, \dots$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$



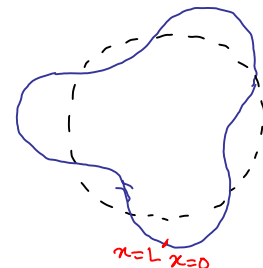
To solve the Schrodinger equ. for Hydrogen atom, we need to do

more algebra, but the physics is the same.

Example The ring (another kind of box)

We sometimes use a ring mode as it is mathematically much easier to manage with solids. This is because we have a periodic boundary condition here.

When in a problem, B.C.'s don't matter, we use a ring-



The ring has eigenfunctions:  $\Psi(x,t) = A \sin(kx) e^{-i\omega t}$  and

$$\Psi(x,t) = A \cos(kx) e^{-i\omega t}$$

we can equally say:  $\Psi(x,t) = A e^{\pm ikx} e^{-i\omega t}$

$$\text{Since } \Psi(x=0) = \Psi(x=L) \Rightarrow 1 = e^{ikL} \Rightarrow k = \frac{2n\pi}{L} \quad n = 1, 2, 3, \dots$$

- Perhaps Carbon Nano tubes are the only real example where the periodic boundary condition is real (and not just a mathematical convenience).

What does  $\Psi$  mean?

$\Psi \Psi^*$  is a probability distribution. So for lots of electrons,

$$\text{electron density is: } n = \sum_i \Psi_i^* \Psi_i$$

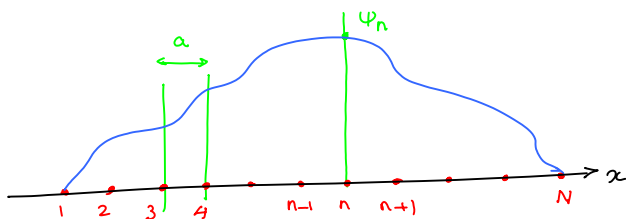
## Finite differences method

Consider 1D Schrödinger eqn:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U(x)\Psi$$

We want to convert the Schrödinger equation to a matrix equation.

First create a lattice for the 1D problem:



$$\Psi(x,t) \rightarrow \begin{bmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_n) \\ \vdots \\ \Psi(x_N) \end{bmatrix} \text{ at a given time } t.$$

So we can write for the Schrödinger equation:

$$i\hbar \frac{d}{dt} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix} = [H] \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix}$$

How do we convert the Hamiltonian into a matrix?

$$H = \frac{p^2}{2m} + U(x) \rightarrow [H] = ?$$

At point  $x_n$  we have:  $i\hbar \left. \frac{d\psi(x,t)}{dt} \right|_{x=x_n} = -\frac{\hbar^2}{2m} \left. \frac{d^2}{dx^2} \psi(x,t) \right|_{x=x_n} + U(x_n) \psi(x_n, t)$

↓  
So this term appears only in diagonal of Hamiltonian.

So expect sth like this:

$$i\hbar \frac{d}{dt} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix} = \begin{bmatrix} U(x_1) & & & \\ & U(x_2) & & \\ & & \ddots & \\ & & & U(x_N) \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{bmatrix}$$