c) Solving the Schrödinger equation using simple 1D examples.

(No system is truly 1D, however in many of systems, 1D properties dominate the behavior).

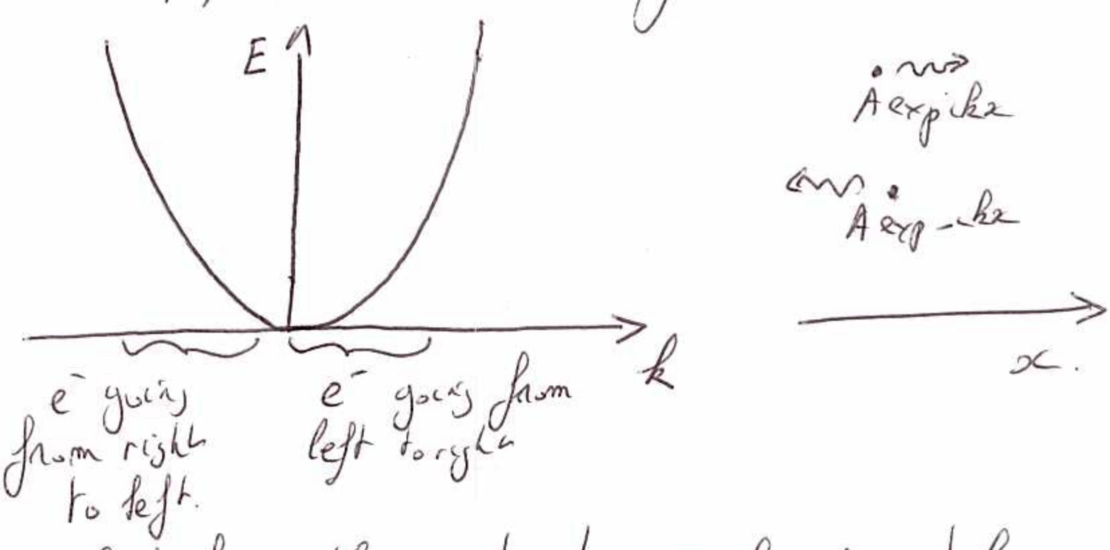
i) free electron model

Here $U(\vec{r})$ does not depend on $\vec{r}$ [we set $U(\vec{r}) \equiv 0$]

$\boxed{\psi_{(x)} = A \exp ikx}$ is solution of the Schrödinger equation.

it comes $\boxed{E = \frac{\hbar k^2}{2m}}$ for the kinetic energy of the e^-.

we call this $E(k)$ relation a dispersion relation.



$\Rightarrow$ the free e^- model is frequently used when analyzing metals.

[illegible]

(ii) e^- into a infinite quantum well.

$$U(x) = \begin{cases} \infty \text{ for } x \leq 0 \\ 0 \text{ for } 0 < x < L \\ \infty \text{ for } x \geq L \end{cases}$$

- Boundary condition $\psi(x) = 0$ for $x = 0$, $x = L$.
since the regions $x \leq 0$ and $x \geq L$ are forbidden for the e^- [i.e. $U(x)\psi(x)$, if $U(x) \to +\infty$, $\psi(x) = 0$]

So $$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \text{ if } x \in]0, L[$$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad \text{with } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Solutions are $\psi(x) = Ae^{ikx} + Be^{-ikx}$ $(A, B \in \mathbb{C})$

with Boundary conditions $\begin{cases} A + B = 0 \Rightarrow A = -B \\ \sin kL = 0 \Rightarrow k = \frac{n\pi}{L} \equiv k_n \end{cases}$ $(n \in \mathbb{N}^*)$

k can take only discrete value.

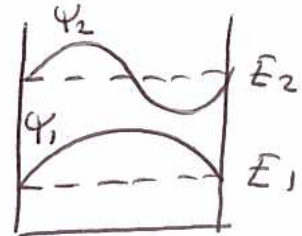
$\psi_n(x) = A' \sin(k_n x)$ with orthonormalization $\int_0^L |\psi_n(x)|^2 = 1$

$$\Rightarrow \boxed{\psi_n(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{L}\right)} \quad \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}}$$

In general if the boundary conditions are equal to zero, the Schrodinger equation become a eigenvalue problems.

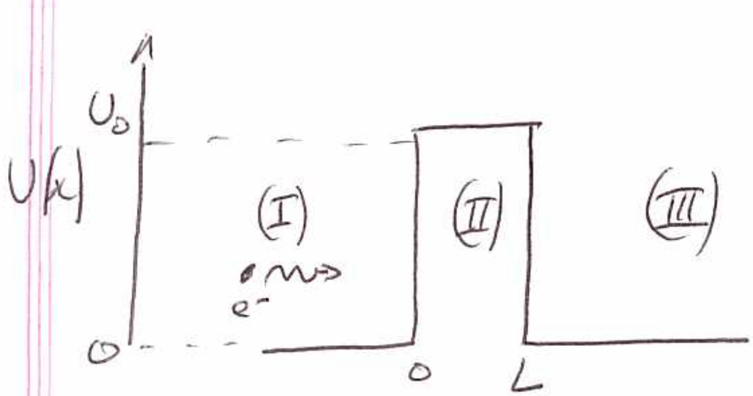
$$\boxed{H\psi_n = E_n \psi_n}$$

The energy spectrum is discrete



$\Rightarrow$ confinement effects in quantum mechanics

(iii). potential wall



$$U(x) = \begin{cases} 0 & \text{if } x \leq 0 \quad (I) \\ U_0 & \text{if } 0 < x < L \quad (II) \\ 0 & \text{if } x \geq L \quad (III) \end{cases}$$

we suppose that $E < U_0 \Rightarrow$ general solution for an e^- coming from the left.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (I) \quad k = \sqrt{\frac{2mE}{\hbar^2}} \\ Ce^{Kx} + De^{Kx} & (II) \quad K = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \\ Ee^{ikx} & (III) \quad k = \sqrt{\frac{2mE}{\hbar^2}} \end{cases}$$

propagating - traveling wave

evanescent wave.

boundary conditions at $x=0$, $x=L$

$$\Psi_{I}\big|_0 = \Psi_{II}\big|_0 \; ; \quad \frac{d\Psi_{I}}{dx}\bigg|_0 = \frac{d\Psi_{II}}{dx}\bigg|_0$$

$$\Psi_{II}\big|_L = \Psi_{III}\big|_L \; ; \quad \frac{d\Psi_{II}}{dx}\bigg|_L = \frac{d\Psi_{III}}{dx}\bigg|_L$$

$\Rightarrow$ we get after calculations A, B, C, D, E [A is already known]

the ratio $R = \dfrac{|B|^2}{|A|^2}$ is the reflexion coefficient.

the ratio $T = \dfrac{|E|^2}{|A|^2}$ is the transmission coefficient.

In contrast to classical mechanics $T \neq 0$!

$\Rightarrow$ tunneling effect. 

Also for the case $E > U_0$, we would find that $R \neq 0$ (also in contrast to classical mechanics)