

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

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

i) free electron model

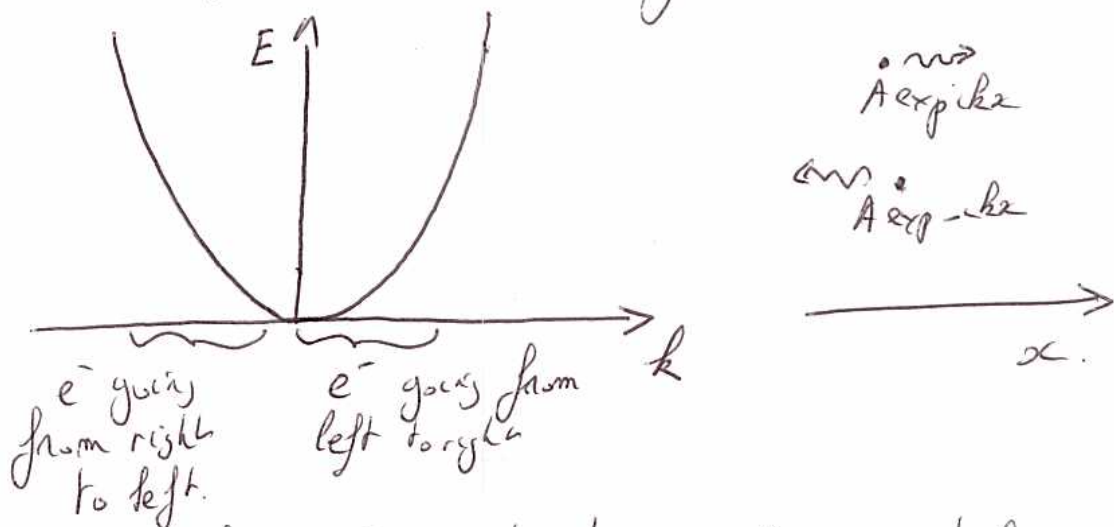
here $U(\vec{r})$ does not depend on \vec{r} [we set $U(\vec{r}) = 0$]

$\Psi_{\vec{k}} = A \exp(i\vec{k}\cdot\vec{r})$ is solution of the Schrödinger equation.

~~it comes from the wave equation~~

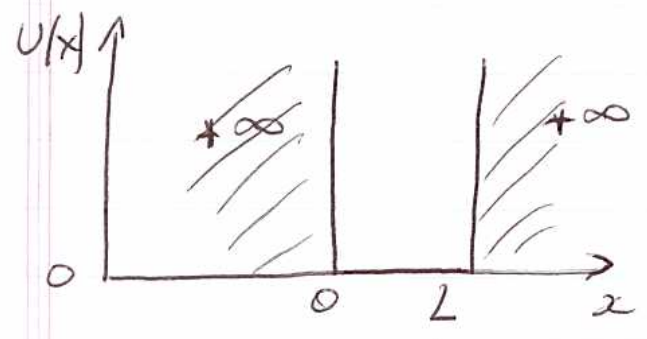
it comes $E = \frac{\hbar^2 k^2}{2m}$ for the kinetic energy of the e^- .

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



⇒ the free e^- model is frequently used when analyzing metals.

(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 $U(x) \rightarrow +\infty, \psi(x) = 0$]

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

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

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 values.

$\psi_n(x) = A' \sin\left(\frac{k_n x}{L}\right)$ with orthonormalization $\int_0^L |\psi_n(x)|^2 dx = 1$

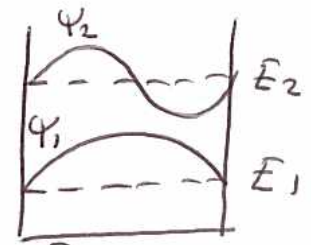
$$\Rightarrow \boxed{\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)} \quad \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2m L^2}}$$

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

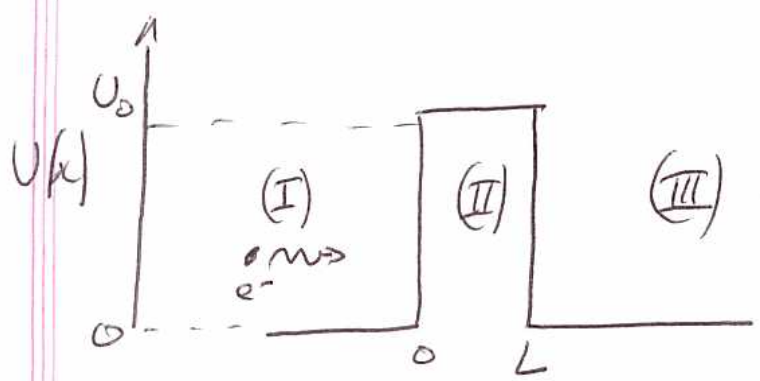
$$H \Psi_m = E_m \Psi_m$$

The energy spectrum is discrete

⇒ confinement effects in quantum mechanics



(iii). potential well



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

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

$$\Psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & \text{(I)} & k = \sqrt{\frac{2mE}{\hbar^2}} \\ C e^{Kx} + D e^{-Kx} & \text{(II)} & K = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \\ E e^{ikx} & \text{(III)} & k = \sqrt{\frac{2mE}{\hbar^2}} \end{cases}$$

propagating -
traveling wave

evanescent wave.

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

$$\Psi_{I/0} = \Psi_{II/0} ; \frac{d\Psi_{II}}{dx}\bigg|_0 = \frac{d\Psi_{III}}{dx}\bigg|_0$$

$$\Psi_{II/L} = \Psi_{III/L} ; \frac{d\Psi_{II}}{dx}\bigg|_L = \frac{d\Psi_{III}}{dx}\bigg|_L$$

⇒ we get after calculations A, B, C, D, E [A is already known]

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

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

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

⇒ tunneling effect. 

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



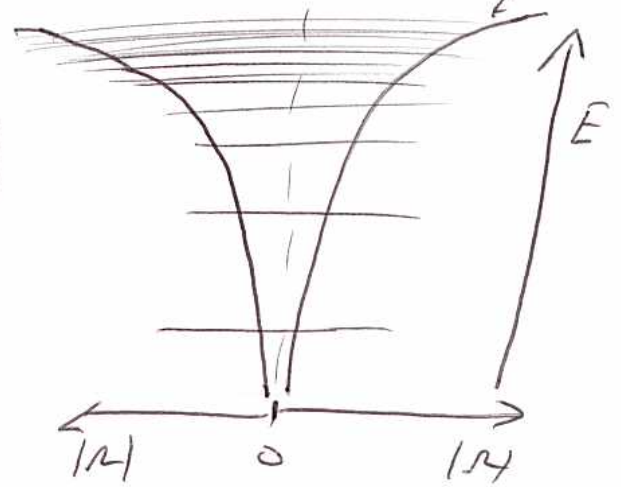
* Application: Schrodinger equation for Hydrogen atom.

Electrostatic potential between 1 proton and 1 electron

$$\Rightarrow V(\vec{r}) = \frac{q}{4\pi\epsilon_0|\vec{r}|}$$

potential "seen" by ke^- $U(\vec{r})$

potential energy $U(\vec{r}) = -qV(\vec{r})$



$$H = -\frac{\hbar^2}{2m} \Delta - \frac{q^2}{4\pi\epsilon_0|r|}$$

$H\psi = E\psi$ + closed boundary conditions [ψ vanishes as $r \rightarrow \infty$]

$$\Rightarrow H\psi_m = E_m\psi_m \Rightarrow \{E_m, \psi_m\}$$

\Rightarrow hydrogen spectrum, consistent with the Bohr model.

*

d) Crystal structure

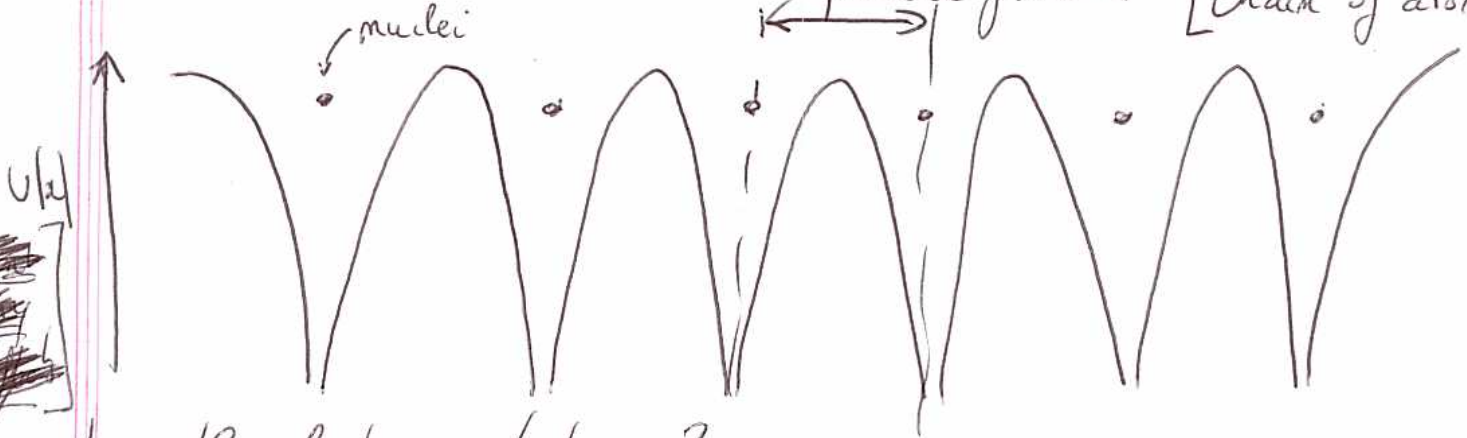
Solid materials are classified by the way the atoms are arranged within the solid; 3 types of materials =

- amorphous = atoms are placed at random, no order
- poly-crystalline = order by segment, no long range order.
- crystalline = atoms are placed in high ordered structure.

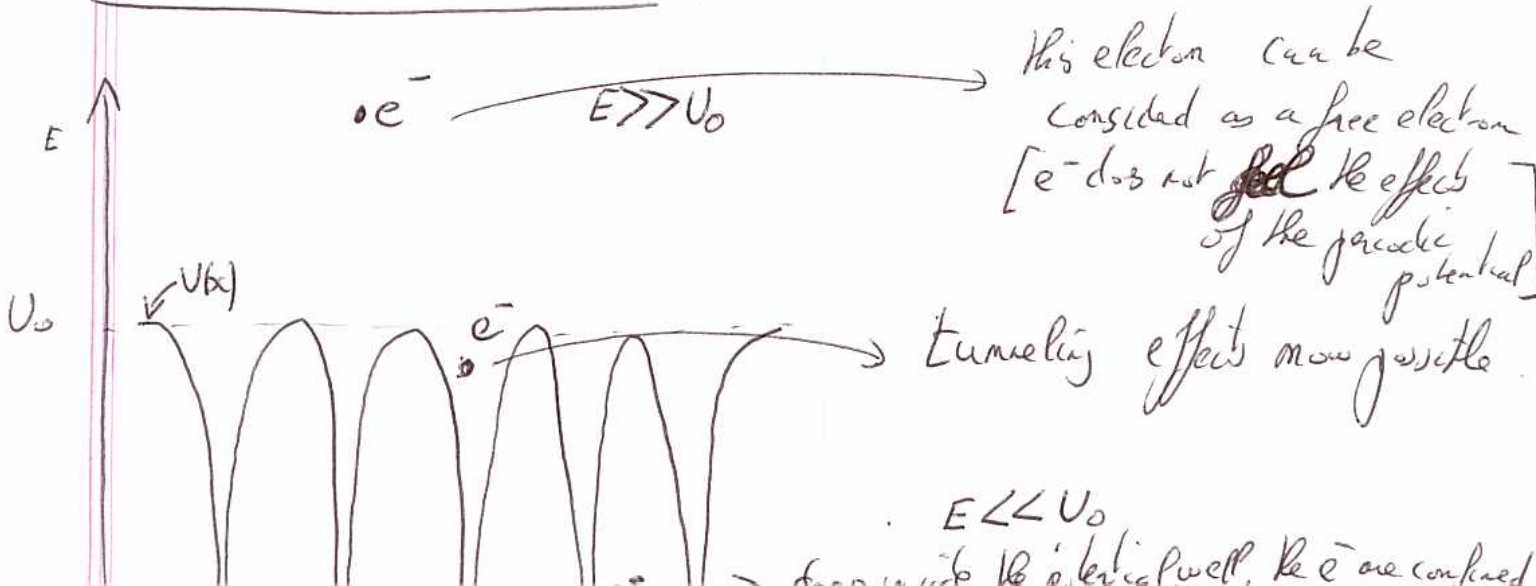
e Annex
A4 of
textbook.

[We will study crystalline semiconductors where a unit cell can be repeated periodically to form the solid.]

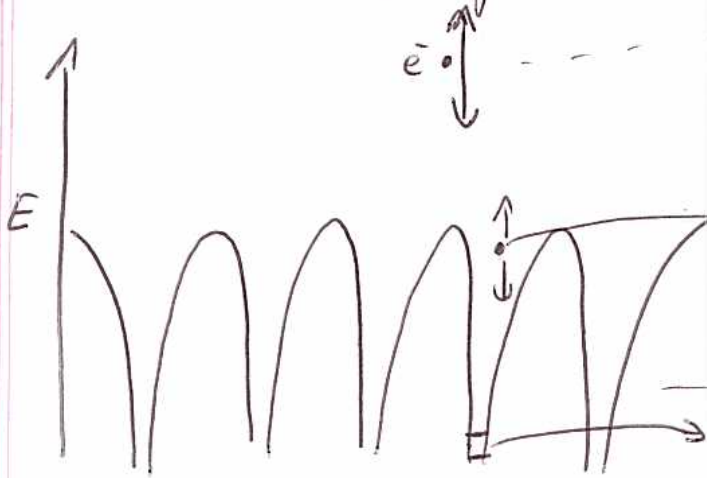
Simple example of potential in the crystal [N number of atoms] periodic potential. [chain of atoms]



how the electrons behave?



What is the energy spectrum ?



continuum, all the energy levels are available
[e⁻ of conduction]

? energy band theory needed to understand the spectrum
[e⁻ of conduction or valence]
discrete level of energy
[core e⁻]

Definition

valence electron = it is an e⁻ in an outer shell of an atom that can participate in forming chemical bonds with other atoms.

core electron = e⁻ occupying completely filled shells under the valence shell.

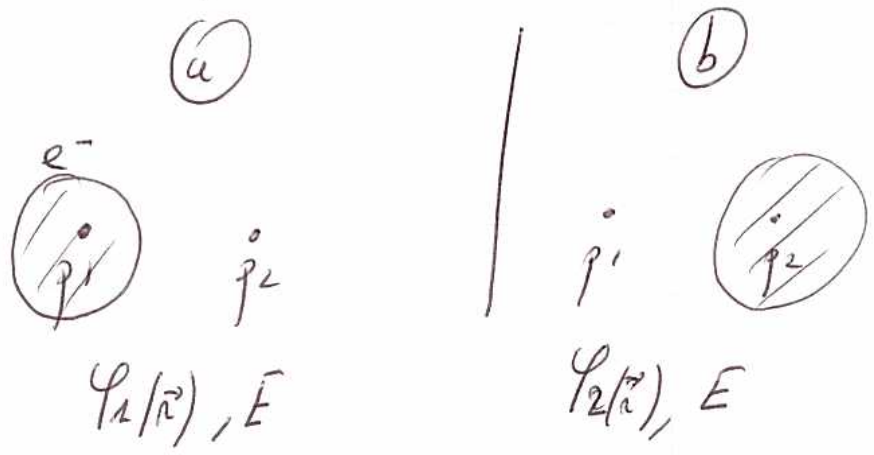
conduction electron = it is an e⁻ that is free, ~~and~~ known as a mobile charge carrier.

II Energy band theory

① Intuitive approach [look abo 1.1.2 in the textbook]

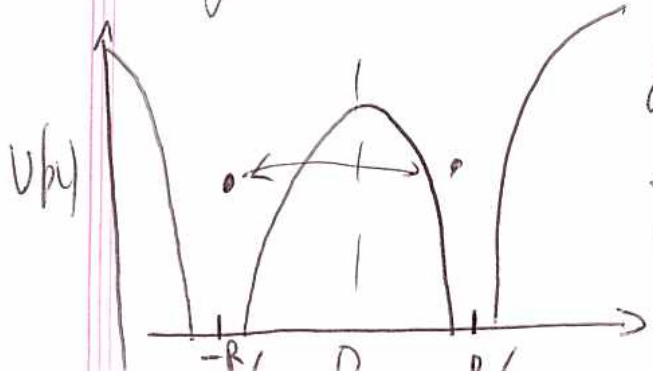
H_2^+ molecule $2p, 1e^-$

2 configurations (a) and (b)

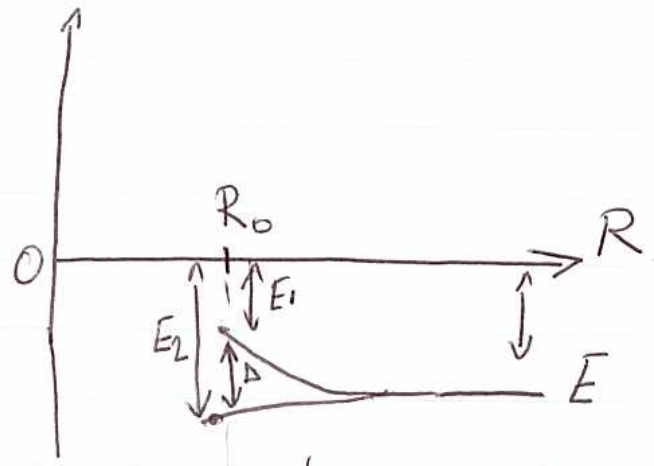


* if $d(p_1, p_2) \gg a_0$ $\Psi_1(\vec{r}), \Psi_2(\vec{r})$ are distinct states associated to one same energy E .
 \Rightarrow the energy level is degenerate.

* if $d(p_1, p_2) \approx a_0$, we bring them close together, the potential that can be seen by the e^- is given by



tunneling effect is now possible
 $\Rightarrow \Psi_1$ and Ψ_2 are coupled
 \Rightarrow lift the degeneracy
 \Rightarrow split the energy E into E_1, E_2

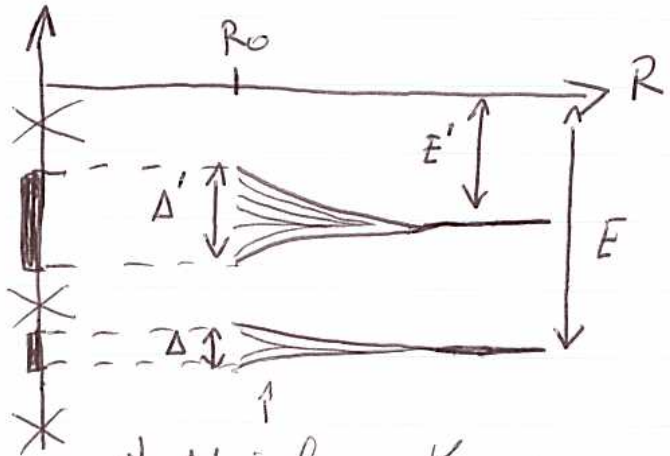


Δ depends on the strength of the coupling.

* generalization for N number of atoms, we have now N 'quantum wells'. [N is large]



Each energy level for a given atom gives rise to N different energy levels (lift the degeneracy)



Actually, it contains $2N$ energy levels due to the spin degeneracy.

* if N is large, the energy levels are so close that they form a continuum \Rightarrow band.

* It also appears some forbidden band of energy between the permitted energy band.

* $\Delta < \Delta'$, the energy bands with smaller energy are also thinner.



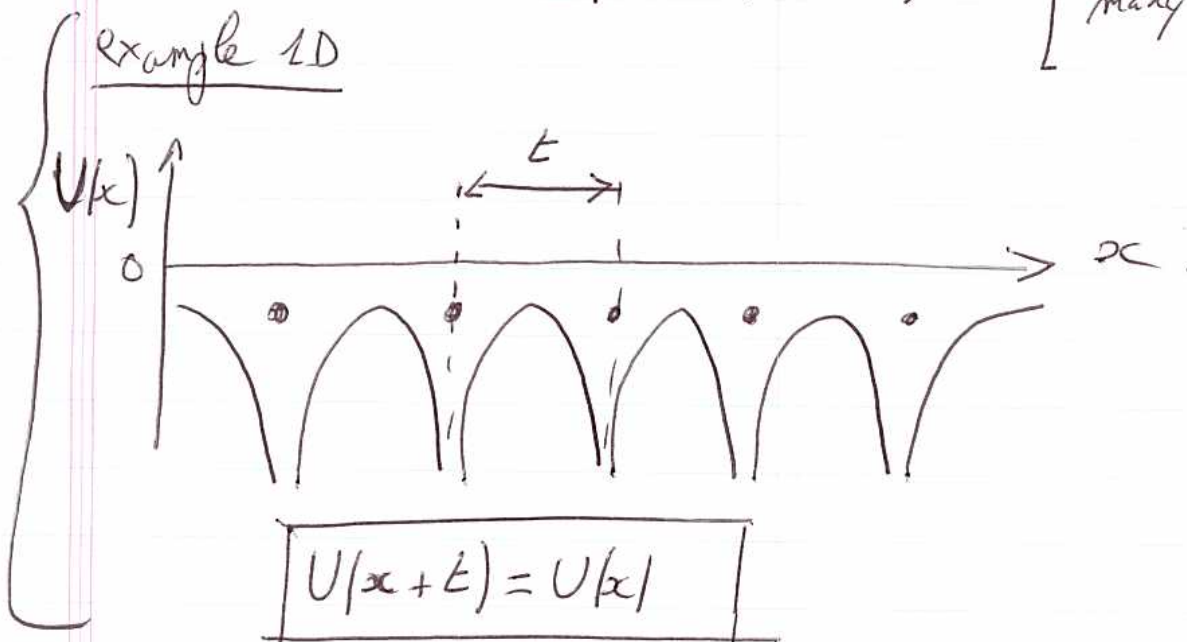
② Analytical approach

periodic nature of the position of the atoms in the crystal \Rightarrow

$$U(\vec{r} + \vec{T}) = U(\vec{r})$$

[$U(x)$ accounts for many body effects]

example 1D



Since the potential is periodic, we can define the boundary conditions for Ψ using the Bloch theorem.

such as $\Psi(x+t) = \Psi(x) e^{ik t}$

or (2nd form of the Bloch theorem)

$$\Psi(x) = u_{\mathbf{k}}(x) e^{i\mathbf{k}x}$$

$$u_{\mathbf{k}}(x+t) = u_{\mathbf{k}}(x)$$