



Solid State Electronics EC210

AAST – Cairo

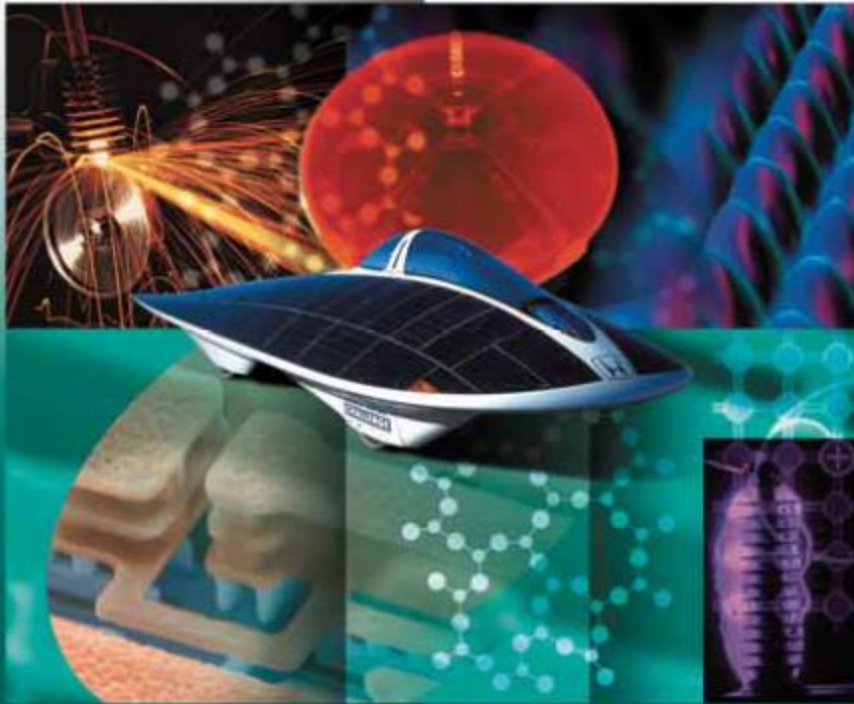
Fall 2016

## **Lec. 7:**

**Hydrogen Potential, Band Theory,  
Kronig-Penny Model, E-k Diagram**

# Principles of Electronic Materials and Devices

Third Edition



S. O. Kasap

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# Pages



P. 231-234: Hydrogen Atom

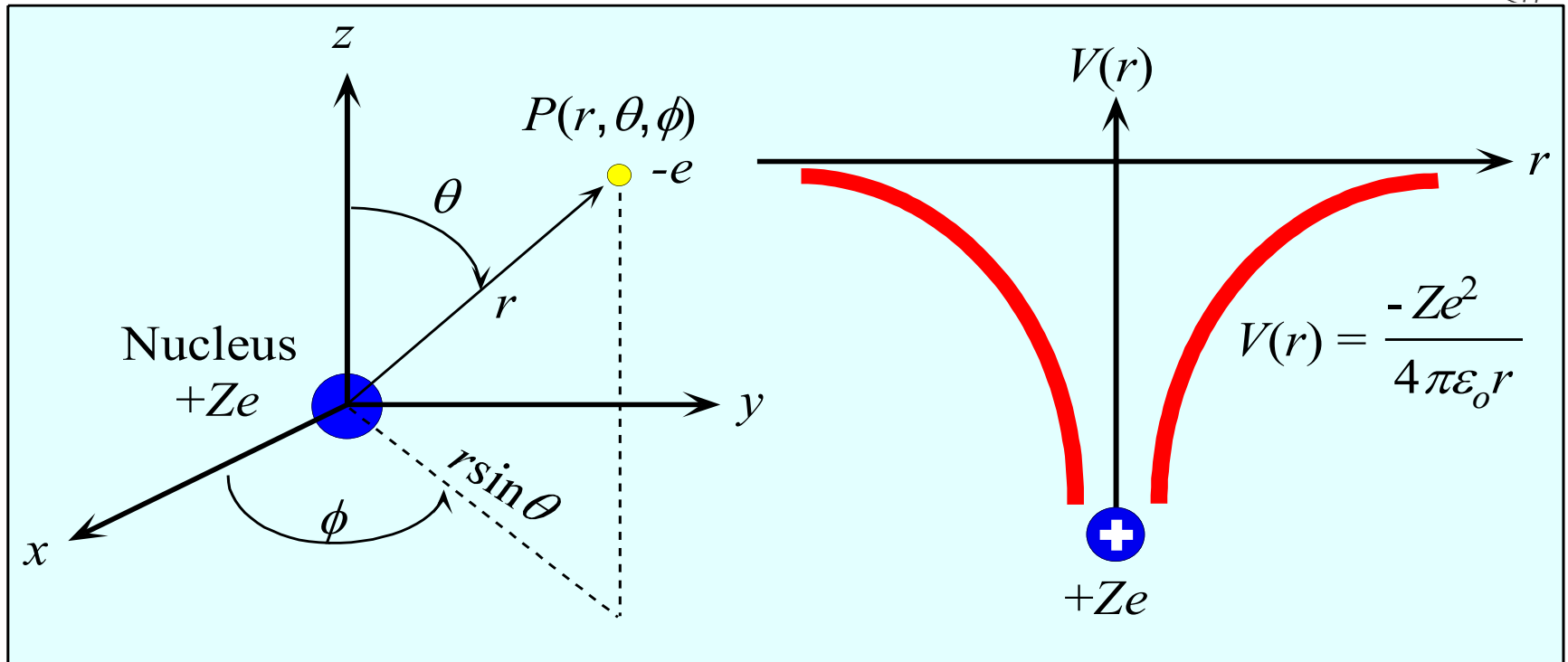
P. 285 – 287, p. 291-297, P.448 (Band Splitting)

# Outline



- Energy Levels in Hydrogen
- Overlap of Hydrogen Atom potential and wavefunction
- Pauli's Exclusion Principle
- Energy Level Splitting
- Band Theory using Hydrogen

# Hydrogen Potential Well



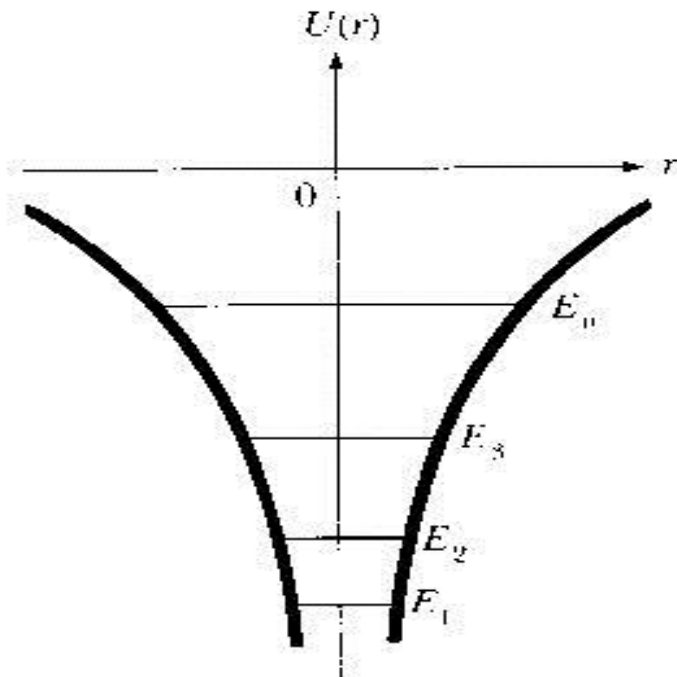
The electron in the hydrogenic atom is attracted by a central force that is always directed towards the positive nucleus. We therefore use spherical coordinates centered at the nucleus to describe the position of the electron. The  $PE$  of the electron depends on  $r$  only.



# Discrete Energy Levels

This is a “Potential Well” where Schrodinger equation has solution inside it (like in 1-D box) and outside it (like in barrier tunneling)

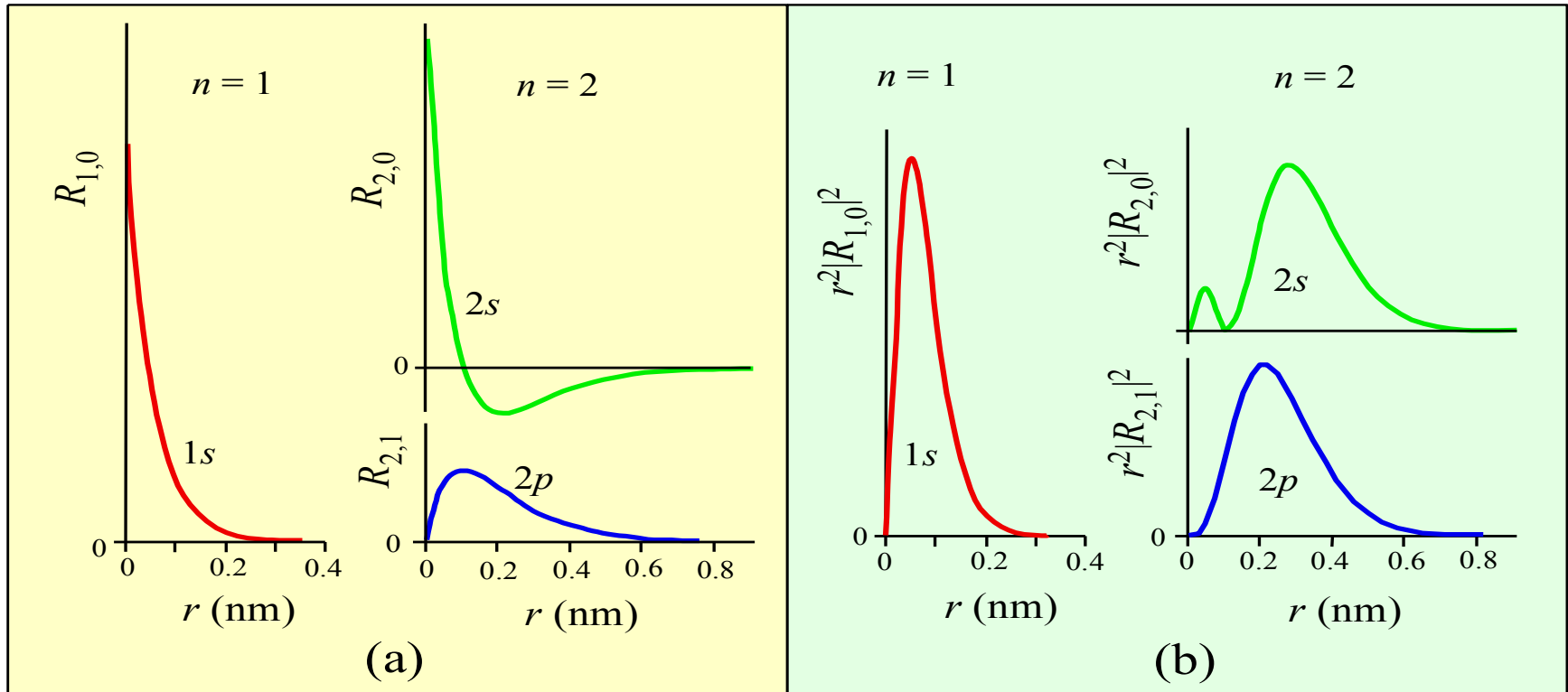
i.e. It has **discrete energy** levels and finite **wavefunctions**



$$U(r) = -\frac{Z}{4\pi\epsilon_0} \frac{e^2}{r}$$

# Hydrogen wavefunction

$$\Psi = R(r) Y(\Theta, \Phi)$$



(a) Radial wavefunctions of the electron in a hydrogenic atom for various  $n$  and  $l$  values. (b)  $r^2|R_{n,l}|^2$  gives the radial probability density. Vertical axis scales are linear in arbitrary units.

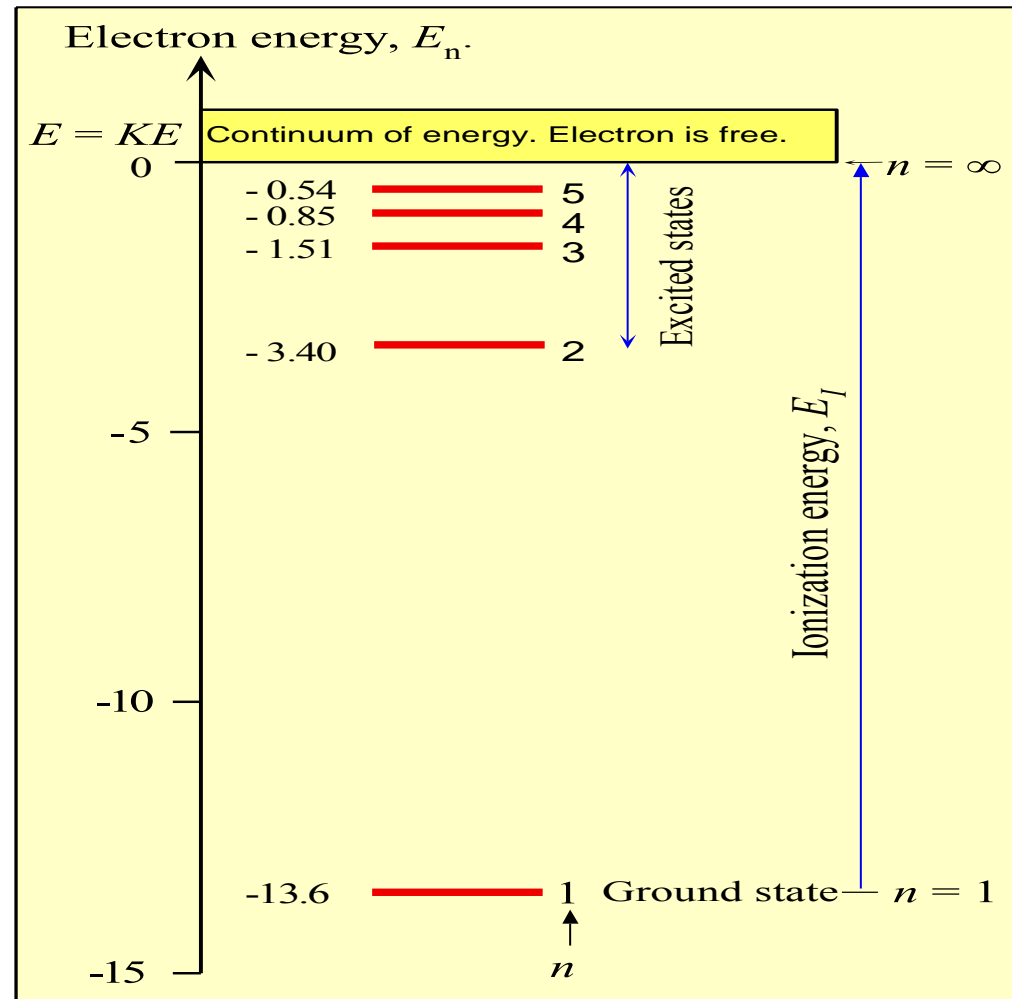
# Energy Levels for H-atom:

Depends on *Principal Quantum Number*



$$E_n = -\frac{Z E_1}{n^2}$$

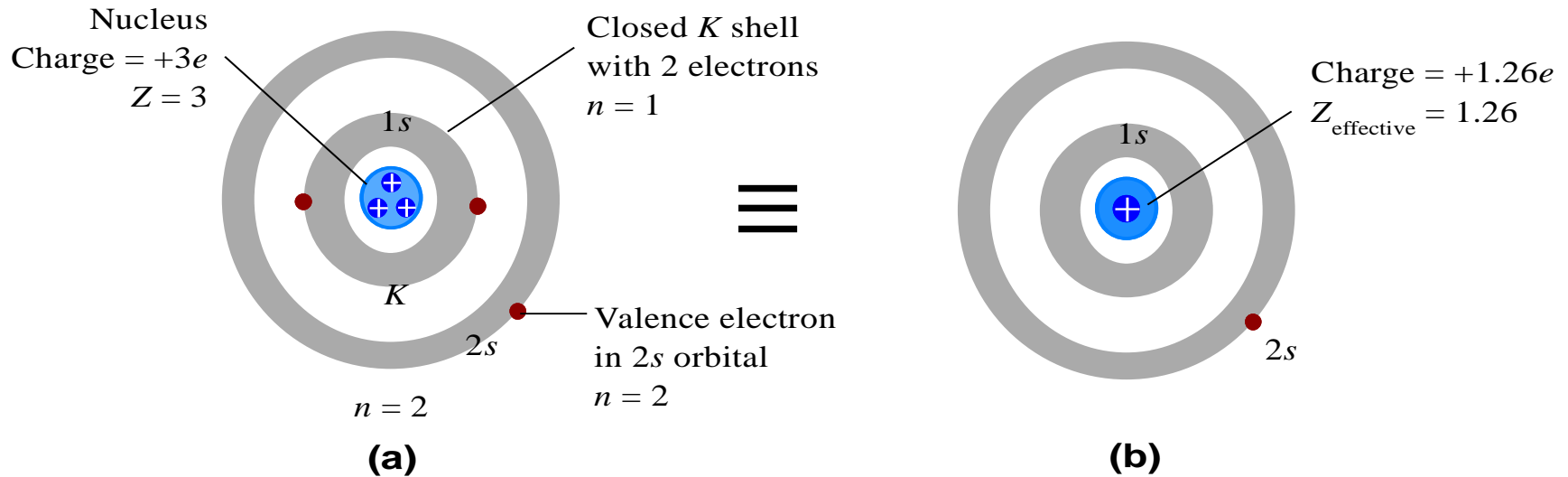
$$E_1 = \frac{me^4}{8\epsilon_0 h^2}$$



The energy of the electron in the hydrogen atom ( $Z = 1$ )



# $Z_{\text{Effective}}$ : (1.26 for Li)

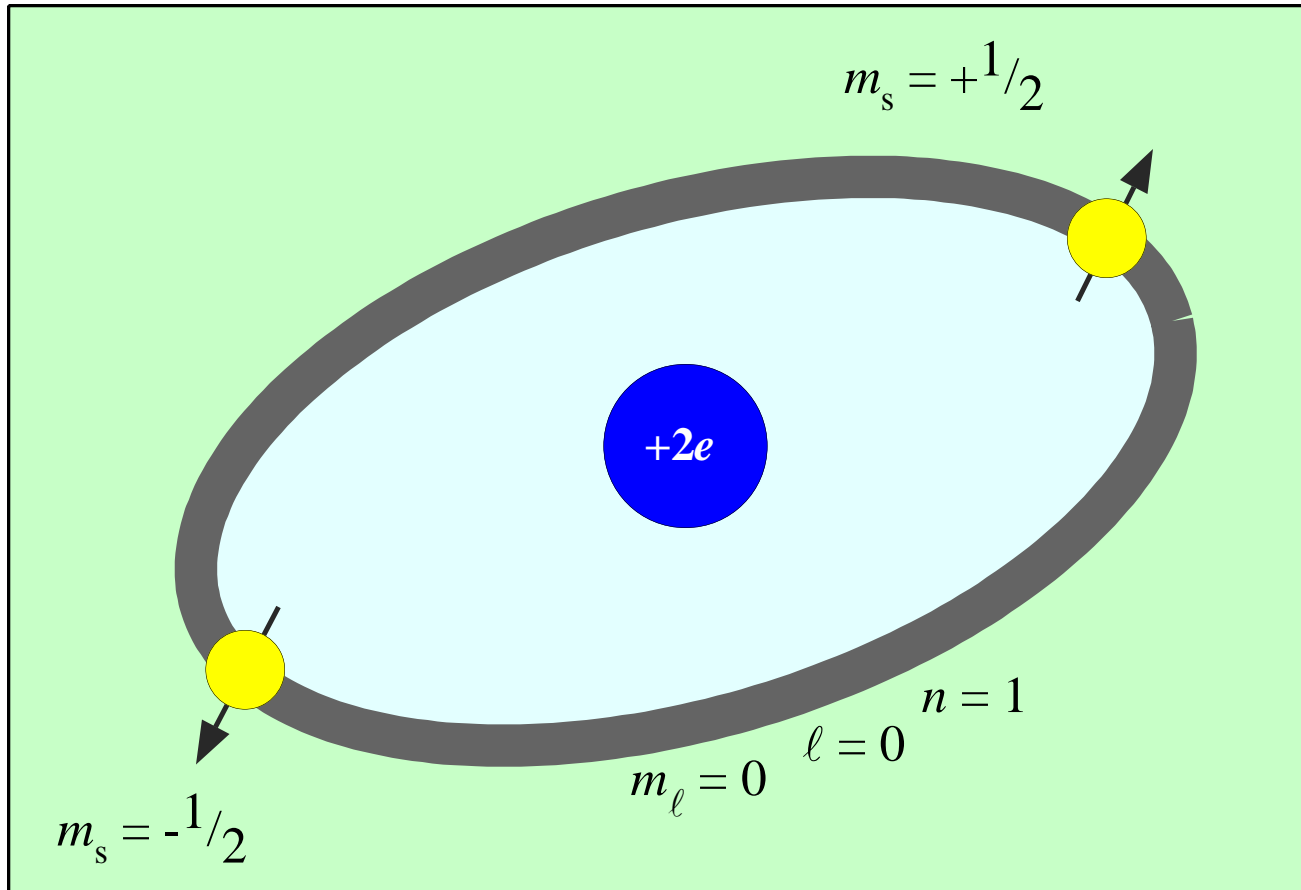


The Li atom has a nucleus with charge  $+3e$ , 2 electrons in the K shell, which is closed, and one electron in the 2s orbital.

(b) A simple view of (a) would be one electron in the 2s orbital that sees a single positive charge,  $Z=1$



# Paired Spins



Paired spins in an orbital.



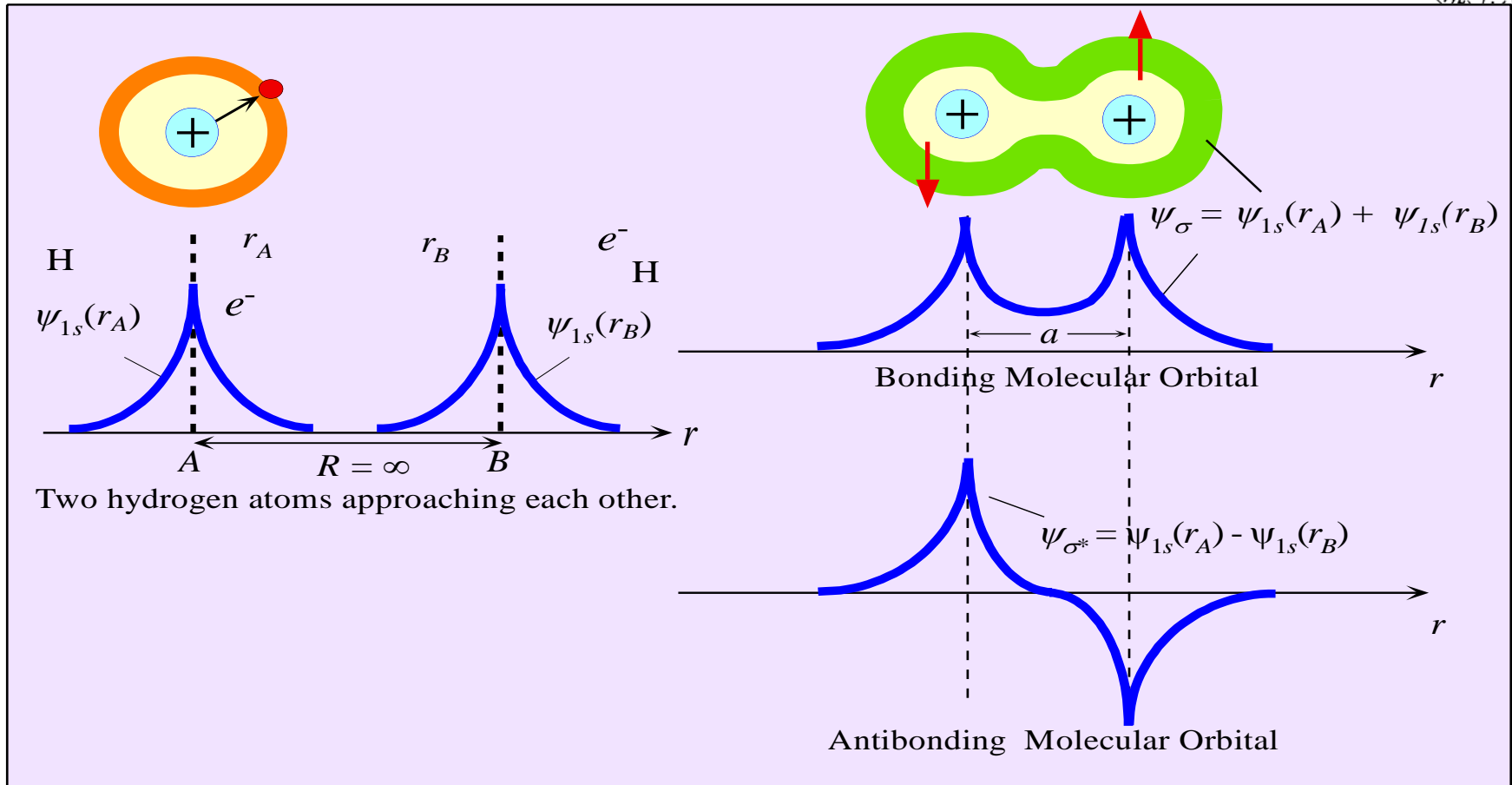
# Pauli's Exclusion Principle:

*No two electrons can have the same four quantum numbers within the same system*

**Table 3.3** The four quantum numbers for the hydrogenic atom

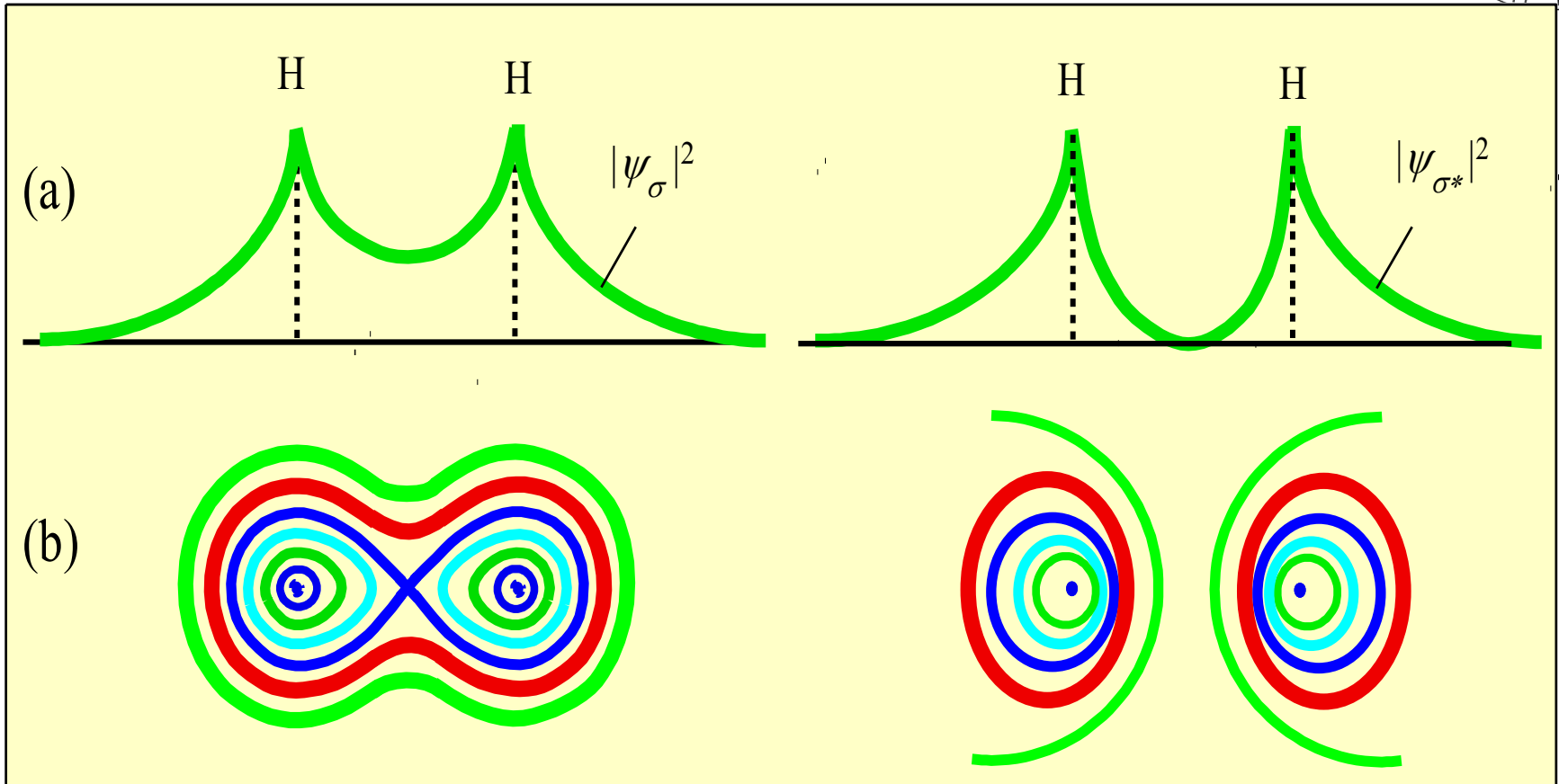
|          |   |   |   |
|----------|---|---|---|
| $n$      | Principal quantum number                | $n = 1, 2, 3, \dots$                        | Quantizes the electron energy   |
| $\ell$   | Orbital angular momentum quantum number | $\ell = 0, 1, 2, \dots (n - 1)$             | Quantizes the magnitude of orbital angular momentum $L$                       |
| $m_\ell$ | Magnetic quantum number                 | $m_\ell = 0, \pm 1, \pm 2, \dots, \pm \ell$ | Quantizes the orbital angular momentum component along a magnetic field $B_z$ |
| $m_s$    | Spin magnetic quantum number            | $m_s = \pm \frac{1}{2}$                     | Quantizes the spin angular momentum component along a magnetic field $B_z$    |

# Wavefunction Interaction: Two H Atoms



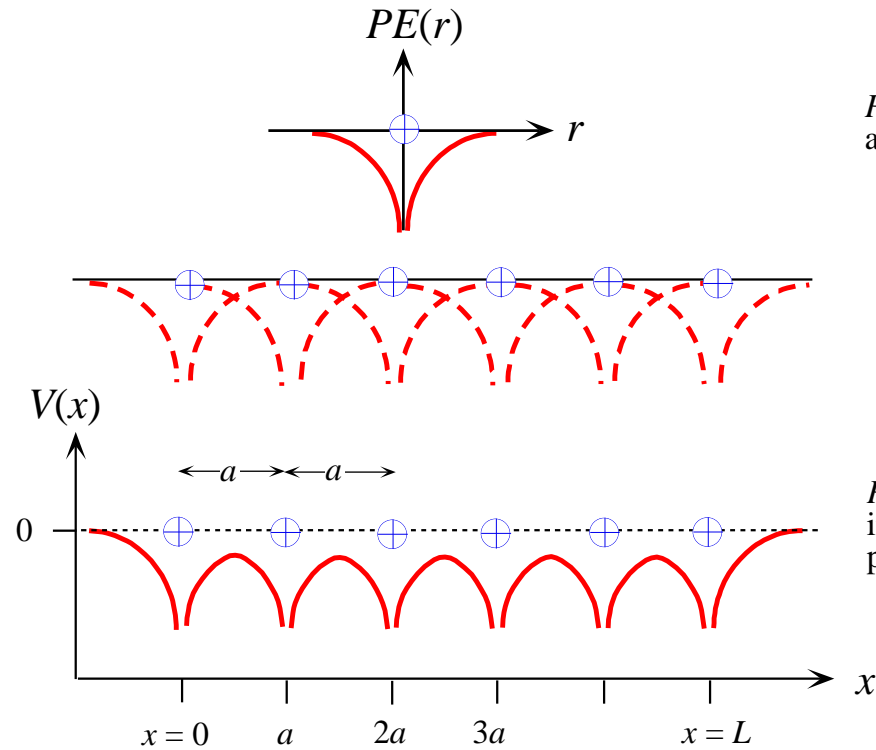
Formation of molecular orbitals, bonding and antibonding ( $\psi_{\sigma}$  and  $\psi_{\sigma^*}$ ) when two H atoms approach each other. The two electrons pair their spins and occupy the bonding orbital  $\psi_{\sigma}$ .

# Wavefunction Interactions: two H Atoms



(a) Electron probability distributions for bonding and antibonding orbitals,  $\psi_\sigma$  and  $\psi_{\sigma^*}$ . (b) Lines represent contours of constant probability.

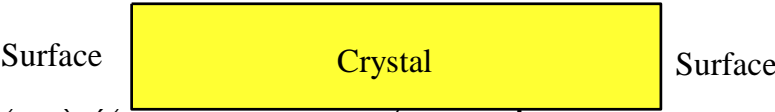
# Superposition of Coulomb Potential for N-Atoms



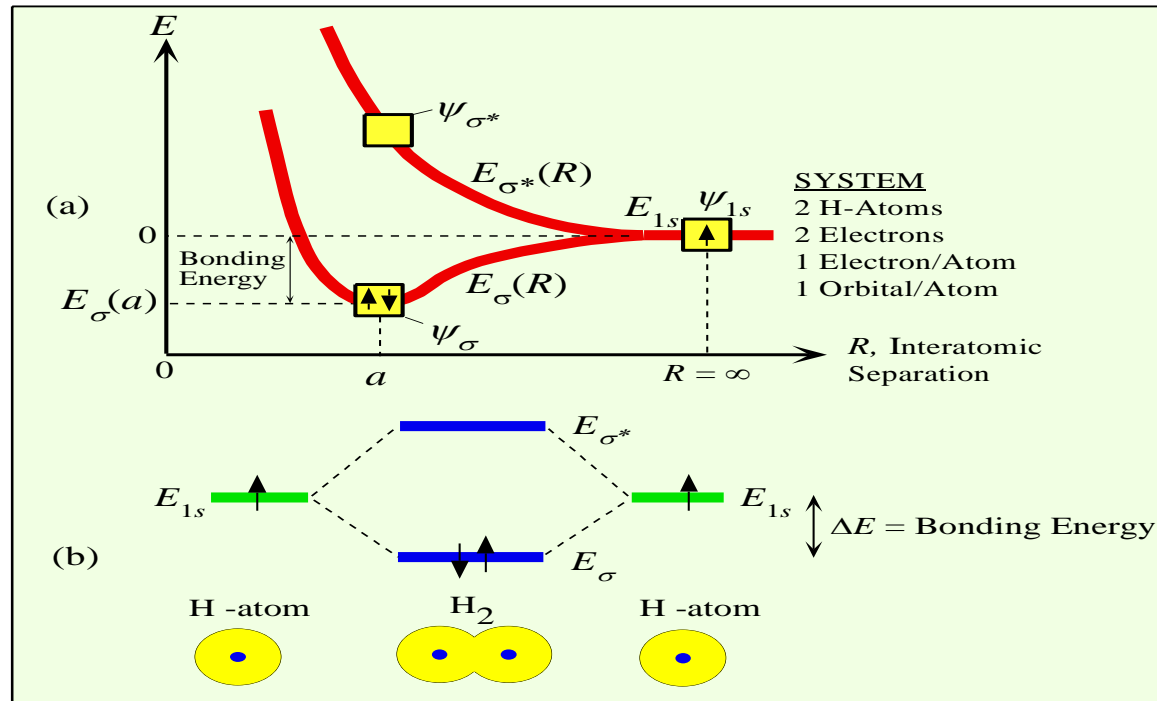
$PE$  of the electron around an isolated atom

When  $N$  atoms are arranged to form the crystal then there is an overlap of individual electron  $PE$  functions.

$PE$  of the electron,  $V(x)$ , inside the crystal is periodic with a period  $a$ .

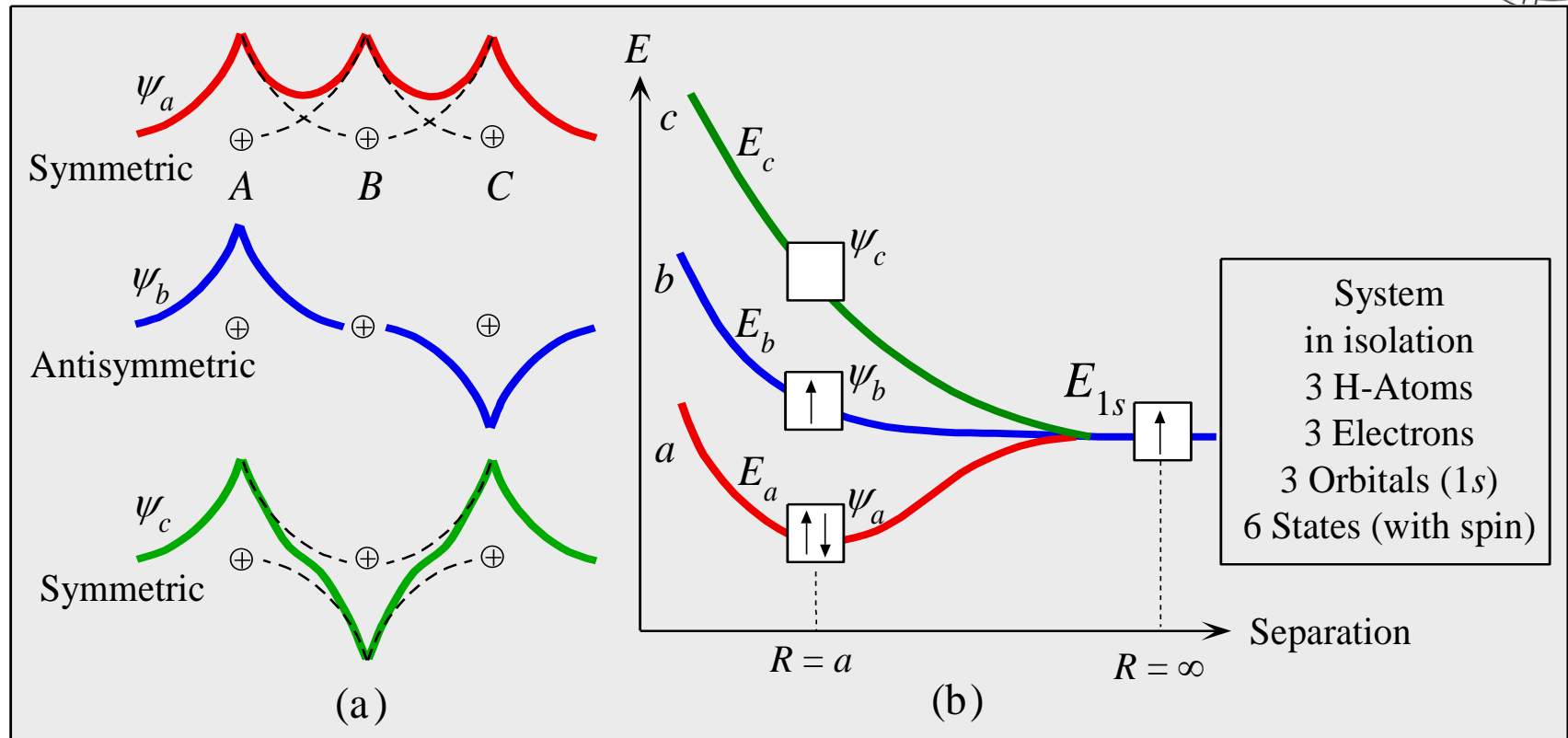
The electron  $P$   periodicity as that of the crystal,  $a$ . Far away outside the crystal, by choice,  $V = 0$  (the electron is free and  $PE = 0$ ).

# Band Splitting



Electron energy in the system comprising two hydrogen atoms. (a) Energy of  $\psi_{\sigma}$  and  $\psi_{\sigma^*}$  vs. the interatomic separation,  $R$ . (b) Schematic diagram showing the changes in the electron energy as two isolated H atoms, far left and far right, come to form a hydrogen molecule.

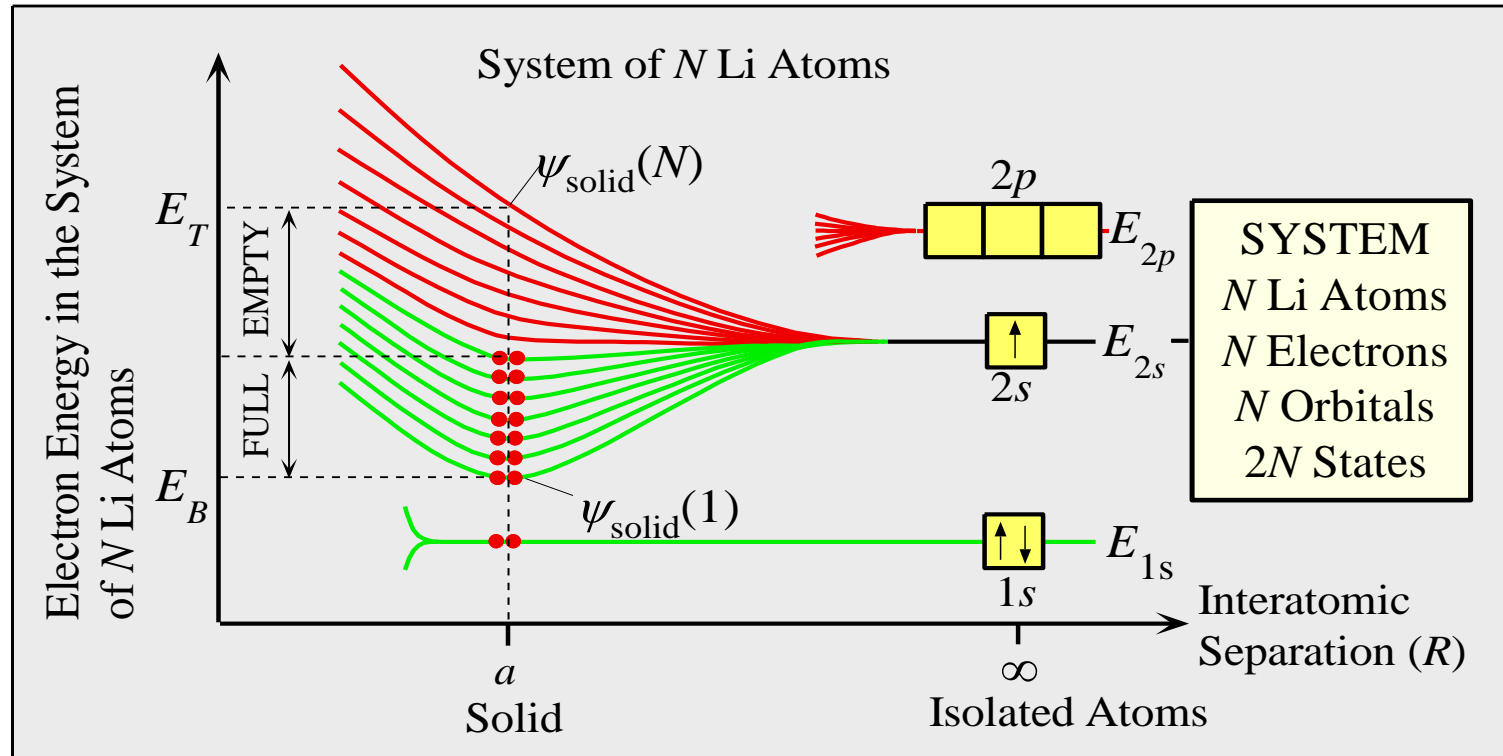
# Three H-Atoms: $\Psi$ Overlap, Band Splitting



(a) Three molecular orbitals from three  $\psi_{1s}$  atomic orbitals overlapping in three different ways. (b) The energies of the three molecular orbitals labeled as  $a$ ,  $b$  and  $c$  in a system with 3 H atoms (highly simplified).

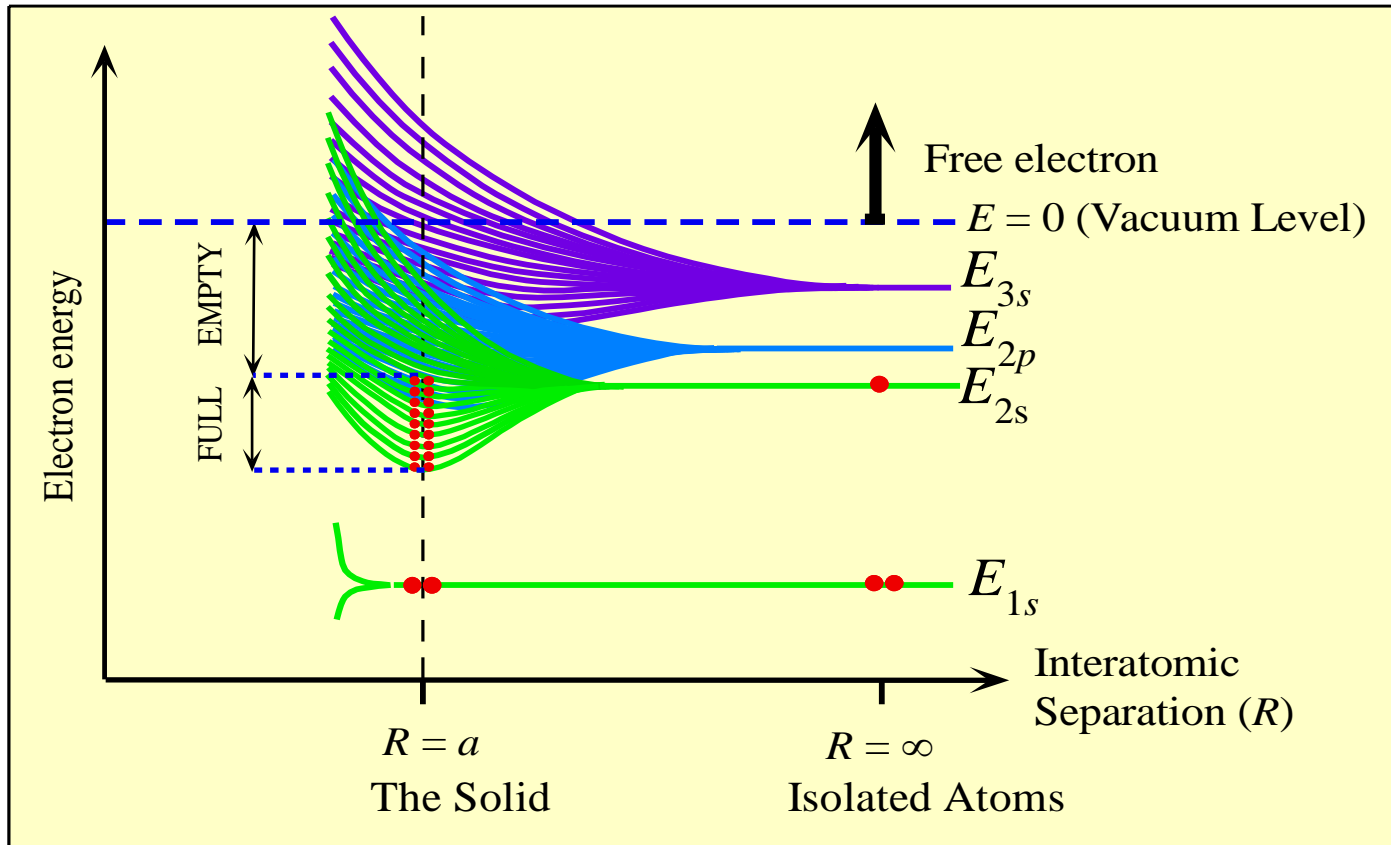


# Band Theory: "N" H-atoms

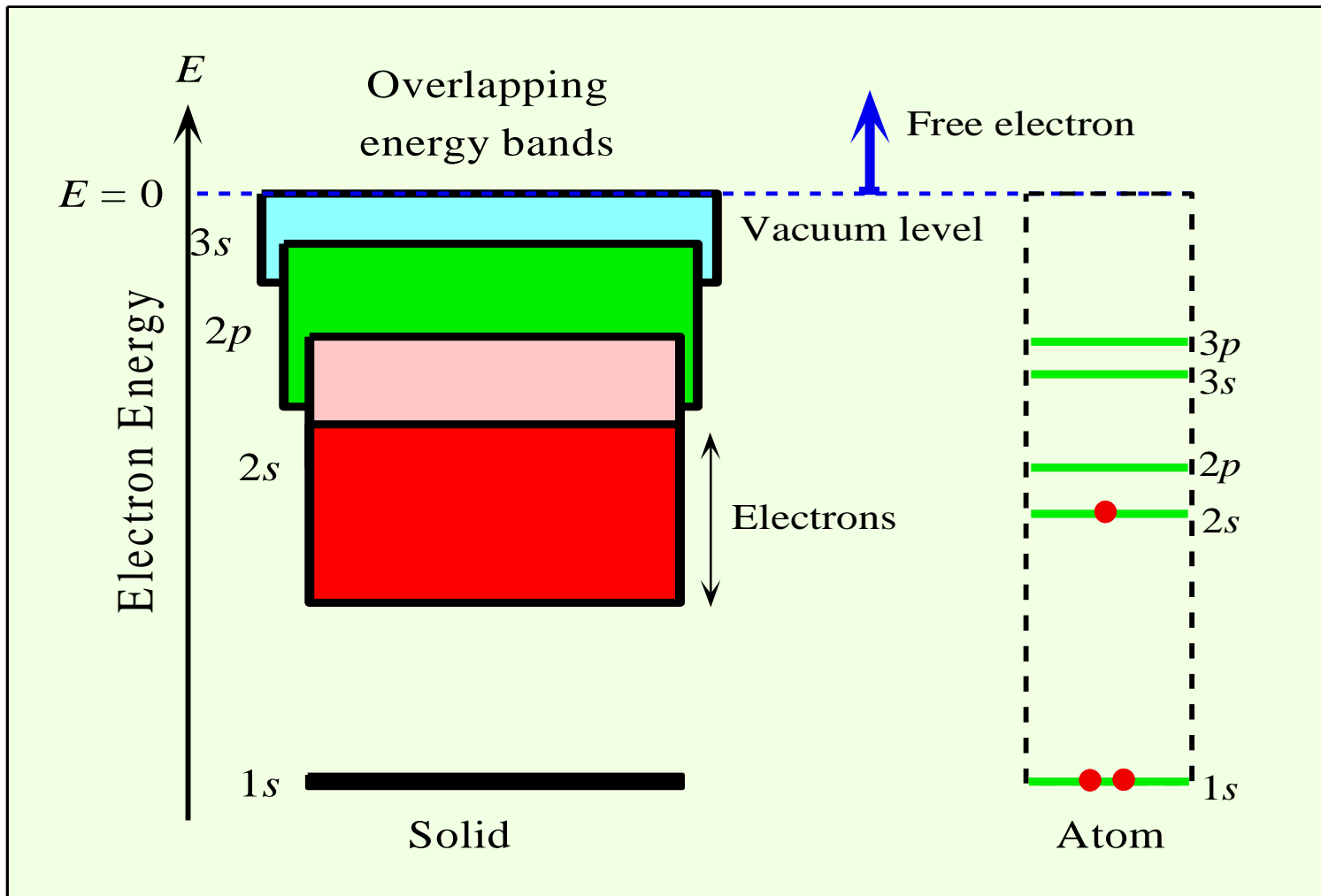


The formation of a  $2s$ -energy band from the  $2s$ -orbitals when  $N$  Li atoms come together to form the Li solid. There are  $N$   $2s$ -electrons but  $2N$  states in the band. The  $2s$ -band therefore is only half full. The atomic  $1s$  orbital is close to the Li nucleus and remains undisturbed in the solid. Thus each Li atom has a closed  $K$ -shell (full  $1s$  orbital).

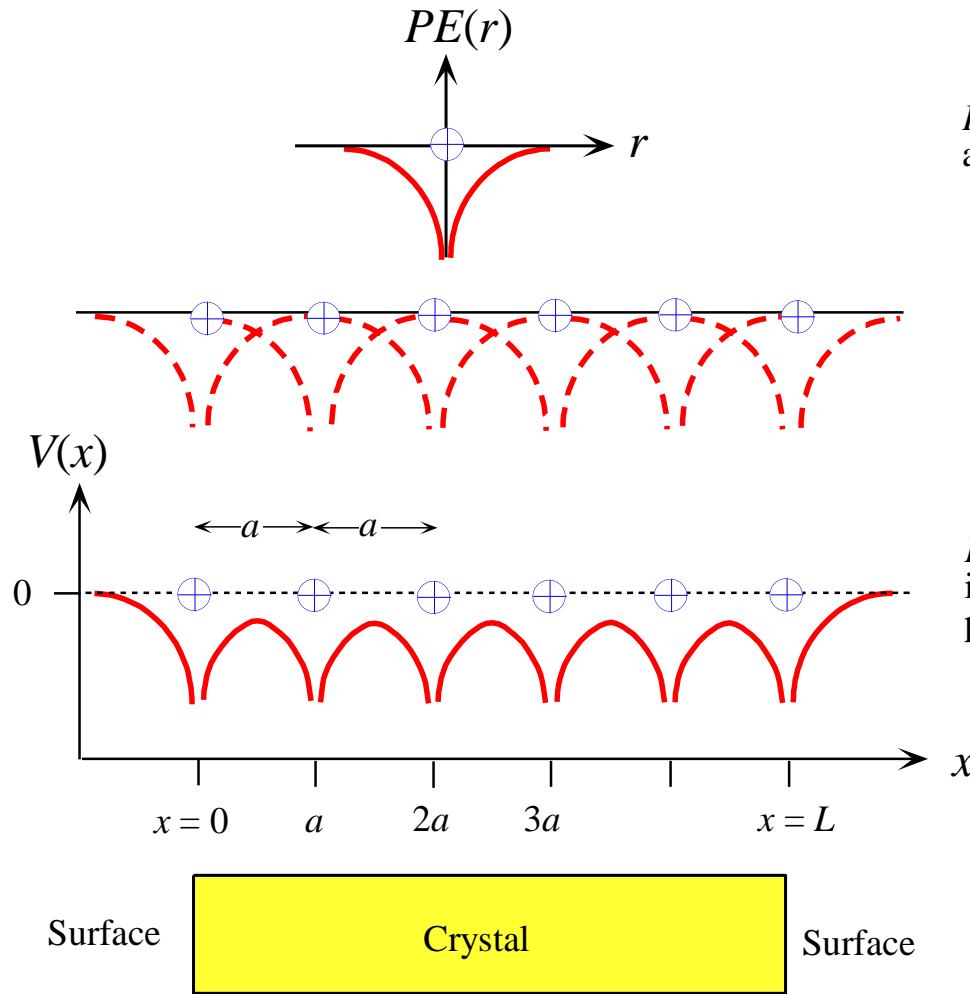
# Band Theory: Bands Overlap



As solid atoms are brought together from infinity, the atomic orbitals overlap and give rise to bands. Outer orbitals overlap first. The  $3s$  orbitals give rise to the  $3s$  band,  $2p$  orbitals to the  $2p$  band and so on. The various bands overlap to produce a single band in which the energy is nearly continuous.



In a metal the various energy bands overlap to give a single band of energies that is only partially full of electrons. There are states with energies up to the vacuum level where the electron is free.



$PE$  of the electron around an isolated atom

When  $N$  atoms are arranged to form the crystal then there is an overlap of individual electron  $PE$  functions.

$PE$  of the electron,  $V(x)$ , inside the crystal is periodic with a period  $a$ .

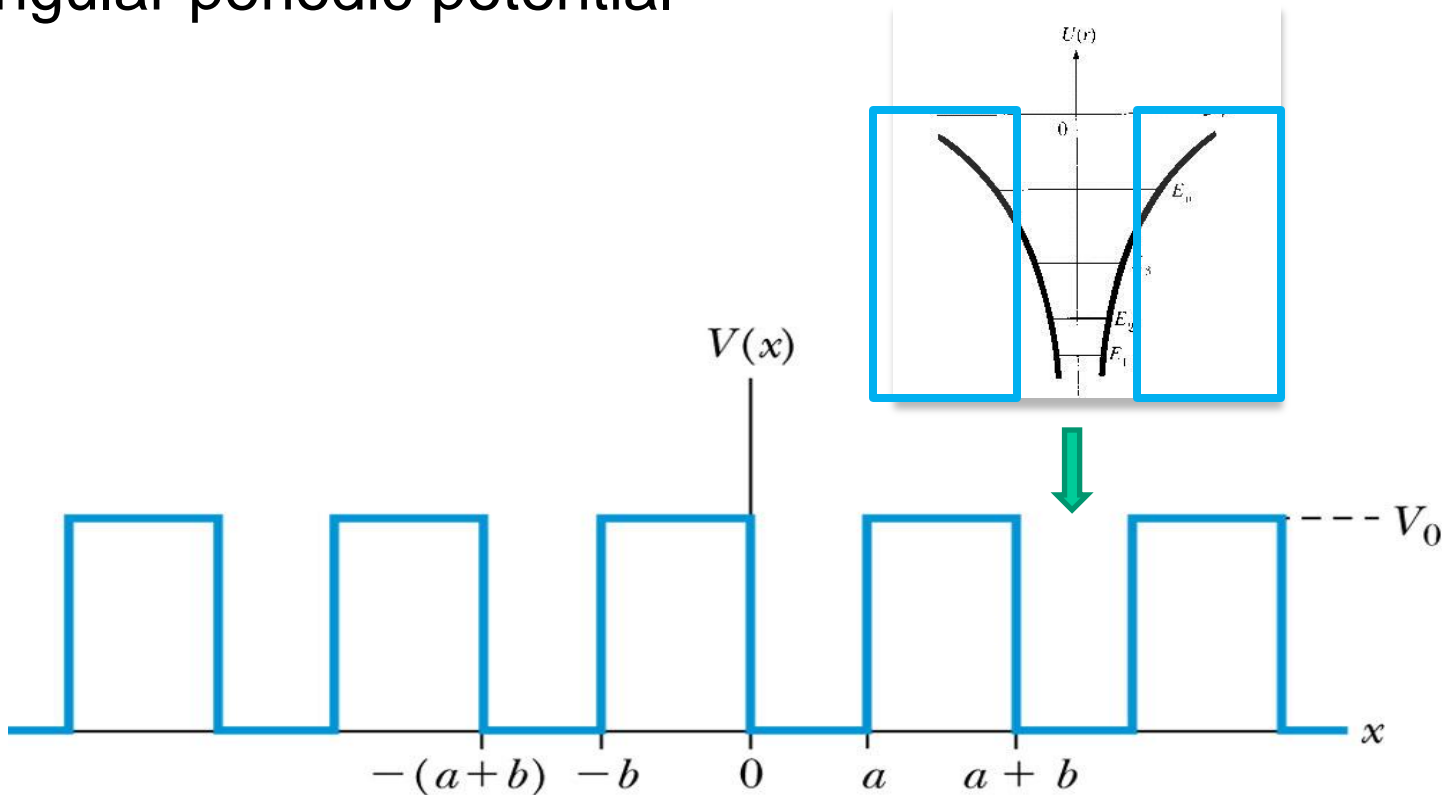
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The electron  $PE$ ,  $V(x)$ , inside the crystal is periodic with the same periodicity as that of the crystal,  $a$ . Far away outside the crystal, by choice,  $V = 0$  (the electron is free and  $PE = 0$ ).



# Kronig-Penney Model

Approximate crystal periodic Coulomb potential by rectangular periodic potential



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# Kronig-Penney Solution: Allowed Energies



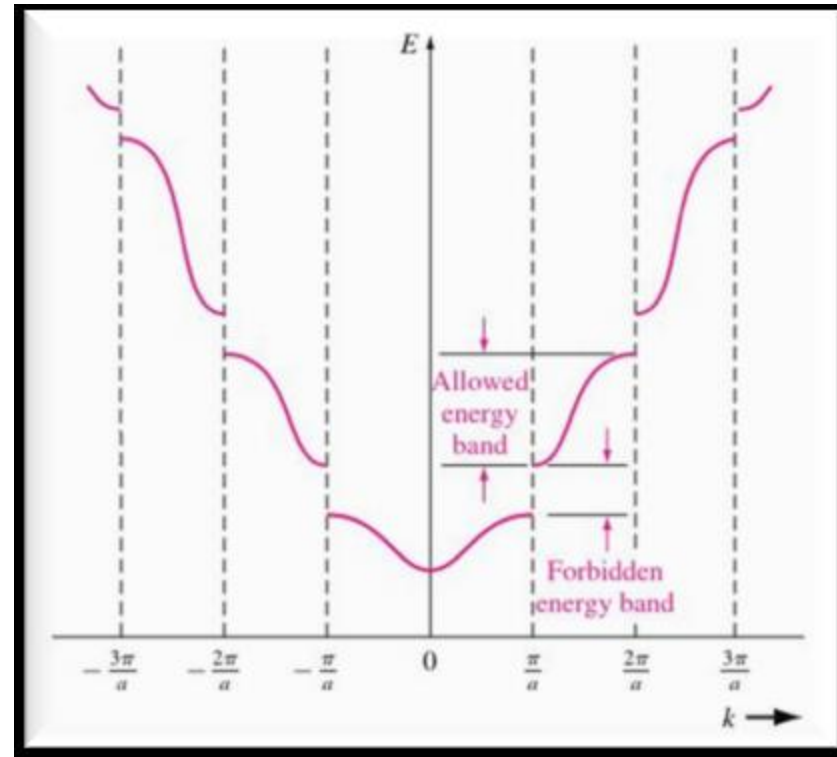
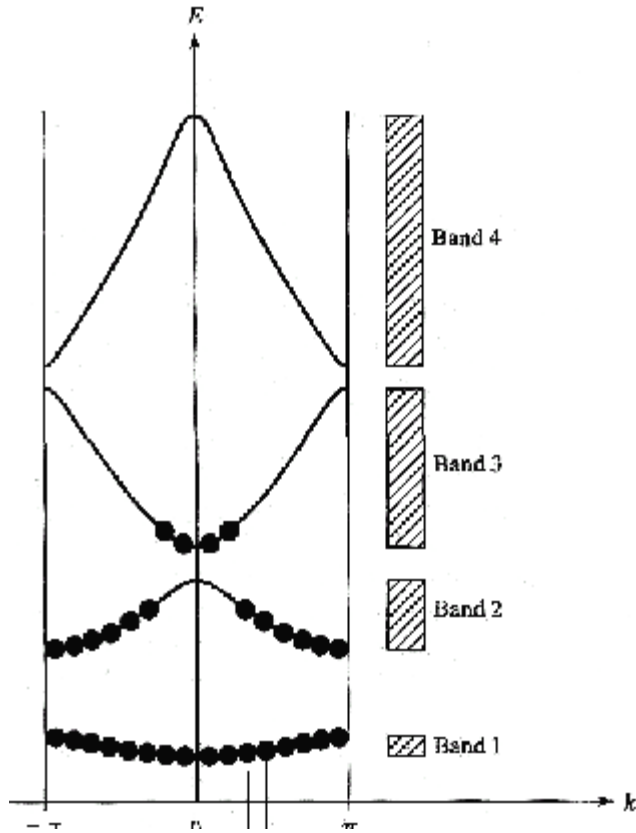
The wavefunctions have solutions only in some allowed “continuous” ranges “or “**Bands**” of  $k$ :

$$\rightarrow E = \frac{k^2 \hbar^2}{2m} \text{ is } \mathbf{allowed}$$

The solution is NOT allowed in other ranges of  $k$ :

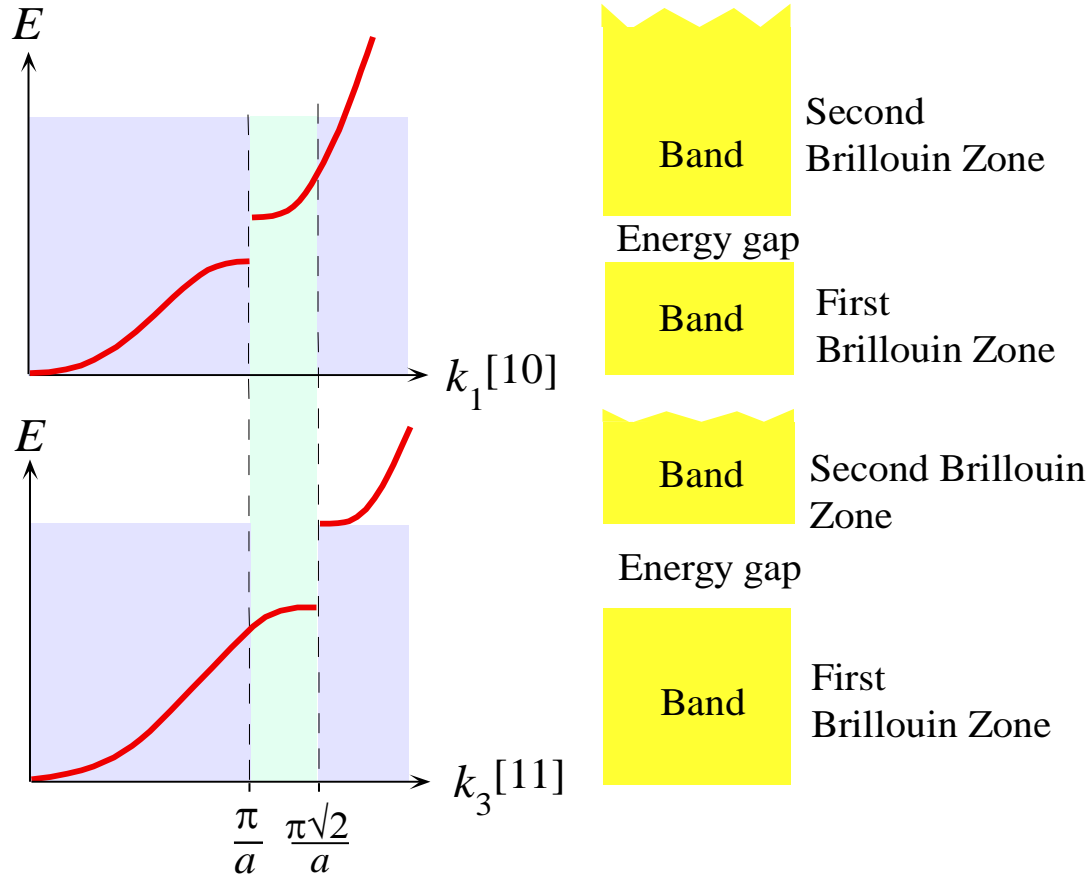
→ Energies corresponding to these  $k$  are “Forbidden”. i.e. form “**Energy Gaps**” in the electron energy range

# Kronig-Penney Model





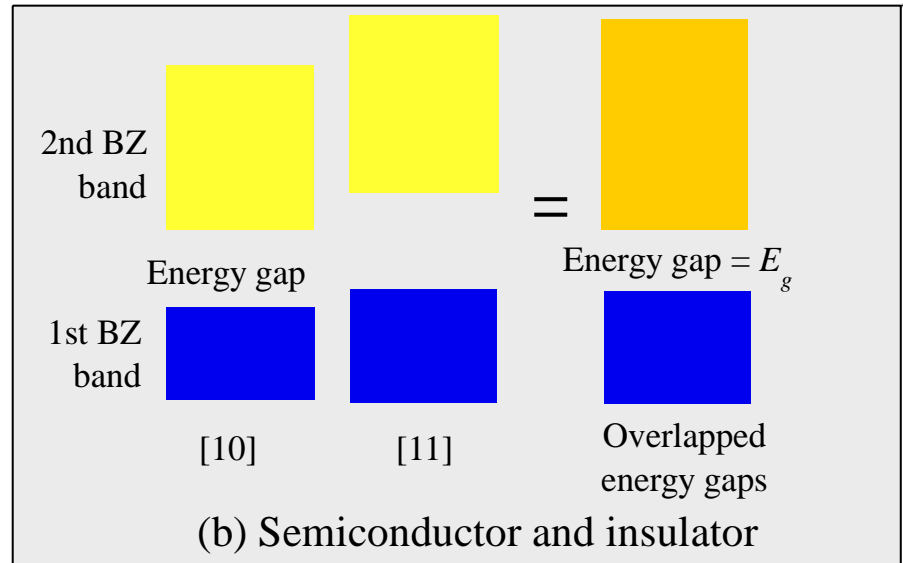
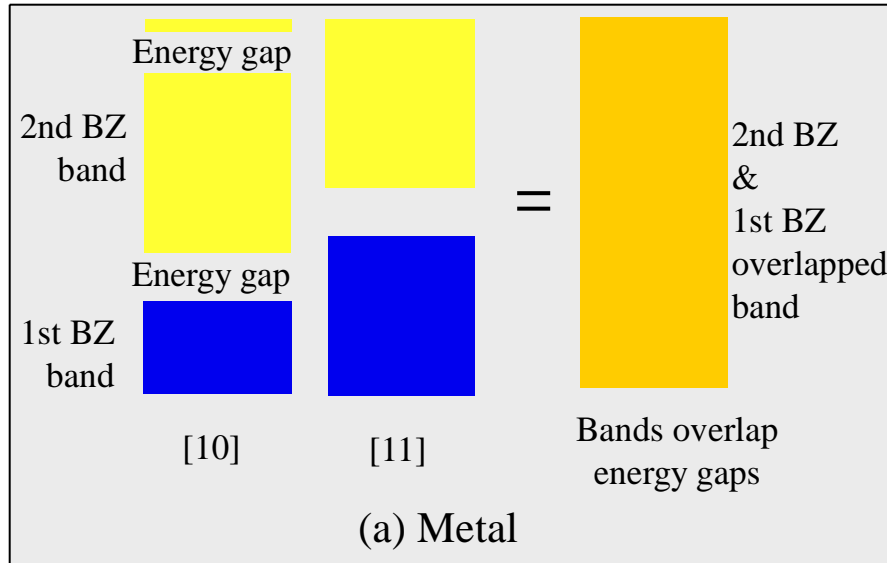
# Energy Gap (Bandgaps, $E_g$ )



The  $E$ - $k$  behavior for the electron along different directions in the two dimensional crystal. The energy gap along  $[10]$  is at  $\pi/a$  whereas it is at  $\pi\sqrt{2}/a$  along  $[11]$ .



# Energy Gaps ( $E_g$ )

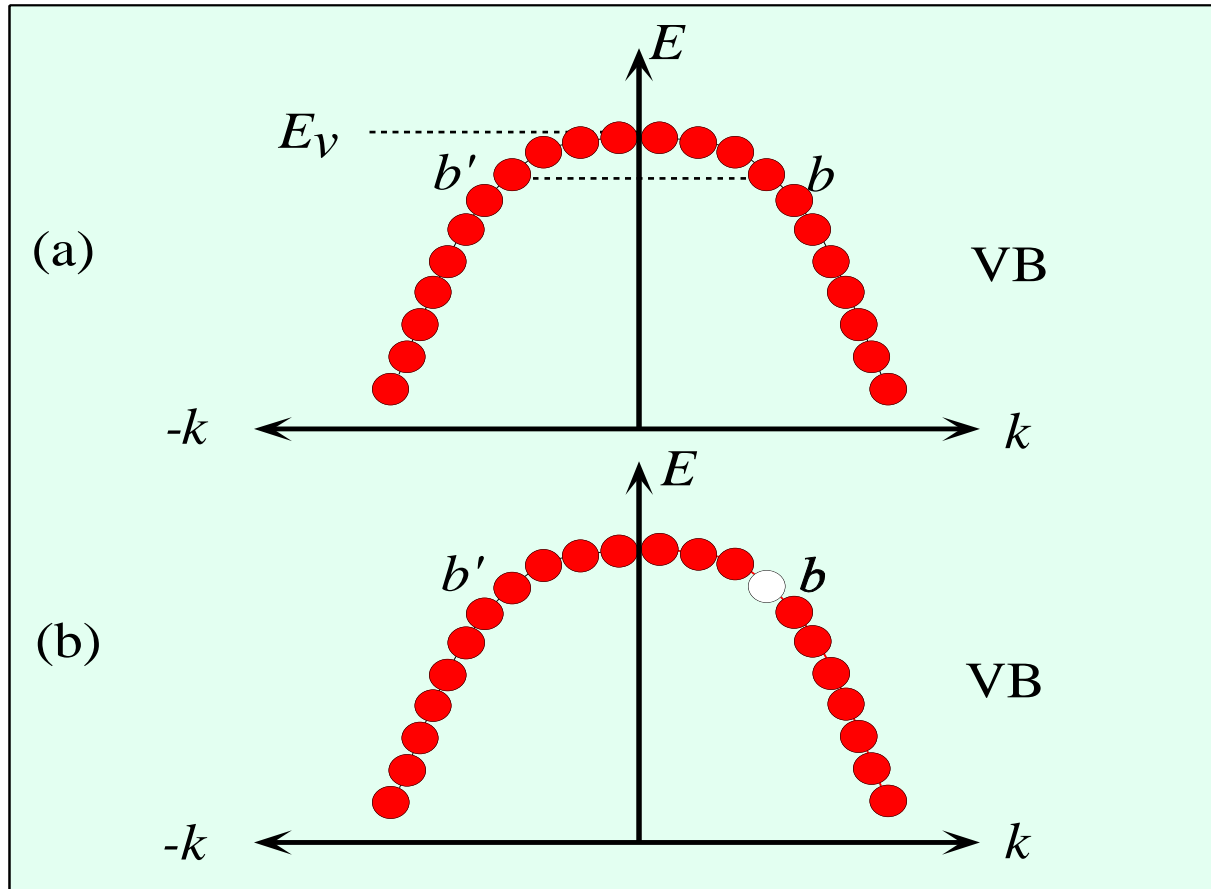


(a) Metal: For the electron in a metal there is no apparent energy gap because the 2nd BZ (Brillouin Zone) along [10] overlaps the 1st BZ along [11]. Bands overlap the energy gaps. Thus the electron can always find any energy by changing its direction.

(b) Semiconductor or insulator: For the electron in a semiconductor there is an energy gap arising from the overlap of the energy gaps along [10] and [11] directions. The electron can never have an energy within this energy gap,  $E_g$ .

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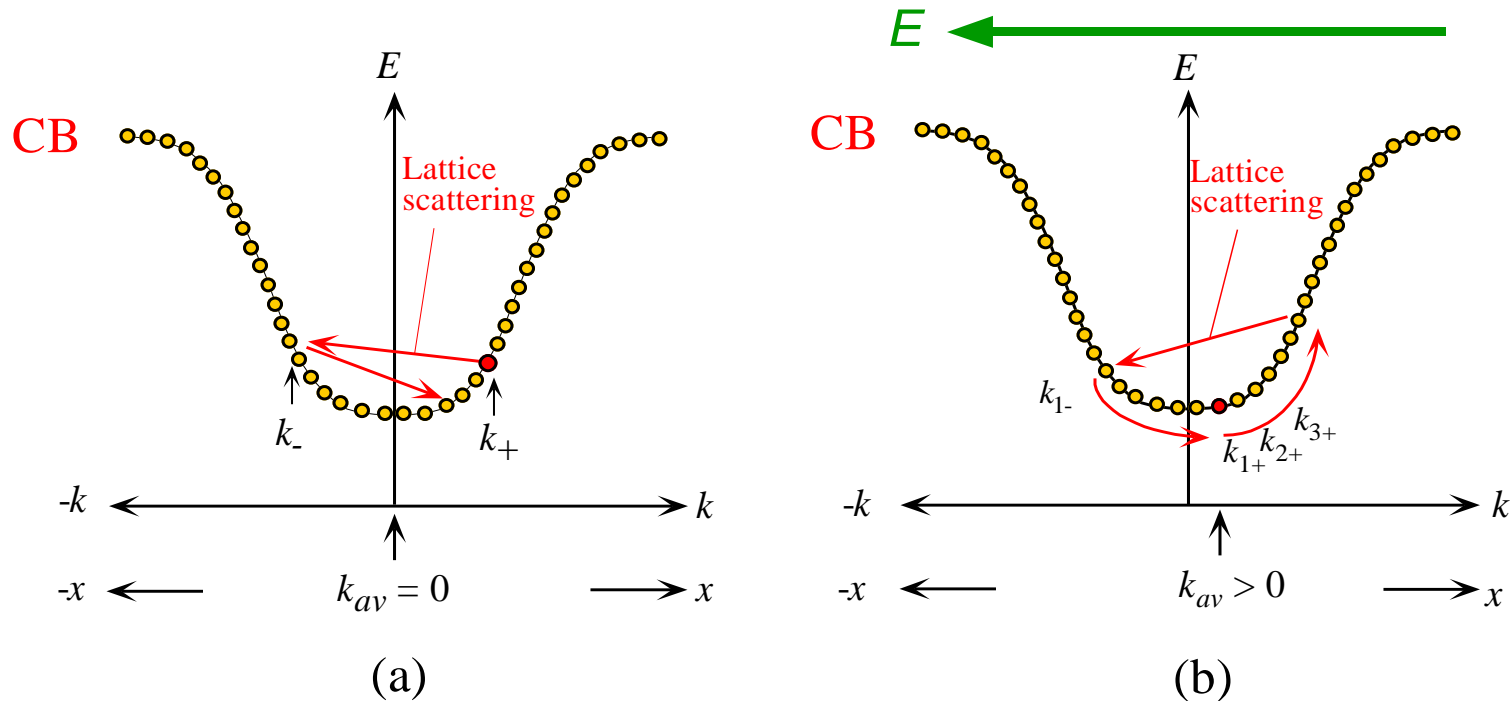
# E-k Diagram for Holes in Valence Band



(a) In a full valence band there is no net contribution to the current. There are equal numbers of electrons (e.g. at  $b$  and  $b'$ ) with opposite momenta. (b) If there is an empty state (*hole*) at  $b$  at the top of the band then the electron at  $b'$  contributes to the current.

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# E-k Diagram for Electrons in Conduction Band



(a) In the absence of a field, over a long time, average of all  $k$  values is zero, there is no net momentum in any one particular direction. (b) In the presence of a field  $E$  in the  $-x$  direction, the electron accelerates in the  $+x$  direction increasing its  $k$  value along  $x$  until it is scattered to a random  $k$  value. Over a long time, average of all  $k$  values is along the  $+x$  direction. Thus the electron drifts along  $+x$ .



# E-k Diagram: Effective Mass

Reminder: Using E-K diagram:

$$m^* = \left[ \frac{1}{\hbar^2} \frac{d^2E}{dk^2} \right]^{-1} = \hbar^2 \left[ \frac{d^2E}{dk^2} \right]^{-1}$$