



Solid State Electronics EC210

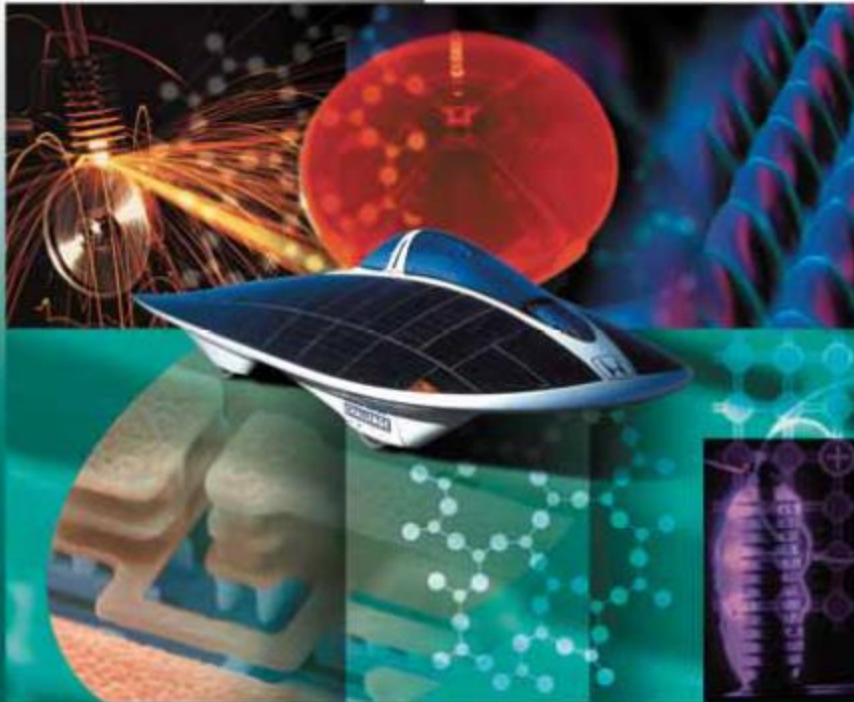
AAST – Cairo

Fall 2014

Lec. 8: Hydrogen Atom and Band Theory

Principles of Electronic Materials and Devices

Third Edition



S. O. Kasap

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Pages



P. 231-234: Hydrogen Atom

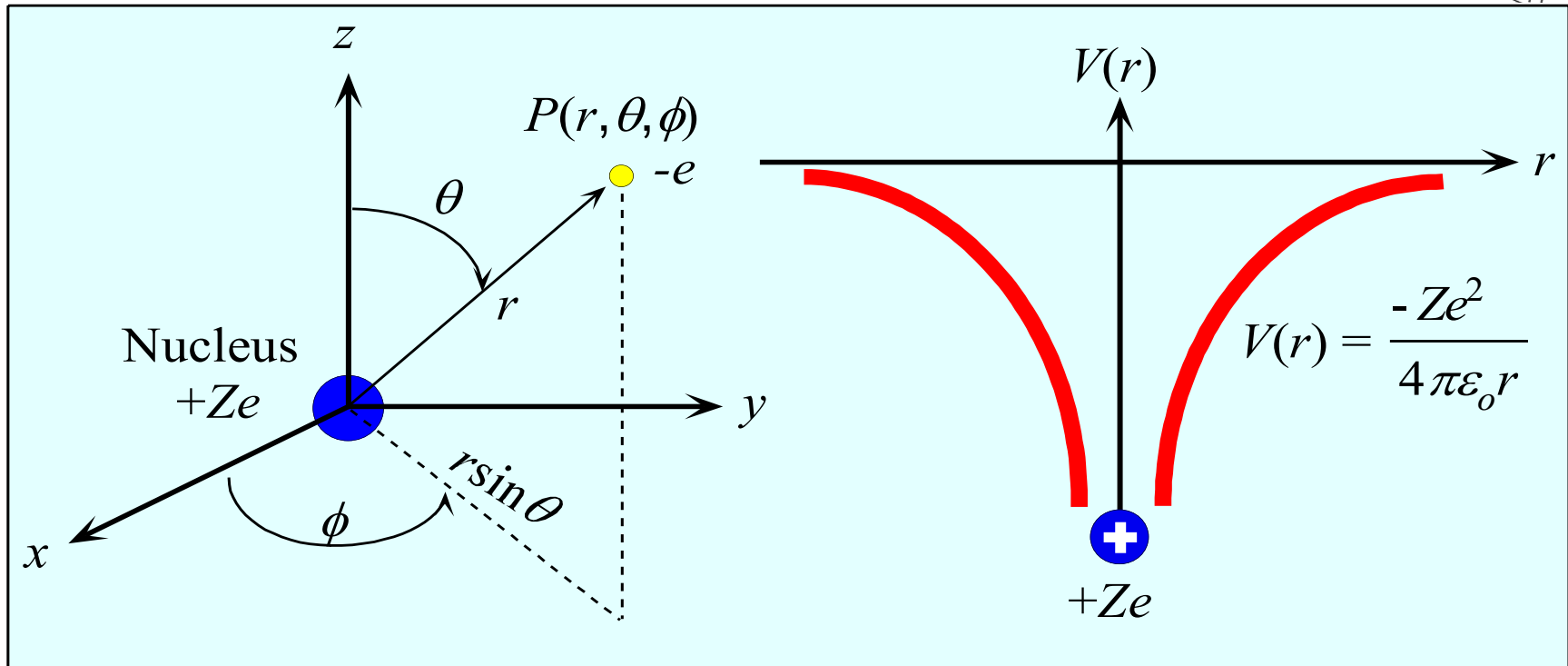
P. 285 – 287, p. 291-297, P.448 (Band Splitting)

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



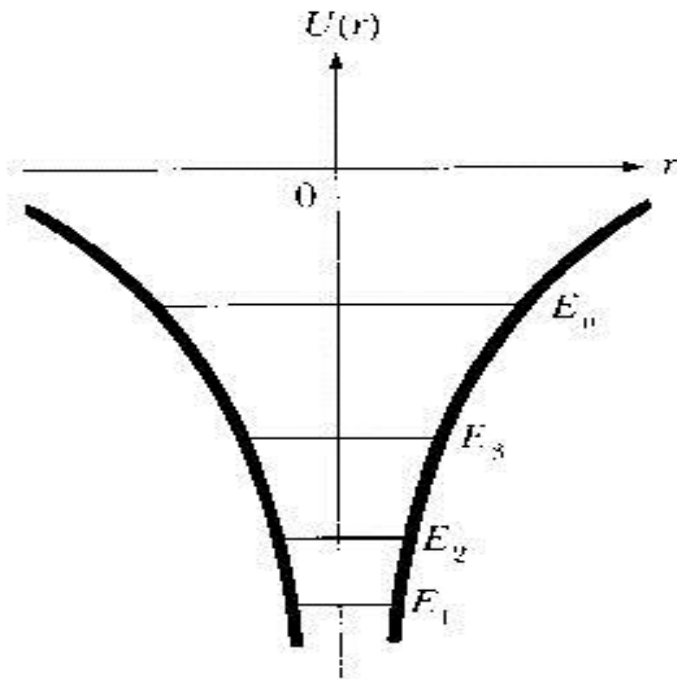
The electron in the hydrogenic atom is attracted by a central force that is always directed towards the positive nucleus. We therefore use spherical coordinates centered at the nucleus to describe the position of the electron. The PE of the electron depends on r only.



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



$$U(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$



Wavefunctions Solutions:

$$\Psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$$

Table 3.2 The radial and spherical harmonic parts of the wavefunction in the hydrogen atom ($a_0 = 0.0529$ nm)

n	ℓ	$R(r)$	m_ℓ	$Y(\theta, \phi)$
1	0	$\left(\frac{1}{a_0}\right)^{3/2} 2 \exp\left(-\frac{r}{a_0}\right)$	0	$\frac{1}{2\sqrt{\pi}}$
2	0	$\left(\frac{1}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) \exp\left(-\frac{r}{2a_0}\right)$	0	$\frac{1}{2\sqrt{\pi}}$
2	1	$\left(\frac{1}{2a_0}\right)^{3/2} \left(\frac{r}{\sqrt{3}a_0}\right) \exp\left(-\frac{r}{2a_0}\right)$	$\left[\begin{array}{l} 0 \\ 1 \\ -1 \end{array} \right]$	$\left\{ \begin{array}{l} \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \theta \\ \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{j\phi} \\ \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{-j\phi} \end{array} \right\} \left\{ \begin{array}{l} \propto \sin \theta \cos \phi \\ \propto \sin \theta \sin \phi \end{array} \right.$

Correspond to $m_\ell = -1$ and $+1$.

$\delta P(r)$: Probability of Finding an Electron at r (within a Spherical Shell of Thickness dr)



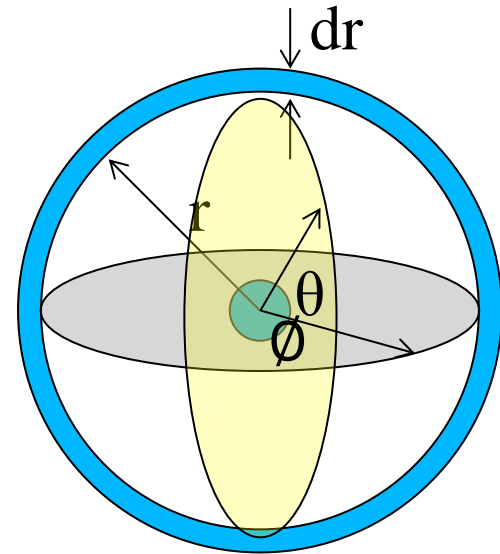
Volume of spherical shell at a distance r and

thickness dr : $dV = 4\pi r^2 dr$

Average of $\overline{Y(\theta, \phi)} = \frac{1}{2\sqrt{\pi}}$

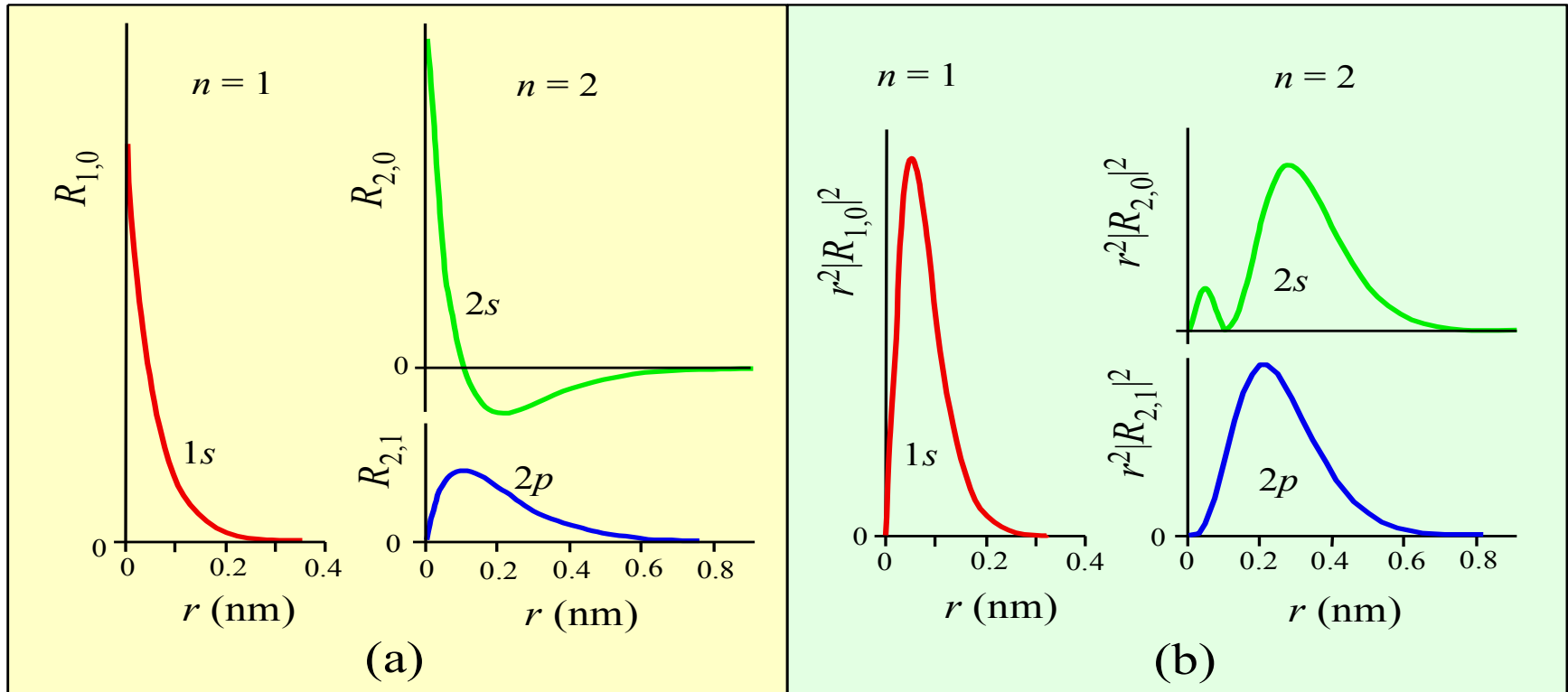
Probability of Finding an Electron at r
within this shell:

$$\begin{aligned}\delta P(r) &= |\Psi(r, \theta, \phi)|^2 dV \\ &= |R(r) \overline{Y(\theta, \phi)}|^2 dV \\ &= \left| R(r) \frac{1}{2\sqrt{\pi}} \right|^2 4\pi r^2 dr = |R(r)|^2 r^2 dr\end{aligned}$$



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.

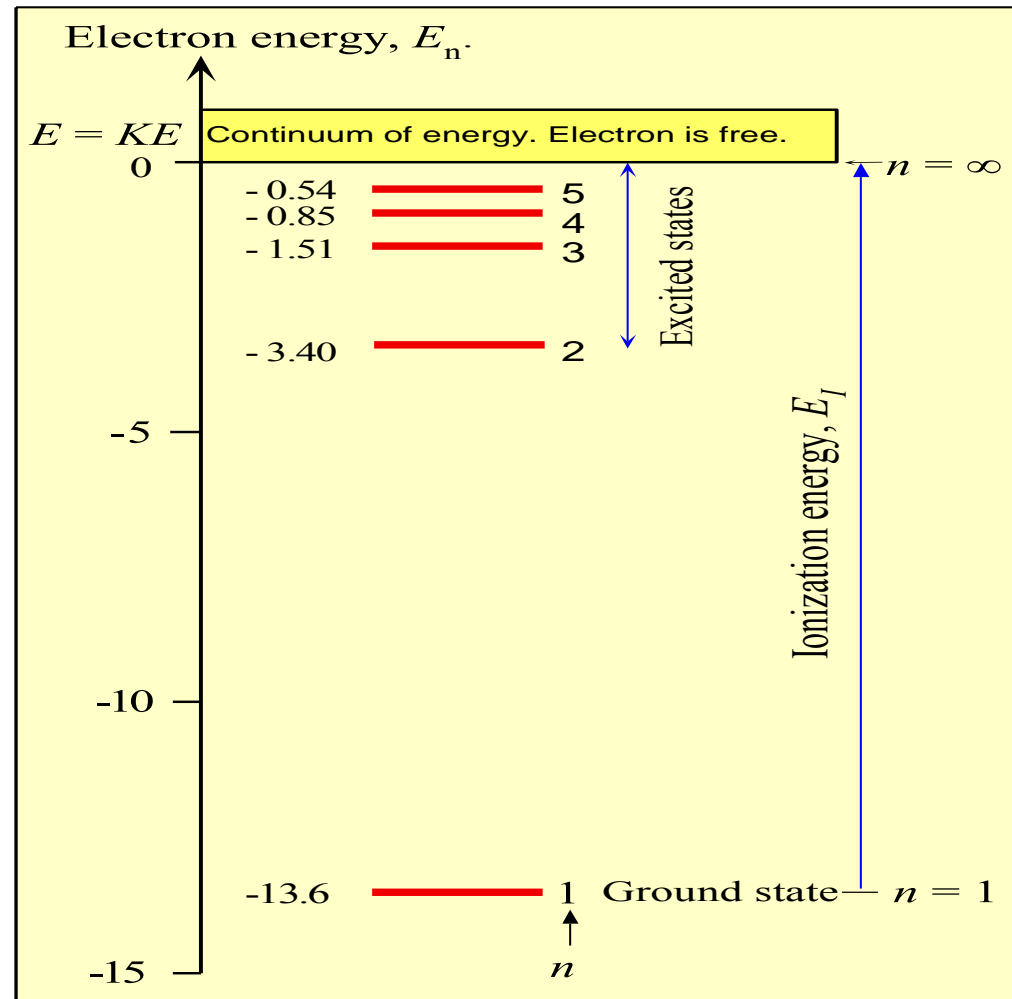
Energy Levels for H-atom:

Depends on *Principal Quantum Number*



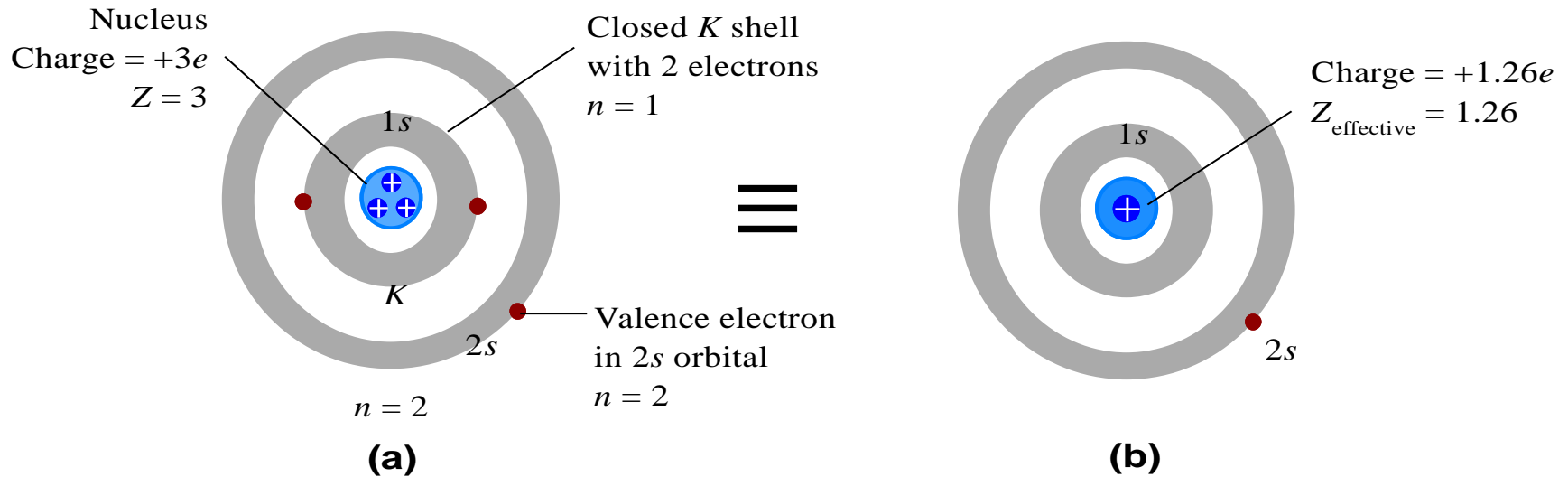
$$E_n = -\frac{Z E_1}{n^2}$$

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



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

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

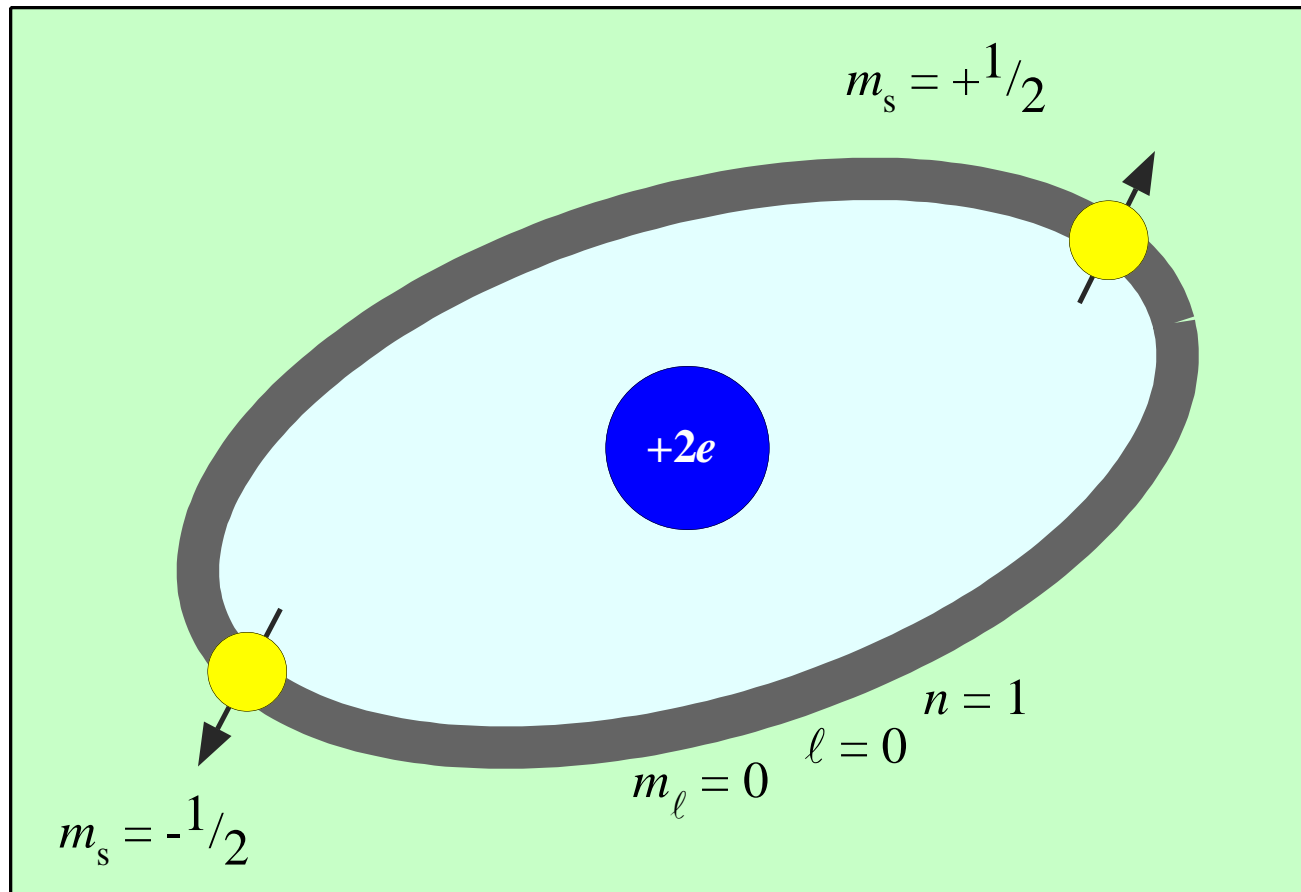


The Li atom has a nucleus with charge $+3e$, 2 electrons in the K shell, which is closed, and one electron in the 2s orbital.

(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.



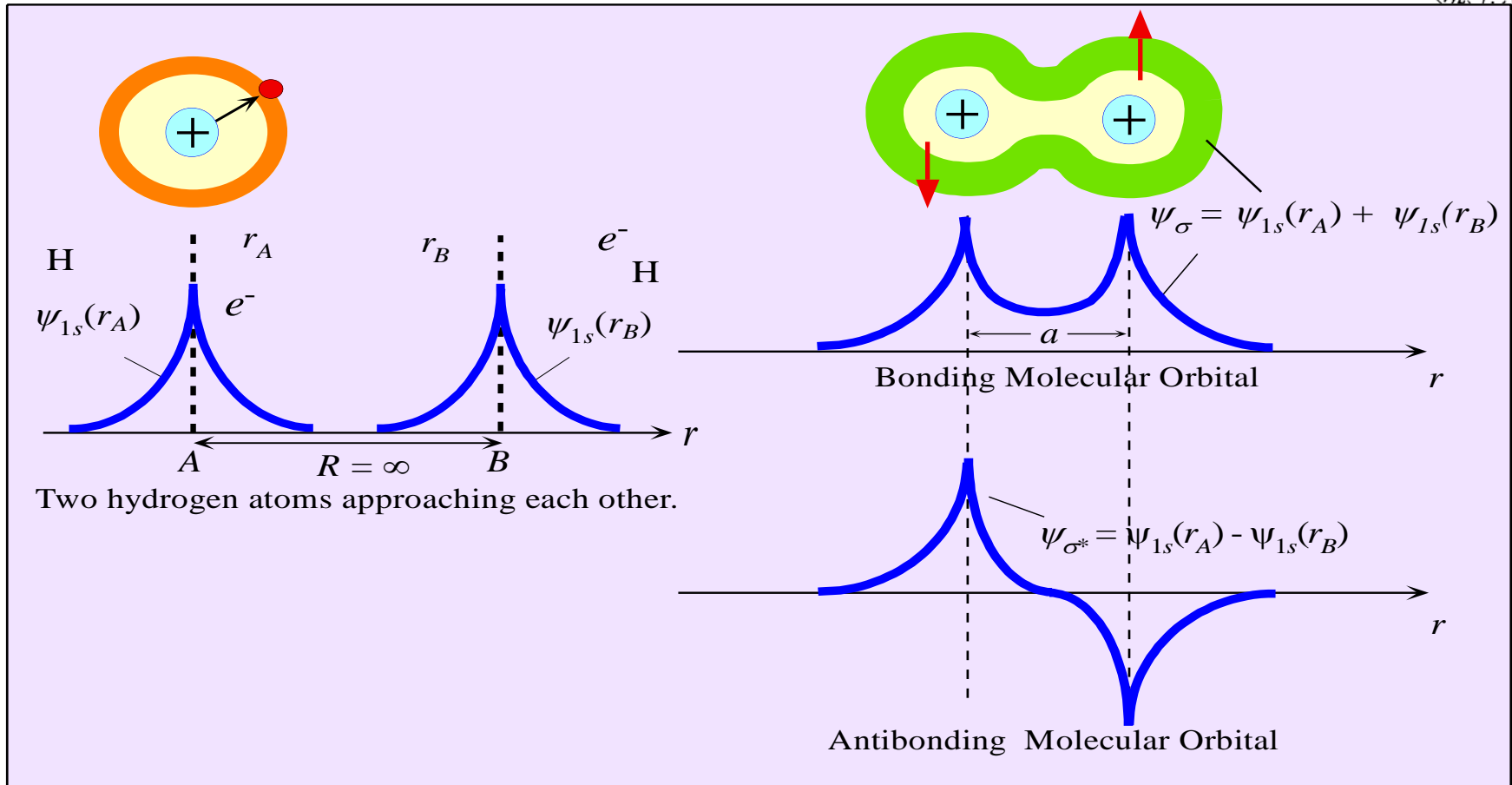
Pauli's Exclusion Principle:

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

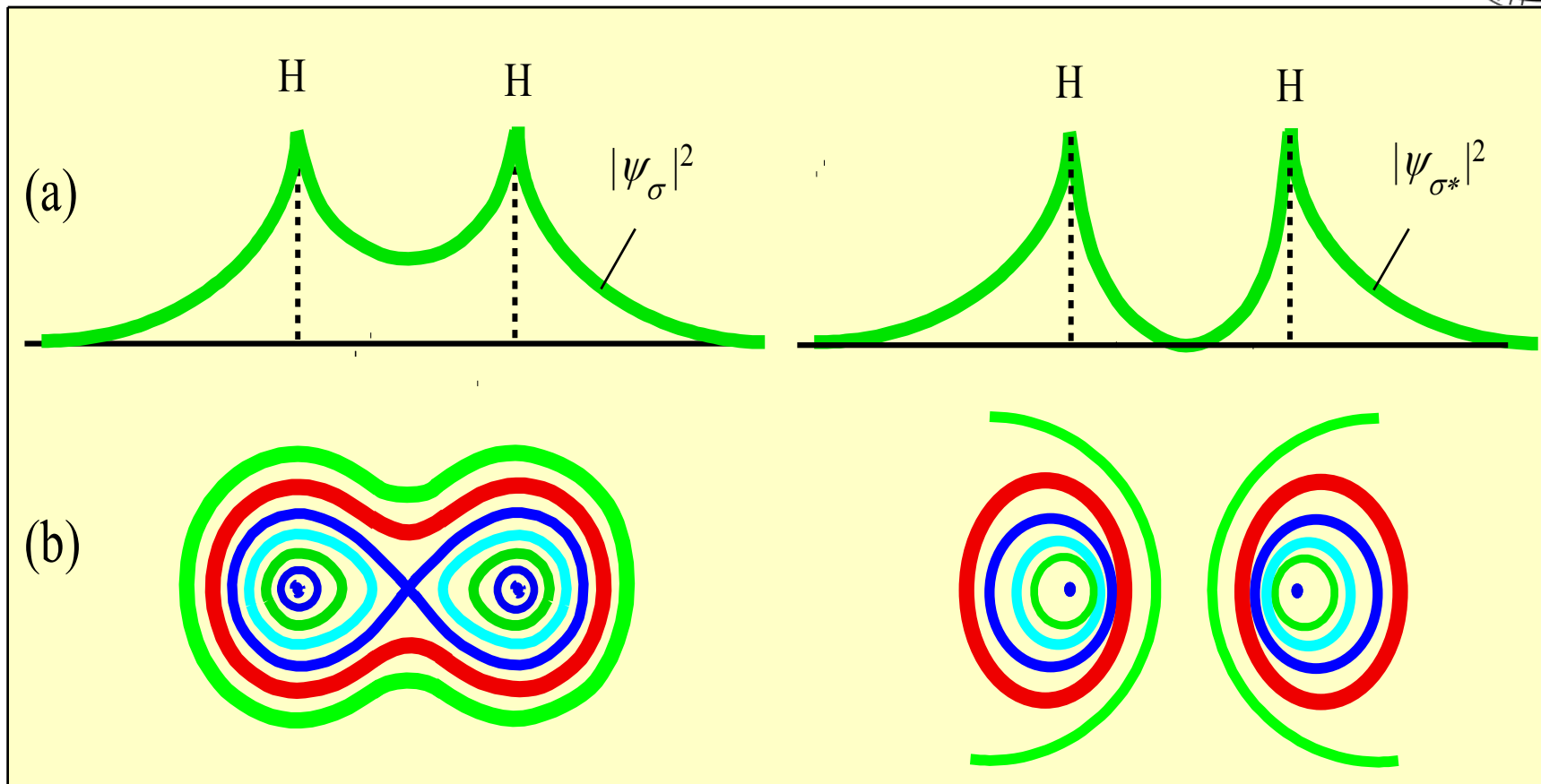
n	Principal quantum number	$n = 1, 2, 3, \dots$	Quantizes the electron energy
ℓ	Orbital angular momentum quantum number	$\ell = 0, 1, 2, \dots (n - 1)$	Quantizes the magnitude of orbital angular momentum L
m_ℓ	Magnetic quantum number	$m_\ell = 0, \pm 1, \pm 2, \dots, \pm \ell$	Quantizes the orbital angular 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



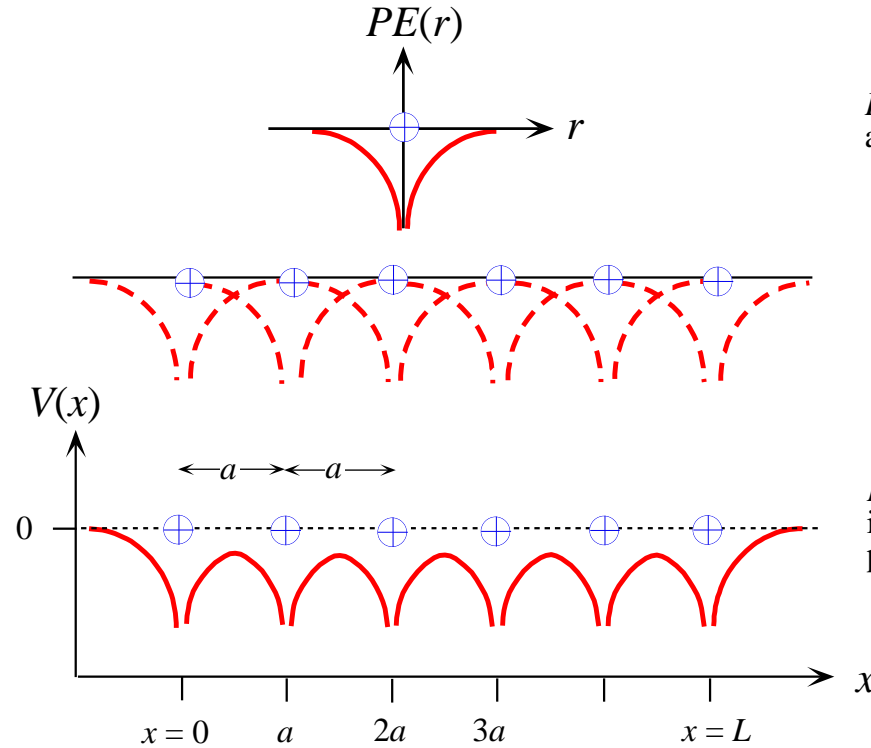
Formation of molecular orbitals, bonding and antibonding (ψ_{σ} and ψ_{σ^*}) when two H atoms approach each other. The two electrons pair their spins and occupy the bonding orbital ψ_{σ} .

Wavefunction Interactions: two H Atoms



(a) Electron probability distributions for bonding and antibonding orbitals, ψ_σ and ψ_{σ^*} . (b) Lines represent contours of constant probability.

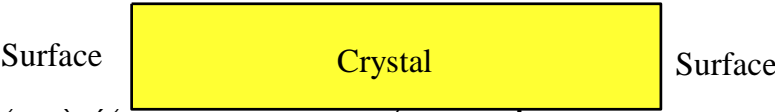
Superposition of Coulomb Potential for N-Atoms



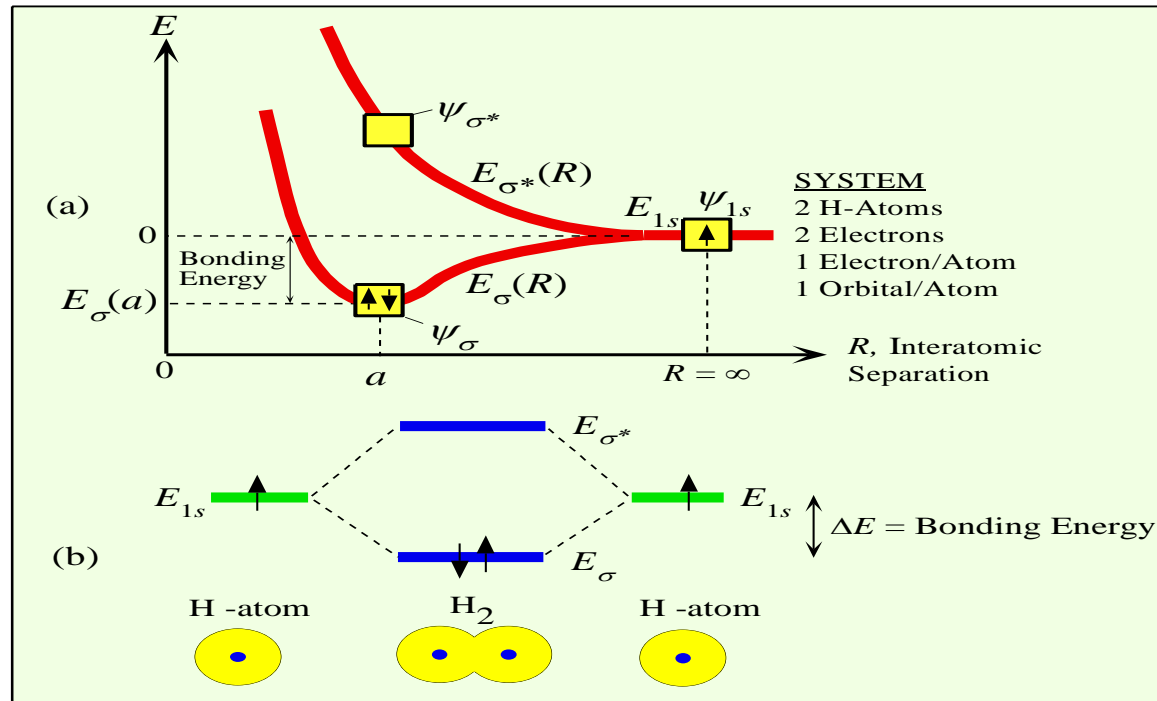
PE of the electron around an isolated atom

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 $PE = 0$).

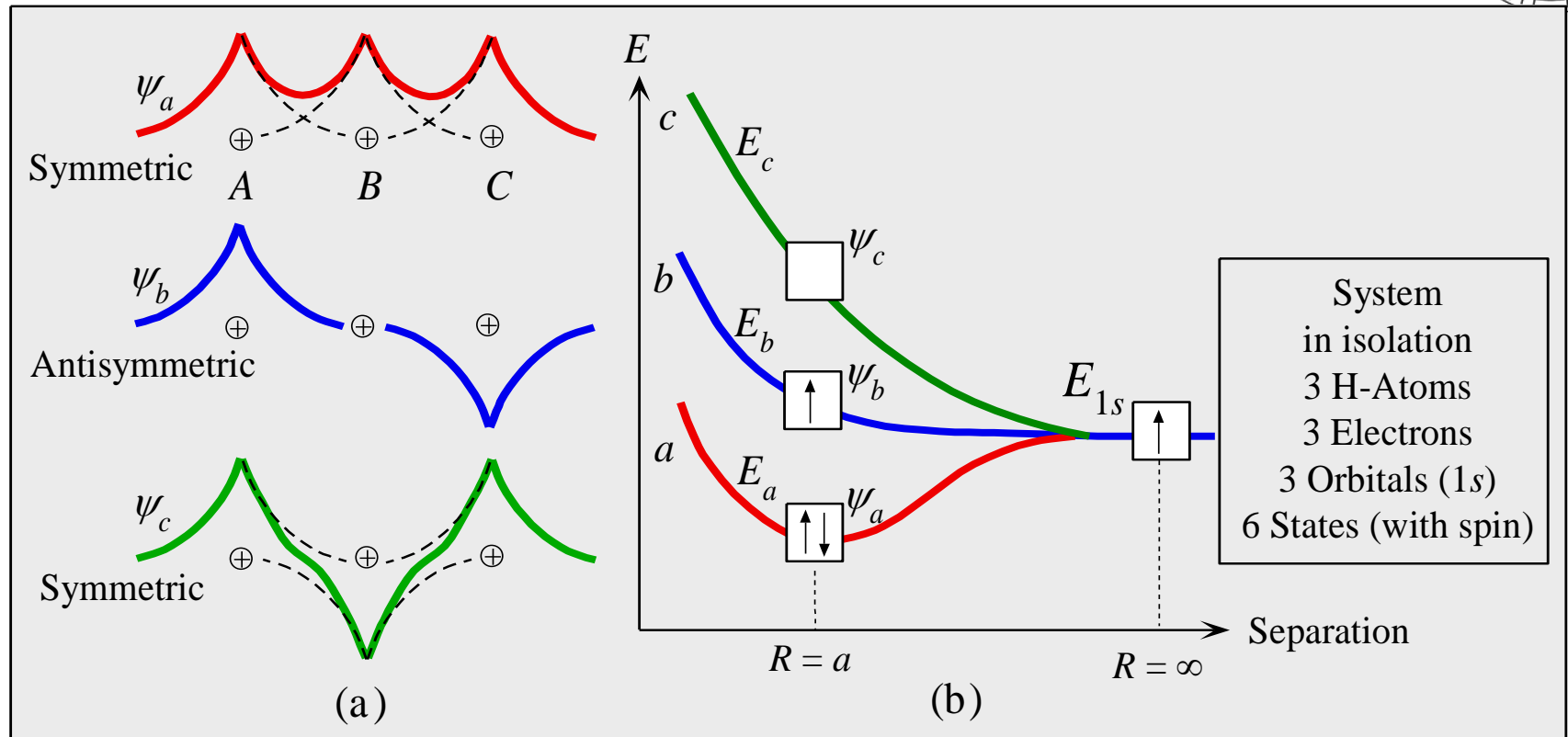
Band Splitting



Electron energy in the system comprising two hydrogen atoms. (a) Energy of ψ_{σ} and ψ_{σ^*} 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.

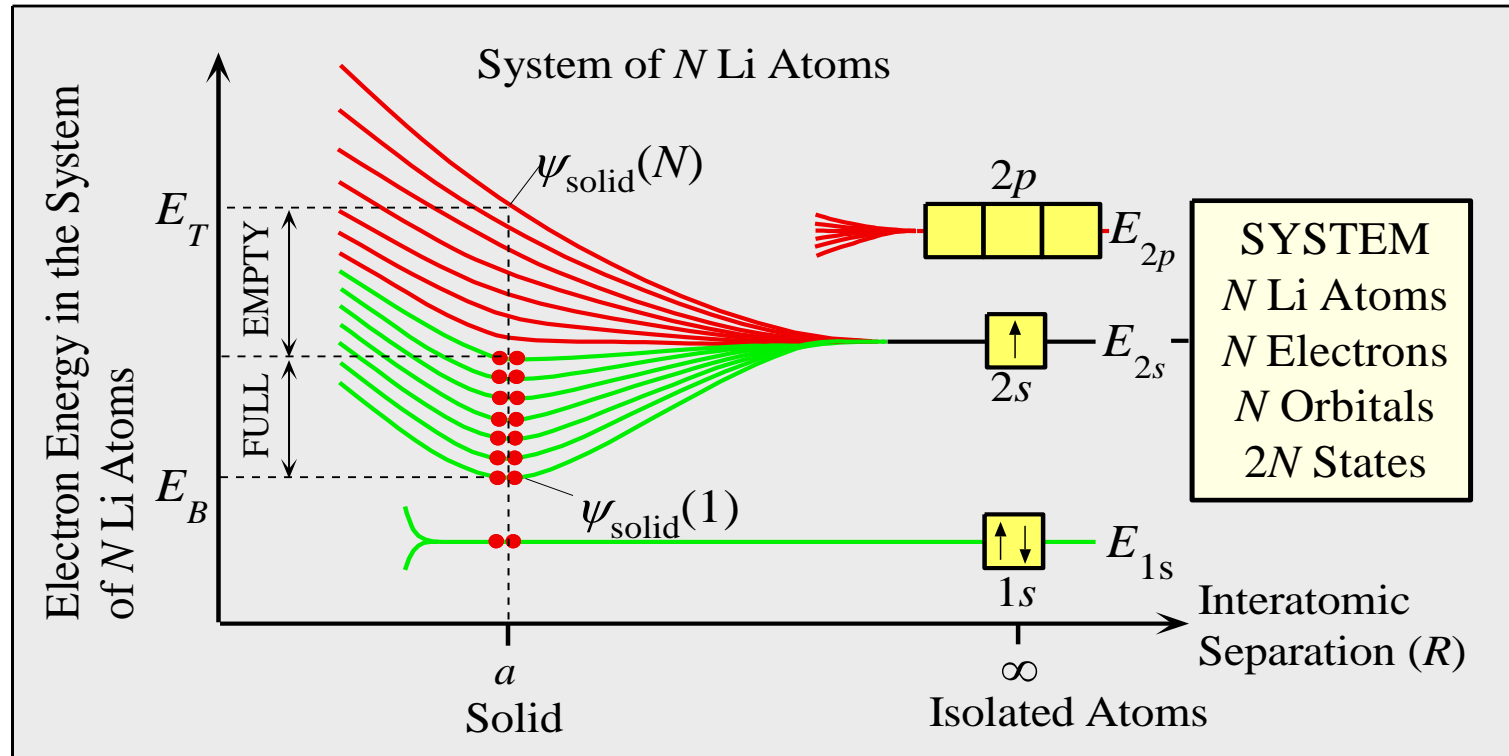


Three H-Atoms: Ψ Overlap, Band Splitting



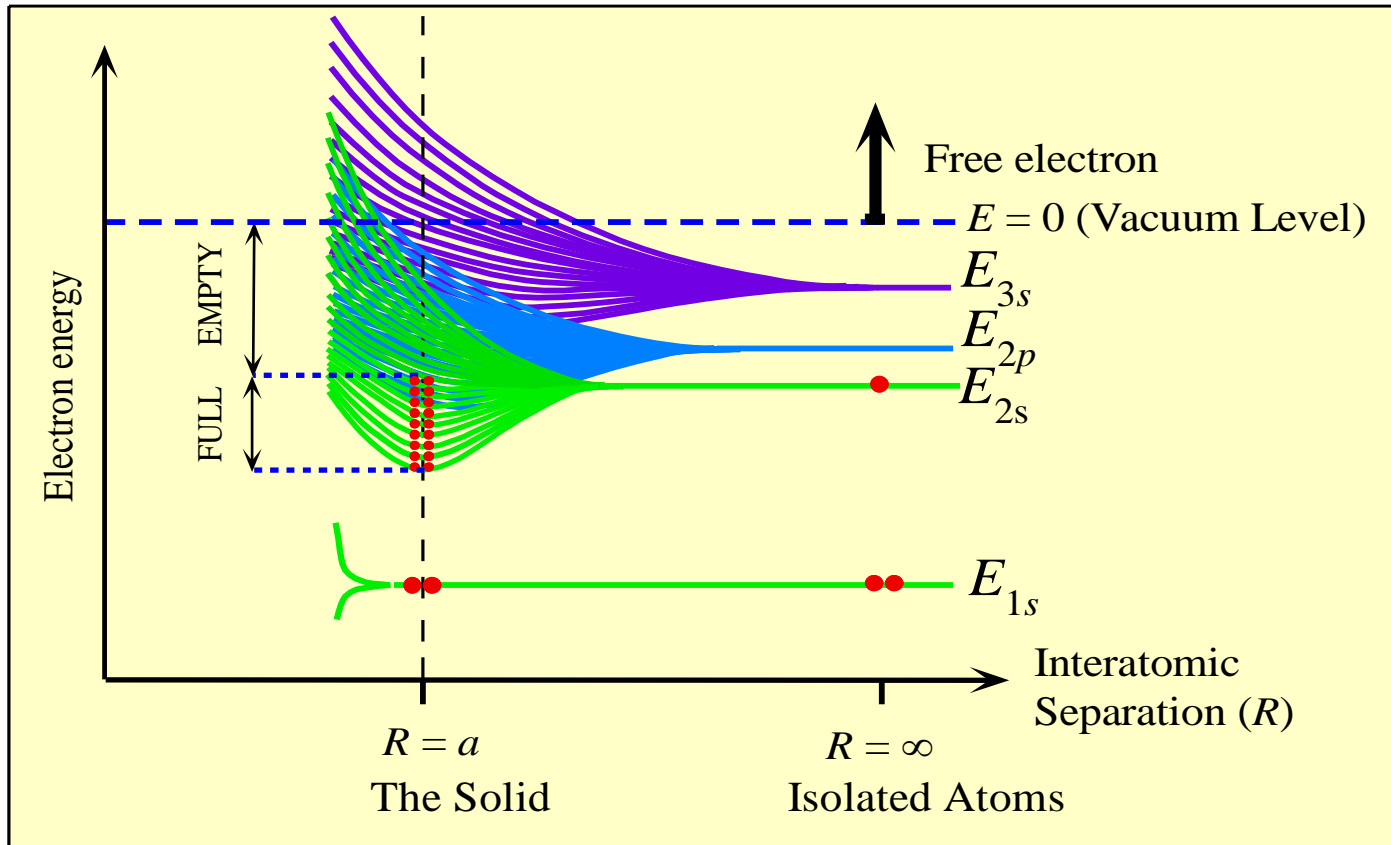
(a) Three molecular orbitals from three ψ_{1s} atomic orbitals overlapping in three different ways. (b) The energies of the three molecular orbitals labeled as a , b and c in a system with 3 H atoms (highly simplified).

Band Theory: "N" H-atoms

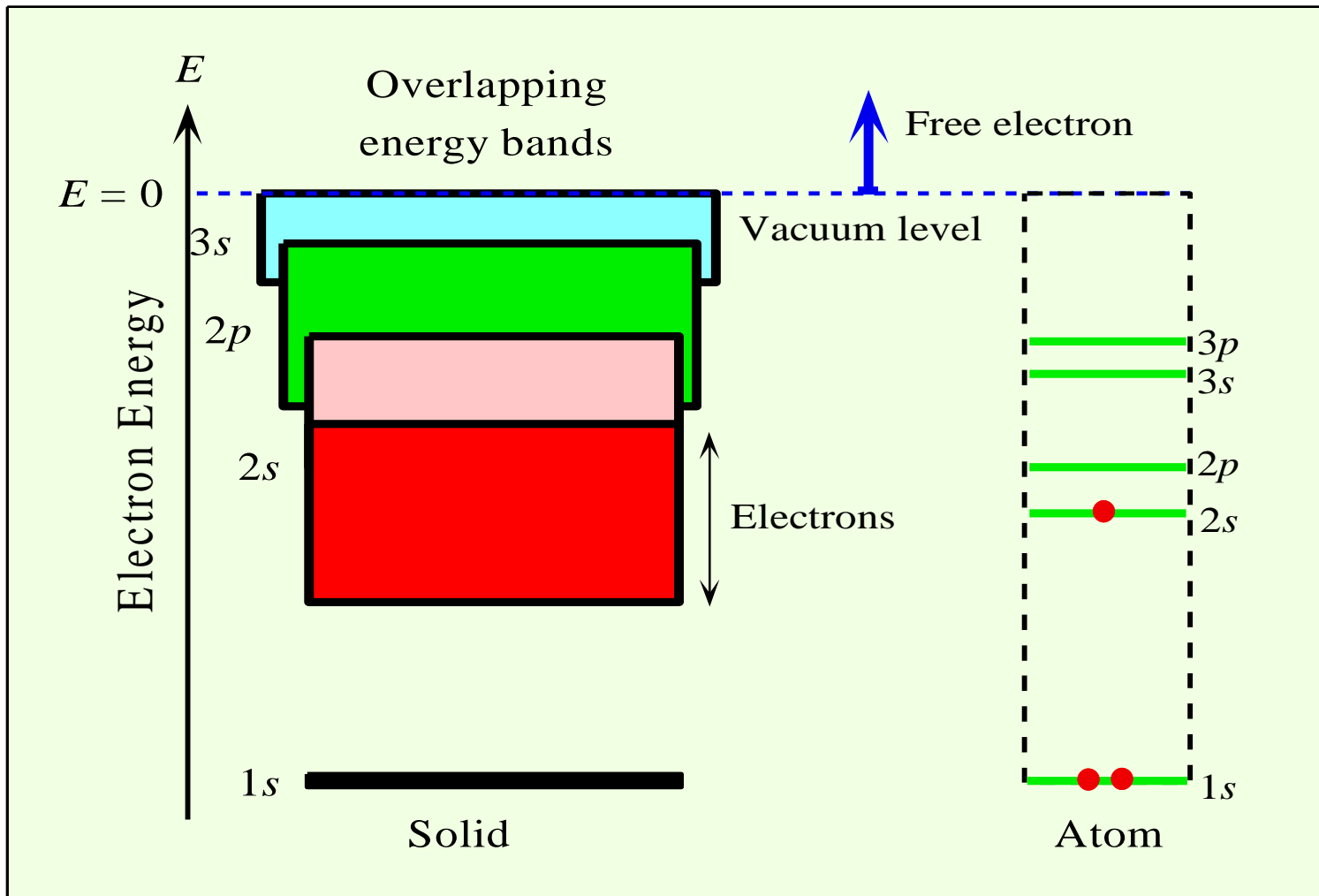


The formation of a $2s$ -energy band from the $2s$ -orbitals when N Li atoms come together to form the Li solid. There are N $2s$ -electrons but $2N$ states in the band. The $2s$ -band therefore is only half full. The atomic $1s$ orbital is close to the Li nucleus and remains undisturbed in the solid.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