Tight Binding Model

→ Ch. 10

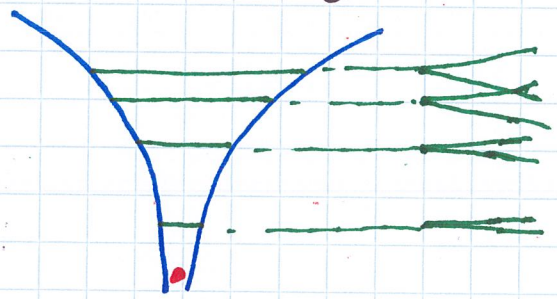
→ opposite of NFEM

→ assume material is composed of (nearly) distinct atoms

→ e^- fill atomic orbitals

→ perturbation comes from overlap of atomic orbitals w neighboring atoms.

↳ lifts the degeneracy of the atomic energy levels.



Atomic Orbitals : degeneracy in N-atom system

$s \rightarrow 2 \times N$ degenerate

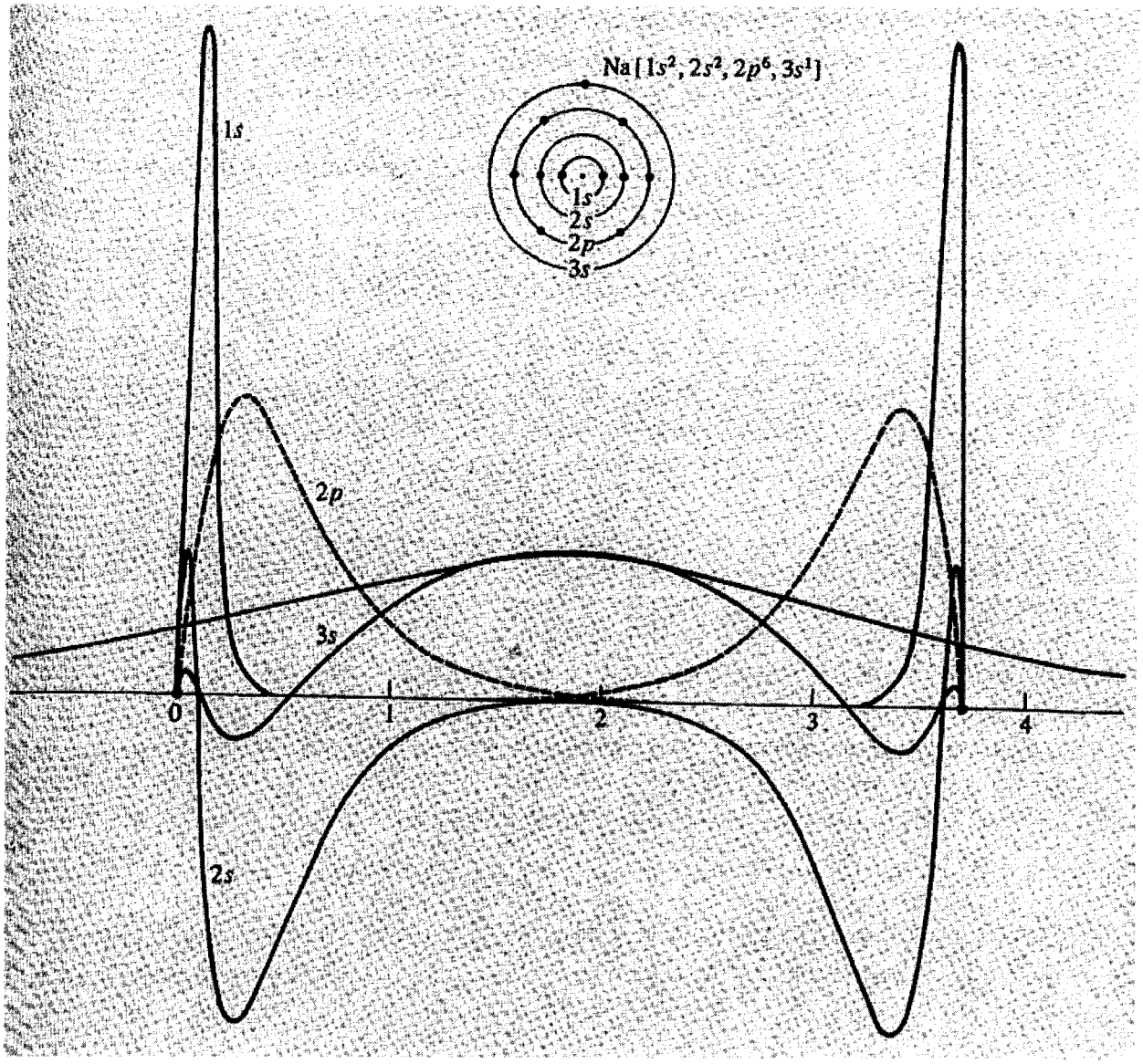
↳ spin ↑,↓ ↳ N atoms

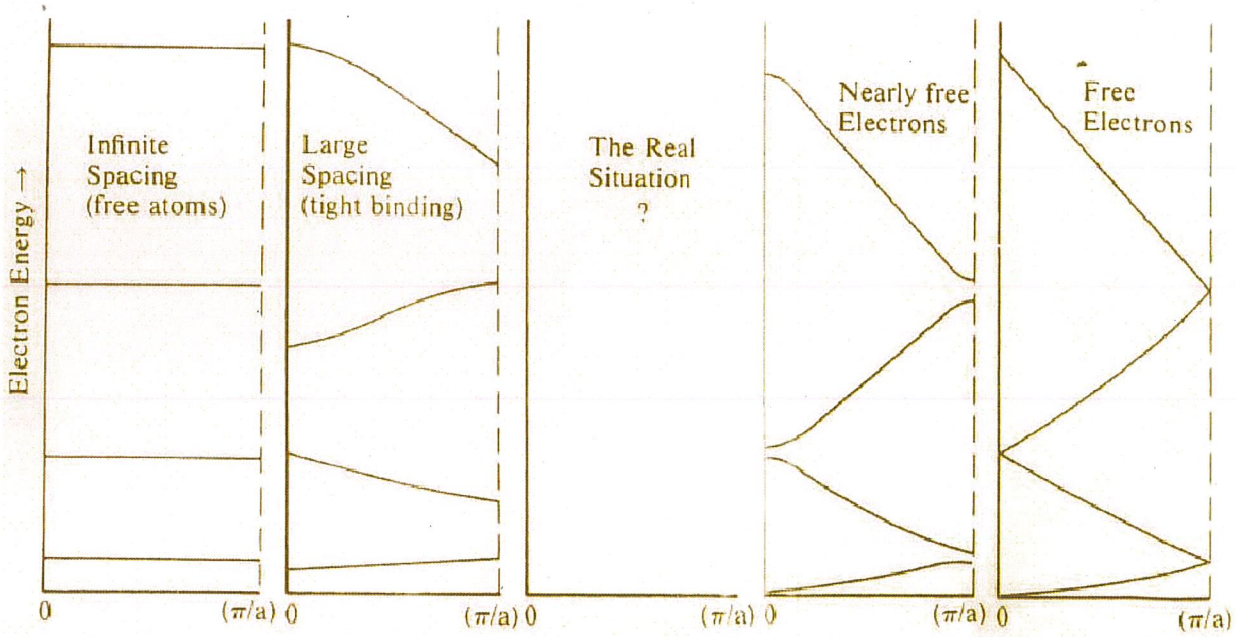
$p \rightarrow 2 \times 3 \times N = 6N$

↳ p_x, p_y, p_z

$d \rightarrow 2 \times 5 \times N = 10N$

→ generally consider "highest" lying orbital to calc. perturbation eg. 3s.


Na[1s², 2s², 2p⁶, 3s¹]
1s
2s
2p
3s
1s
2p
3s
2s
0
1
2
3
4


Electron Energy →
Infinite
Spacing
(free atoms)
Large
Spacing
(tight binding)
The Real
Situation
?
Nearly free
Electrons
Free
Electrons
0
(π/a)
0
(π/a)
0
(π/a)
0
(π/a)
0
(π/a)