

Looking to the end of the quarter:

- **Problem Set 5 due today...to next Thursday, with answers back when you hand in**
- **Course review summary to be handed out at the end of this week**
- **Review sessions by Skype from Baltimore APS Meeting: Wednesday and Thursday, 8:00-9:30 PM in room 285, Tanat Kissikov presiding**
- **Questions by e-mail, but a busy week at conference**
- **Tanat also available, will schedule office hour(s)**

Physics 140A-Introduction to Solid State Physics
Winter, 2016
Problem Set 5

**Due anytime from Thursday, March 10th until Thursday, March 17th,
with answers returned by e-mail whenever you turn this in.
Final examination is on Saturday, March 19th**

Reading in Omar: Chapter 4--Sections 4.1-4.9, Chapter 5--Sections 5.1-5.8,5.9, 5.11, in 5.4 read on Brillouin zones only, not Symmetry Properties, in 5.6-5.7 don't worry about detailed mathematics

Optional parallel reading in Ibach and Luth: Chapter 6-Sections 6.1-6.4, Chapter 7-Sections 7.1-7.5, and Panel 5. This book presents a more concise version of the same material.

Problems in Omar:

[1] Chapter 4, Problem 1

[2] Chapter 4, Problem 7 (for Cu only)

[3] Chapter 5, Problem 8(a) only. Do this via suitable sketches, not a math. problem.

[4] Chapter 5, Problem 11(a) only.

[5] Chapter 5, Problem 12

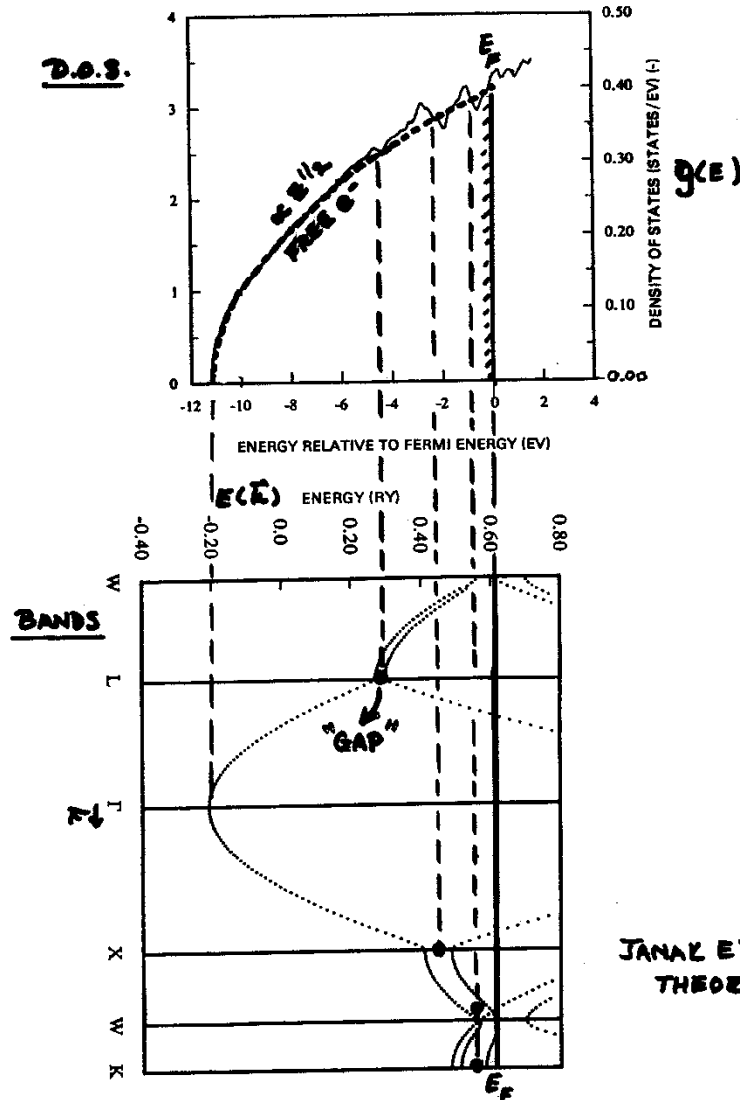
[6] Chapter 5, Problem 14(a) only.

[7] Special problem: On the next page is shown a theoretical electronic band structure calculation for aluminum, together with the corresponding density of states. The energy is in Rydbergs = $Ry = 13.605 \text{ eV}$. The electronic configuration of atomic aluminum is $1s^2 2s^2 2p^6 3s^2 3p^1$. It is fcc with lattice constant 4.05 \AA .

- (a) Which are the core electrons and which are the valence electrons in aluminum?
- (b) Show, by numerical check at five equally spaced points, that the band extending from Γ to X actually is very close to that expected for a totally free electron (what your text calls the empty lattice model). Note that you will need to use the correct magnitude for the wave vector along this direction.
- (c) Show, also by numerical check at five points, that the calculated density of states curve follows on average that expected for a free electron.
- (d) Do an approximate numerical integration of the density of states (given in states/eV) from the bottom of the bands to the Fermi level, and show that it yields an answer consistent with the number of valence electrons.
- (e) What is the group velocity of an electron in a state just beyond L and going toward W?
- (f) Bragg reflection from which set of planes is responsible for the gap at X?
- (g) Qualitatively explain the little peaks and valleys in the density of states centered on the dashed lines.

From 7: Special problem

ALUMINUM - ELECTRONIC BANDS & D.O.S.



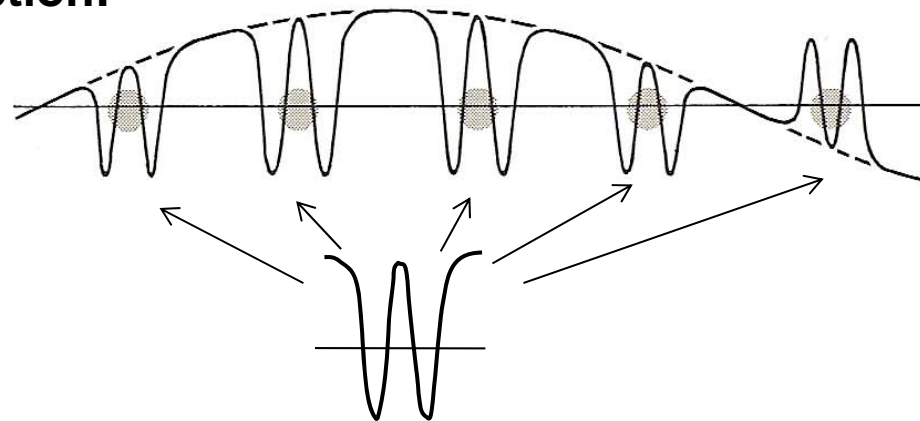
Electrons in crystalline solids—are everywhere

For all states in crystalline (ordered) solids:

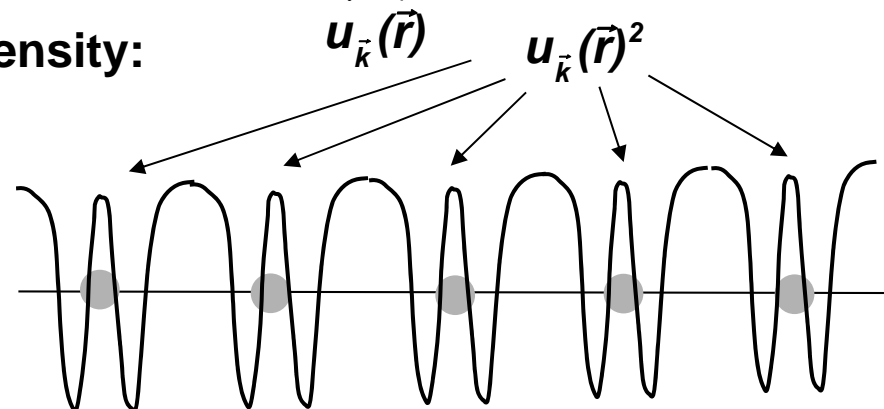
$\Psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}$, where $u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{A})$, this is a "Bloch function" with probability density of

$\Psi_{\vec{k}}^*(\vec{r})\Psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}^*(\vec{r})e^{-i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}} = u_{\vec{k}}(\vec{r})^2$, the same on every atom!

A typical Bloch function: *Re or Im part of $e^{i\vec{k}\cdot\vec{r}}$: $\cos kr$ or $\sin kr$*



And its probability density:

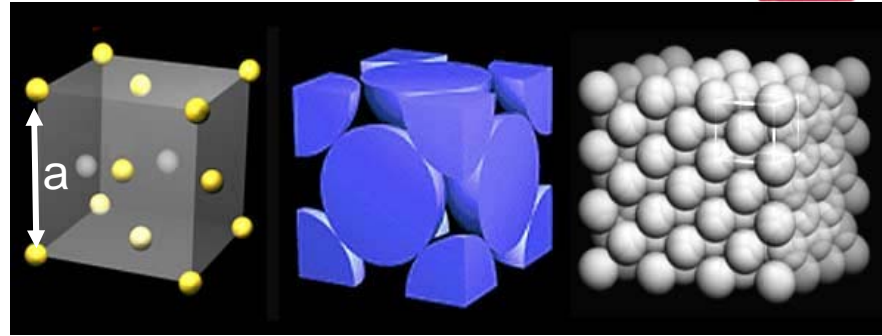


Omar, Sections
5.1-5.3

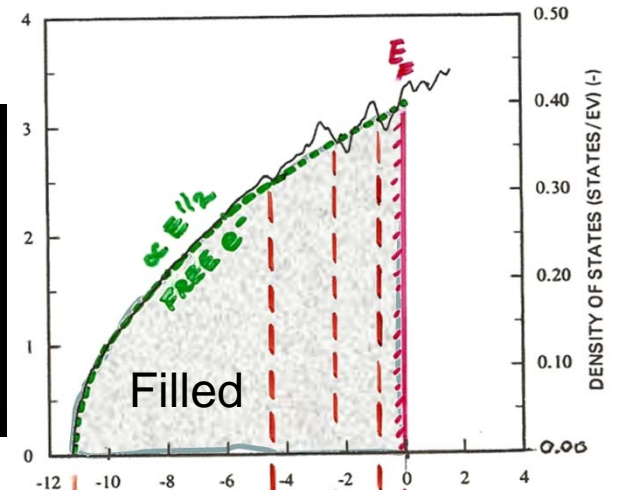
Electronic bands and density of states for “free-electron” metals-

Rydberg = 13.605 eV

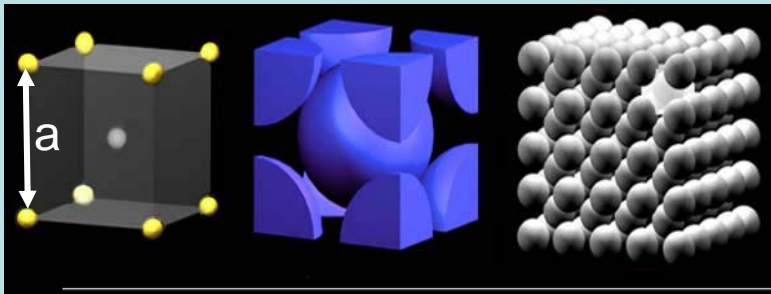
Aluminum—fcc,
 $a = 4.05 \text{ \AA}$
 $1s^2 2s^2 2p^6 3s^2 3p^1$



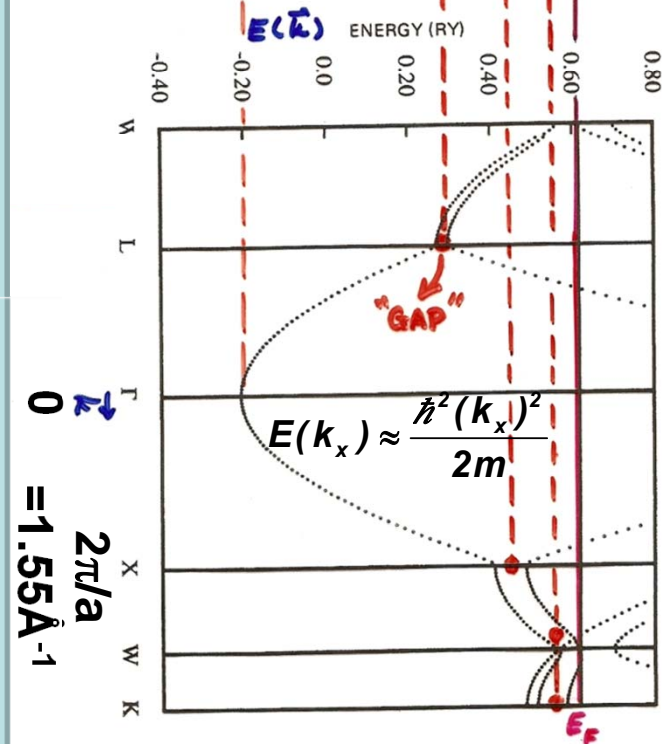
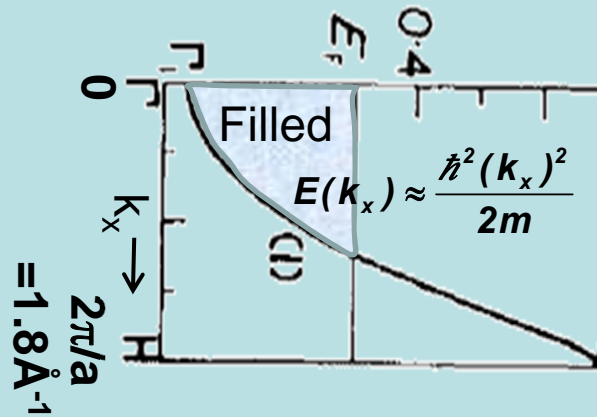
D.O.S.



Lithium—bcc, $a = 3.49 \text{ \AA}$
 $1s^2 2s^1$



E (Ryd) Ryd = 13.6 eV



ELECTRONS IN SOLIDS:

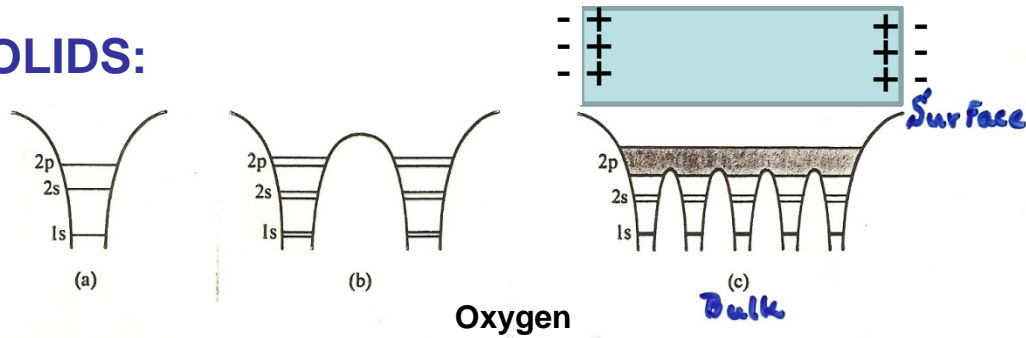


Fig. 5.1 The evolution of the energy spectrum of ~~O~~ from an atom (a), to a molecule (b), to a solid (c).

+ Successive Approximations:



Forget the surfaces

Treat as free-particle in a box

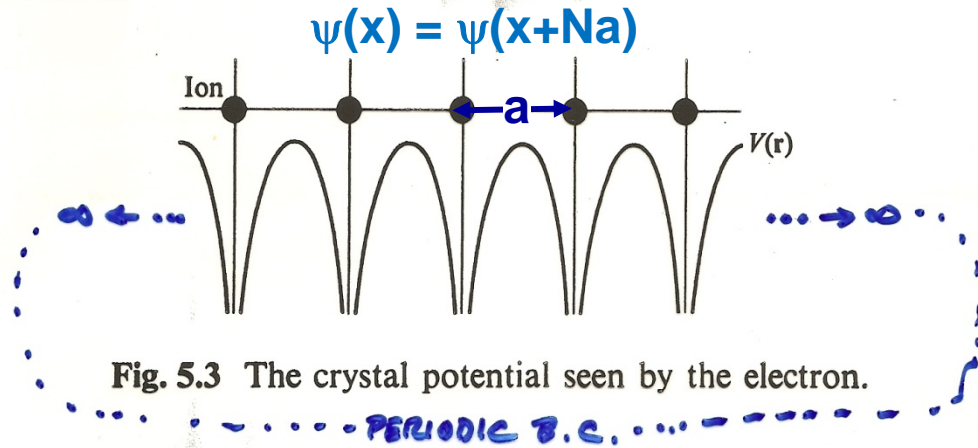
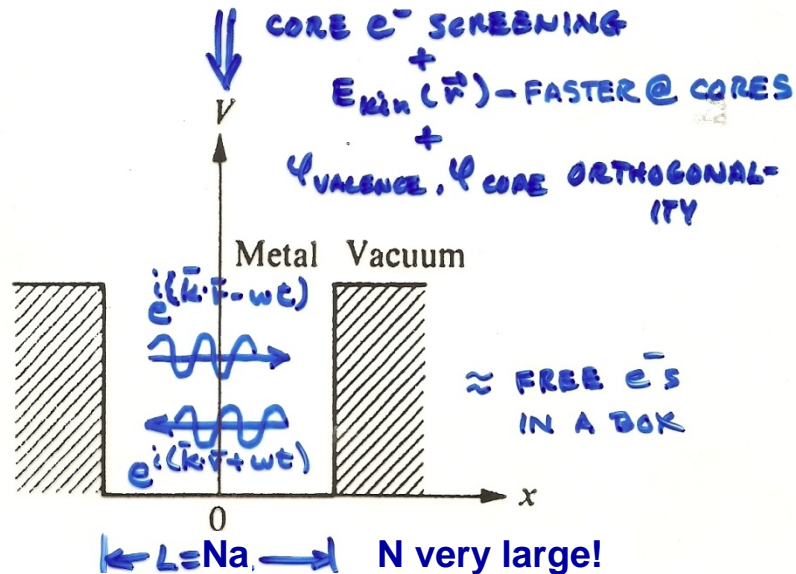
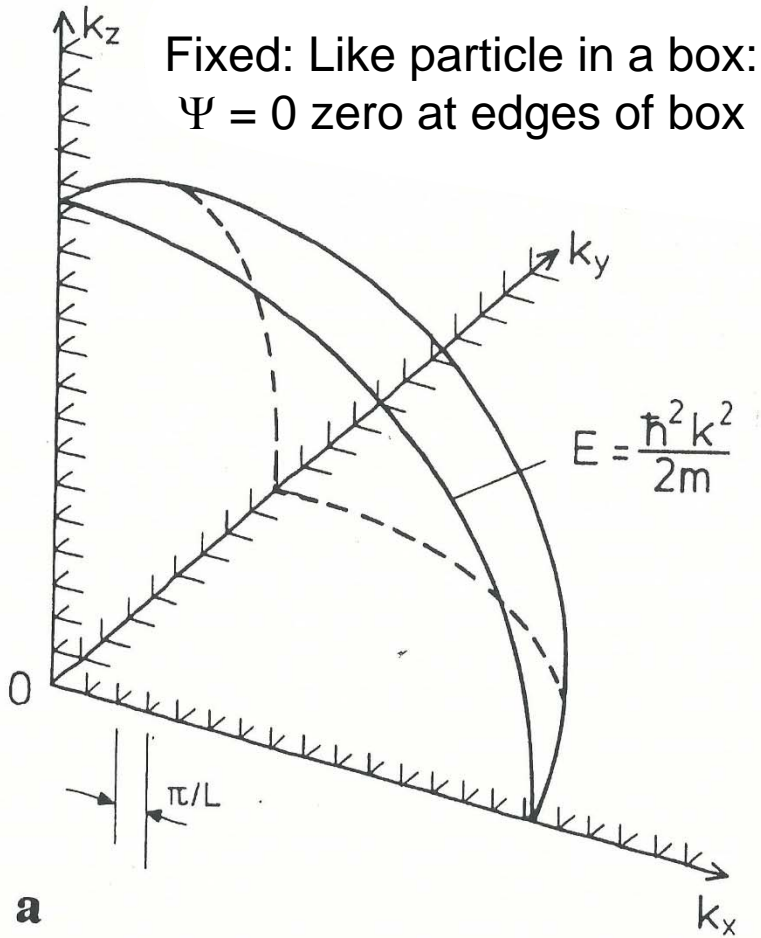


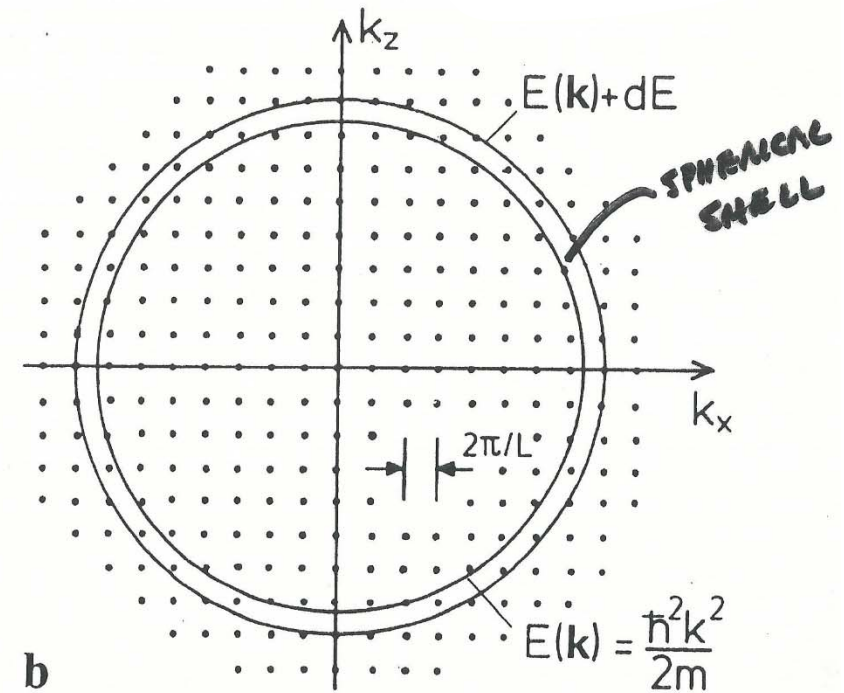
Fig. 5.3 The crystal potential seen by the electron.



3D counting of particle-in-a-box density of states, with fixed and periodic boundary conditions



Periodic: Like vibrational waves or electrons in a solid: $\psi(x) = \psi(x+L)$



$$3D: g(\epsilon) = g(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{4\pi k^2}{\hbar} \left| \frac{d\omega}{dk} \right|$$

+ two different spins!

3D free-electron density of states

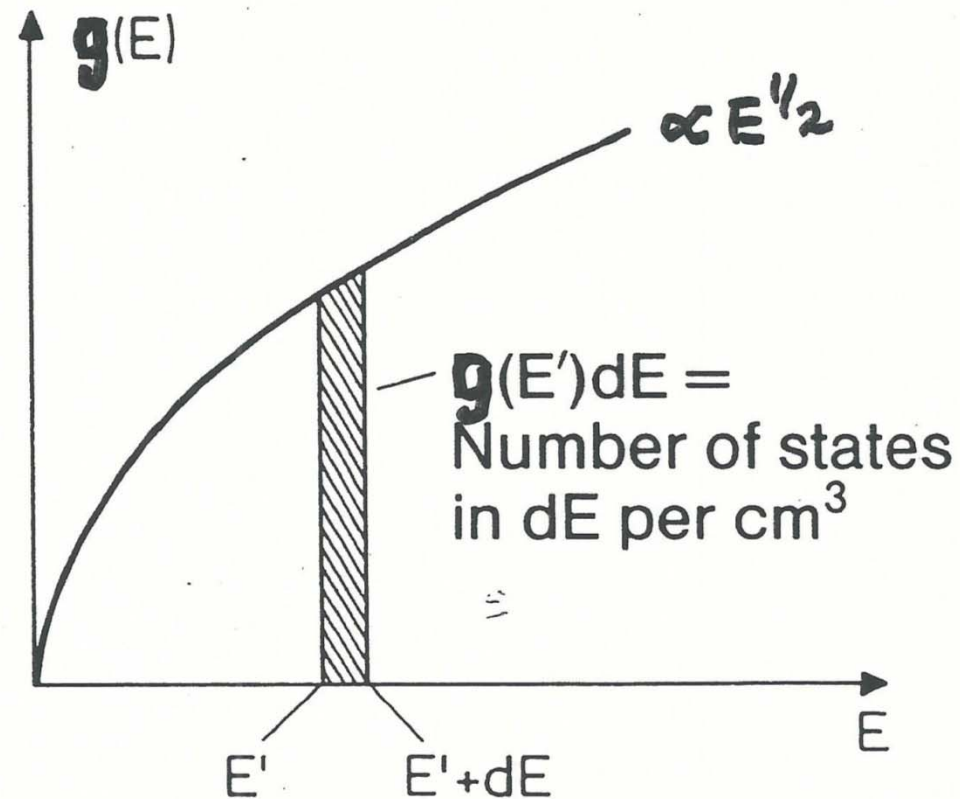
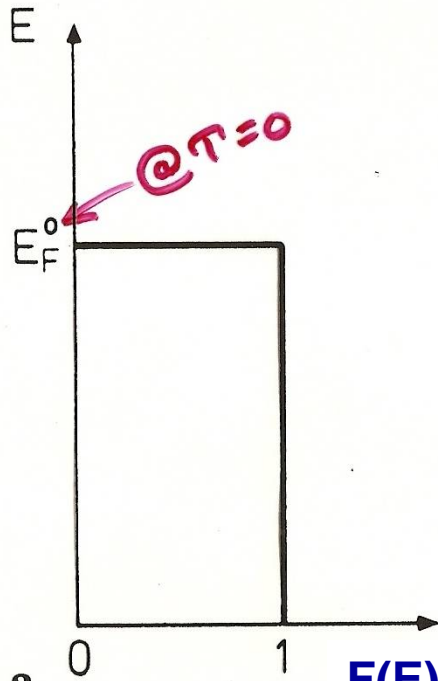


Fig. 6.4. Density of one-particle states $g(E)$ for a free electron gas in three dimensions

The free-electron solid at absolute zero:

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m_e} = 3.81(k(\text{in } \text{\AA}^{-1}))^2 \text{ (in eV)}$$



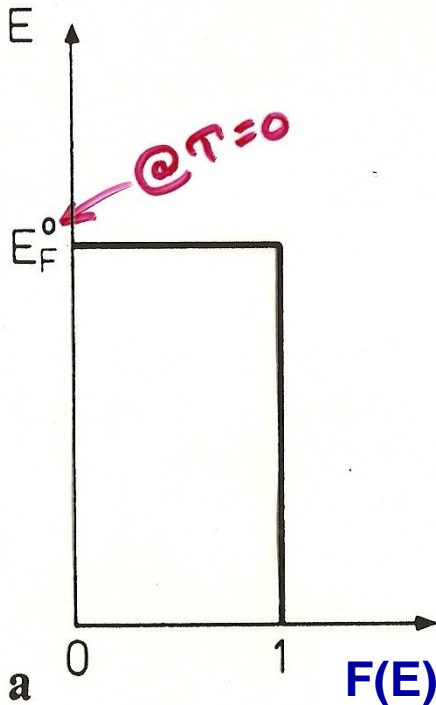
a

F(E):
FERMI-
DIRAC

$$F(E, T) = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

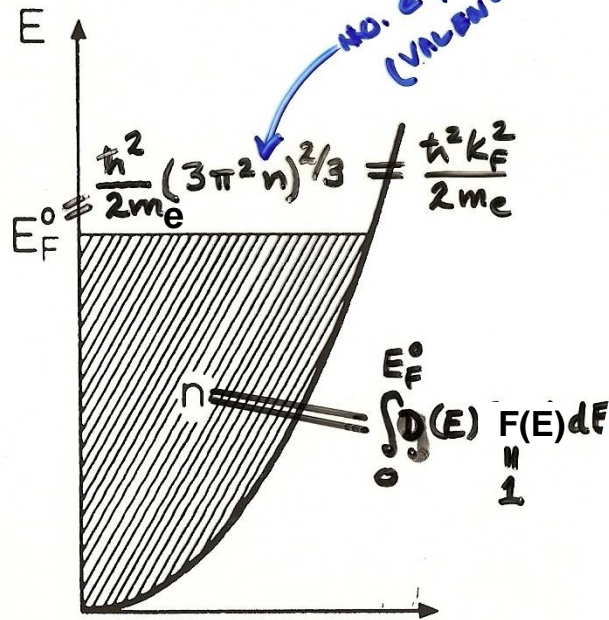
The free-electron solid at absolute zero

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m_e} = 3.81(k(\text{in } \text{\AA}^{-1}))^2 \text{ (in eV)}$$



$F(E)$:
FERMI-
DIRAC

$$F(E, T) = \frac{1}{e^{(E-E_F^0)/k_B T} + 1}$$



$g(E) \cdot F(E)$

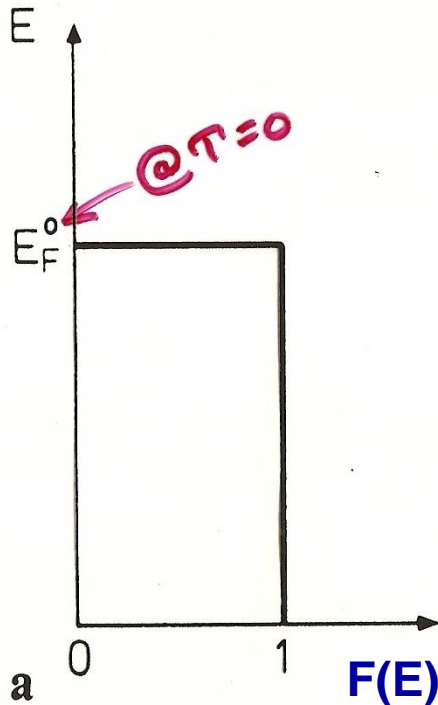
$$\frac{(2m_e)^{3/2}}{2\pi^2 \hbar^3} E^{1/2}$$

= the density of states

In Energy
Space

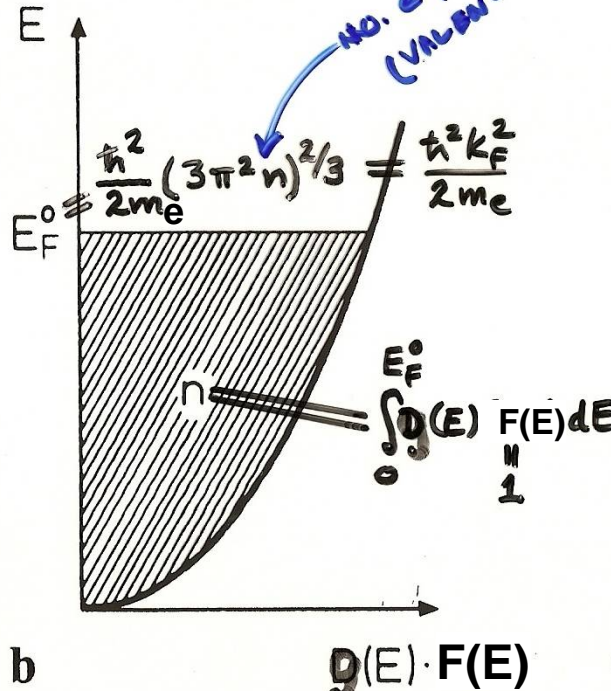
The free-electron solid at absolute zero

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m_e} = 3.81(k(\text{in } \text{\AA}^{-1}))^2 \text{ (in eV)}$$



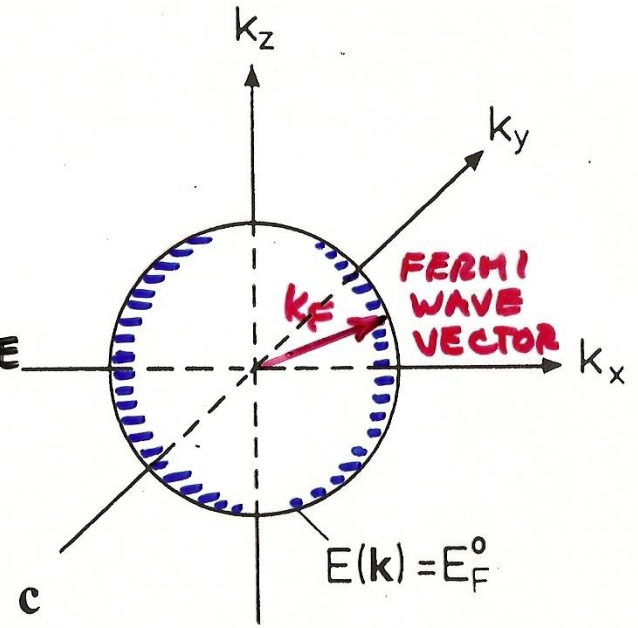
**F(E):
FERMI-
DIRAC**

$$F(E, T) = \frac{1}{e^{(E-E_F^0)/k_B T} + 1}$$



**$g(E) \cdot F(E)$
= the density of states**

**In Energy
Space**



**$k_F = (3\pi^2 n)^{1/3}$
 $v_F = p_F/m_e = \hbar k_F/m_e$
 $= \hbar(3\pi^2 n)^{1/3}/m_e$**

**In k- or
"Reciprocal"
Space**

Table 9.4 Fermi Energies ($T = 300$ K), Fermi Temperatures, and Fermi Velocities for Selected Metals

Element	E_F (eV)	T_F ($\times 10^4$ K)	u_F ($\times 10^6$ m/s)
Li	4.74	5.51	1.29
Na	3.24	3.77	1.07
K	2.12	2.46	0.86
Rb	1.85	2.15	0.81
Cs	1.59	1.84	0.75
Cu	7.00	8.16	1.57
Ag	5.49	6.38	1.39
Au	5.53	6.42	1.40
Be	14.3	16.6	2.25
Mg	7.08	8.23	1.58
Ca	4.69	5.44	1.28
Sr	3.93	4.57	1.18
Ba	3.64	4.23	1.13
Nb	5.32	6.18	1.37
Fe	11.1	13.0	1.98
Mn	10.9	12.7	1.96
Zn	9.47	11.0	1.83
Cd	7.17	8.68	1.62
Hg	7.13	8.29	1.58
Al	11.7	13.6	2.03
Ga	10.4	12.1	1.92
In	8.63	10.0	1.74
Tl	8.15	9.46	1.69
Sn	10.2	11.8	1.90
Pb	9.47	11.0	1.83
Bi	9.90	11.5	1.87
Sb	10.9	12.7	1.96

Two nearly-free
electron metals

Fermi velocities
about 0.01c,
pretty fast

Electrical Conductivity:

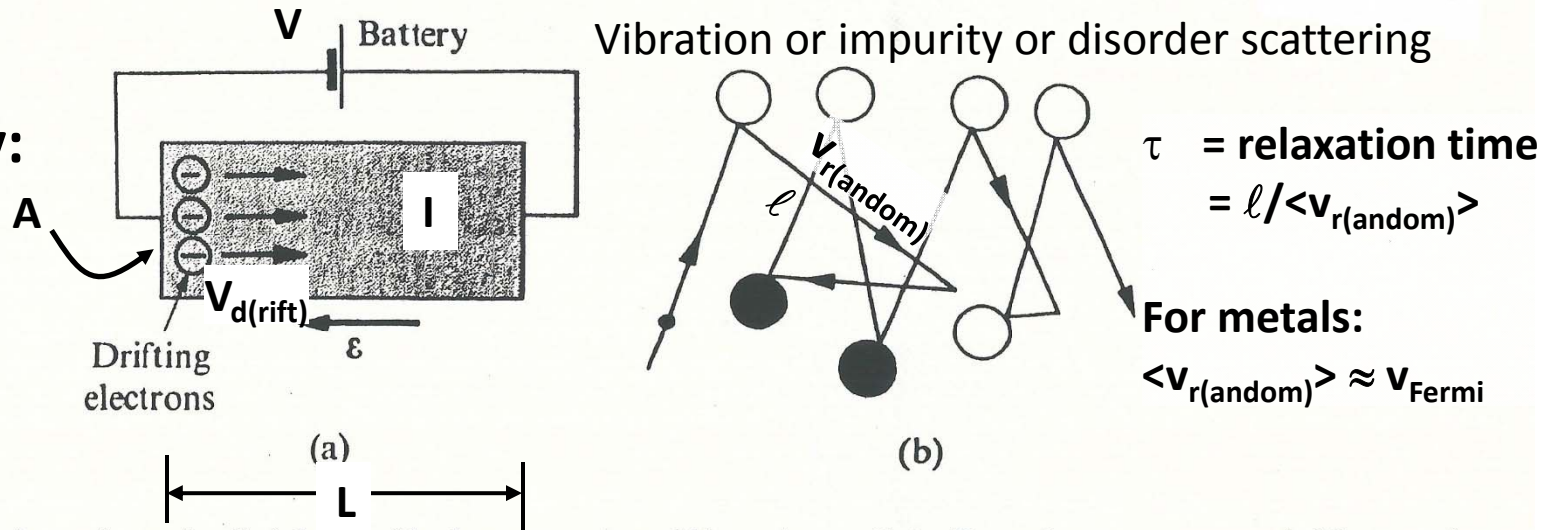


Fig. 4.4 (a) An electric field applied to a metallic wire. (b) Random versus drift motion of electrons. Circles represent scattering centers.

Vibration or impurity or disorder scattering

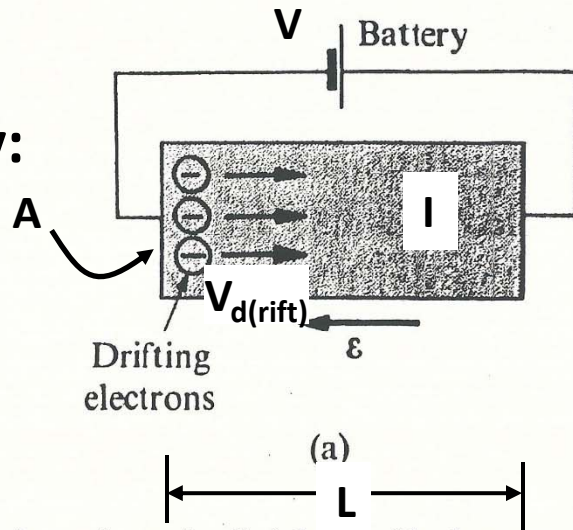
$$J = \frac{I}{A}, \quad \mathcal{E} = \text{DUEC. FIBLA} = \frac{V}{L}, \quad R = \frac{L\rho}{A} \rightarrow \text{RESISTIVITY}$$



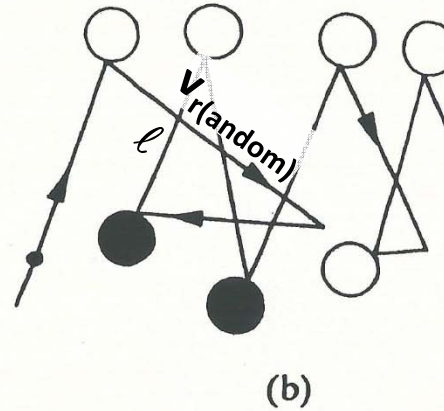
$$J = \sigma \mathcal{E} = (-Ne)v_d$$

$$\sigma \equiv \frac{1}{\rho} = \text{CONDUCTIVITY}$$

Electrical Conductivity:



Vibration or impurity or disorder scattering



$$\tau = \text{relaxation time} = l / \langle v_{r(\text{andom})} \rangle$$

For metals:

$$\langle v_{r(\text{andom})} \rangle \approx v_{\text{Fermi}}$$

Fig. 4.4 (a) An electric field applied to a metallic wire. (b) Random versus drift motion of electrons. Circles represent scattering centers.

$$J = \frac{I}{A}, \quad E = \text{ELEC. FIELD} = \frac{V}{L}, \quad R = \frac{L\rho}{A} \quad \rho \rightarrow \text{RESISTIVITY}$$



$$\sigma \equiv \frac{1}{\rho} = \text{CONDUCTIVITY}$$

$$J = \sigma E = (-Ne)v_d = \frac{Ne^2\tau}{m^*} E \Rightarrow \boxed{\sigma = \frac{Ne^2\tau}{m^*}}$$

ELECTRON EQU. OF MOTION: $m^* = \text{EFFECTIVE MASS} = m_e$ IF FREE

$$0 \equiv m^* \frac{dv_d}{dt} = -eE - m^* \frac{v_d}{\tau}$$

STEADY STATE

$$v_d = -\frac{e\tau}{m^*} E$$

FRICTION FORCE DUE TO COLLISIONS:
 $\tau = \text{COLL. TIME}$

Electrical conductivity and the free-electron gas

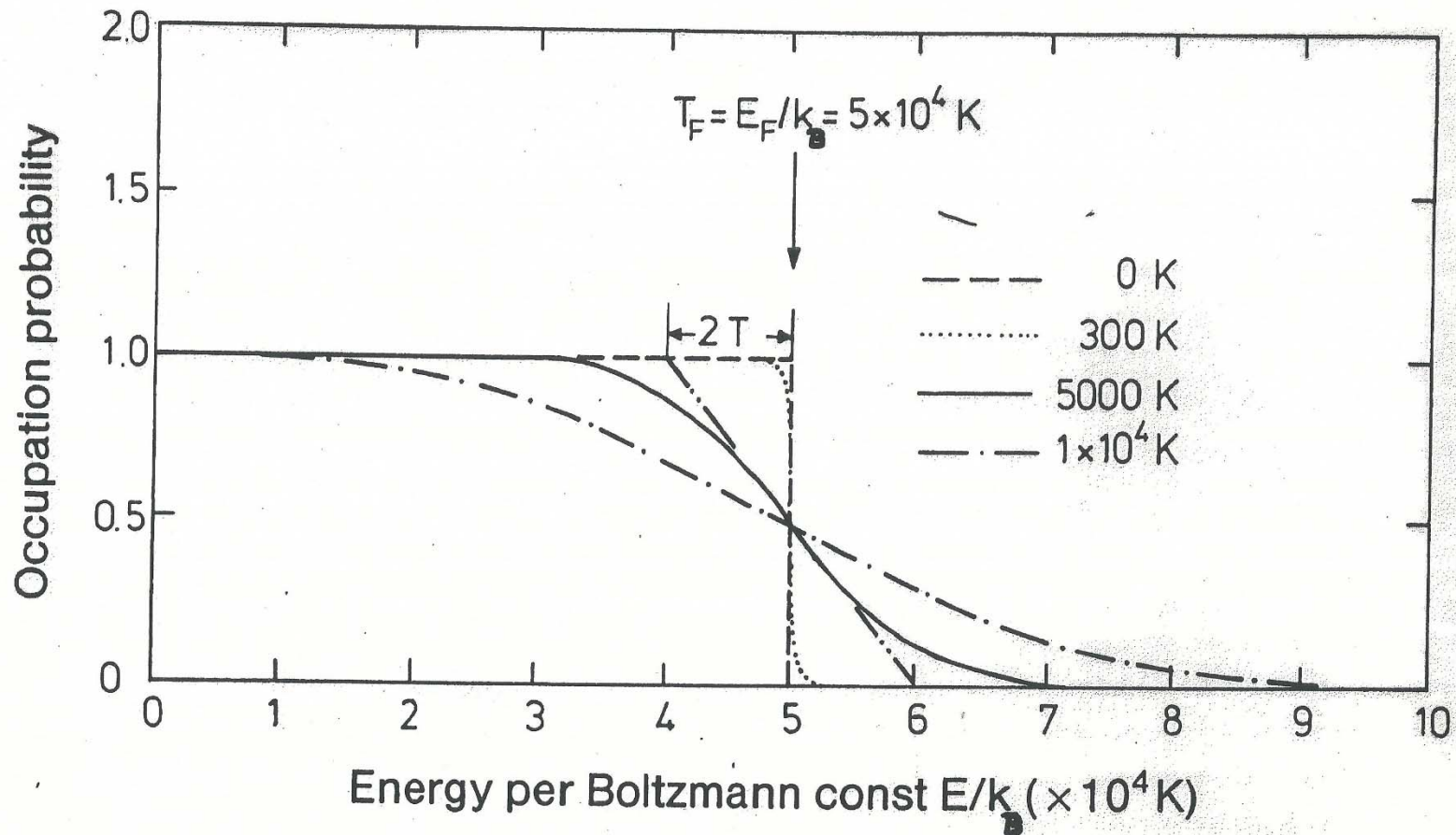
Table 4.1

Electrical Conductivities and Other Transport Parameters for Metals

Element	σ , $\text{ohm}^{-1} \text{m}^{-1}$	N , m^{-3}	τ , s	v_F , m/s	l , Å	E_F , eV	E_F (obs.), eV	m^*/m_0
Li	1.07×10^7	4.6×10^{28}	0.9×10^{-14}	1.3×10^6	110	4.7	3.7	1.2
Na	2.11	2.5	3.1	1.1	350	3.1	2.5	1.2
K	1.39	1.3	4.3	0.85	370	2.1	1.9	1.1
Rb	0.80	1.1	2.75	0.80	220	1.8	—	—
Cs	0.50	0.85	—	0.75	160	1.5	—	—
Cu	5.88	8.45	2.7	1.6	420	7.0	7.0	1.0
Ag	6.21	5.85	4.1	1.4	570	5.5	—	—
Au	4.55	5.90	2.9	1.4	410	5.5	—	—
Zn	1.69	13.10	—	1.82	—	9.4	11.0	0.85
Cd	1.38	9.28	—	1.62	—	7.5	—	—
Hg	0.10	—	—	—	—	—	—	—
Al	3.65	18.06	—	2.02	—	11.6	11.8	—
Ga	0.67	15.30	—	1.91	—	10.3	—	—
In	1.14	11.5	—	1.74	—	8.6	—	—

Values quoted are for metals at room temperature. The concentration is found by using the usual chemical valences. The Fermi velocity v_F and E_F are evaluated by using $m^* = m_0$ and the appropriate equation from Section 4.6. The Fermi energy E_F (observed) is the experimentally determined value as discussed in Chapter 6. The effective mass m^* is determined by using the experimental value E_F (observed) and the relation $E_F = (\hbar^2/2m^*)(3\pi^2N)^{2/3}$, Eq. (4.34).

Fermi-Dirac Distribution as a Function of Temperature



Free-electron density of states at finite temperature

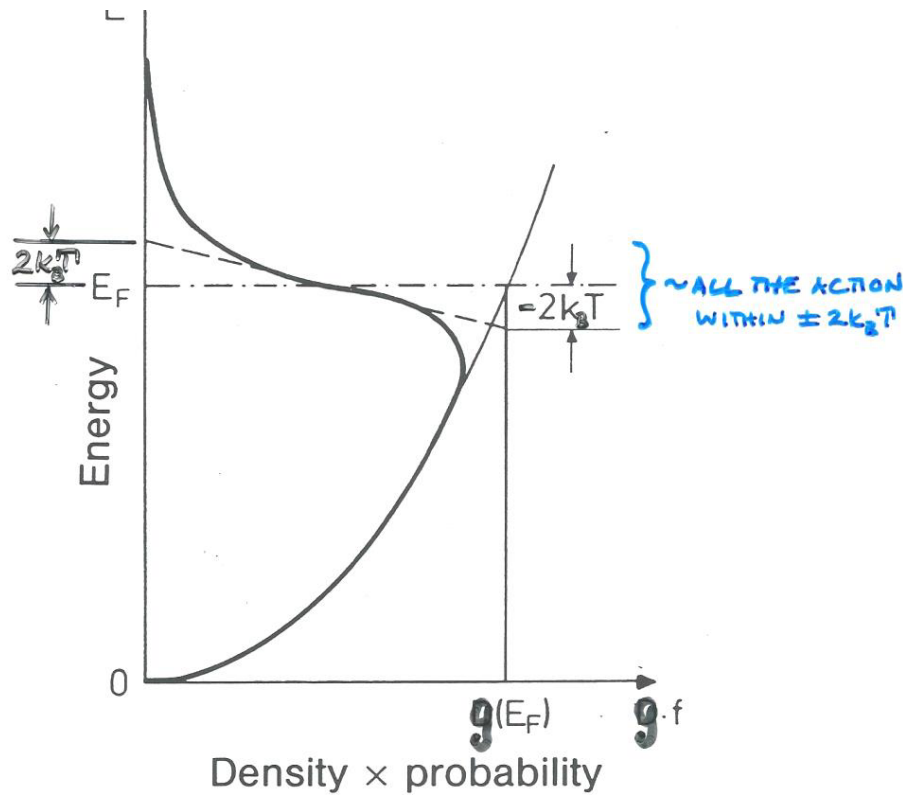


Fig. 6.7. Explanation of the specific heat capacity of quasi-free metal electrons. The effect of raising the temperature from 0K to T is to allow electrons from $\leq 2kT$ below the Fermi energy to be promoted to $\leq 2kT$ above E_F . The tangent (---) intersects the energy axis at $E_F + 2kT$

Heat capacity: Debye model combined with low-T electronic contributions

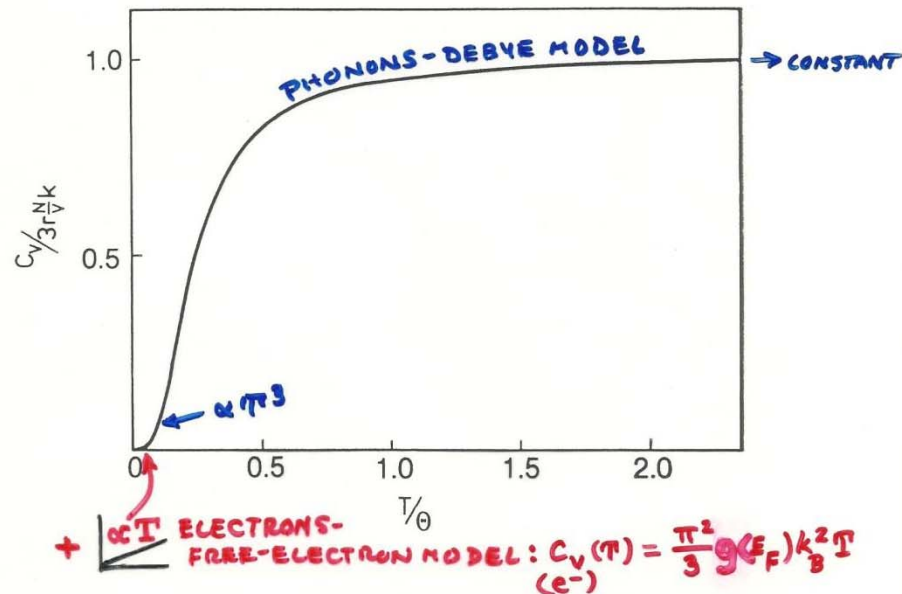
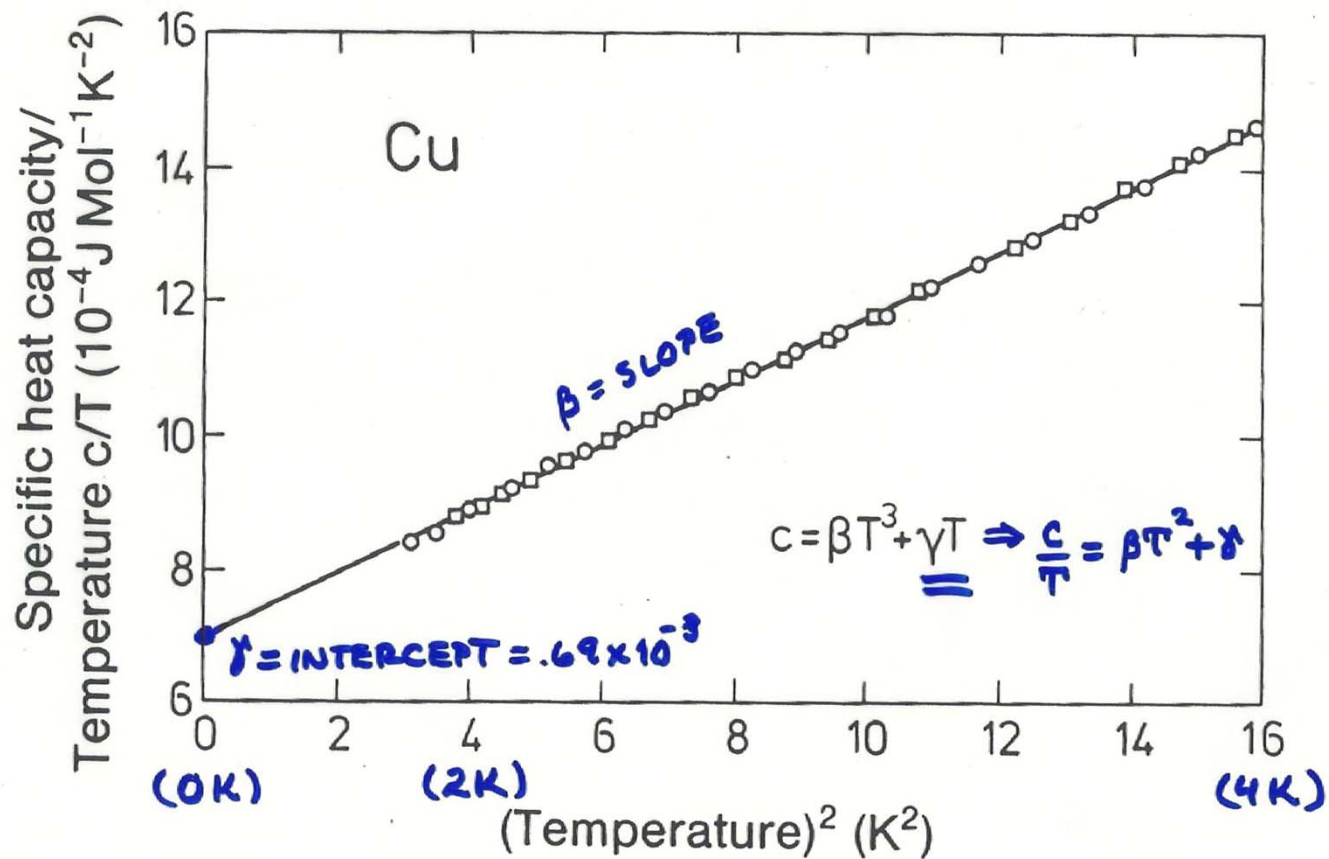


Fig. 5.3. The specific heat capacity per unit volume according to the Debye model. The specific heat is normalized to the Boltzmann constant k , the density of unit cells N/V and the number of atoms in the unit cell r . In this model different materials are only distinguished by their values of Debye temperature Θ

$$C_v(T) = \frac{3rNk}{V} 3 \left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{\left(\frac{\hbar\omega}{kT}\right)^4 e^{\frac{\hbar\omega}{kT}} d\left(\frac{\hbar\omega}{kT}\right)}{\left(e^{\frac{\hbar\omega}{kT}} - 1\right)^2}$$

$\frac{N}{V} = \frac{1}{V_{\text{cell}}}$

Heat capacity: the low-T regime



The nearly-free electron model

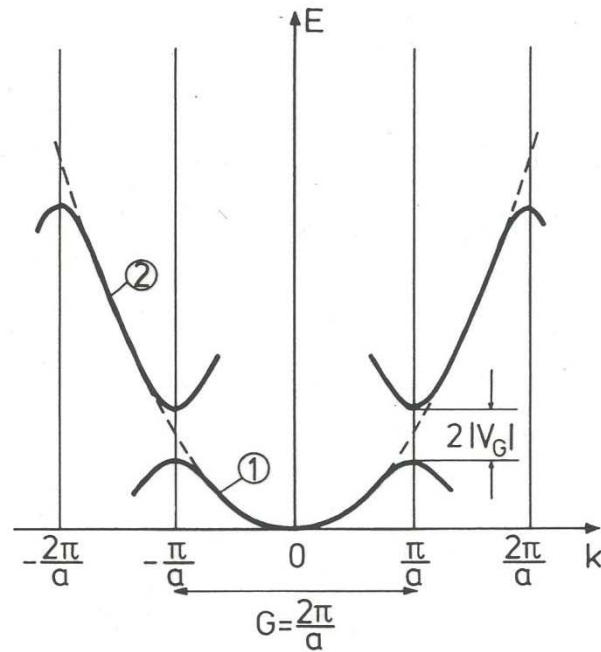


Fig. 7.5. Splitting of the energy parabola of the free electron (---) at the edges of the first Brillouin zone ($k = \pm\pi/a$ in the one-dimensional case). To a first approximation the gap is given by twice the corresponding Fourier coefficient V_G of the potential. Periodic continuation over the whole of k -space gives rise to continuous bands ① and ②, shown here only in the vicinity of the original energy parabola

The nearly-free electron model

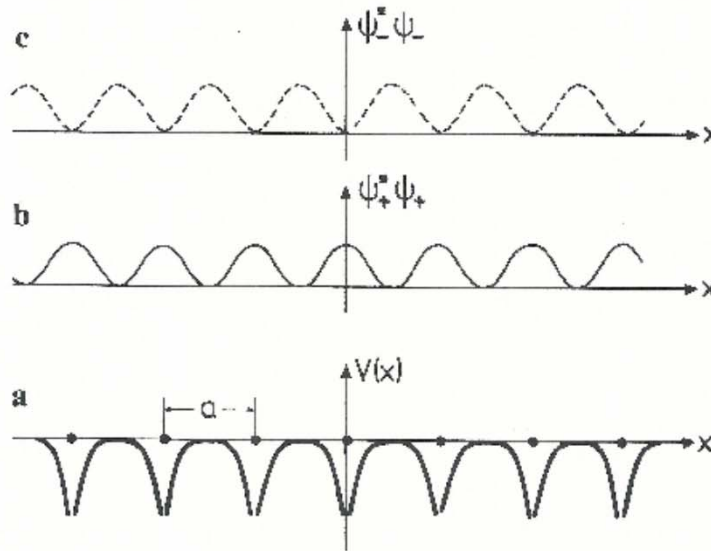


Fig. 7.4 a. Qualitative form of the potential energy $V(x)$ of an electron in a one-dimensional lattice. The positions of the ion cores are indicated by the points with separation a (lattice constant). b Probability density $\rho_+ = \psi_+^* \psi_+$ for the standing wave produced by Bragg reflection at $k = \pm \pi/a$ (upper edge of band ① in Fig. 7.5). c Probability density $\rho_- = \psi_-^* \psi_-$ for the standing wave at the lower edge of band ② (Fig. 7.5) at $k = \pm \pi/a$

Higher energy:

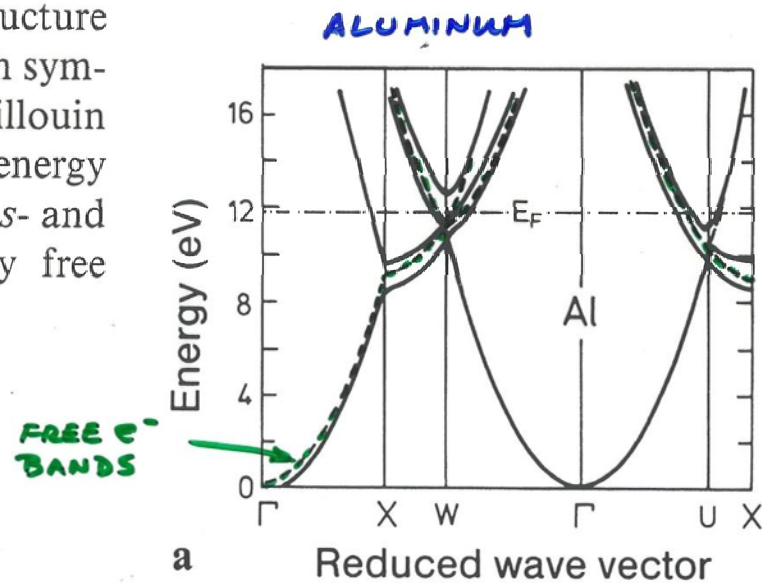
$$\psi_- \approx e^{iGx/2} - e^{-iGx/2} \propto \sin(\pi x/a)$$

Lower energy:

$$\psi_+ \approx e^{iGx/2} + e^{-iGx/2} \propto \cos(\pi x/a)$$

Aluminum band structure compared to free-electron states

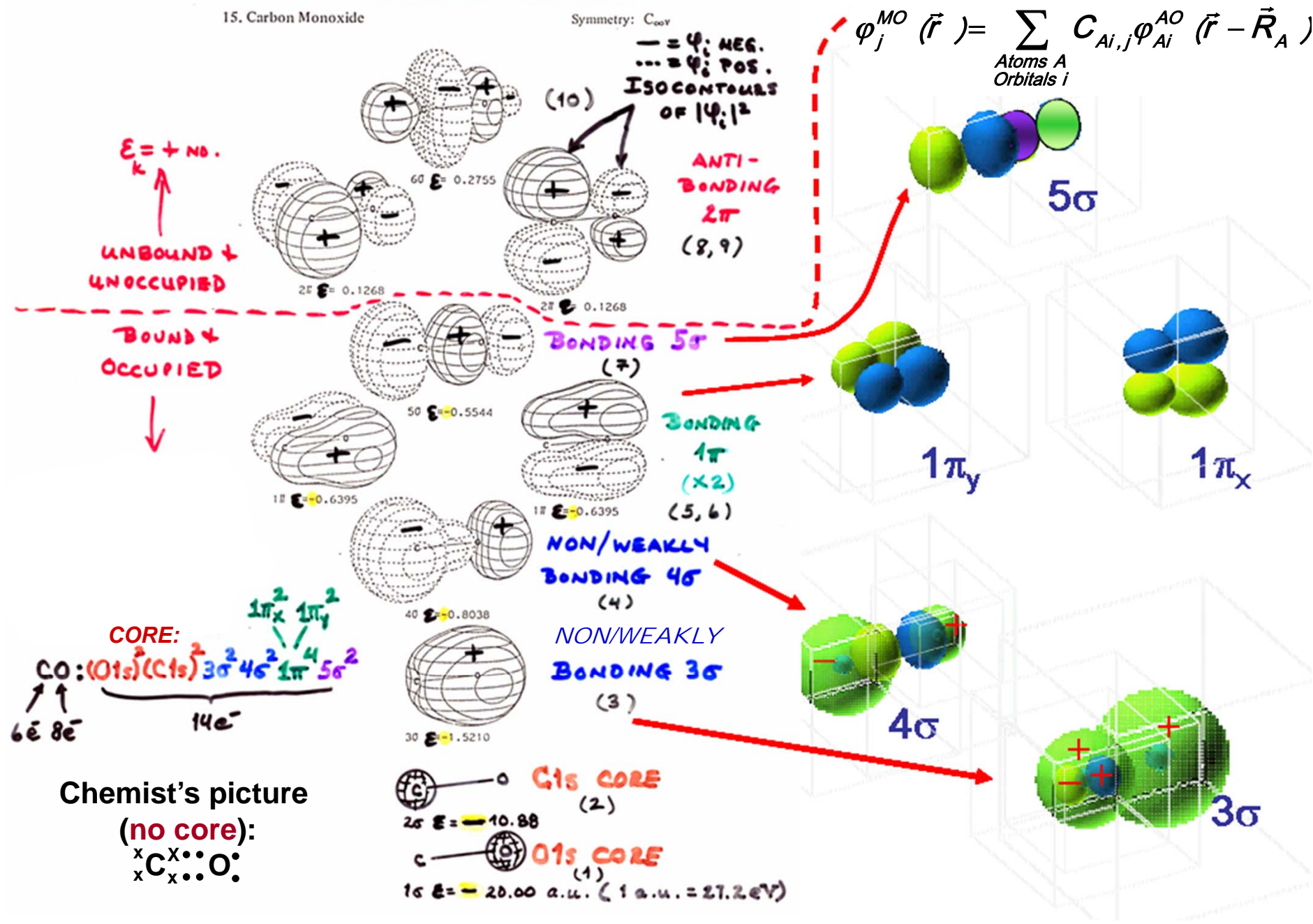
Fig. 7.11a. Theoretical bandstructure $E(k)$ for Al along directions of high symmetry (Γ is the center of the Brillouin zone). The dotted lines are the energy bands that one would obtain if the s - and p -electrons in Al were completely free (“empty” lattice). After [7.3].



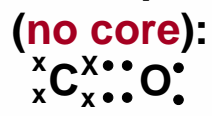
The LCAO-MO or tight-binding picture for CO:

Atomic orbital makeup

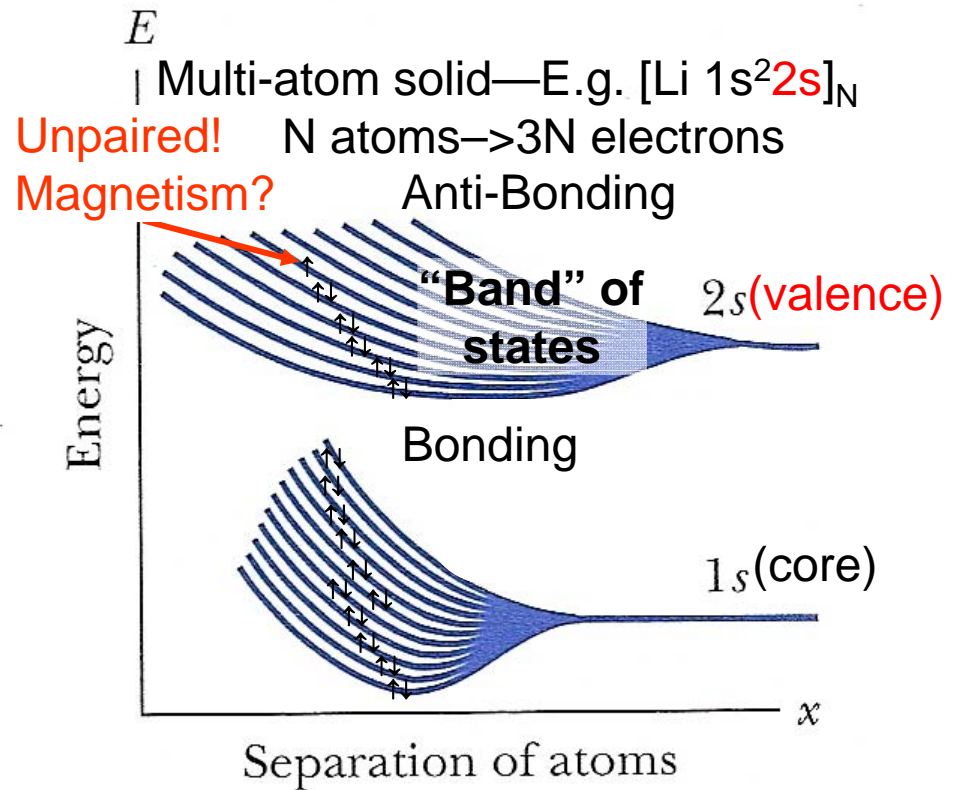
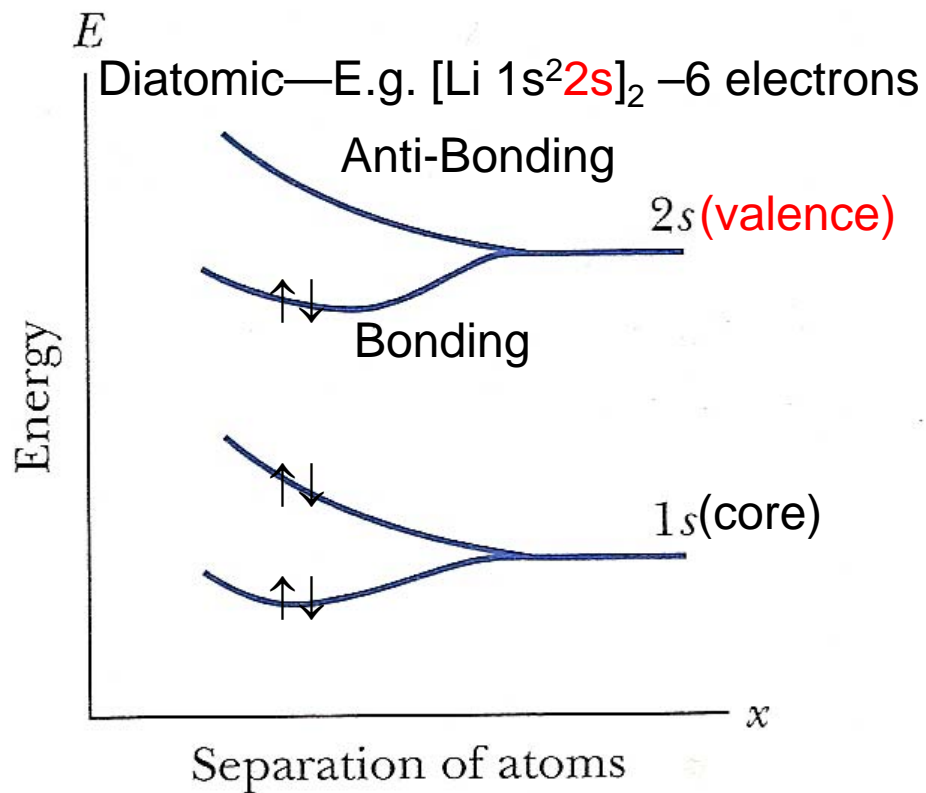
$$\varphi_j^{MO}(\vec{r}) = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}} C_{Ai,j} \varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$



Chemist's picture



Bonding in solids/solid-state devices as an extension of that in molecules



Example: $N = 11$: 22 e^- in 1s-derived
11 e^- in 2s-derived

For many cases, we can again use atomic orbitals as the basis functions: the Tight Binding Model

Recall for a molecule:

$$\varphi_j^{MO}(\vec{r}) = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^N C_{Ai,j} \varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

For a solid with N atoms: (Omar, Section 5.8)

$$\varphi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^N e^{i\vec{k}\cdot\vec{R}_A} C_{Ai,\vec{k}} \varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

Is it Bloch?

$$= e^{i\vec{k}\cdot\vec{r}} \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^N e^{-i\vec{k}\cdot(\vec{r}-\vec{R}_A)} C_{Ai,\vec{k}} \varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

Yes!

The Tight-Binding Model

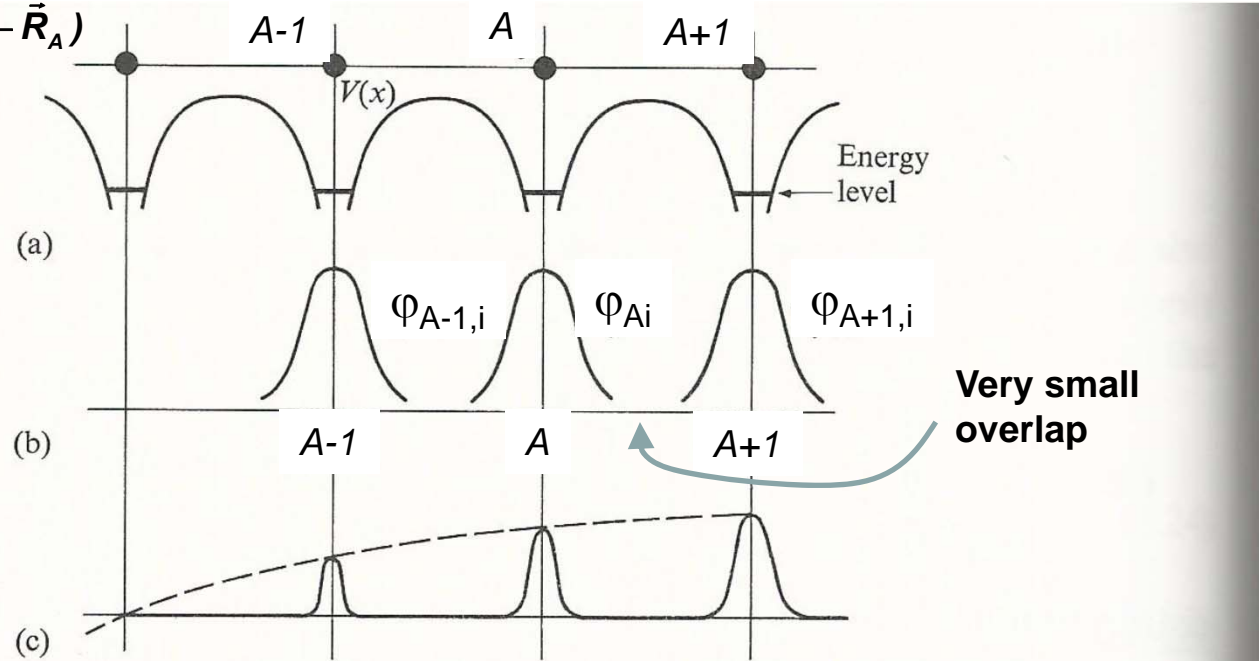


Fig. 5.14 The tight-binding model. (a) The crystal potential. (b) The atomic wave functions. (c) The corresponding Bloch function.

1D Tight-Binding Model: The potential

$$V(x) = v(x) + V'(x), \quad (5.35)$$

where $v(x)$ is the atomic potential due to the atom at the origin and $V'(x)$ is that due to all the other atoms. These potentials are plotted in Figs. 5.15(a) and (b).

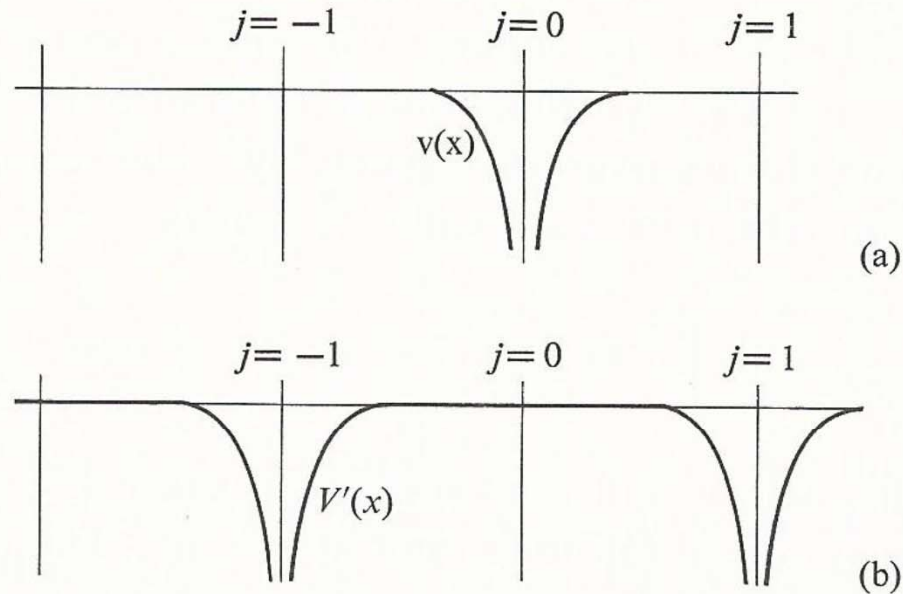


Fig. 5.15 The splitting of the crystal potential into (a) an atomic potential and (b) the remainder of the crystal potential.

1D Tight-Binding Model

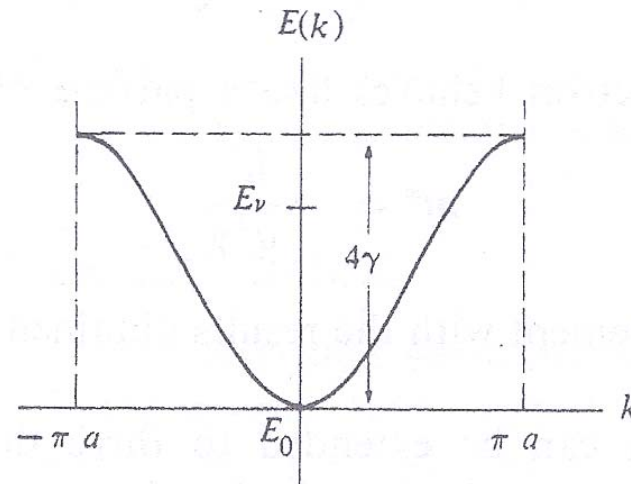


Fig. 5.16 The dispersion curve in the tight-binding model.

$$E(k) = E_v - \beta - 2\gamma \cos ka.$$

$$\langle \phi_{v,atom}(x) | \hat{H}_{solid}(x) | \phi_{v,atom}(x) \rangle = E_{v,atom} - \beta (+no.)$$

$$\beta = -\langle \phi_{v,atom}(x) | V'_{solid}(x) | \phi_{v,atom}(x) \rangle$$

$$\gamma (\text{the bonding interaction}) = -\langle \phi_{v,atom}(x) | \hat{H}_{solid}(x) | \phi_{v,atom}(x-a) \rangle$$

$$\approx \langle \phi_{v,atom}(x) | V'_{solid}(x-a) | \phi_{v,atom}(x-a) \rangle, \text{ an "overlap integral"}$$

3D Tight-Binding Model

$$E(k) \approx E_i - A_i - 2B_i(\cos k_x a + \cos k_y a + \cos k_z a)$$

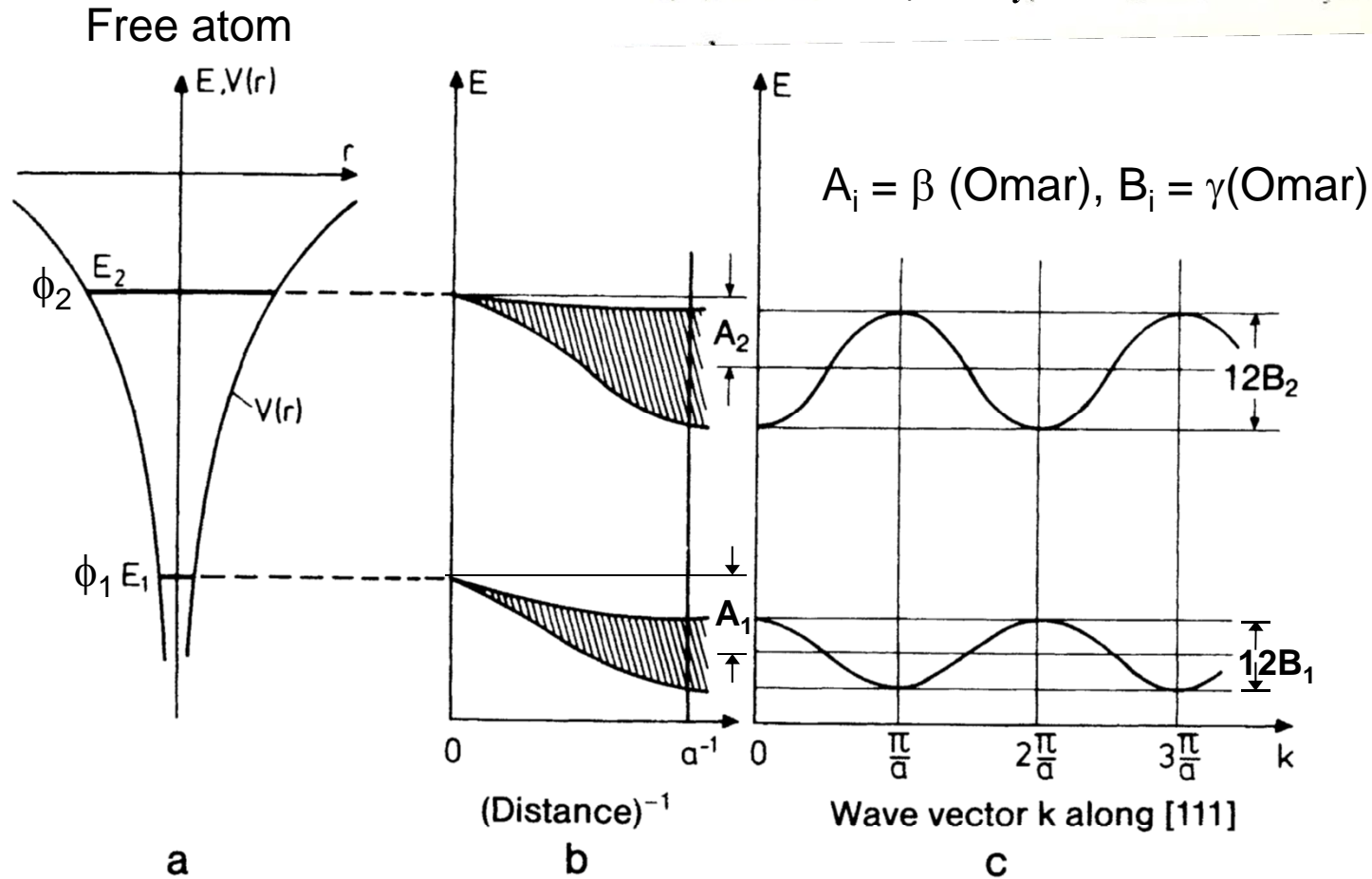


Fig. 7.8a–c. Qualitative illustration of the result of a tight-binding calculation for a primitive cubic lattice with lattice constant a . (a) Position of the energy levels E_1 and E_2 in the potential $V(r)$ of the free atom. (b) Reduction and broadening of the levels E_1 and E_2 as a function of the reciprocal atomic separation r^{-1} . At the equilibrium separation a the mean energy decrease is A and the width of the band is $12B$. (c) Dependence of the one-electron energy E on the wave vector $k(1, 1, 1)$ in the direction of the main diagonal [111]

Ibach and Luth

Electronic bands and density of states for a transition metal-Copper

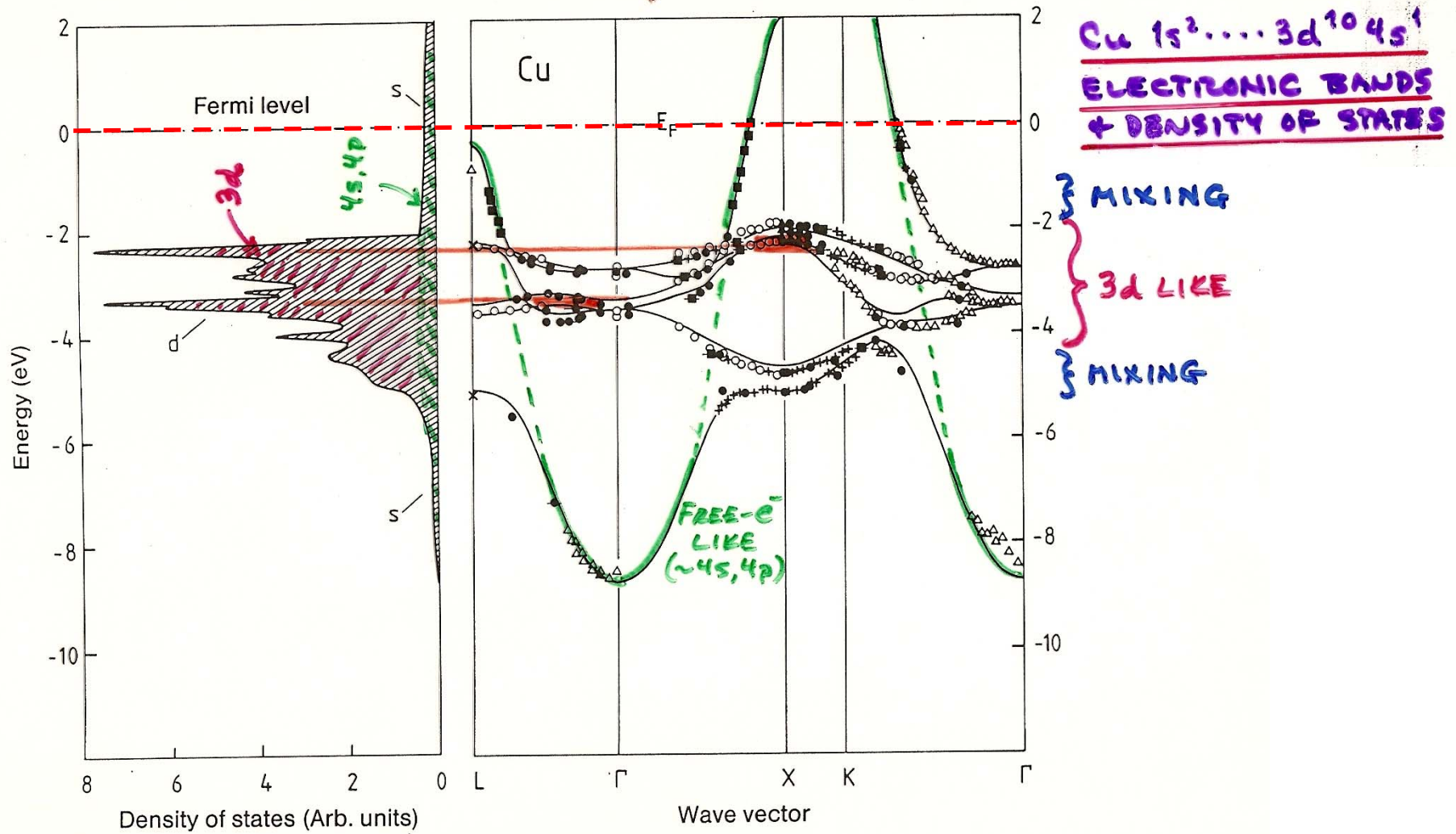
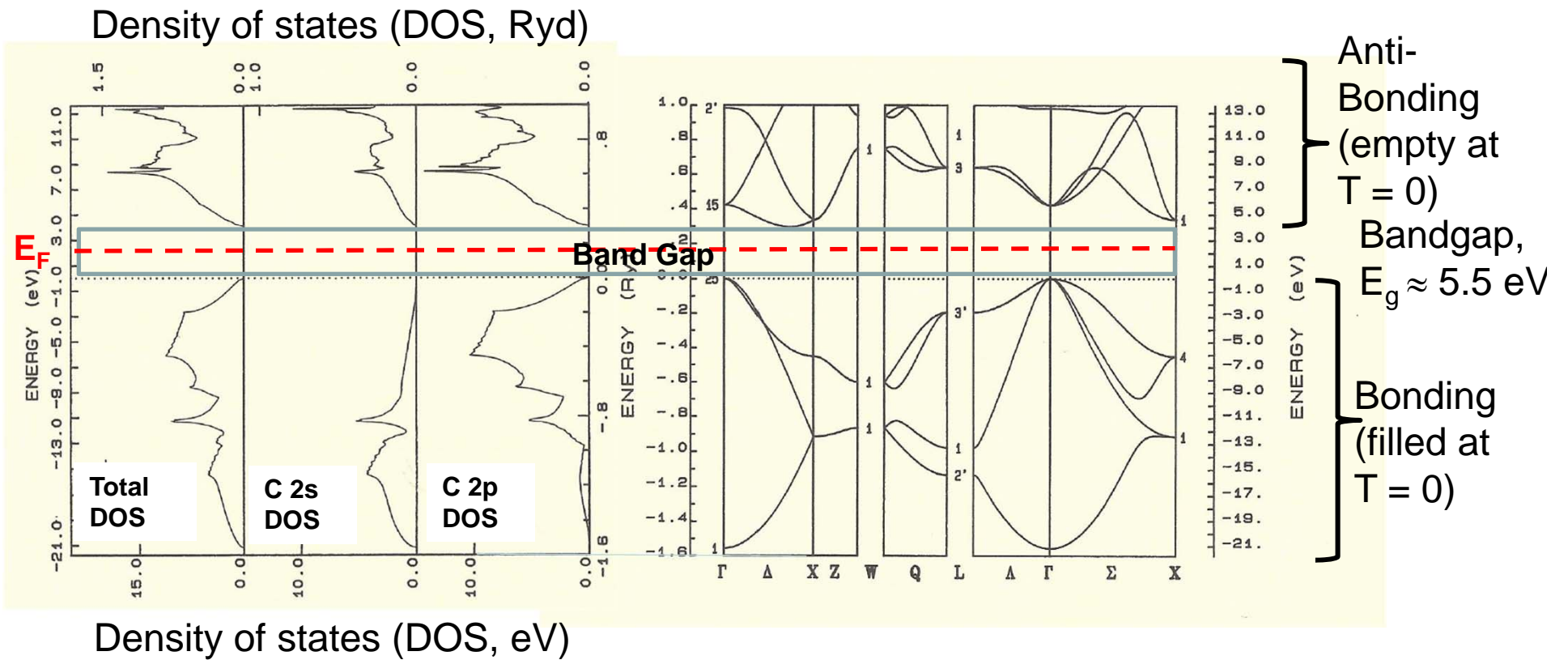
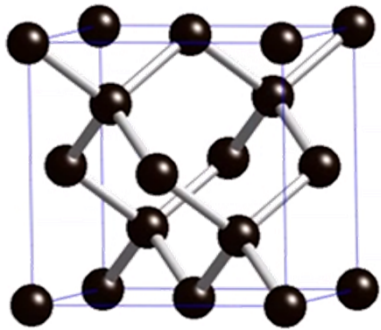


Fig. 7.12. Bandstructure $E(k)$ for copper along directions of high crystal symmetry (right). The experimental data were measured by various authors and were presented collectively by Courths and Hüfner [7.4]. The full lines showing the calculated energy bands and the density of states (left) are from [7.5]. The experimental data agree very well, not only among themselves, but also with the calculation

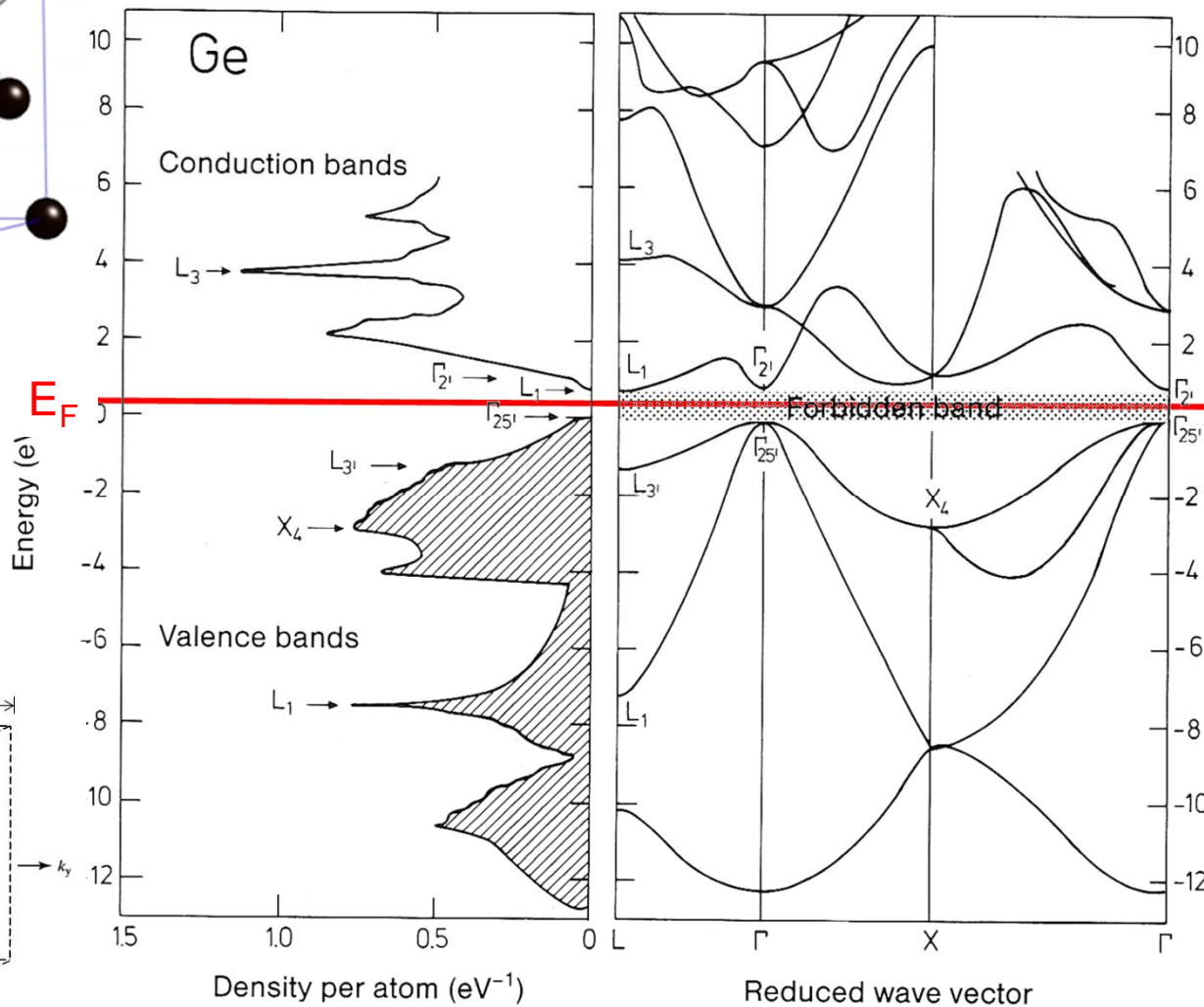
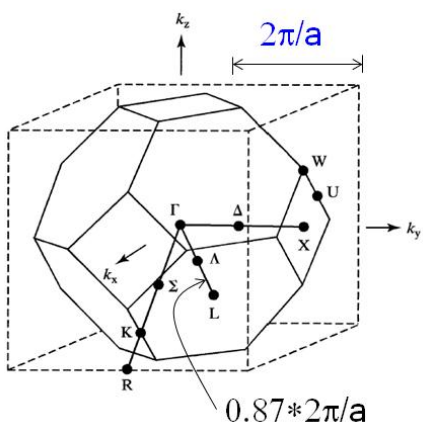
Electronic bands and density of states for an insulator-Carbon: Diamond—
 $1s^2 2s^2 2p^2$



Electronic bands and density of states for a semiconductor-Germanium—
 $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$



Diamond Structure = fcc + 2-atom basis

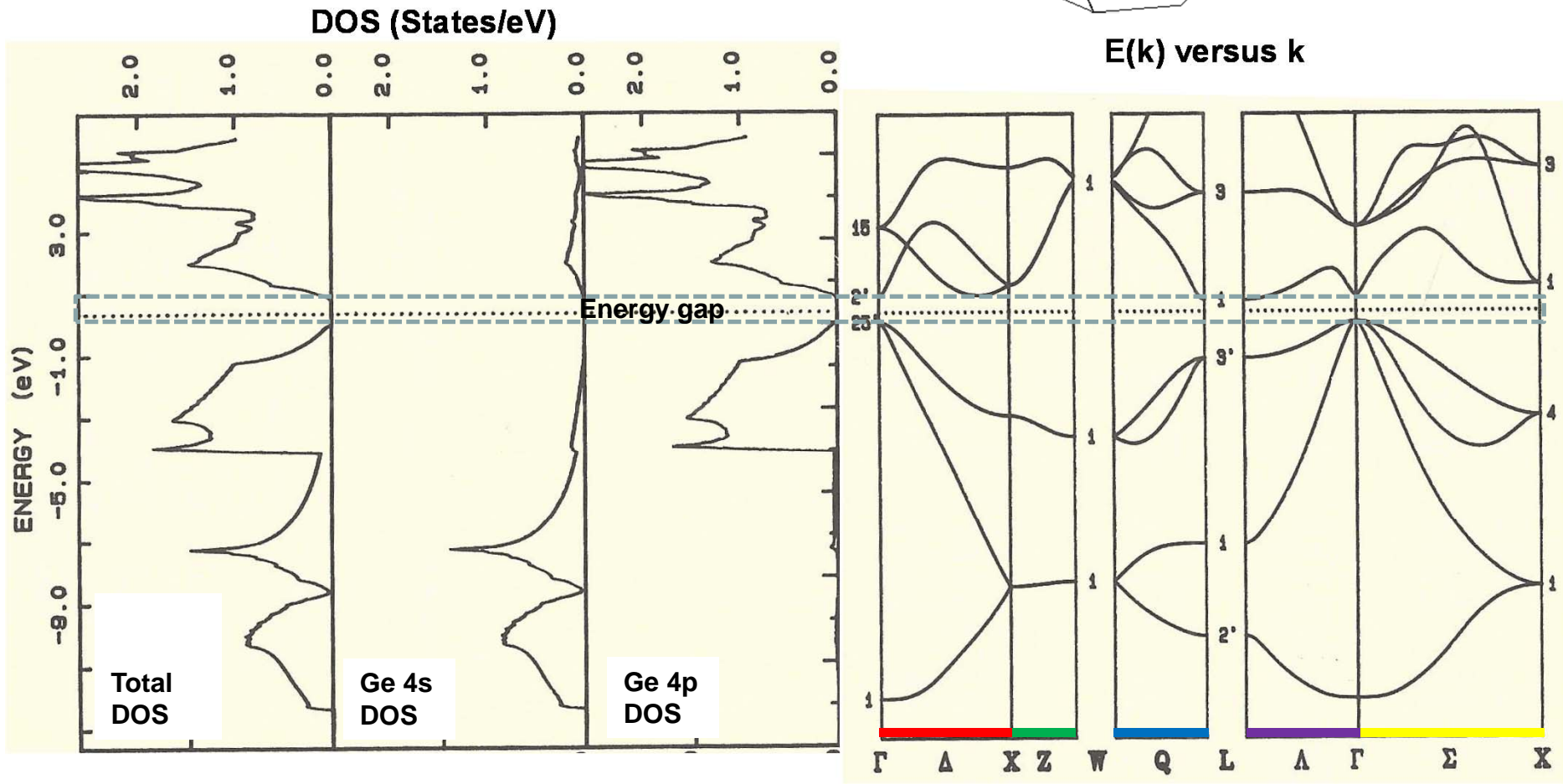
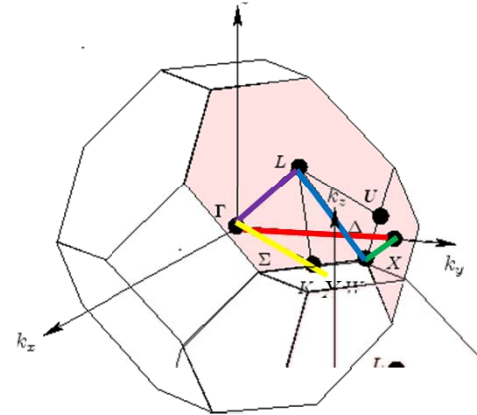


Anti-Bonding (empty at $T = 0$)

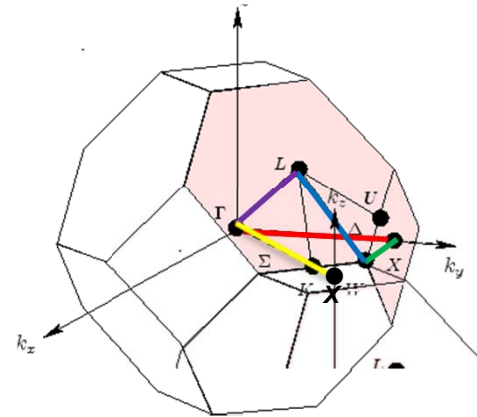
Bandgap, $E_g \approx 0.7$ eV

Bonding (filled at $T = 0$)

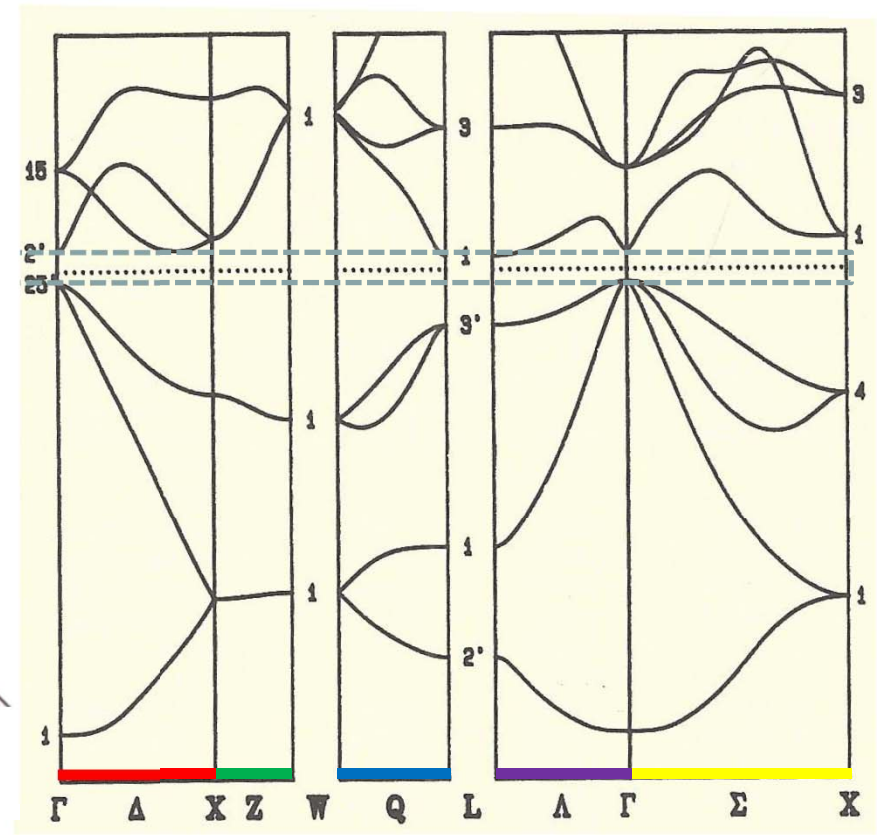
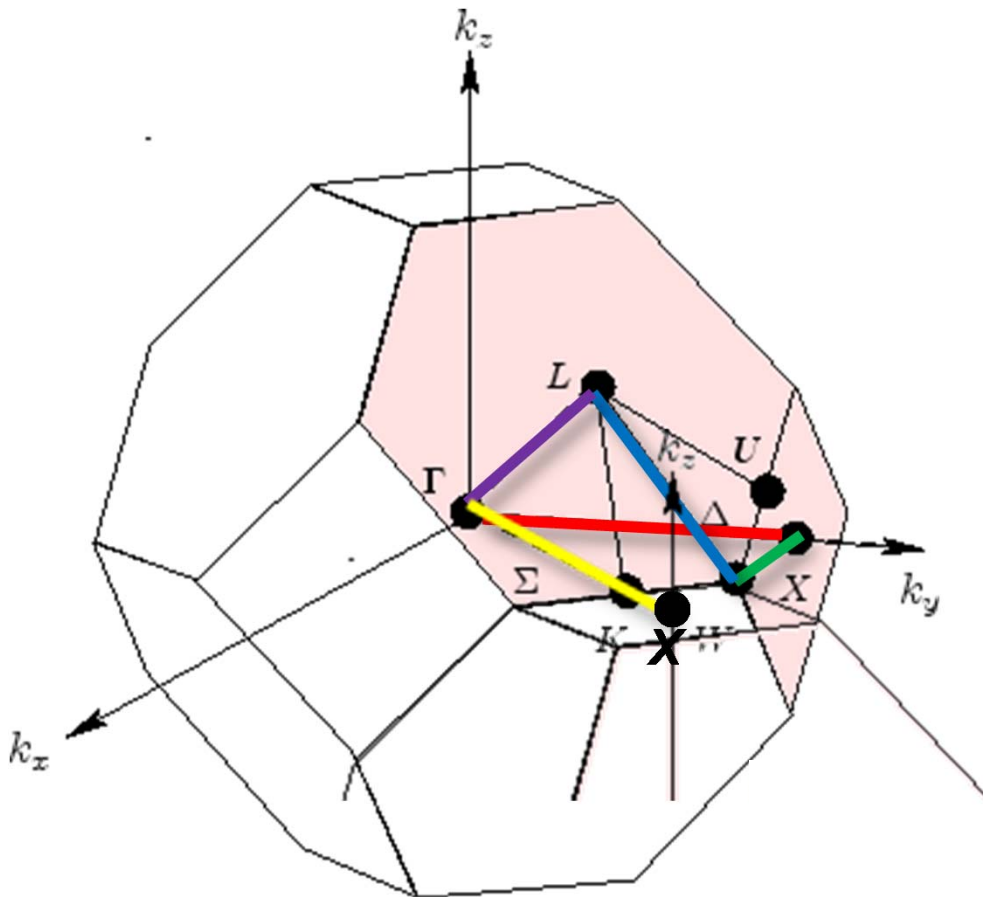
Electronic bands and density of states for a semiconductor-Germanium (cont'd)



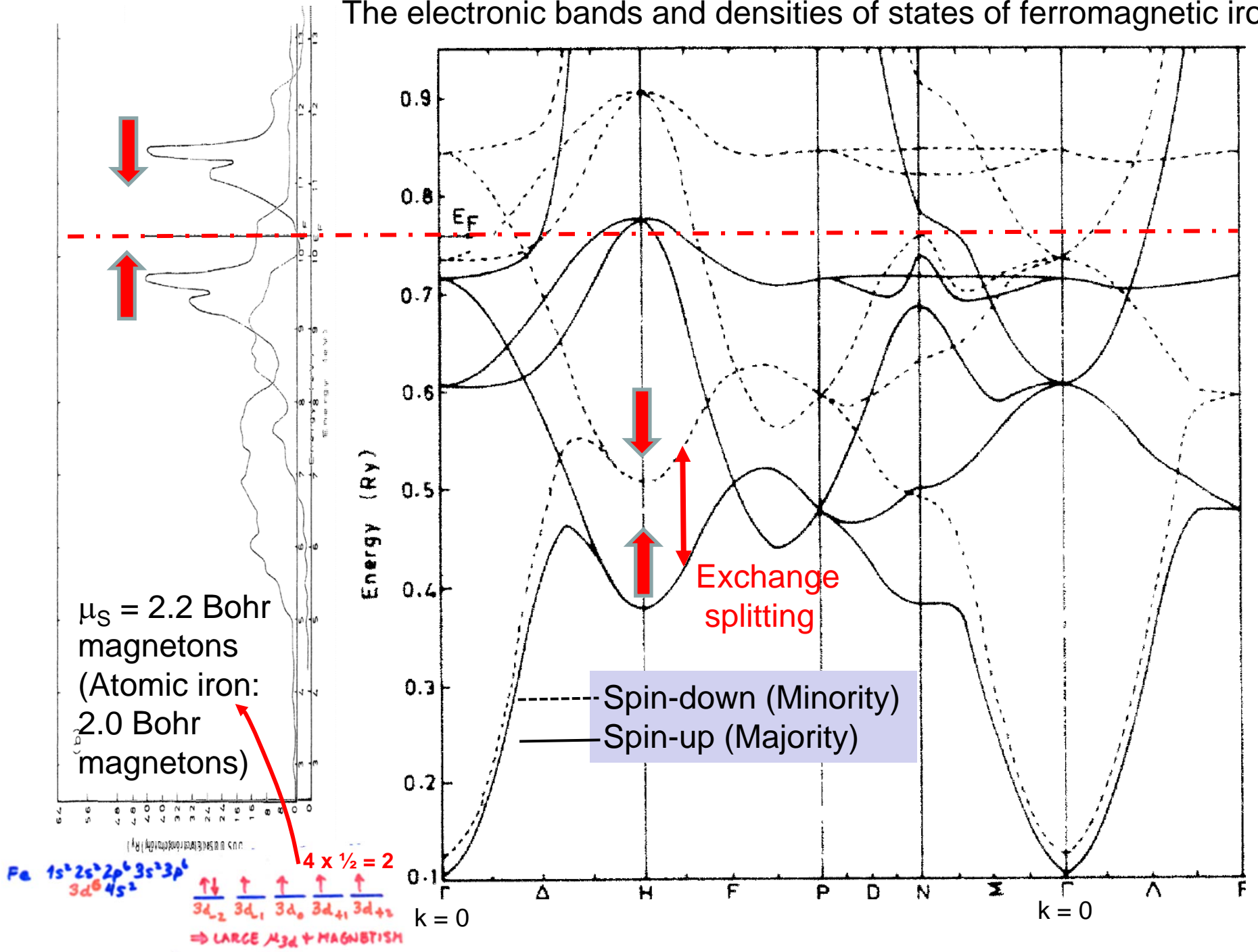
Electronic bands and density of states for a semiconductor-Germanium (cont'd)



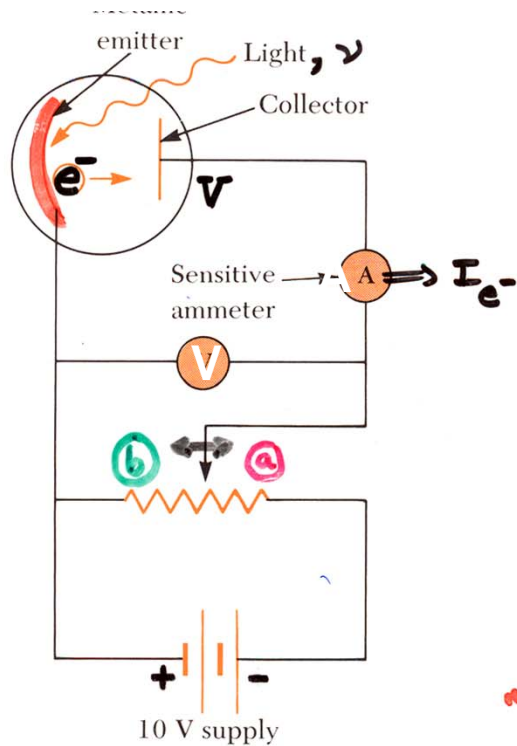
E(k) versus k



The electronic bands and densities of states of ferromagnetic iron



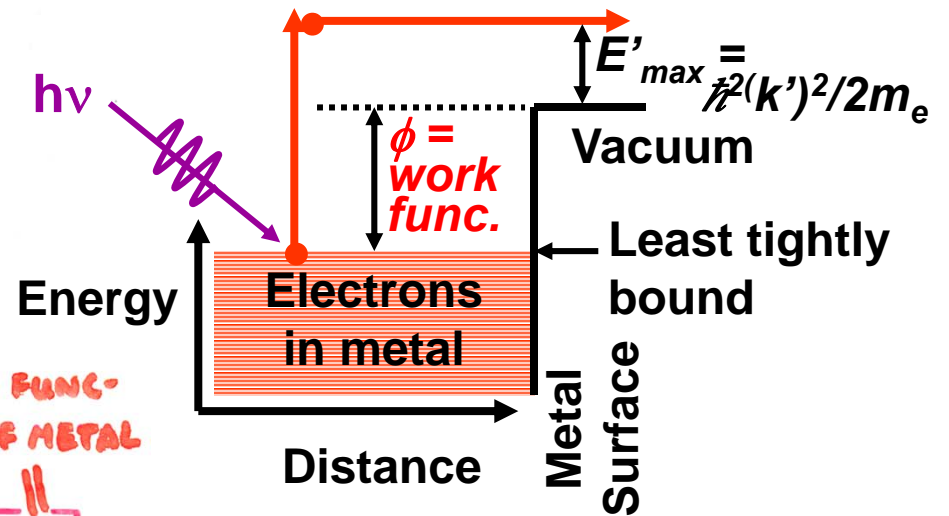
The Photoelectric Effect:



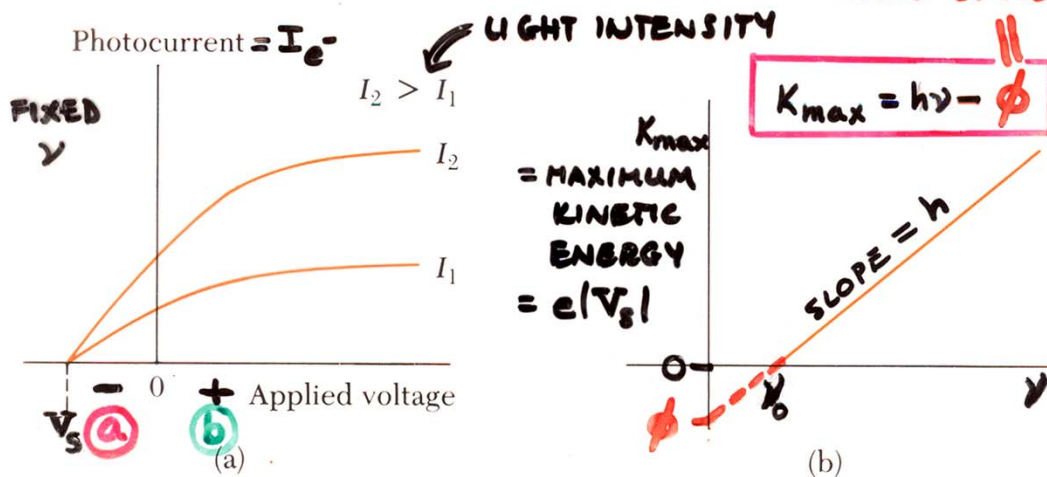
Einstein, 1905:
Light can only emit or absorb energy in quantized units:

$$E_{\text{photon}} = h\nu$$

$h = \text{Planck's constant!}$

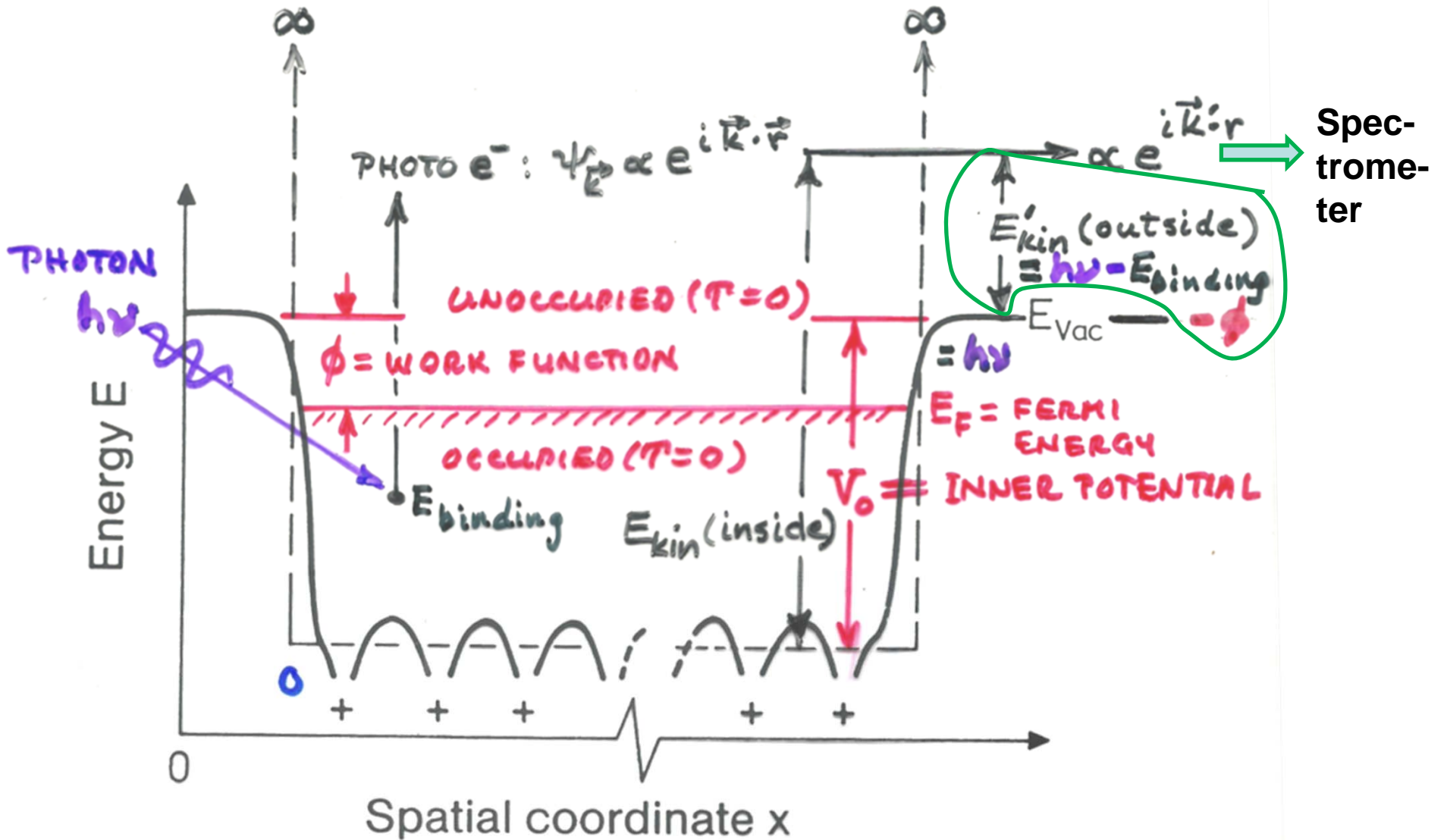


"WORK FUNCTION" OF METAL

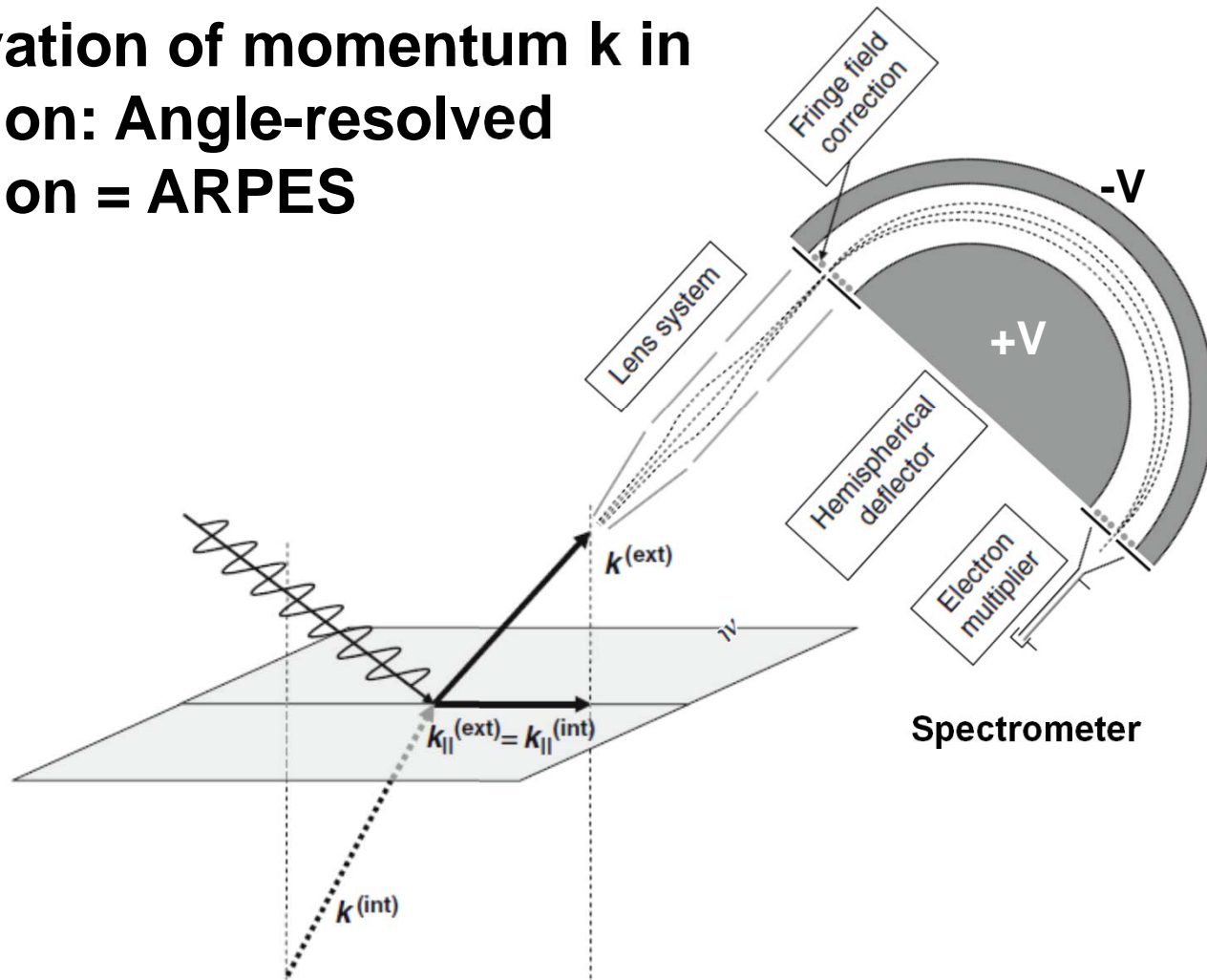
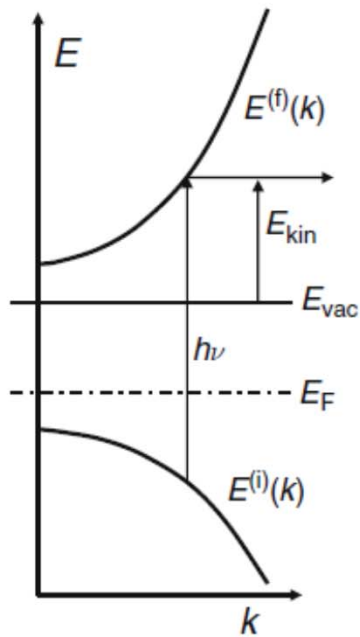


Light behaves in some ways like a particle of zero rest mass and:
 $E_{\text{photon}} = h\nu$

The conservation of energy in photoelectron spectroscopy = "photoemission:"



The conservation of momentum k in photoemission: Angle-resolved photoemission = ARPES



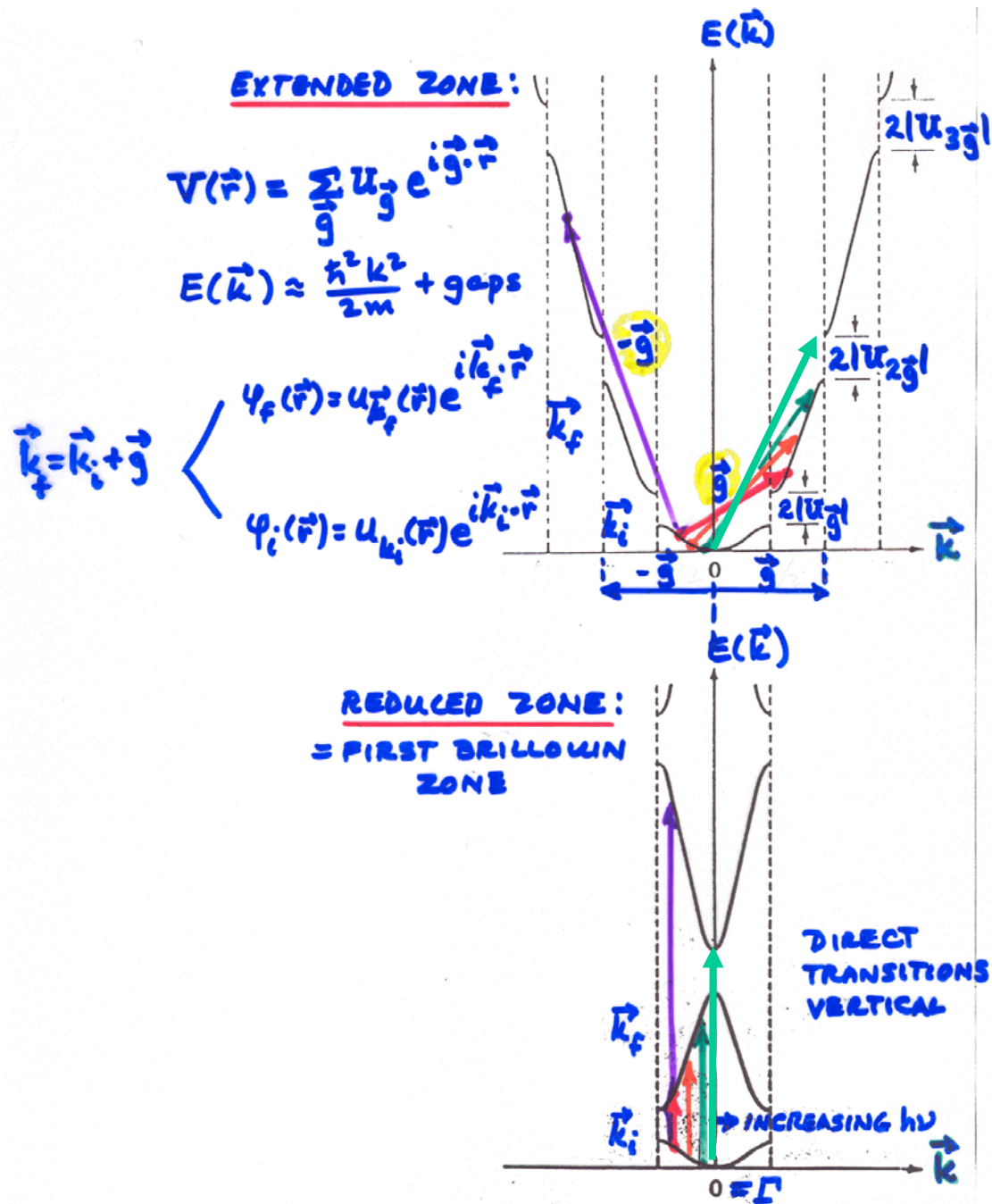
$$\Psi_{\vec{k}^i}(\vec{r}) = u_{\vec{k}^i}(\vec{r}) e^{i\vec{k}^i \cdot \vec{r}}$$

$$\Psi_{\vec{k}^f}(\vec{r}) = u_{\vec{k}^f}(\vec{r}) e^{i\vec{k}^f \cdot \vec{r}}$$

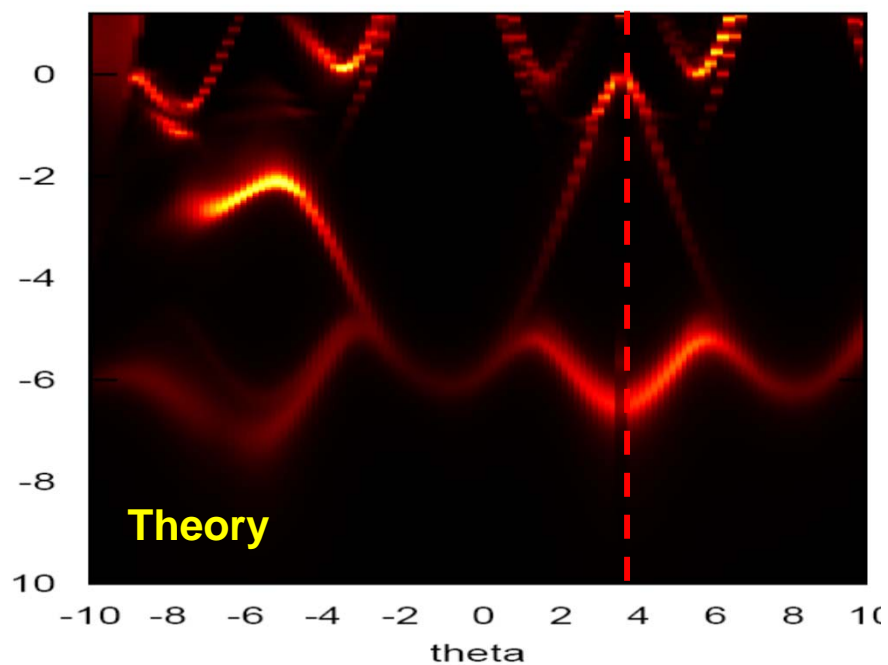
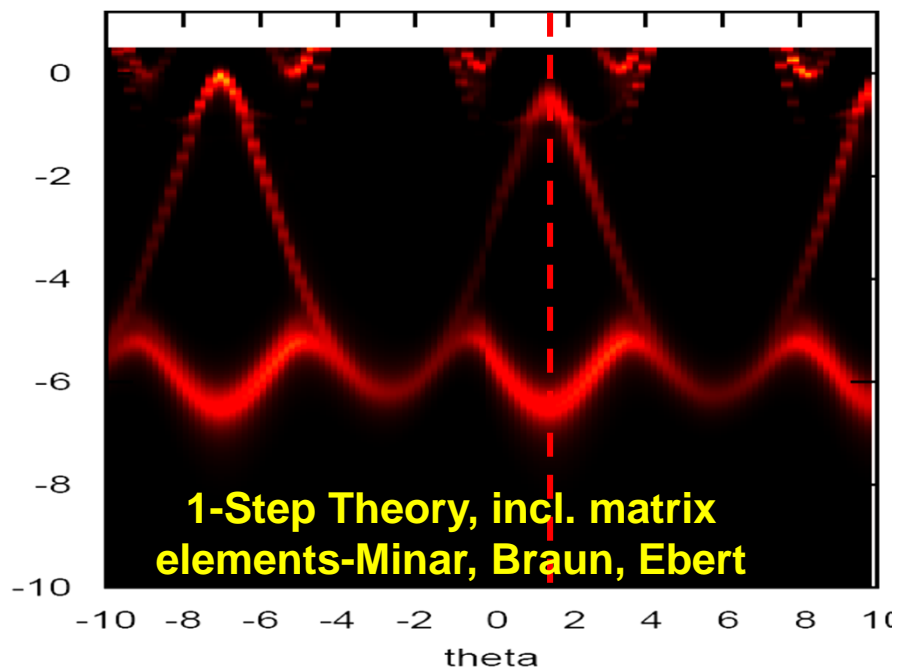
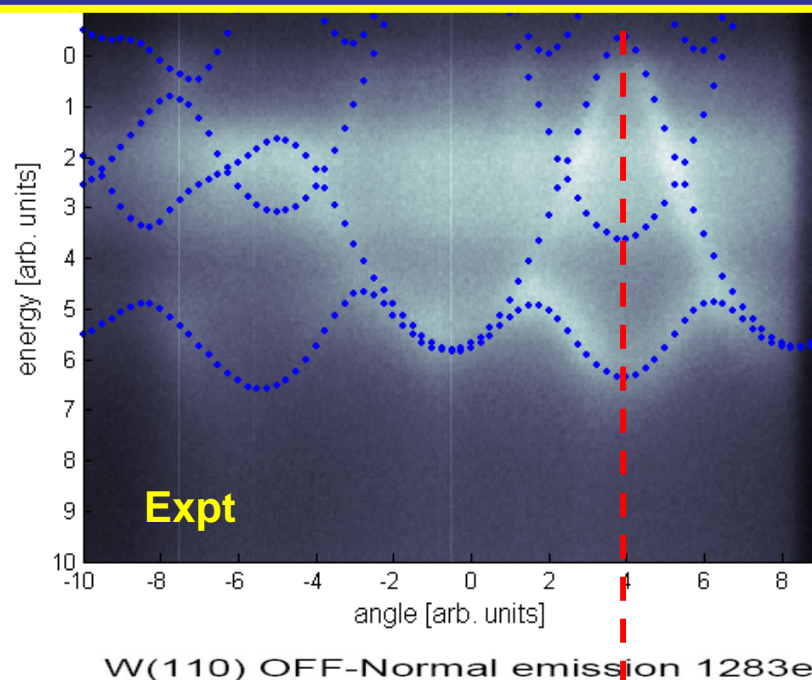
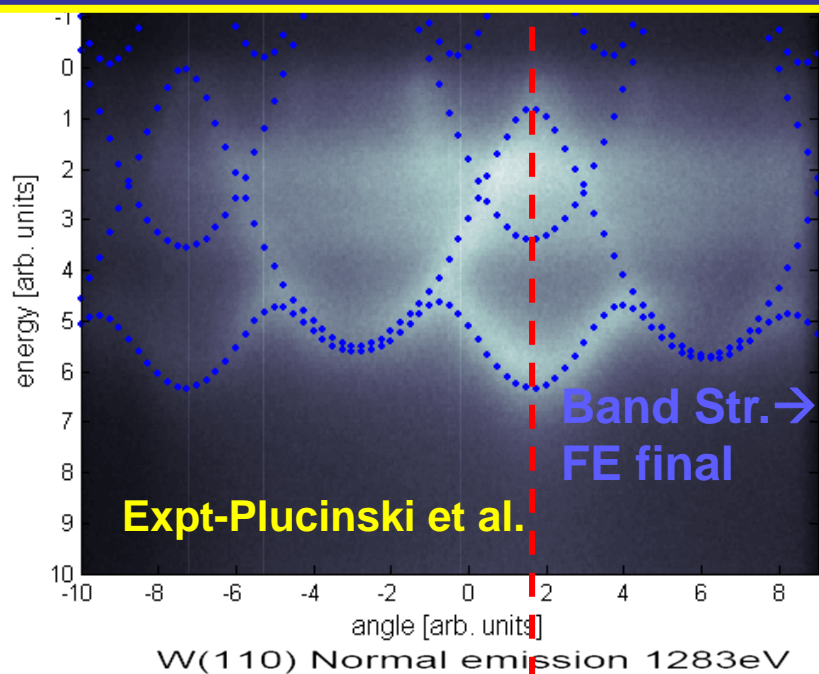
Selection rule: $\vec{k}_f = \vec{k}_i + \vec{g}_{hk\ell}$

Ibach & Luth
Chap. 7, Panel V

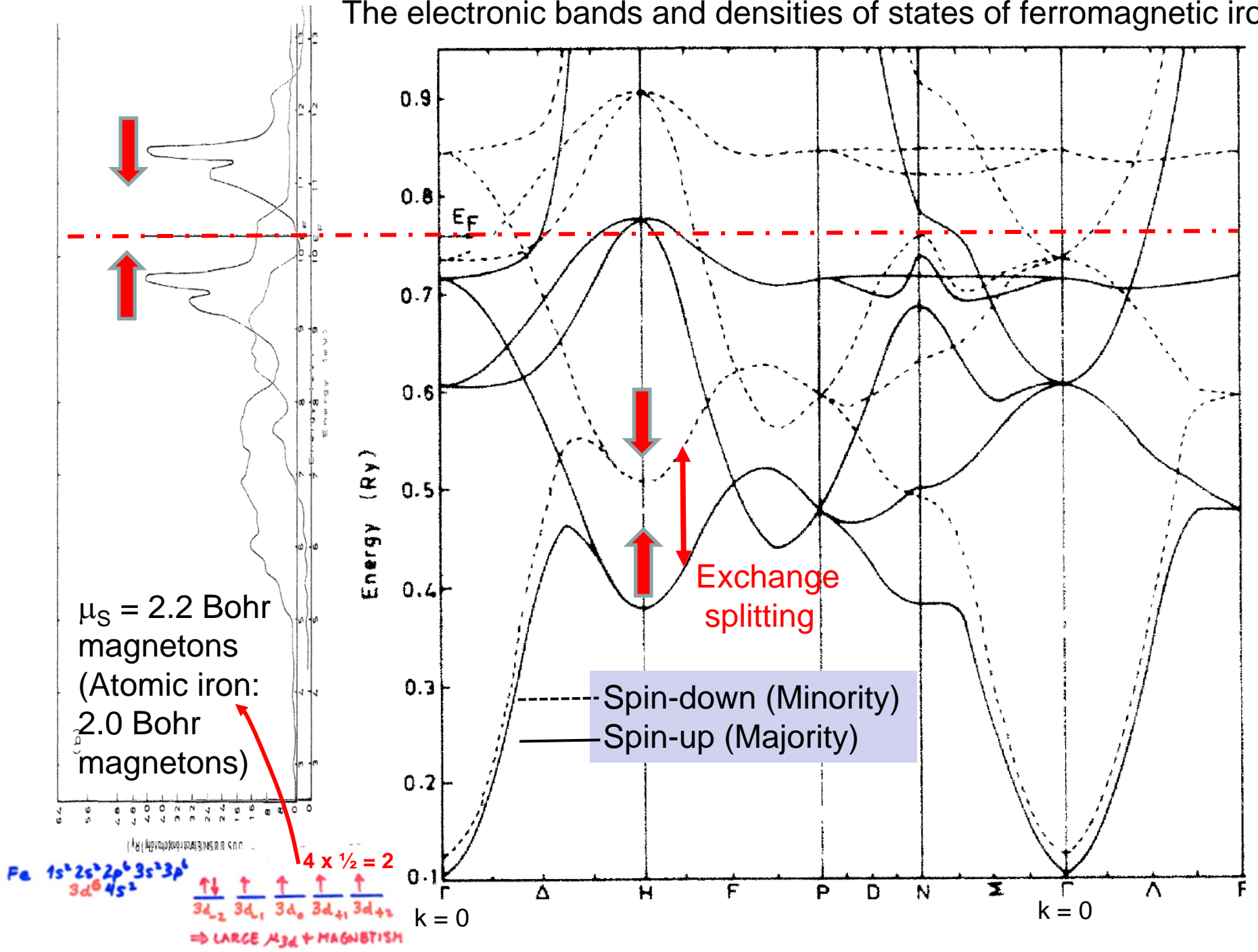
NEARLY-FREE ELECTRONS IN A WEAK PERIODIC POTENTIAL—1 DIM.



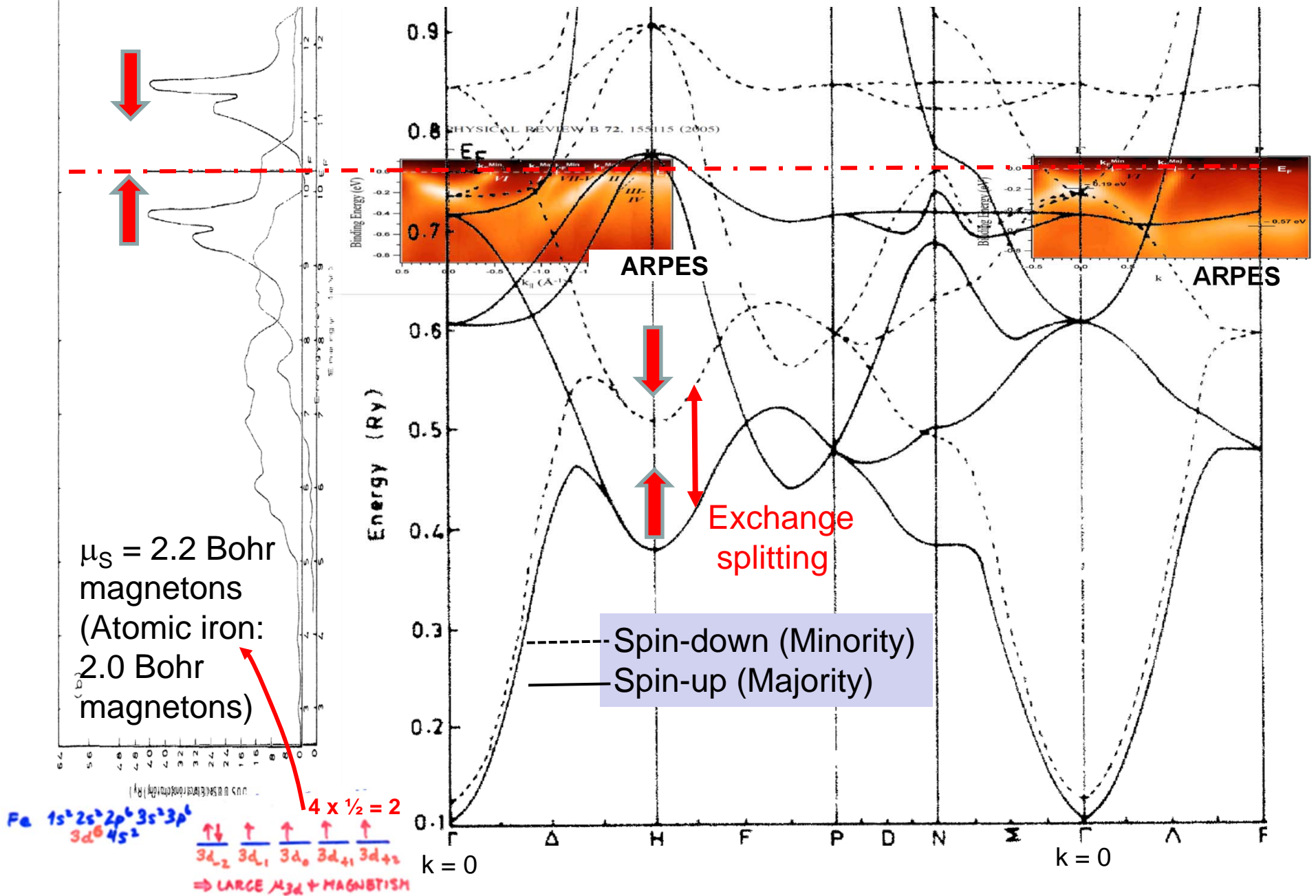
Measuring the band structure of tungsten with photoelectrons: $h\nu = 1253.6$ eV, $T = \sim 77$ K,



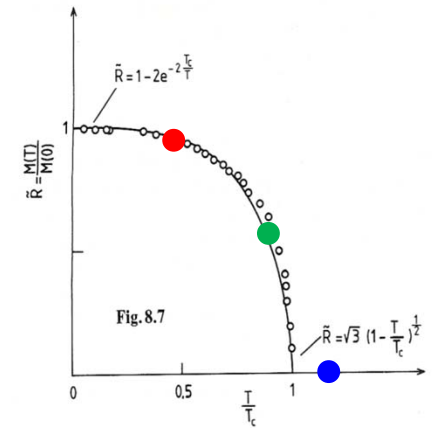
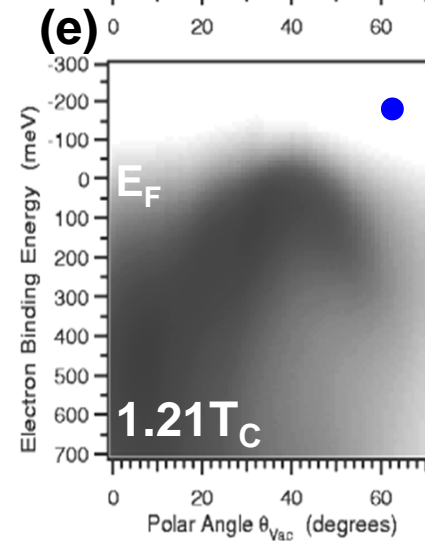
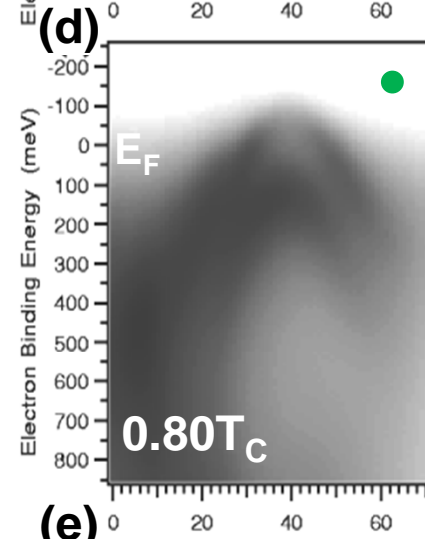
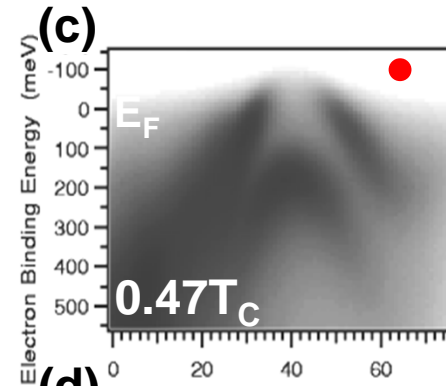
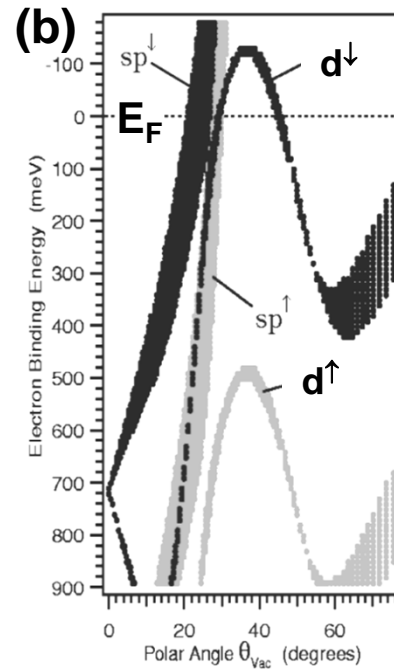
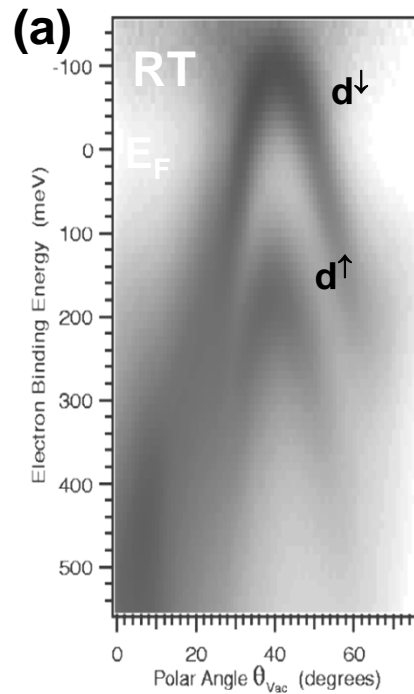
The electronic bands and densities of states of ferromagnetic iron



The electronic bands and densities of states of metallic ferromagnetic iron (face-centered cubic)

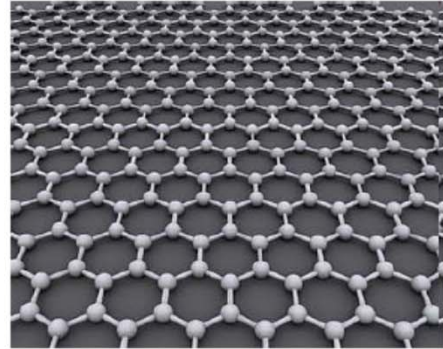


Measuring the magnetic (exchange) splitting of bands with photoelectrons

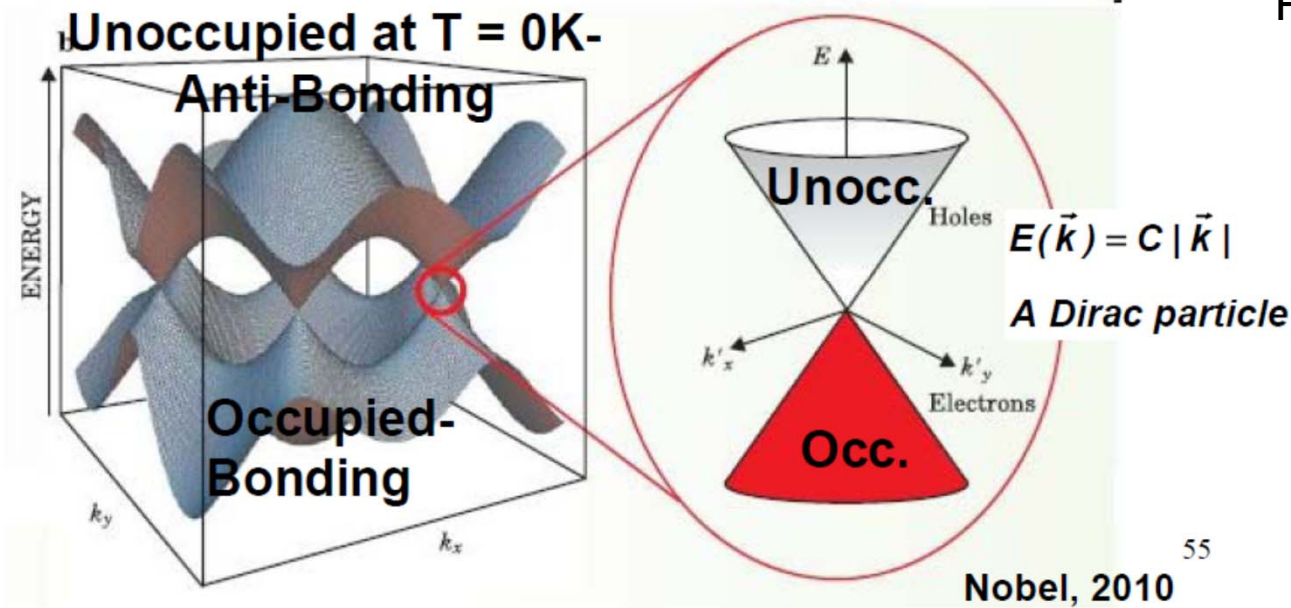


Kreutz et al.,
Phys. Rev. B 58 (1998) 1300

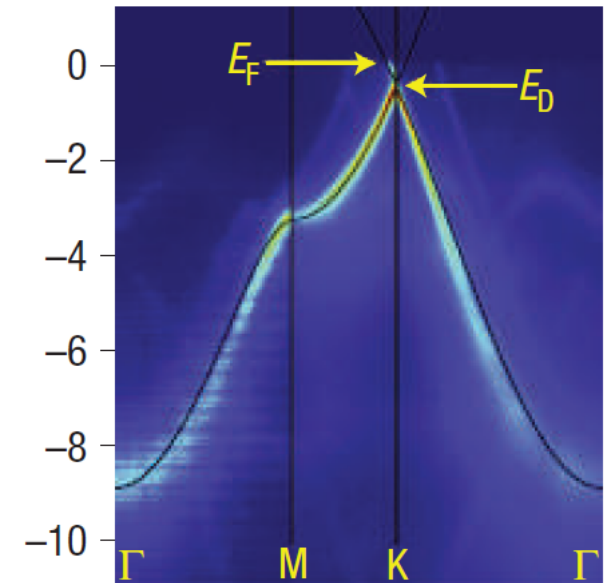
Graphene- A very special 2D case



The Nobel Prize in Physics 2010
 Andre Geim, Konstantin Novoselov
 ... "for groundbreaking experiments regarding the two-dimensional material graphene"



Photoelectron spectroscopy



Bostwick et al., Nature Physics 3, 36 - 40 (2007)

Looking to the end of the quarter:

- **Problem Set 5 due today...to next Thursday, with answers back when you hand in**
- **Course review summary to be handed out at the end of this week**
- **Review sessions by Skype from Baltimore APS Meeting: Wednesday and Thursday, 8:00-9:30 PM in room 285, Tanat Kissikov presiding**
- **Questions by e-mail, but a busy week at conference**
- **Tanat also available, will schedule office hour(s)**