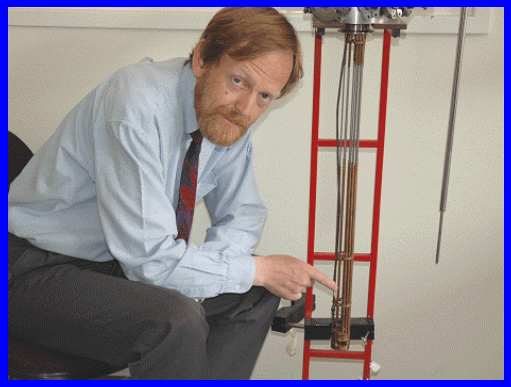
UvA-VU Master Course: Advanced Solid State Physics

Contents in 2005:

- Diffraction from periodic structures (week 6, AdV)
- **Electronic band structure of solids** (week 7, AdV)
- Motion of electrons and transport phenomena (week 8, AdV)
- Superconductivity (week 9&10, RW)
- Magnetism (week 11&12,JB)

Anne de Visser



Rinke Wijngaarden

Jürgen Buschow

Literature, software and homework

The course is based on the book:

H. Ibach and H. Lüth: Solid State Physics

3rd edition (Springer-Verlag, Berlin, 2003)

ISBN 3-540-43870-X

See also:

N.W. Ashcroft and N.D. Mermin: Solid State Physics

(Saunders College Publ.)

ISBN 0-03-083993-9

Computer simulations form an essential part of the course:

R.H. Silsbee and J. Dräger:

Simulations for Solid State Physics

(Cambridge University Press, Cambridge 1997)

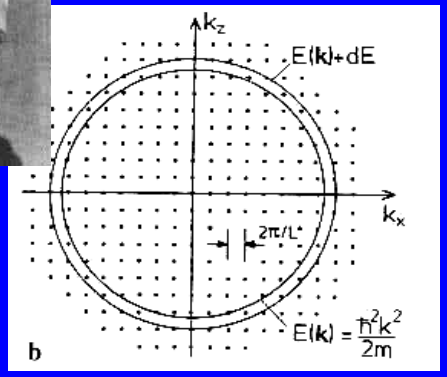
ISBN 0-521-59911-3

Software (freeware): www.physics.cornell.edu/sss/

Homework exercises will be distributed throughout the course

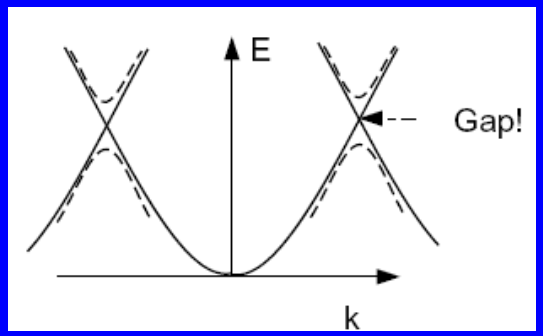
Completing the course gives 6 ECTS → ~ 6 x 28 hours

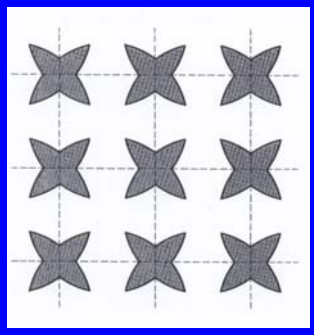
Course 2: Electronic band structure of solids

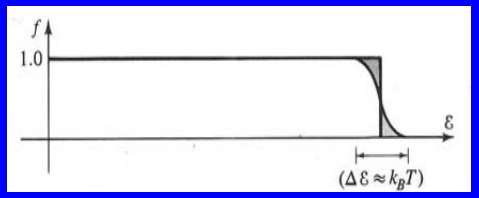


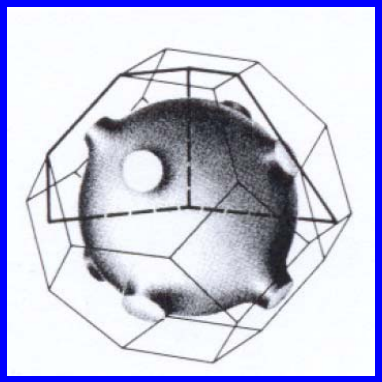
$$\psi_{\vec{k}}(\vec{r}) = u_k(\vec{r})e^{i\vec{k}\cdot\vec{r}}$$

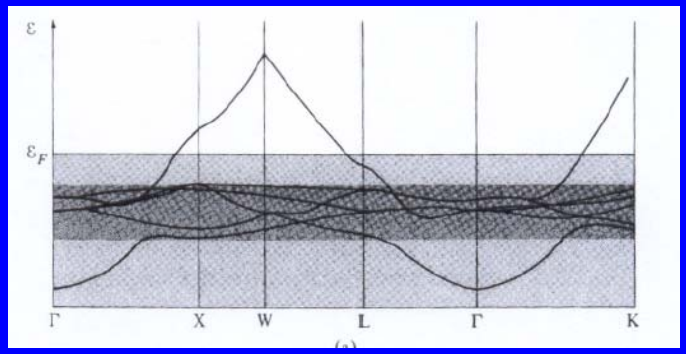
$$u_{\vec{k}}(\vec{r}) = u_k(\vec{r} + \vec{r}_n)$$











Pictures are taken from the Solid State Course by Mark Jarrel (Cincinnati University), from the book of Ibach and Lüth, from the book of Ashcroft and Mermin and from several sources on the web.

Course 2: Electronic band structure of solids

- Reminder: Coupled quantum wells
- Reminder: Free electrons in solids
- Effect of the lattice potential
- General symmetry – Bloch states
- The nearly-free electron approximation
- The tight binding approximation
- Examples: Fermi surfaces / Band structure

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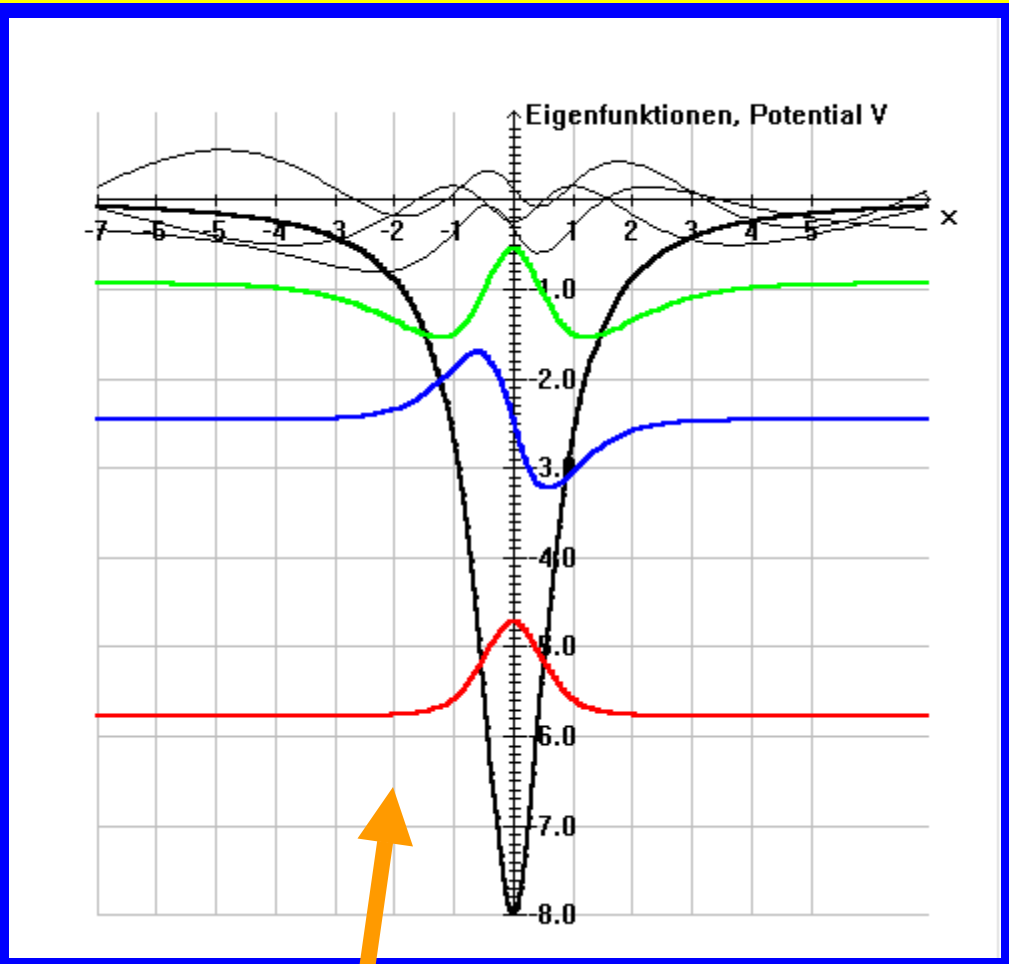
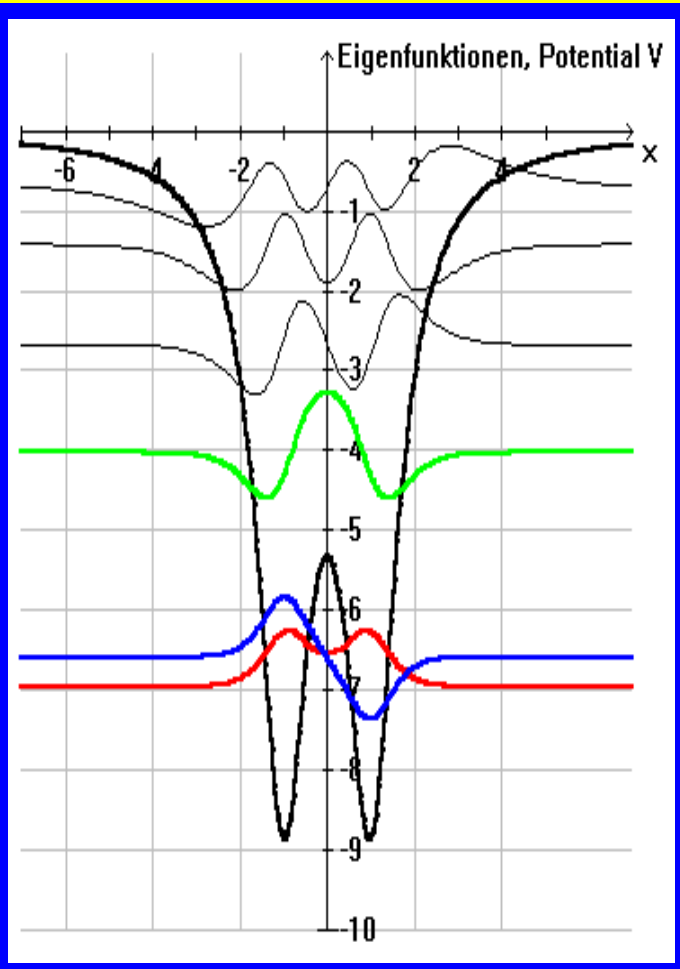
Reminder: Coupled QWs; 1- and 2-atom electron states

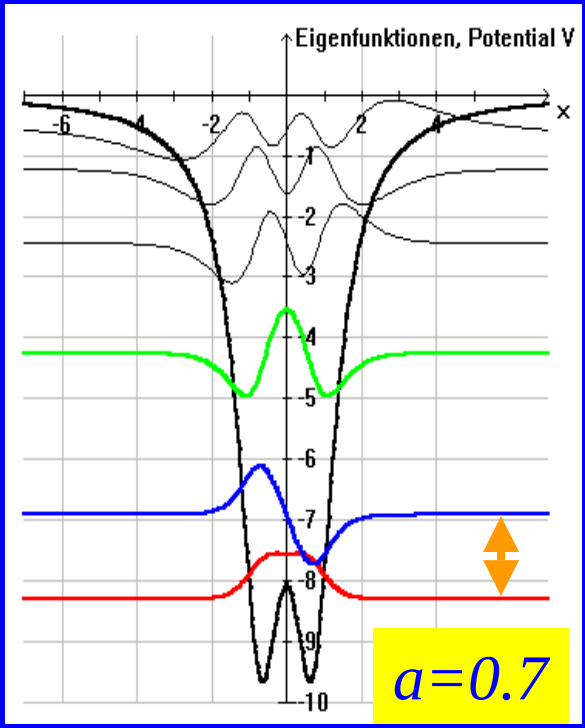


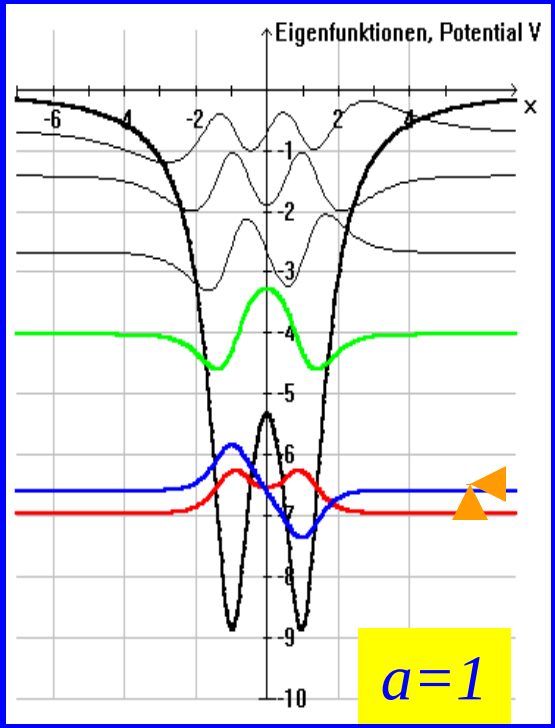


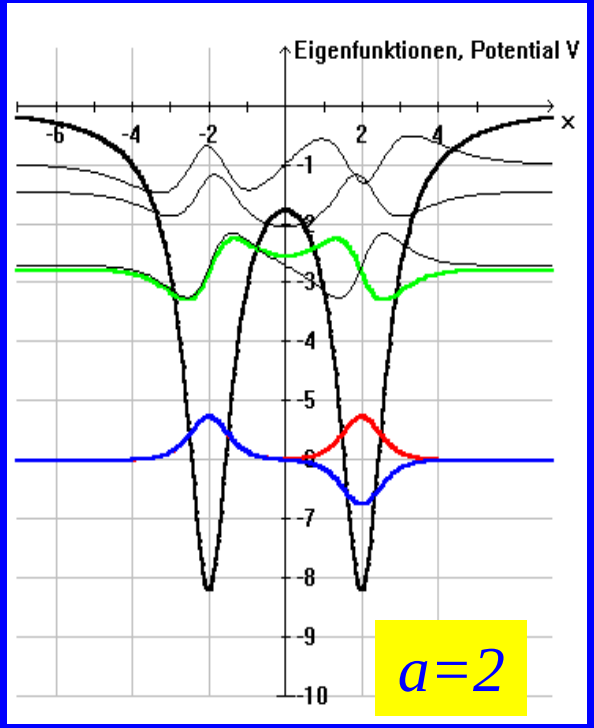
$$H\psi = [\nabla^2 + V]\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi - \frac{4}{x^2 + 0.5}\psi = E\psi$$

Schrödinger eq.

Effect of lattice spacing on electron states

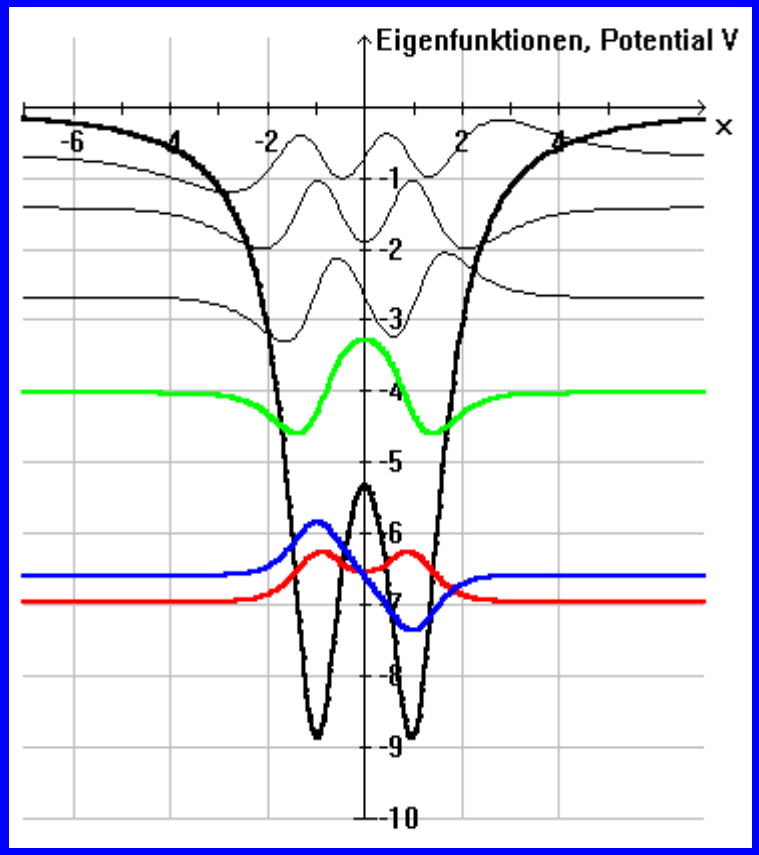




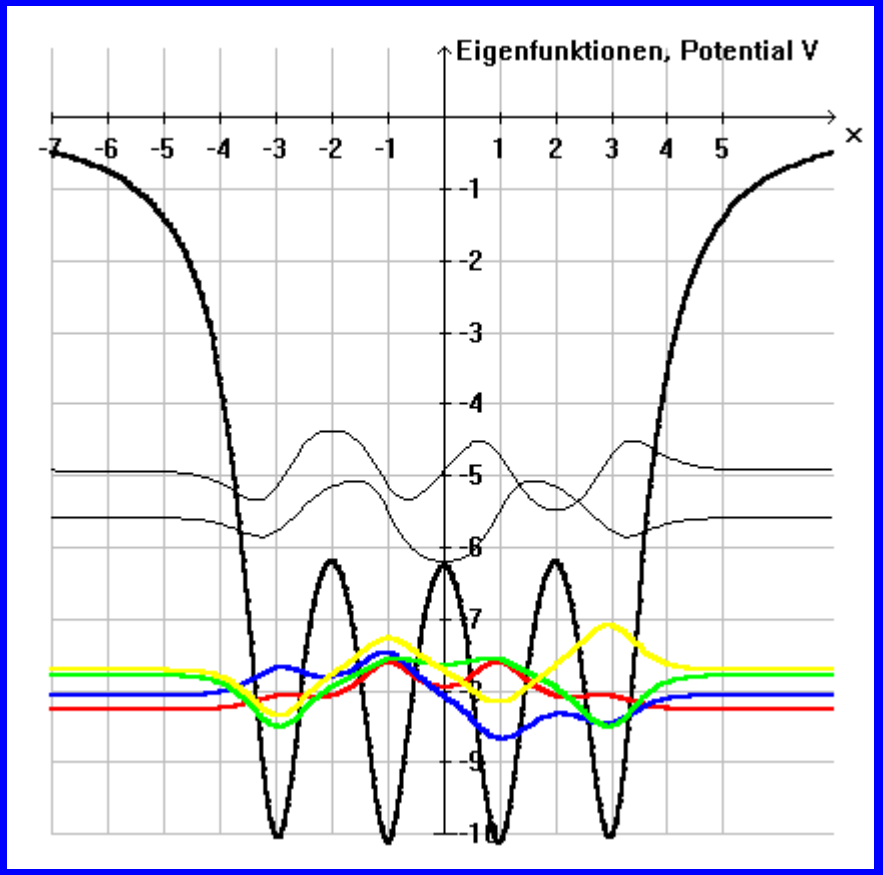


$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi-\frac{4}{(x-a)^2+0.5}\psi-\frac{4}{(x+a)^2+0.5}\psi=E\psi$$

N states for N atoms



2 states

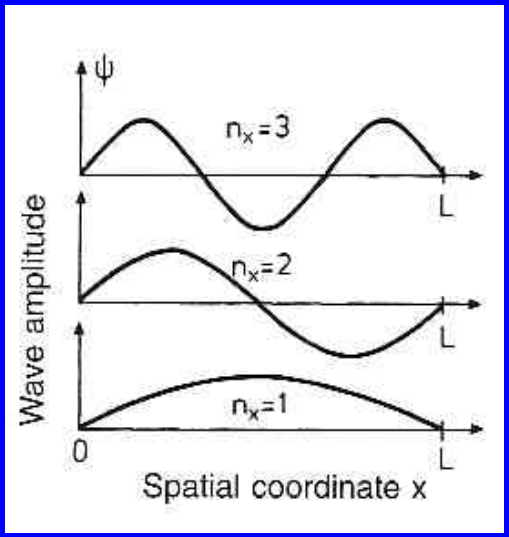


4 states

Reminder: Free electrons in solids

- Free electron gas
- Pauli exclusion principle
- Quantum Fermi-Dirac distribution
- N electrons in volume $V=L^3$
- Hamiltonian with potential(**r**) = 0
- Periodic boundary conditions
- Propagating electron waves

Arnold J.W. Sommerfeld
(1868-1951)



(fixed boundary conditions)

Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) = E\,\psi(\vec{r})$$

General solution:

$$\psi(\vec{r}) = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}$$

Periodic boundary conditions:

$$\psi(x+L, y+L, z+L) = \psi(x, y, z)$$

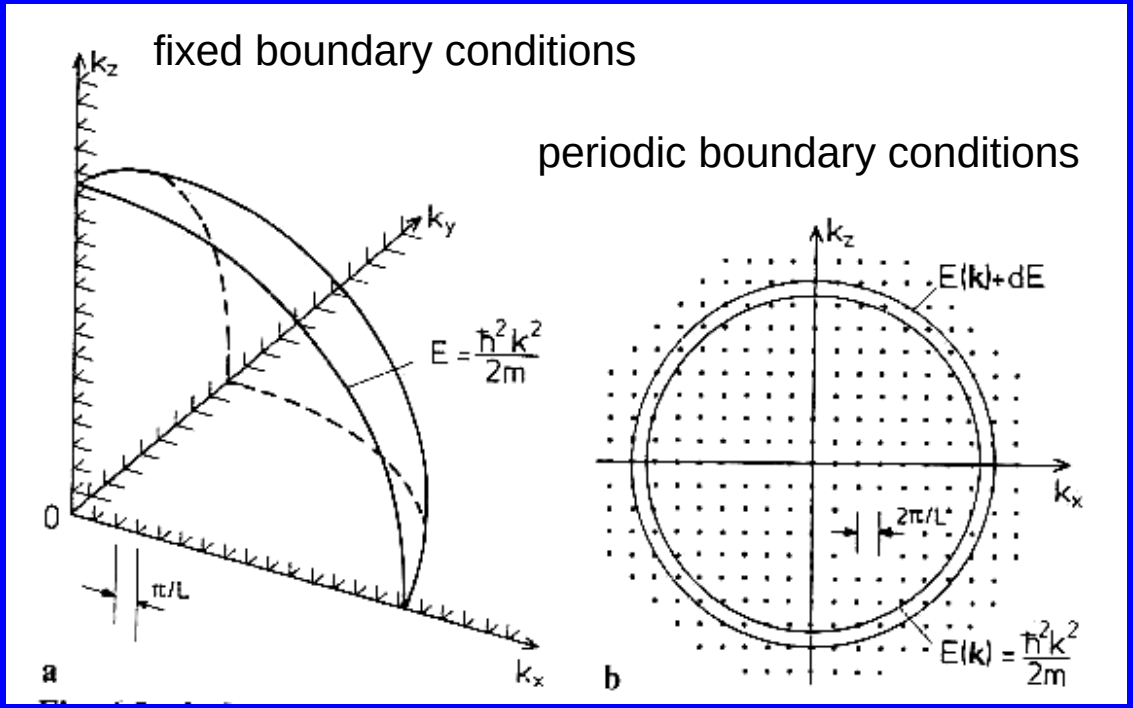
Components wave vector:

$$k_x = \frac{2\pi n_x}{L},\ k_y = \frac{2\pi n_y}{L},\ k_z = \frac{2\pi n_z}{L}$$

Eigenenergies:

$$E(\vec{k}) = \frac{\hbar^2}{2m}(k_x^{\,2} + k_y^{\,2} + k_z^{\,2})$$

Fermi sphere in k-space



Fermi energy:

$$E_F = \frac{\hbar^2}{2m} k_F^{\,2}$$

Fermi wave vector:

$$k_F = \left(\frac{3\pi^2 N}{V} \right)^{1/3}$$

Fermi temperature:

$$T_F = E_F / k_B$$

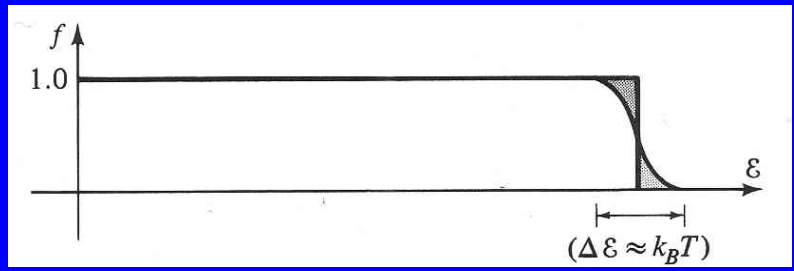
Fermi velocity:

$$\vec{v}_F = \left(\frac{\hbar}{m} \right) \vec{k}_F$$

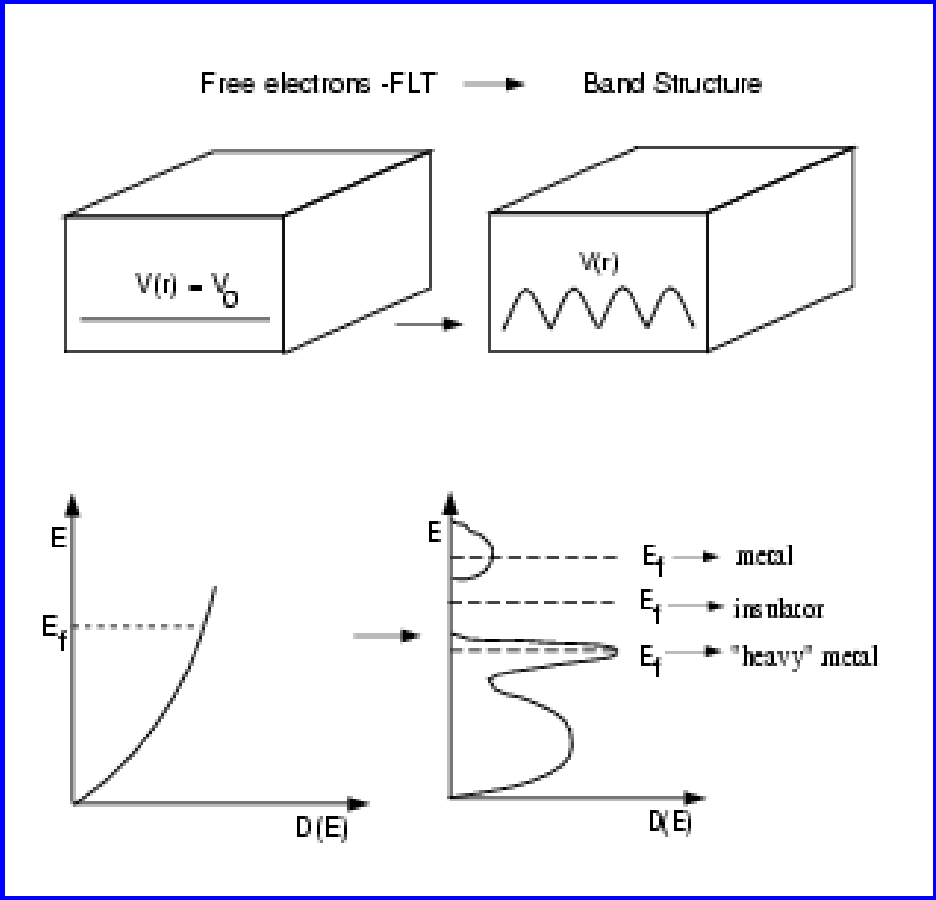
Fermi-Dirac distribution:

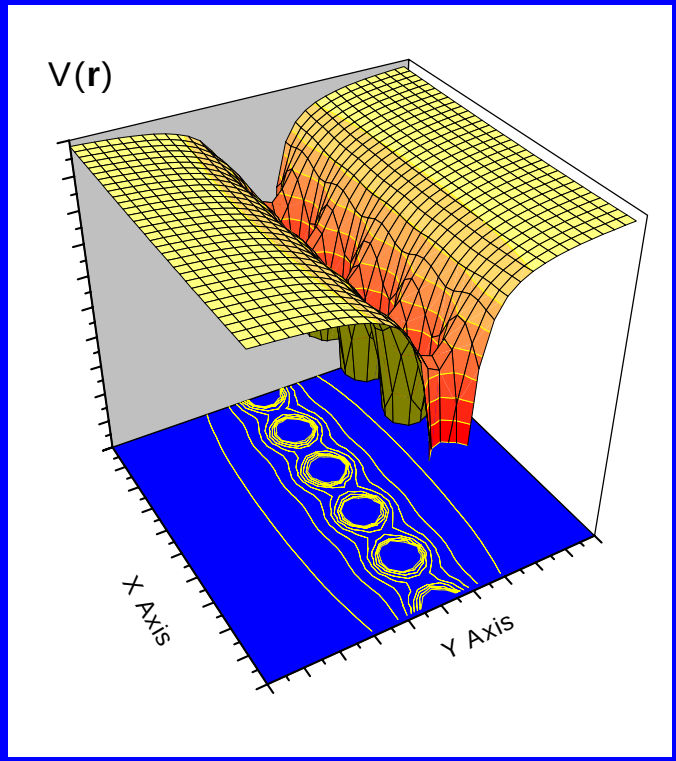
$$f_{FD}(\vec{v}) = \frac{(m/\hbar)^3}{4\pi^3} \frac{1}{\exp[(\frac{1}{2} mv^2 - \mu)/k_B T] + 1}$$

μ is chemical potential



Effect of the lattice potential





Fermi gas +
constant potential
$V(r)=V_0$

Fermi gas +
periodic potential
V(r)

General symmetry – Bloch states

Solve Schrödinger eq. with potential

$$V(\vec{r}) = V(\vec{r} + \vec{r}_n)$$

$$H\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r})$$

$\mathbf{r}_n$ direct lattice vector

with potential as Fourier series

$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

G reciprocal lattice vector

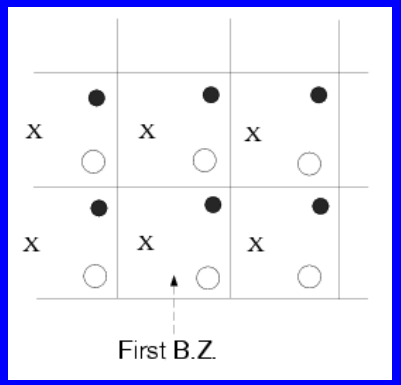
and general solution

$$\psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

→ Schrödinger eq. in reciprocal space

$$\left(\frac{\hbar^2 k^2}{2m} - E \right) C_k + \sum_{\vec{G}} V_{\vec{G}} C_{\vec{k}-\vec{G}} = 0$$

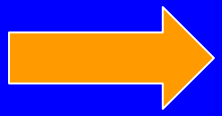
couples $C_{\mathbf{k}}$ only with $C_{\mathbf{k}-\mathbf{G}}$, $C_{\mathbf{k}-\mathbf{G}'}$, $C_{\mathbf{k}-\mathbf{G}''}$, etc.
for each k-vector in unit cell → N problems
index eigenvalues by **k**: $E_{\mathbf{k}}=E(\mathbf{k})$



solution for each **k**

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i(\vec{k}-\vec{G})\cdot\vec{r}} = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{-i\vec{G}\cdot\vec{r}} e^{i\vec{k}\cdot\vec{r}}$$

Fourier series over reciprocal lattice points $u_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{-i\vec{G}\cdot\vec{r}}$



solution is modulated plane wave (Bloch theorem)

$$\psi_{\vec{k}}(\vec{r}) = u_k(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$
$$u_{\vec{k}}(\vec{r}) = u_k(\vec{r} + \vec{r}_n)$$

Bloch waves

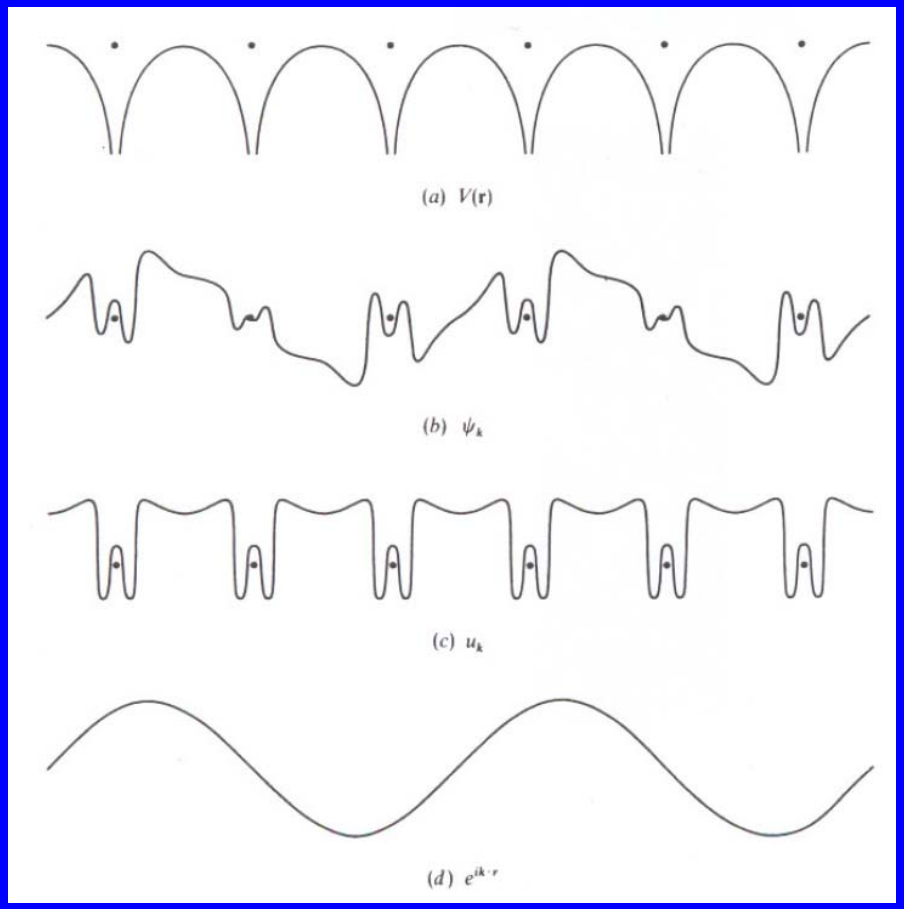
Periodic in **k** $\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}+\vec{G}}(\vec{r})$

Periodicity **G**

$$H\psi_{\vec{k}} = E(\vec{k})\psi_{\vec{k}}$$
$$E(\vec{k}) = E(\vec{k} + \vec{G})$$

knowledge in 1st Brillouin zone is sufficient

Example Bloch wave



periodic lattice potential V(r)

Bloch wave $\psi_k = u_k e^{ikr}$ (real part)

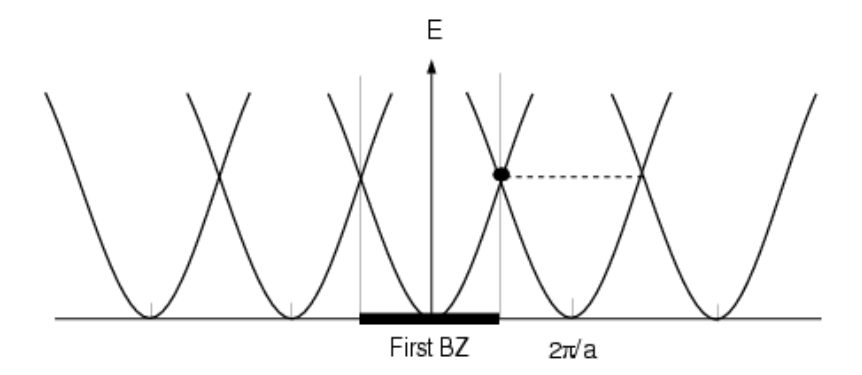
Bloch function u_k

plane wave e^{ikr} (real part)

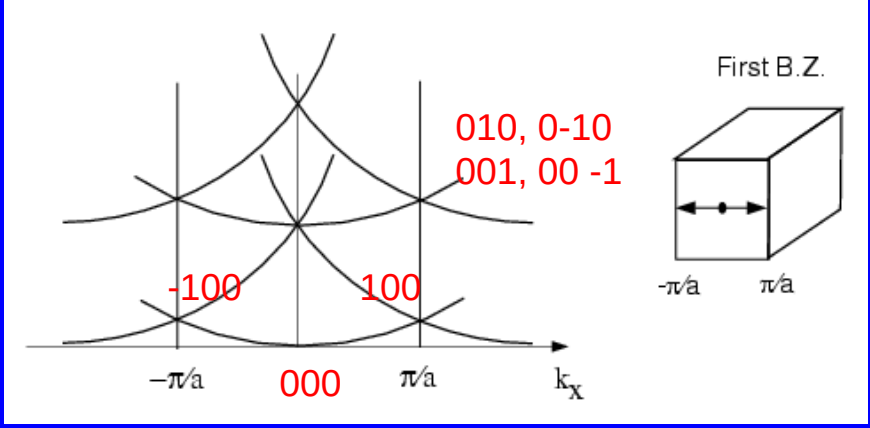
The nearly-free electron approximation: empty lattice case

V_G=0; symmetry requires:

$$E(\vec{k}) = E(\vec{k}+\vec{G}) = \frac{\hbar^2}{2m}\left|\vec{k}+\vec{G}\right|^2$$



1 D case; G=h2π/a
E(k) for vanishing potential (empty lattice)
→ reduction to 1st BZ



3D cubic case;
E(k) revolving parabola's → complex behaviour in 1st BZ

Case of weak V_G

Degeneracy: At ZB ($k=\pi/a$) electron state involves at least two G values: $G=0,\ 2\pi/a$

$\rightarrow$ plane waves $\quad e^{ikx},\ e^{i(k-G)x} \rightarrow e^{iGx/2},\ e^{-iGx/2}$

for exact solution (many **G**) solve: $\left(\frac{\hbar^2 k^2}{2m} - E_{\vec{k}}\right) C_{\vec{k}} + \sum_{\vec{G}} V_{\vec{G}} C_{\vec{k}-\vec{G}} = 0$

largest contributions for $\mathbf{G}=\mathbf{G}_1$ for which: $E_{\vec{k}} = E_{\vec{k}-\vec{G}_1} \approx \frac{\hbar^2 k^2}{2m}$

$$C_{\vec{k}} = \frac{\sum_{\vec{G}} V_{\vec{G}} C_{\vec{k}-\vec{G}}}{E_{\vec{k}} - \frac{\hbar^2 k^2}{2m}}$$

$$C_{\vec{k}-\vec{G}_1} = \frac{\sum_{\vec{G}} V_{\vec{G}} C_{\vec{k}-\vec{G}_1-\vec{G}}}{E_{\vec{k}-\vec{G}_1} - \frac{\hbar^2 \left|\vec{k}-\vec{G}_1\right|^2}{2m}}$$

$$C_{\vec{k}} \approx C_{\vec{k}-\vec{G}_1} >> other\ C_{\vec{k}-\vec{G}} \quad ;\ V_0 = 0\ ;$$

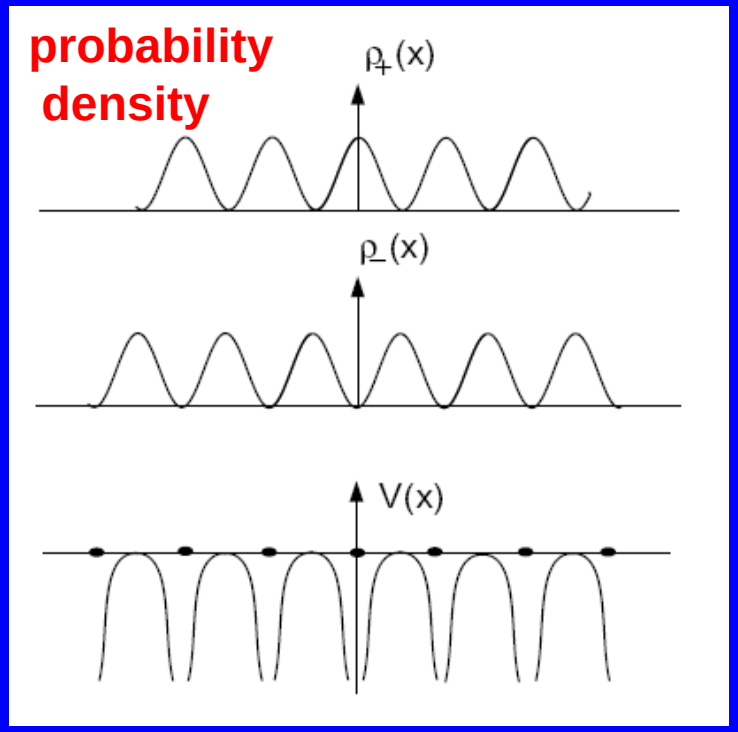
$|\mathbf{k}|^2 \cong |\mathbf{k}-\mathbf{G}|^2$ $\leftarrow$ Bragg condition

Case of weak V_G

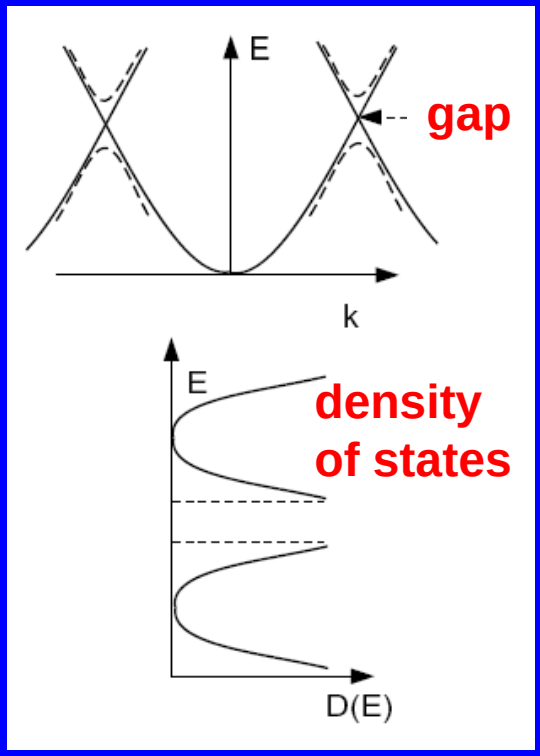
Standing waves: superposition of incoming and Bragg reflected wave

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

$$\rho_+ = \psi_+^* \psi_+ \sim \cos^2 \pi x/a$$
$$\rho_- = \psi_-^* \psi_- \sim \sin^2 \pi x/a$$



energy $E_+ < E_-$ → gap



General treatment

Largest deviation from free electron model at ZB when
$|\mathbf{k}|^2 \cong |\mathbf{k}-\mathbf{G}|^2$ ← Bragg condition
retain largest terms with C_k and C_{k-G}

$$\left(E - \frac{\hbar^2 k^2}{2m}\right) C_{\vec{k}} - V_{\vec{G}} C_{\vec{k}-\vec{G}} = 0$$

$$\left(E - \frac{\hbar^2 \left|\vec{k}-\vec{G}\right|^2}{2m}\right) C_{\vec{k}-\vec{G}} - V_{-\vec{G}} C_{\vec{k}} = 0$$

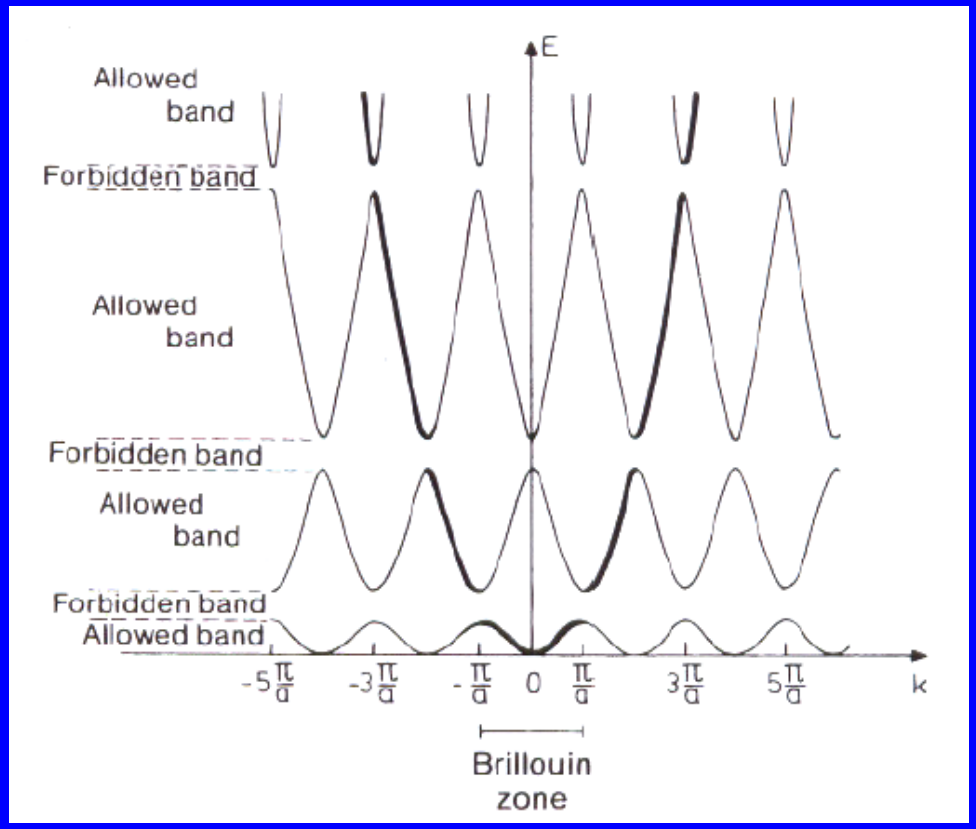
$$\begin{vmatrix} \left(\frac{\hbar^2 k^2}{2m} - E\right) & V_{\vec{G}} \\ V_{-\vec{G}} & \left(\frac{\hbar^2 \left|\vec{k}-\vec{G}\right|^2}{2m} - E\right) \end{vmatrix} = 0$$

with $E_{\vec{k}-\vec{G}} = \frac{\hbar^2 \left|\vec{k}-\vec{G}\right|^2}{2m}$

$$E_{\pm} = \tfrac{1}{2}(E^0_{\vec{k}-\vec{G}} + E^0_{\vec{k}}) \pm \left[\tfrac{1}{4}(E^0_{\vec{k}-\vec{G}} - E^0_{\vec{k}})^2 + \left|V_G\right|^2\right]^{1/2}$$

At ZB $E^0_{\vec{k}-\vec{G}} = E^0_{\vec{k}}$ gap $\Delta E = E_+ - E_- = 2\left|V_{\vec{G}}\right|$

Energy dispersion E(k) 1 D lattice in extended zone scheme



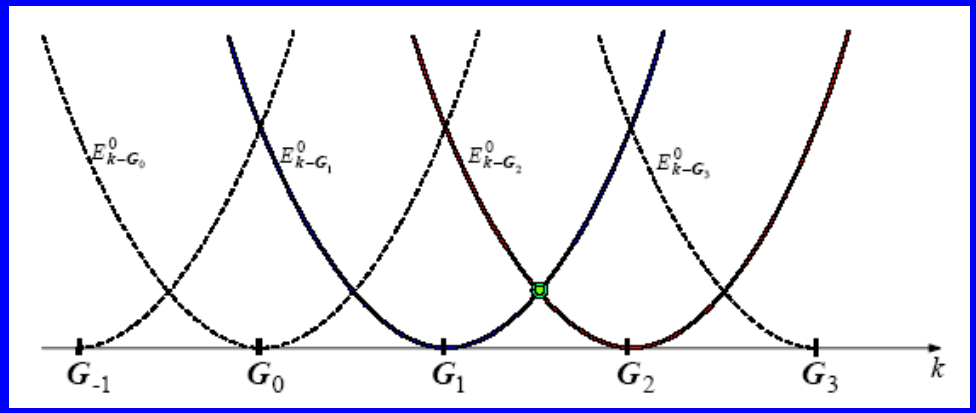
- Bragg condition at BZ → backscattering destroys electronic states
- 2N independent states in each energy band

Example - Exercise

Consider a square lattice in two dimensions with a background potential

- V_0 = 2.0 eV
- V(x,y) disturbs the system
- gaps are formed at the intersection of free electron bands

$$V(x,y) = V_0 \cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)$$

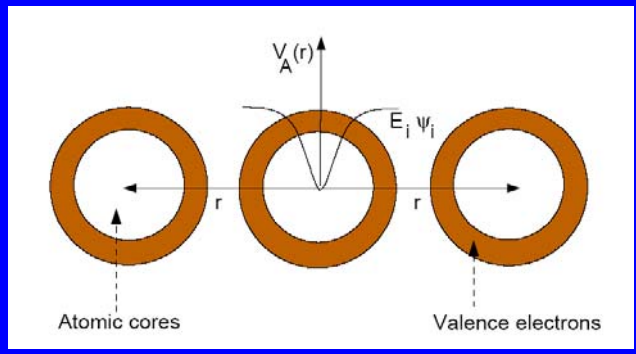


- Set up a 2x2 secular eq. to calculate the bandgap at the point (π/a, π/a) of the Brillouin zone

solve Schrödinger eq.: $$H\psi(\vec{r}) = (H_0 + V(x,y))\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

The tight-binding approximation

- crystal electron state is linear superposition of atomic orbitals
- potential V_A of free atom at $\mathbf{r}_n$
- start from atomic problem with valence eigenstates φ_i and energy E_i



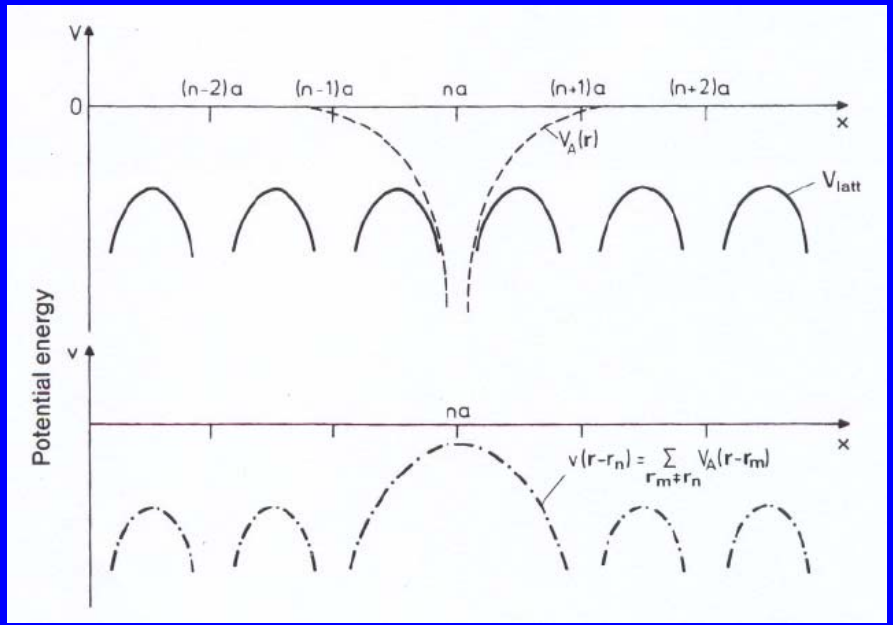
unperturbed Schrödinger eq. for atom n

$$H_A(\vec{r}-\vec{r}_n)\varphi_i(\vec{r}-\vec{r}_n)=E_i\varphi_i(\vec{r}-\vec{r}_n)$$

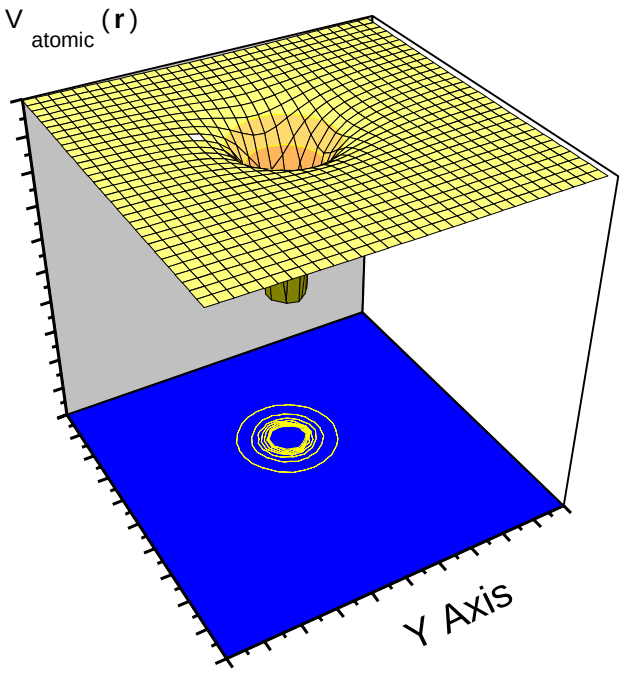
include perturbation due to atomic potential of all other atoms

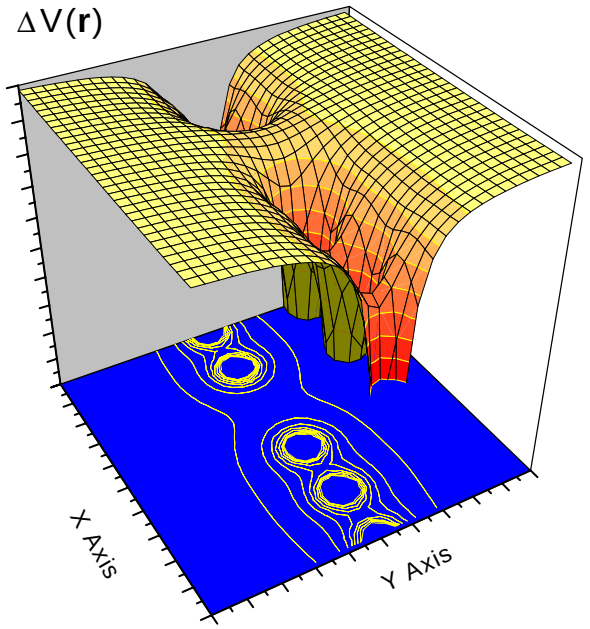
$$H=H_A+v=-\frac{\hbar^2}{2m}\Delta+V_A(\vec{r}-\vec{r}_n)+v(\vec{r}-\vec{r}_n)$$

$$v(\vec{r}-\vec{r}_n)=\sum_{m\neq n}V_A(\vec{r}-\vec{r}_n)$$



The tight-binding approximation





task: solve Hamiltonian

$$H\psi_{\vec{k}}(\vec{r}) = E(\vec{k})\psi_{\vec{k}}(\vec{r})$$

$$E(\vec{k}) = \frac{\left\langle \psi_{\vec{k}} \middle| H \middle| \psi_{\vec{k}} \right\rangle}{\left\langle \psi_{\vec{k}} \middle| \psi_{\vec{k}} \right\rangle}$$

$\rightarrow$ solve for $\phi_{\mathbf{k}} \cong \psi_{\mathbf{k}}$ with $E'(\mathbf{k}) \rightarrow E(\mathbf{k})$

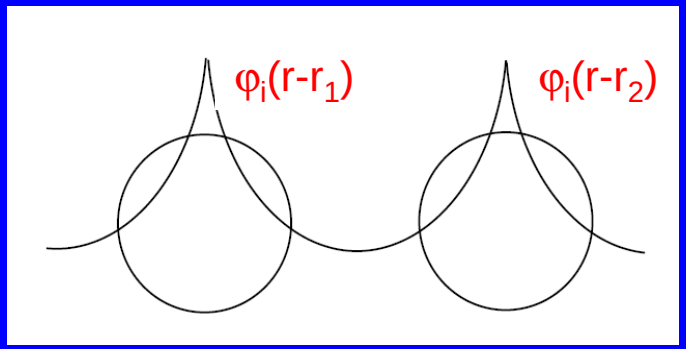
with $\phi_{\mathbf{k}}$ is Bloch state: $\phi_{\mathbf{k+G}} = \phi_{\mathbf{k}}$

write $\phi_{\mathbf{k}}$ as linear combination of atomic orbitals φ_i

$$\psi_{\vec{k}} \approx \phi_{\vec{k}} = \sum_n a_n \varphi_i(\vec{r} - \vec{r}_n) = \sum_n e^{i\vec{k}\cdot\vec{r}_n} \varphi_i(\vec{r} - \vec{r}_n) \;\; ; \;\; a_n = e^{i\vec{k}\cdot\vec{r}_n}$$

$$\left\langle \phi_{\vec{k}} \middle| \phi_{\vec{k}} \right\rangle = \sum_{n,m} e^{i\vec{k}\cdot(\vec{r}_n - \vec{r}_m)} \int \varphi_i^*(\vec{r} - \vec{r}_m)\varphi_i(\vec{r} - \vec{r}_n)d\vec{r}$$

$$\cong \sum_n \varphi_i^*(\vec{r} - \vec{r}_n)\varphi_i(\vec{r} - \vec{r}_n)d\vec{r} = N$$



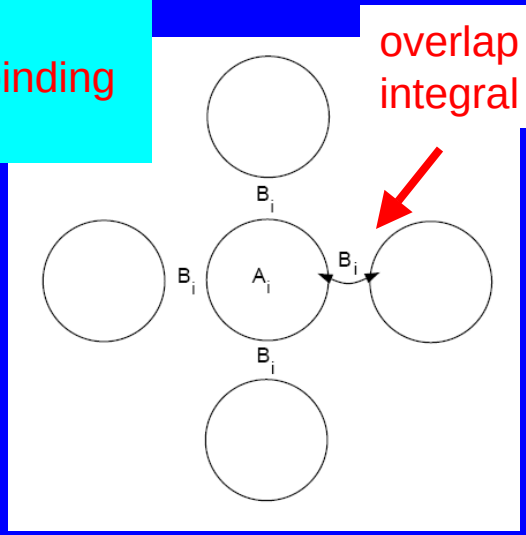
neglect nn interaction: n=m

$$E(\vec{k}) \approx \frac{1}{N} \sum_{n,m} e^{i\vec{k}\cdot(\vec{r}_n - \vec{r}_m)} \int \varphi_i^*(\vec{r} - \vec{r}_m)[E_i + v(\vec{r} - \vec{r}_n)]\varphi_i(\vec{r} - \vec{r}_n)d\vec{r}$$

include (only) nearest neighbour interaction

Simple cubic case:
- isotropic hybridization
- φ_i spherical symmetry, s-wave

cubic tight-binding lattice



$$E(\vec{k}) \approx E_i - A - B\sum_m e^{i\vec{k}\cdot(\vec{r}_n - \vec{r}_m)}$$

with $\mathbf{r}_m$ only nearest neighbour of $\mathbf{r}_n$

$$A = -\int \varphi_i^*(\vec{r} - \vec{r}_n) v(\vec{r} - \vec{r}_n) \varphi_i(\vec{r} - \vec{r}_n) d\vec{r}$$

$$B = -\int \varphi_i^*(\vec{r} - \vec{r}_m) v(\vec{r} - \vec{r}_n) \varphi_i(\vec{r} - \vec{r}_n) d\vec{r}$$

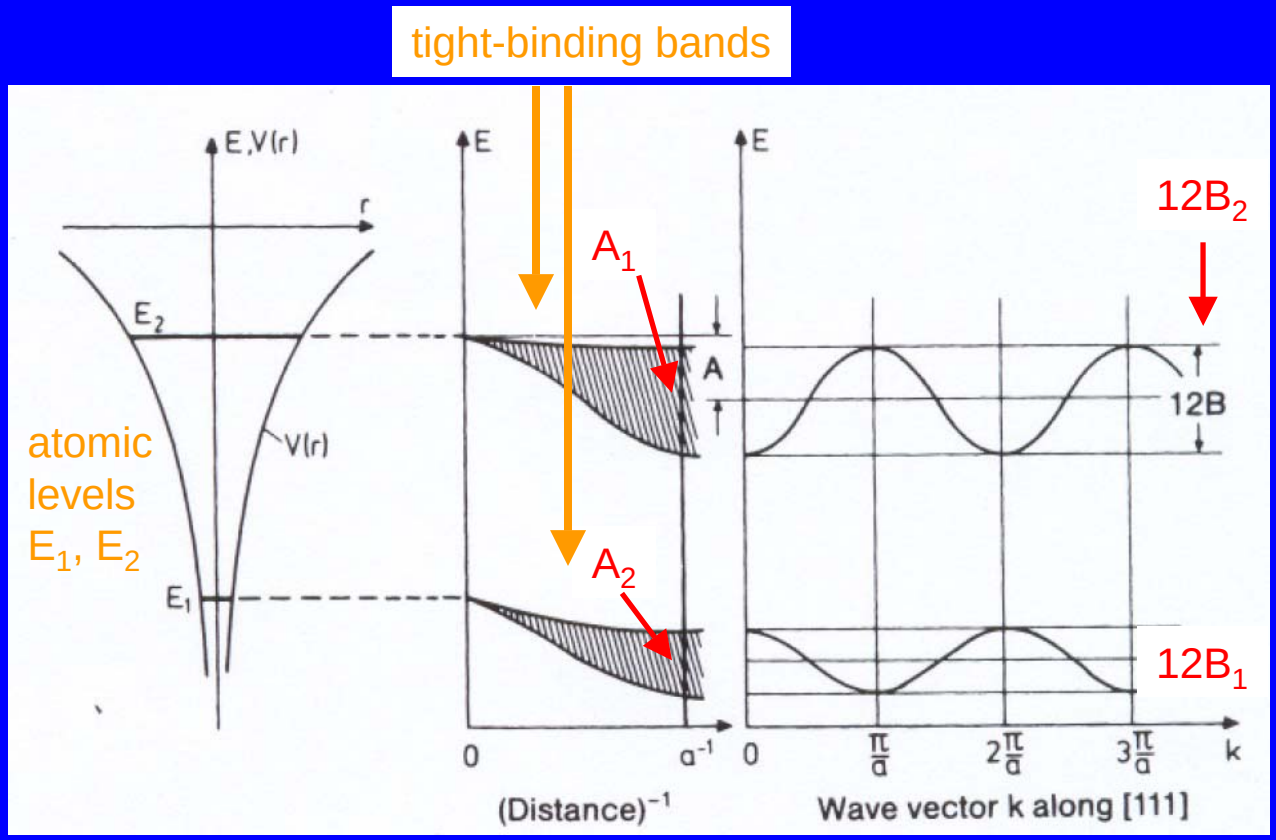
in the case of simple cubic lattice → $\vec{r}_n - \vec{r}_m = (\pm a,0,0);(0,\pm a,0);(0,0,\pm a)$

$$E(\vec{k}) \approx E_i - A - 2B(\cos k_x a + \cos k_y a + \cos k_z a)$$

- A, B >0; band center E_i-A_i
- width of the band 12B
- for small k (near Γ-point): with $k^2 = k_x^2 + k_y^2 + k_z^2$

$$E(\vec{k}) = E_i - A - 6B + Ba^2k^2$$

Simple cubic case: $E(\vec{k}) \approx E_i - A - 2B(\cos k_x a + \cos k_y a + \cos k_z a)$

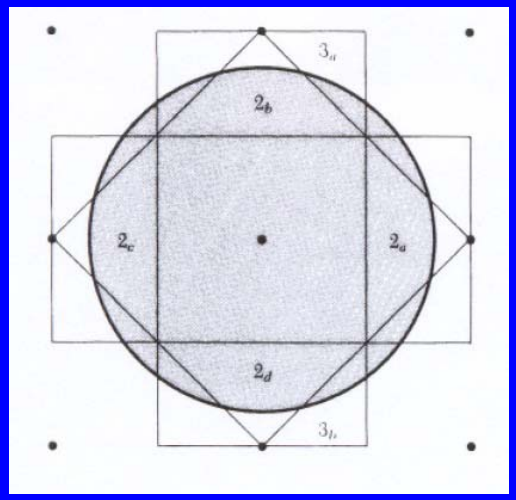


- energy width larger as overlap (hybridization) increases
- 2N electrons per band

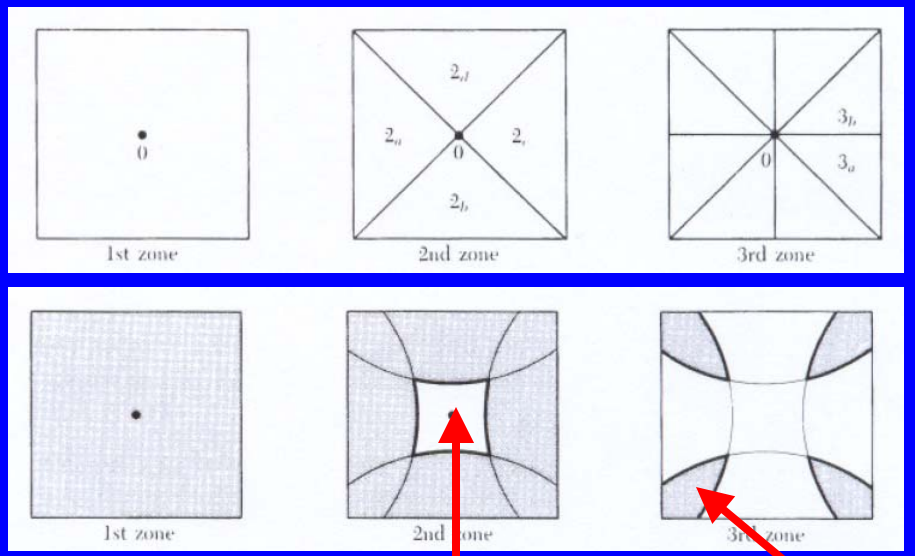
Examples: Fermi surfaces / Band structure

2D square lattice free electron gas with large Fermi sphere

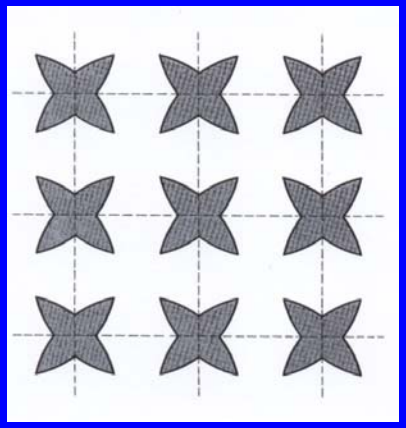
extended zone scheme



Brillouin zones in reduced zone scheme



hole like electron like FS

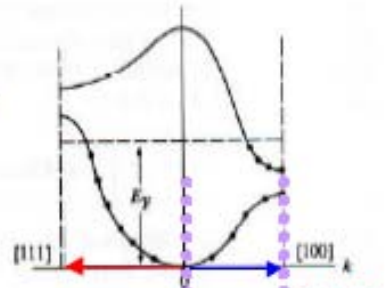


3rd zone in periodic zone scheme

2D square lattice
effect of lattice potential

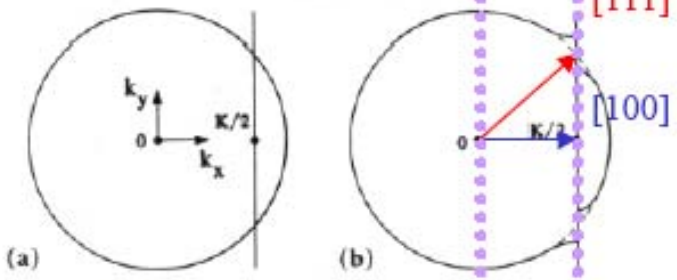
■ Because the energy band is distorted near the zone boundary, the FS near the ZB is distorted as a result.

band structure



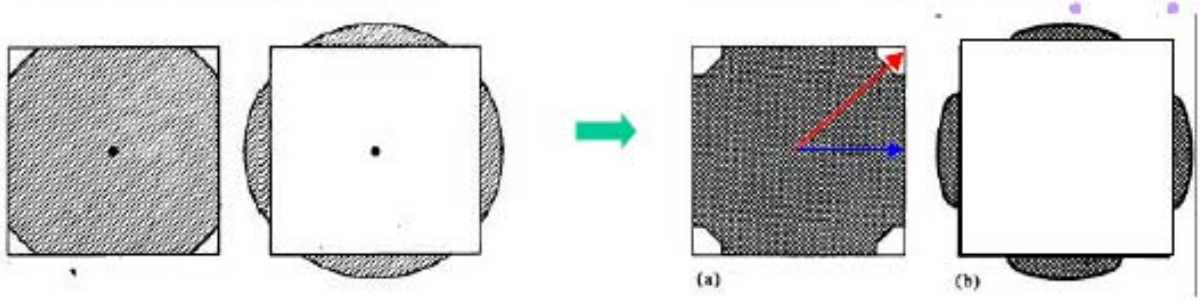
[111]

[100]



Without lattice potential

With lattice potential

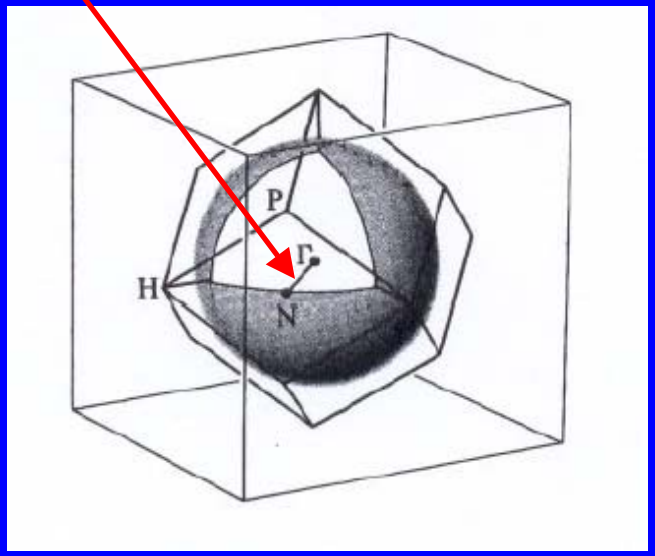


Monovalent metals

Alkali metals: Li $1s^2s^1$, Na [Ne]$3s^1$, K [Ar]$4s^1$, Rb [Kr]$5s^1$, Cs [Xe]$6s^1$

bcc lattice: density $n = 2/a^3 = k_F^3/(3\pi^2) \rightarrow k_F = 0.62\ (2\pi/a)$

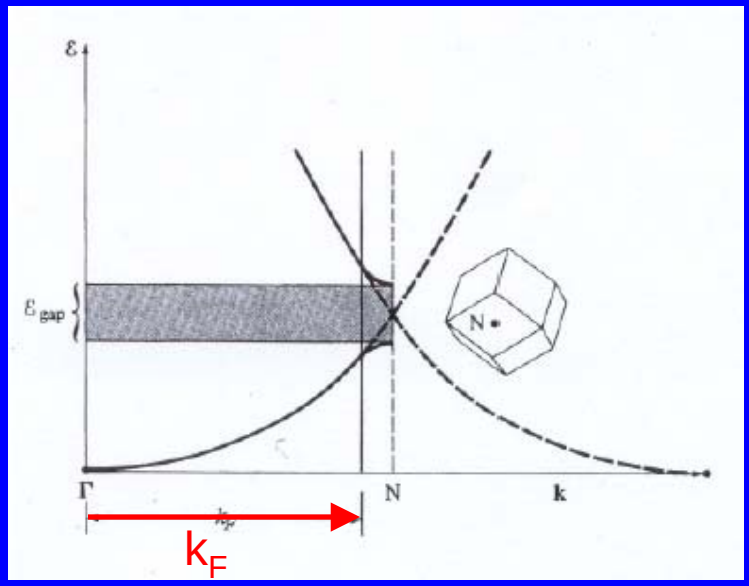
$$\Gamma N = \frac{2\pi}{a}\sqrt{\left(\tfrac{1}{2}\right)^2 + \left(\tfrac{1}{2}\right)^2 + 0^2} = 0.707\,\frac{2\pi}{a}$$



Fermi sphere contained in first BZ

$$\text{number of states}\quad \frac{4\pi k_F^3}{3}\frac{V}{8\pi^3} = \frac{k_F^3}{6\pi^2}V$$

$$\text{density of electrons}\quad n = \frac{N}{V} = 2\times\frac{k_F^3}{6\pi^2} = \frac{k_F^3}{3\pi^2}$$



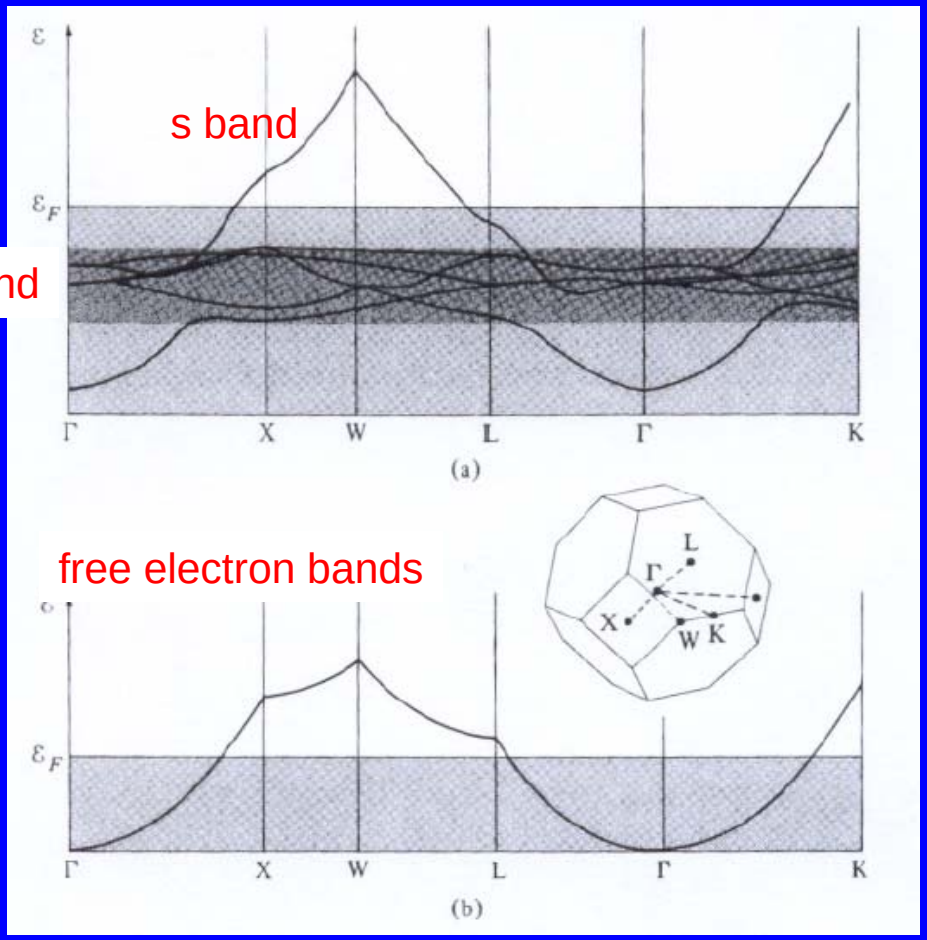
Monovalent metals

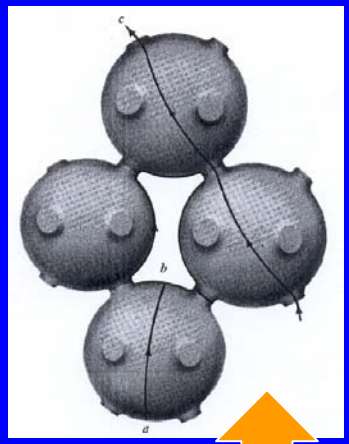
Noble metals: Cu $[Ar]3d^{10}4s^{1}$

Ag $[Kr]4d^{10}4s^{1}$

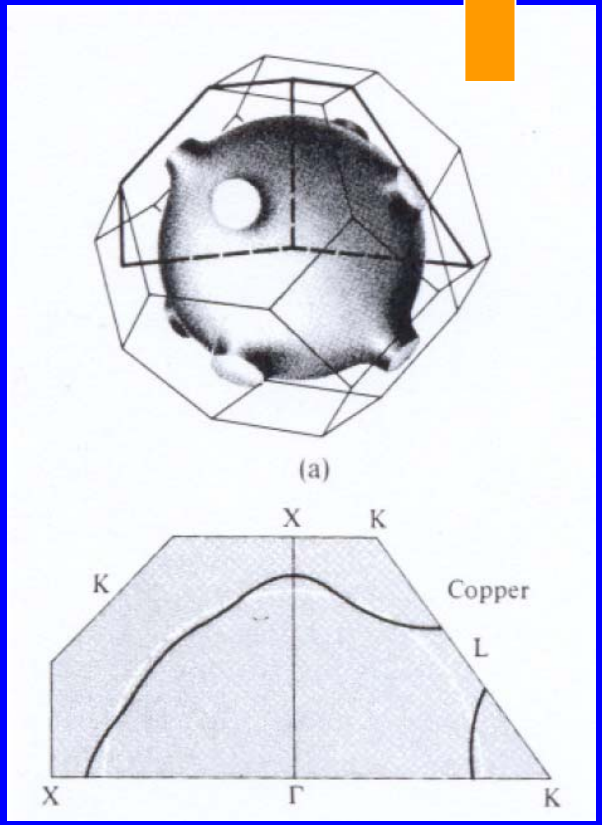
Au $[Xe]4f^{14}3d^{10}4s^{1}$

Bandstructure of copper (fcc lattice): 6 bands





free electron-like FS



A tetravalent fcc free electron metal

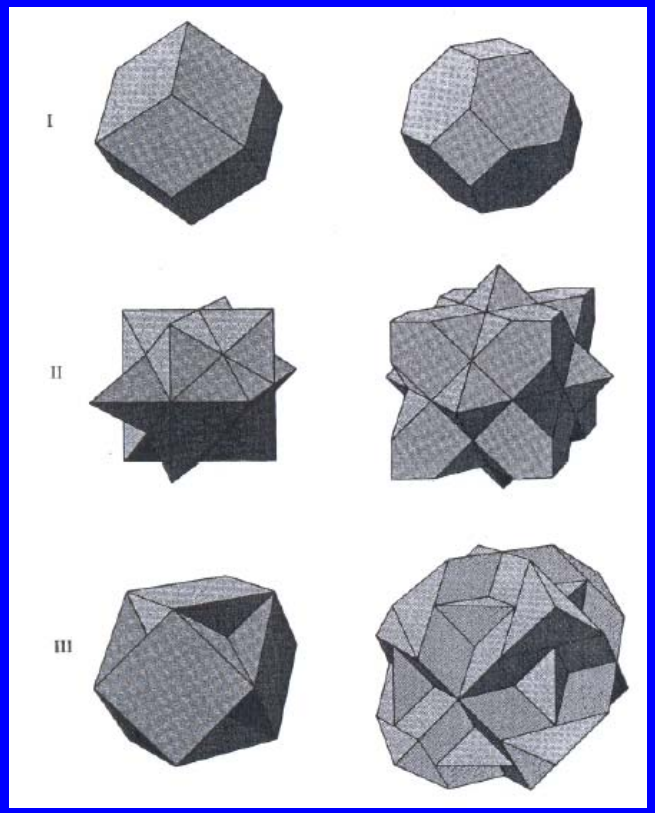
bcc

fcc

1st

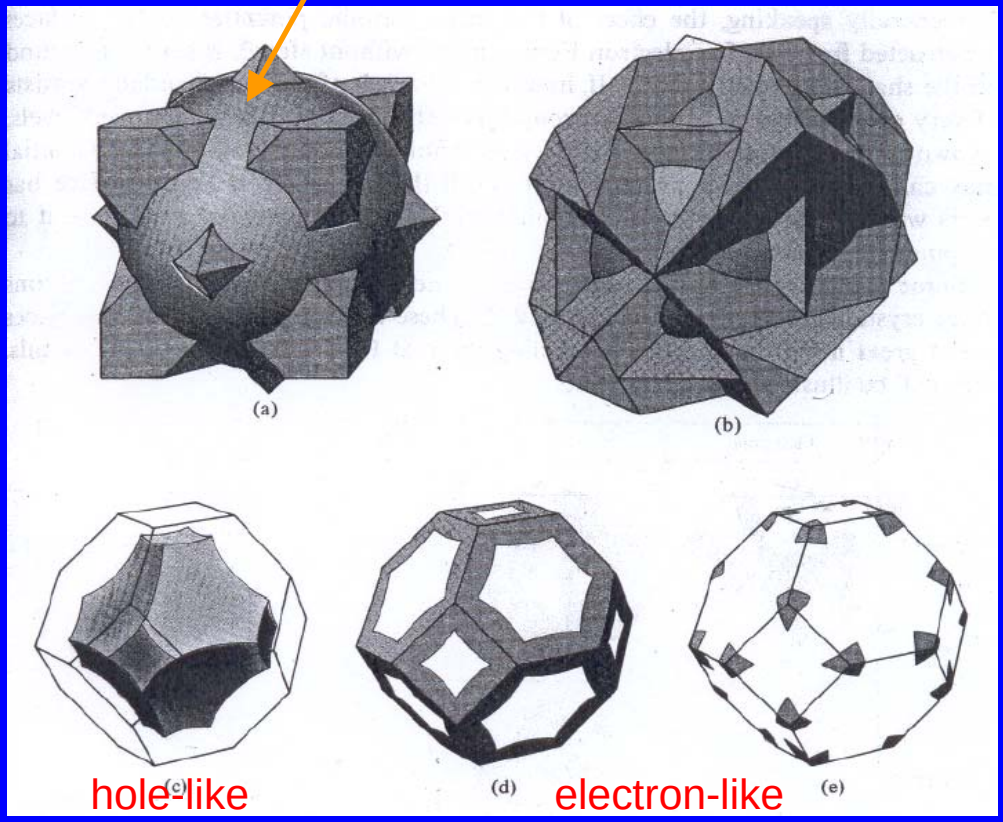
2nd

3rd



exterior surfaces
Brillouin zones

Fermi sphere



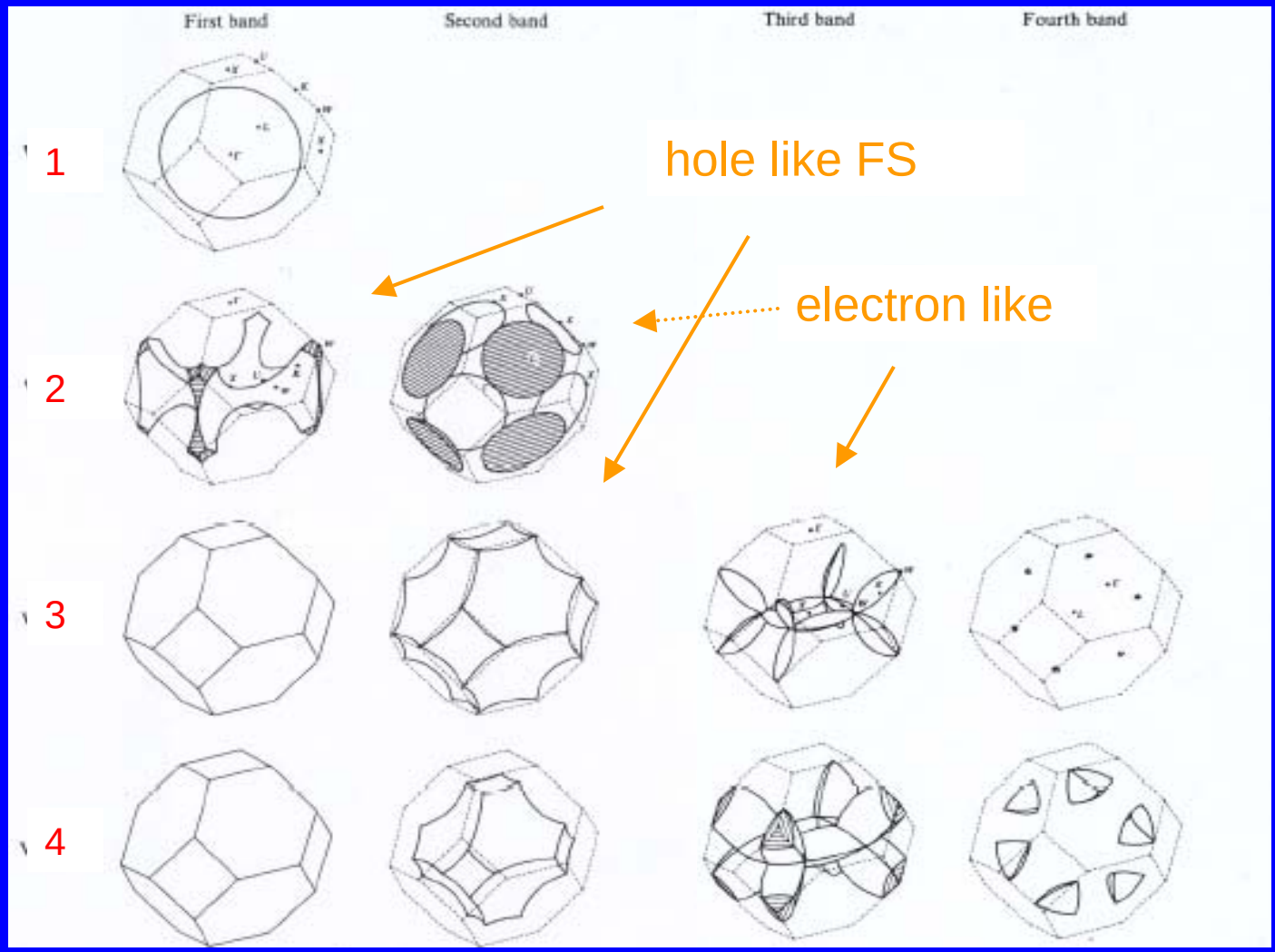
hole-like

electron-like

Fermi surfaces for fcc lattice
in reduced zone scheme

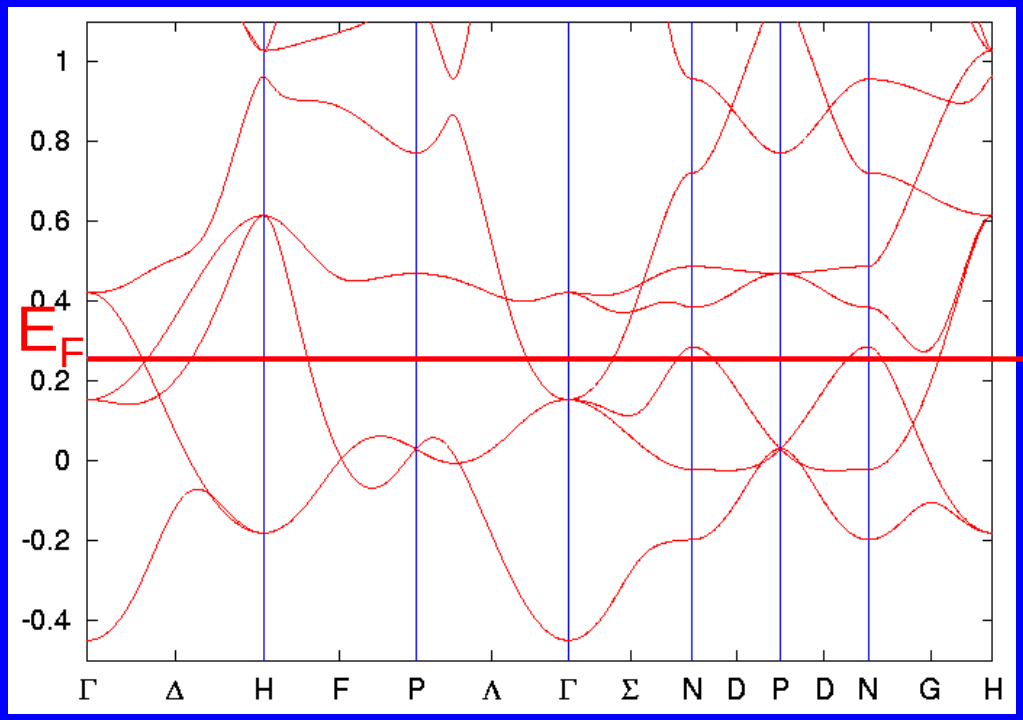
valence

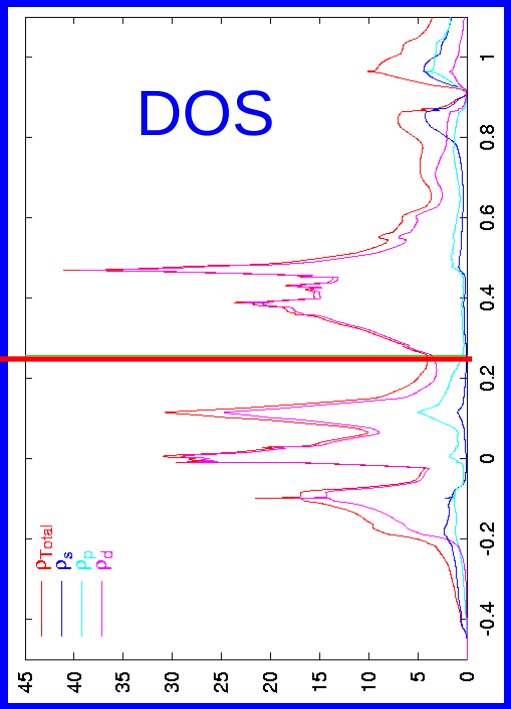
1-4 valent free electron surfaces

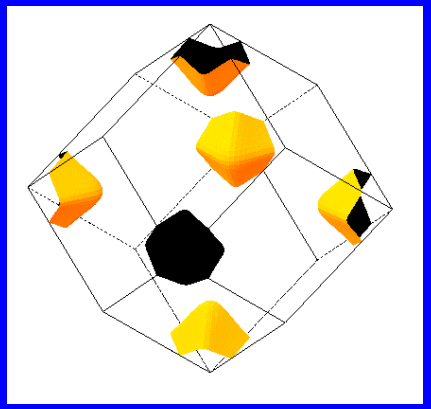


Fermi surfaces for fcc lattices in reduced zone scheme

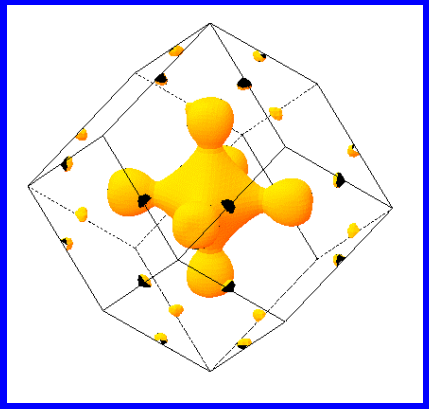
Example bandstructure: 5d metal tungsten (bcc lattice)



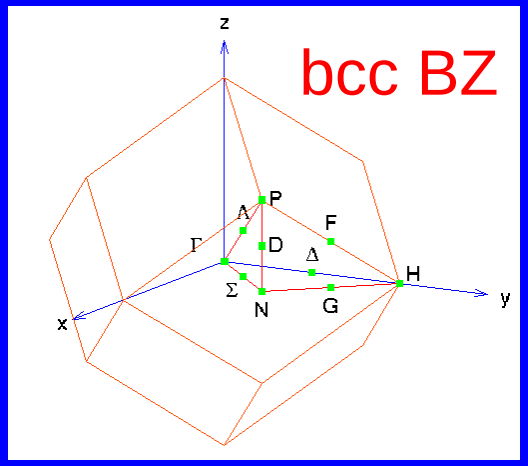




3rd band



4th band



Periodic Table of the Fermi Surfaces of Elemental Solids

http://www.phys.ufl.edu/fermisurface

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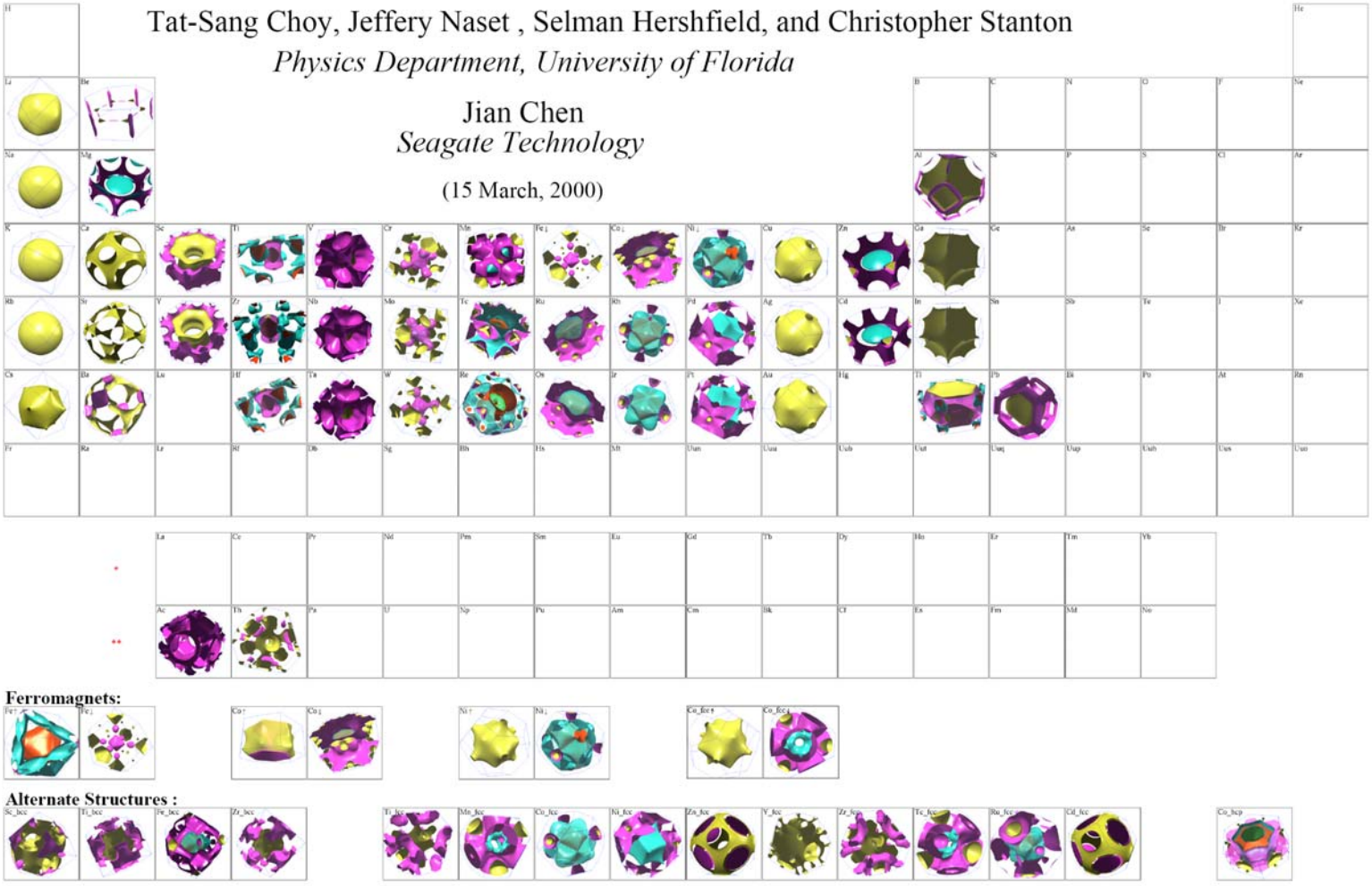
Physics Department, University of Florida

Jian Chen

Seagate Technology

(15 March, 2000)



Source of tight binding parameters (except for fcc Co ferromagnet): D.A. Papaconstantopoulos, *Handbook of the band structure of elemental solids*, Plenum 1986.

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another nice Fermi surface website: http://www.phy.tu-dresden.de/~fermisur/