Condensed Matter Physics I

Prof. Dr. Ir. Paul H.M. van Loosdrecht

II Physikalisches Institut, Room 312

E-mail: pvl@ph2.uni-koeln.de

Website: http:/www.loosdrecht.net/

Previously

- Free electron model
- Density of states, Fermi-Dirac distribution
- Pressure, Bulk modulus, Heat capacity, Thermal mass
- Charge conductivity

Today

- Transport
- Failures of the free electron model
- Incorporating periodicity

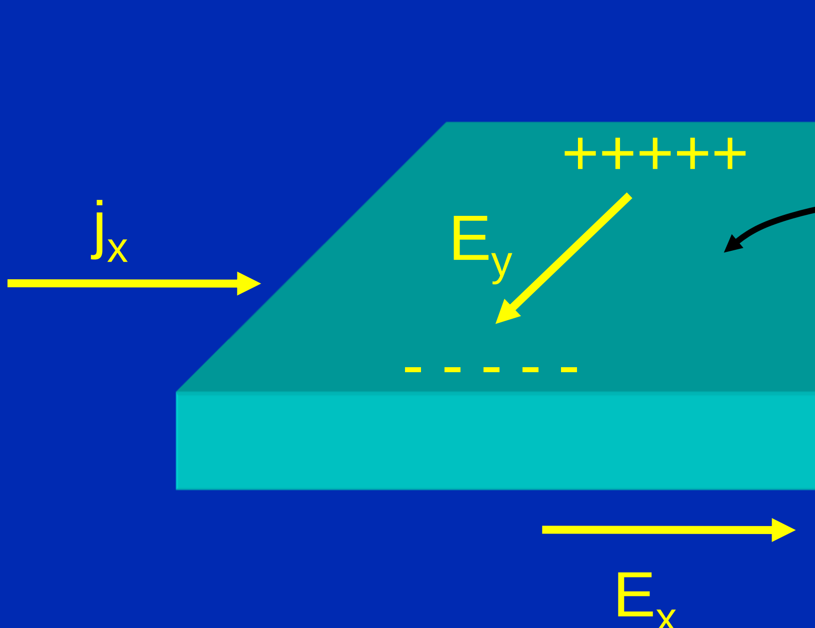
Classical Hall effect

Transport equation: $\hbar\left(\frac{d}{dt}+\frac{1}{\tau}\right)k = F = q\left(E+\frac{k}{m}\times B\right)$

Steady state: $\hbar\vec{k} = -e\tau\left(\vec{E}+\frac{\hbar}{m}\vec{k}\times\vec{B}\right)$

$E_y = R_H \cdot j_x B_\perp$

$R_H = \frac{1}{ne}$



Thermal conductivity

$$J = -\kappa \cdot \nabla T$$

Electronic heat conductivity: $\kappa = \frac{1}{3} C_{el} \cdot v \cdot l = \frac{\pi^2 k_b^2 n \tau}{3m} T$

Wiedemann-Franz law: $\frac{\kappa}{\sigma} = \frac{\pi^2 k_b^2 n \tau}{3m} T \cdot \frac{m}{n e^2 \tau} = L \cdot T$

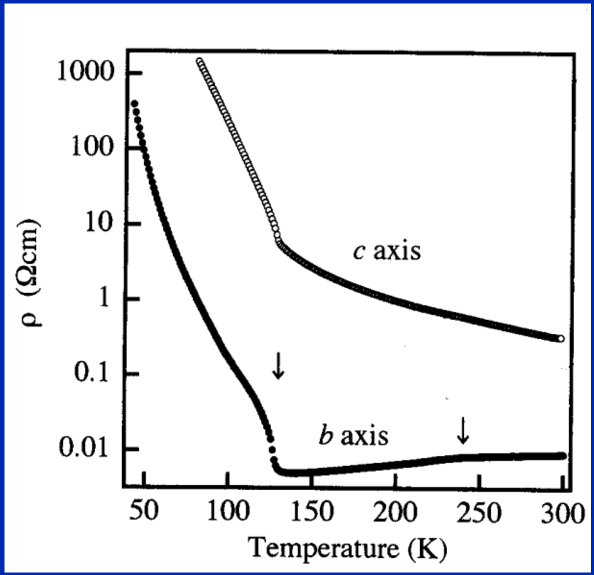
Lorenz number $L = \frac{\pi^2}{3} \left(\frac{k_b}{e}\right)^2 = 2.45 \cdot 10^{-8} \ \frac{\mathrm{W \cdot \Omega}}{K^2}$

Table 10-2 Lorentz number $L = K/\sigma T$ in units of 10^{-8} W·Ω/K², for several metals at 0°C and 100°C

Metal	0°C	100°C	Metal	0°C	100°C
Ag	2.31	2.37	Pb	2.47	2.56
Au	2.35	2.40	Pt	2.51	2.60
Cd	2.42	2.43	Sn	2.52	2.49
Cu	2.23	2.33	W	3.04	3.20
Mo	2.61	2.79	Zn	2.31	2.33

Free electron model: failures

- Hall coefficient
- Magnetoresistance
- Wiedemann-Franz law
- T-dependence of cond., thermal cond.
- Direction dependence of conductivity →
- AC conductivity
- Linear term in specific heat
- Compressibility of metals



NaV_6O_{15}

Yamada,Ueda JPSJ **68,** 2735 (1999)

- What determines the electron density
- Why are some materials bad metals or even isolators

e^- in a periodic potential

- Bragg scattering of free electrons, gaps
- Effect of translational symmetry, Bloch theorem
- Reduced Brillouin zone, Energy bands
- Weak potentials, perturbation theory
- Photo emission

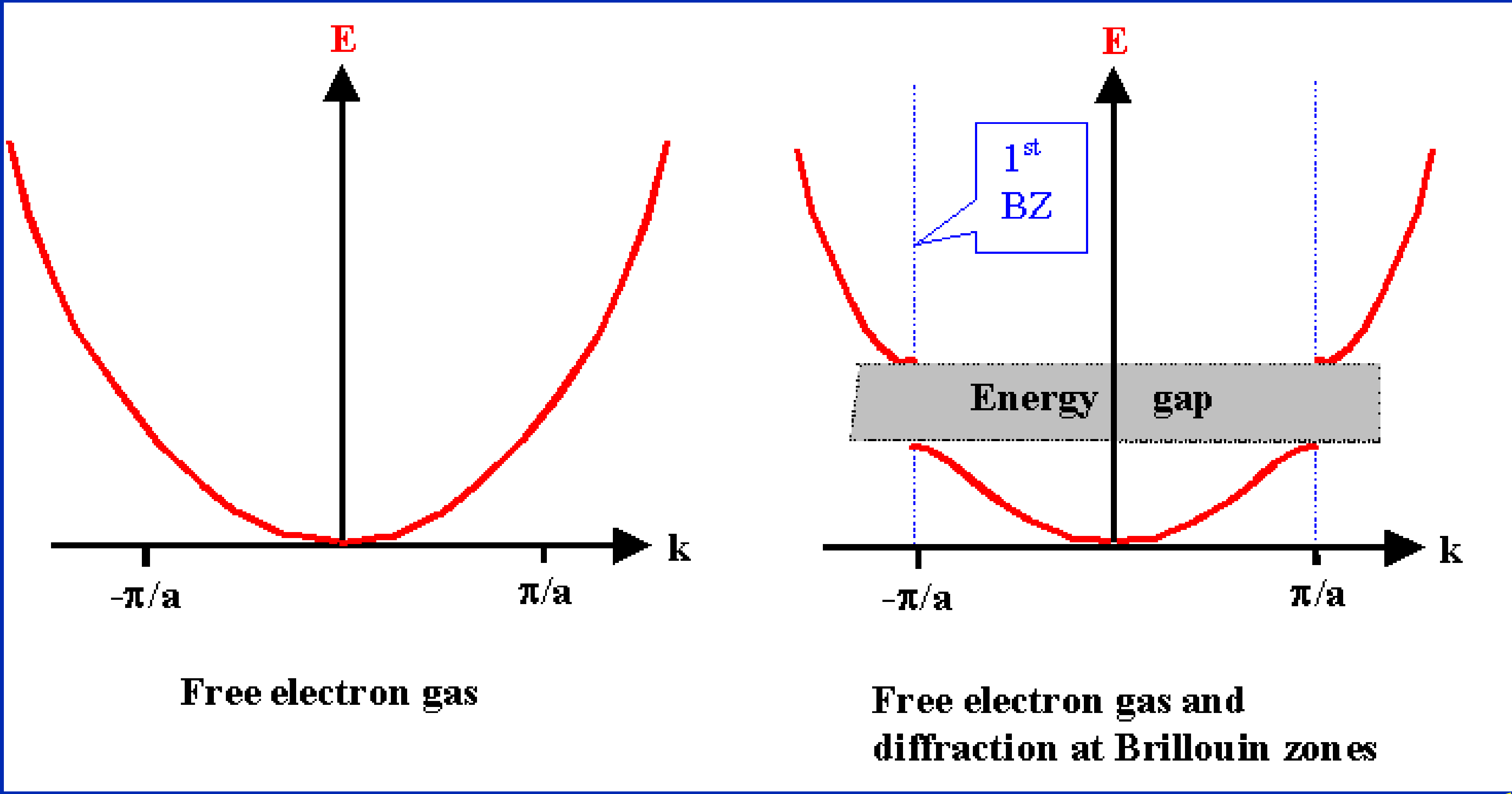
Incorporating the periodic potential

$$V(\vec{r}) = V(\vec{r} + \vec{R}_{\vec{n}}) \qquad \vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) \Psi_\lambda = E_\lambda \Psi_\lambda$$

- Empty lattice
- Weak potential (nearly free electron model, perturbation)
- Strong potential (tight binding (LCAO))

Bragg scattering



TRANSLATIONAL SYMMETRY

When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal….
By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation

F. BLOCH

Translational symmetry

$$V(\vec{r}) = V(\vec{r} + \vec{R}_{\vec{n}}) \qquad \vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\Psi_\lambda = E_\lambda \Psi_\lambda$$

Translation operator: $T_{\vec{n}}\psi(\vec{r}) \equiv \psi(\vec{r} + \vec{R}_{\vec{n}})$

Translationally invariant Hamiltonian: $[H, T_{\vec{n}}] = 0$

$$T_{\vec{n}} \cdot H\Psi_\lambda = H \cdot T_{\vec{n}}\Psi_\lambda = E_\lambda\, T_{\vec{n}}\Psi_\lambda$$

⇒ If Ψ_λ is an eigenstate with energy E_λ, so is $T_{\vec{n}}\Psi_\lambda$!

Bloch theorem

$$T_{100}\left|\psi_\lambda\right\rangle = e^{i\phi_{\lambda,1}}\left|\psi_\lambda\right\rangle \quad T_{200}\left|\psi_\lambda\right\rangle = e^{i\phi_{\lambda,1}}e^{i\phi_{\lambda,1}}\left|\psi_\lambda\right\rangle \ \ldots.$$

$$\Rightarrow T_{nml}\left|\psi_\lambda\right\rangle = e^{i\left(n\phi_{\lambda,1}+m\phi_{\lambda,2}+l\phi_{\lambda,3}\right)}\left|\psi_\lambda\right\rangle = e^{i\left(n\vec{a}_1+m\vec{a}_2+l\vec{a}_3\right)\cdot\vec{k}}\left|\psi_\lambda\right\rangle$$

The vectors *k* label the eigenstates: $\left|\psi_\lambda\right\rangle = \left|\psi_{\vec{k}}\right\rangle$

<u>Bloch Theorem (form II)</u>

$$T_{\vec{n}}\Psi_{\vec{k}}(\vec{r}) = \Psi_{\vec{k}}(\vec{r}+\vec{R}_{\vec{n}}) = e^{i\vec{k}\cdot\vec{R}_{\vec{n}}}\Psi_{\vec{k}}(\vec{r})$$

Bloch theorem

<u>Bloch Theorem</u>

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

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

The eigenstates of a periodic one-electron Hamiltonian can be chosen to have the form of a plane wave times a function with the periodicity of the Hamiltonian

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

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

The functions $u_{\vec{k}}(\vec{r})$ are translational invariant

$\Rightarrow$ 3D fourier expansion of a periodic function

$$u_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} \tilde{u}_{\vec{k},\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

$$\Rightarrow \boxed{\Psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} \tilde{u}_{\vec{k},\vec{G}} \cdot e^{i(\vec{k}+\vec{G})\cdot\vec{r}}}$$

Electrons in a periodic potential

$$H = \frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})$$

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

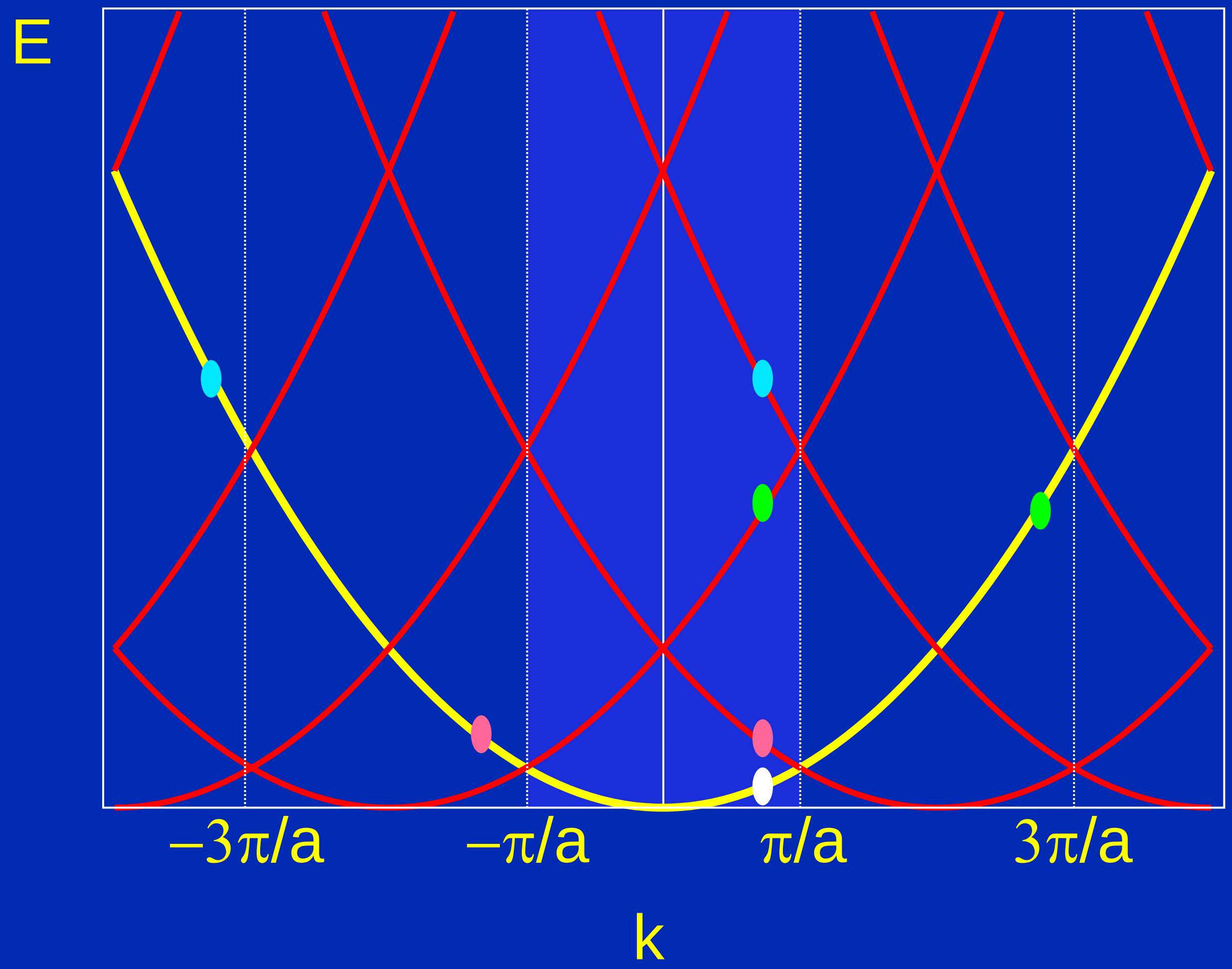
$$\Rightarrow \langle \vec{q} | H | \vec{k} \rangle = \frac{\hbar^2 k^2}{2m}\delta_{\vec{q},\vec{k}} + \sum_{\vec{G}} V_{\vec{G}} \delta_{\vec{q},\vec{k}+\vec{G}}$$

Each free e$^-$ state k couples to all states k+G !

Eigenstates $\quad |\psi_{\vec{k}}\rangle = \sum_{\vec{G}} \alpha_{\vec{G}} |\vec{k}+\vec{G}\rangle$

Energies $\quad E_{\vec{k}} = \frac{\hbar^2}{2m}\sum_{\vec{G}} |\alpha_{\vec{G}}|^2 |\vec{k}+\vec{G}|^2 + \sum_{\vec{G},\vec{Q}} \alpha_{\vec{G}} \alpha^*_{\vec{Q}} V_{\vec{Q}-\vec{G}}$

Reduced Brillouin zone



Perturbation theory

$$\left|\psi_k\right\rangle = \frac{1}{C}\left\{\left|\vec{k}\right\rangle + \sum_{\vec{G}\neq 0} \frac{V_{\vec{G}}}{E_{\vec{k}}^{(0)} - E_{\vec{k}+\vec{G}}^{(0)}} \left|\vec{k}+\vec{G}\right\rangle\right\}$$

$$\left|C\right|^2 = 1 + \sum_{\vec{G}\neq 0} \left|\frac{V_{\vec{G}}}{E_{\vec{k}}^{(0)} - E_{\vec{k}+\vec{G}}^{(0)}}\right|^2$$

$$\left|C\right|^2 E_{\vec{k}} = E_{\vec{k}}^{(0)} + V_{\vec{0}} + \sum_{\vec{G}\neq 0} \frac{\left|V_{\vec{G}}\right|^2}{E_{\vec{k}}^{(0)} - E_{\vec{k}+\vec{G}}^{(0)}}$$

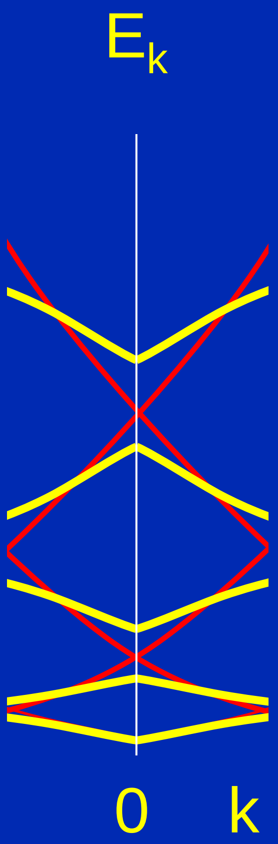
Large contribution when $E^0_k \approx E^0_{k+G}$

Near zone boundary

$$\left|\psi_k\right\rangle \approx a_0\left|\vec{k}\right\rangle + a_{\vec{b}}\left|\vec{k}+\vec{b}\right\rangle$$

$$H \approx \begin{bmatrix} E_k^{(0)} & V_{\vec{b}} \\ V_{\vec{b}} & E_{k+\vec{b}}^{(0)} \end{bmatrix}$$

$$\Rightarrow E_k = \frac{1}{2}\left[E_k^{(0)} + E_{k+\vec{b}}^{(0)}\right] \pm \frac{1}{2}\sqrt{\left(E_k^{(0)} - E_{k+\vec{b}}^{(0)}\right)^2 + 4V_b^{\,2}}$$



If $E^0_k = E^0_{k+b} \;\rightarrow\; E_k = E^0_k \pm V_b$

Band structure: Approaches

- Empty lattice (only periodicity)
- Perturbation theory (nearly free electrons, weak potential)
- Tight binding method (LCAO)
- Exact models (Kronig-Penney model, see for instance Kittel)
- ‘advanced’ methods: see for instance
  ashcroft and mermin, chapter 11

Band structure: Approaches

- Empty lattice (only periodicity)
- Perturbation theory (nearly free electrons, weak potential)
- Tight binding method (LCAO)
- Exact models (Kronig-Penney model, see for instance Kittel)
- ‘advanced’ methods: see for instance
  ashcroft and mermin, chapter 11

Diamond band structure

VOLUME 16, NUMBER 9 PHYSICAL REVIEW LETTERS 28 FEBRUARY 1966

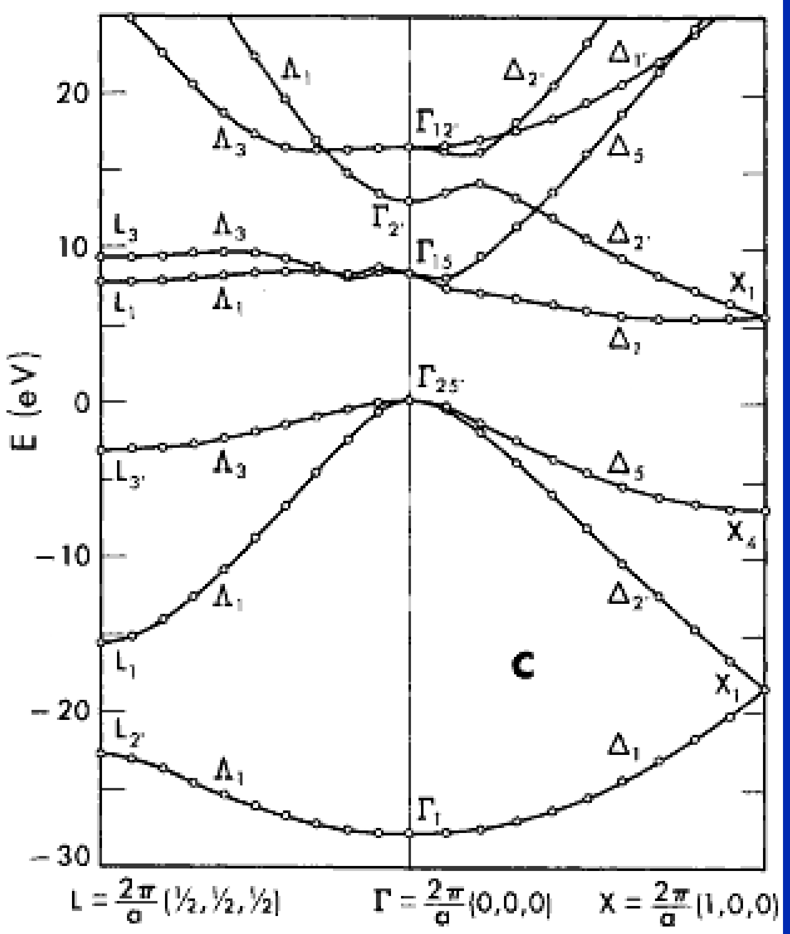


FIG. 1. The electronic band structure of diamond.

BAND STRUCTURE AND OPTICAL PROPERTIES OF DIAMOND*

W. Saslow,† T. K. Bergstresser, and Marvin L. Cohen‡
Department of Physics, University of California, Berkeley, California
(Received 27 January 1966)

PHYSICAL REVIEW B VOLUME 51, NUMBER 2 1 JANUARY 1995-II

Electronic band structure of the superconductor Sr_2RuO_4

Tamio Oguchi
Department of Materials Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 724, Japan
(Received 28 September 1994; revised manuscript received 8 November 1994)

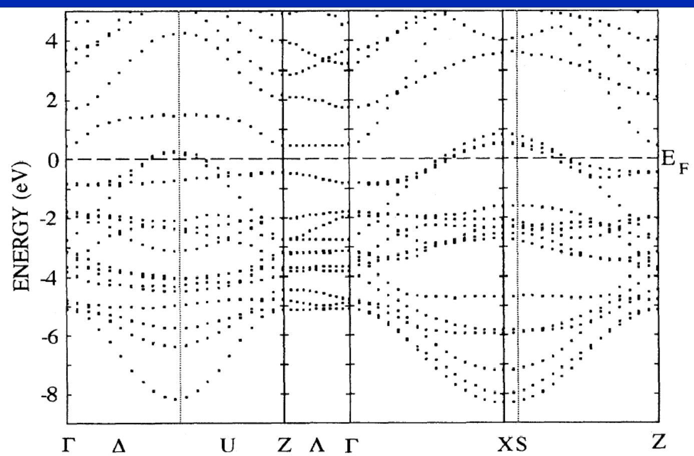


FIG. 1. Calculated energy band structure of Sr_2RuO_4 along high-symmetry lines. A horizontal broken line denotes the Fermi energy.

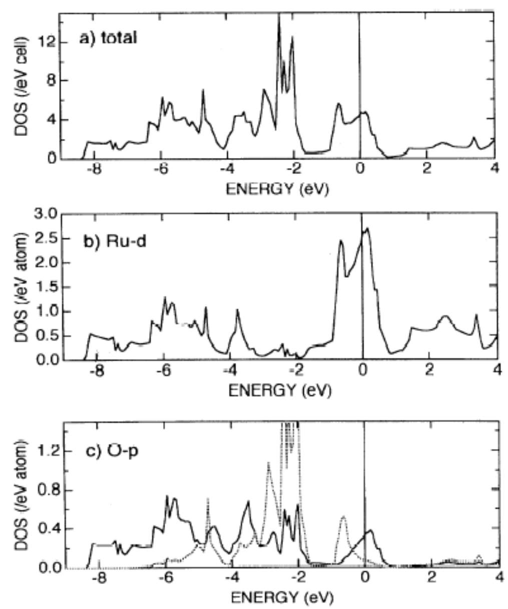


FIG. 3. Calculated density of states (DOS) of Sr_2RuO_4: (a) total DOS, (b) partial Ru d DOS, and (c) partial O p DOS. In panel (c), solid and dotted curves represent the partial p DOS of the O(I) and O(II) atoms, respectively. A vertical line denotes the Fermi energy.

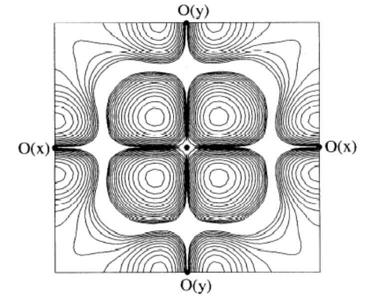


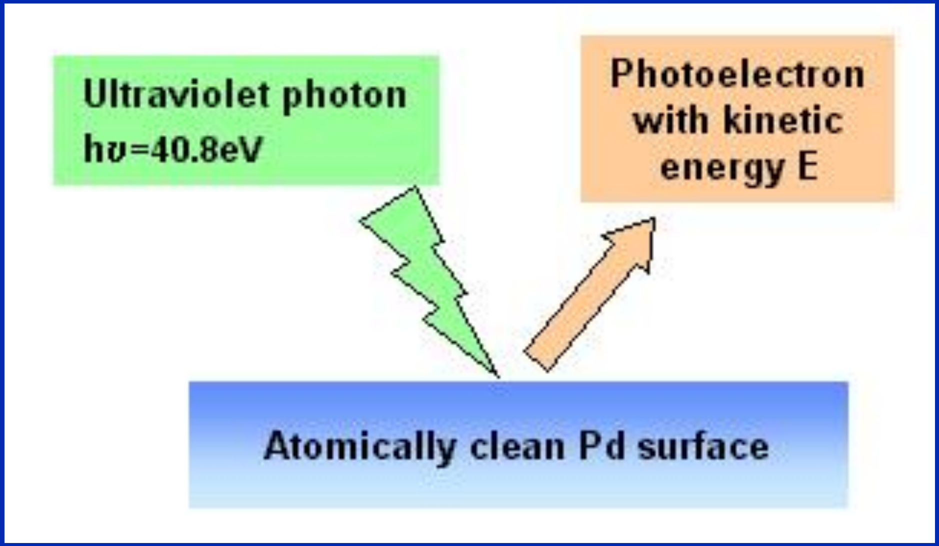
FIG. 2. An ab-plane contour map of the pseudocharge density of the antibonding $d\varepsilon(xy)$-$p\pi$ band at the X point (the 15th band in Fig. 1). Contours of charge density are plotted as $(2)^{n/2}\times 10^{-3}$ electrons/bohr^3 ($n=0,1,\ldots$). A clear node (zero amplitude of the wave function) between the Ru (at center) and four O(I) atoms indicates the antibonding character of the state.

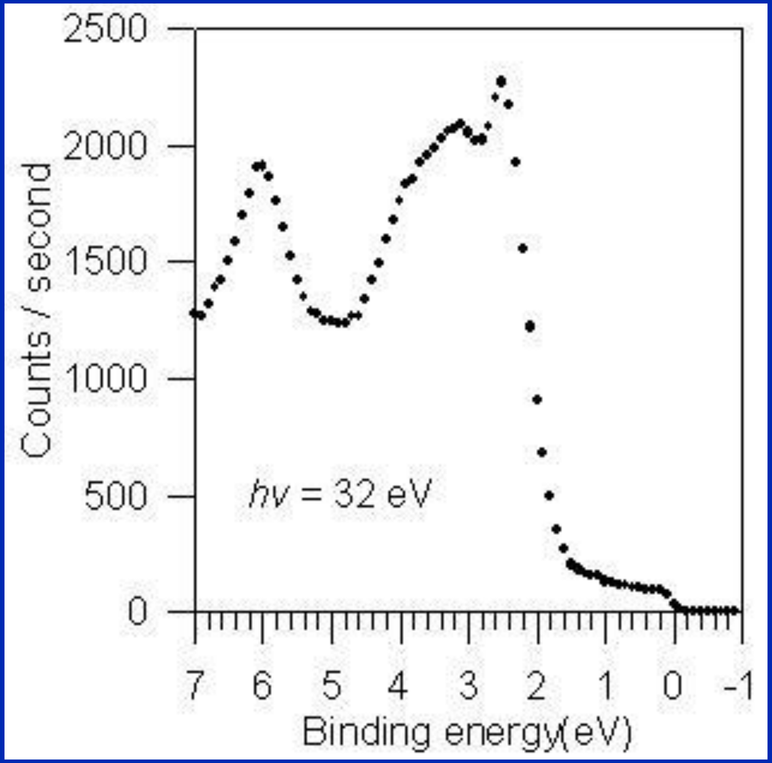
PvL CMP-I
WS 16/17

Photoemission

$$E_{bind} = \hbar\omega - E_{kin} - \phi$$

$$\hbar k_{||}^{i} = \hbar k_{||}^{f} = \sqrt{2mE_{kin}}\sin\theta$$





Gold, U. Johansson, R. Nyholm

Photoemission

VOLUME 89, NUMBER 15 PHYSICAL REVIEW LETTERS 7 OCTOBER 2002

Bulk Band Gaps in Divalent Hexaborides

J. D. Denlinger
Advanced Light Source, Lawrence Berkeley National Laborato

J. A. Clack, J. W. Allen, and G.-H. G
Randall Laboratory, University of Michigan, Ann Arbo

D. M. Poirier* and C. G. Olso
Ames Laboratory, Iowa State University, Ame

J. L. Sarrao,† A. D. Bianchi,† and Z
National High Magnetic Field Lab and Department of Physics, Florida St

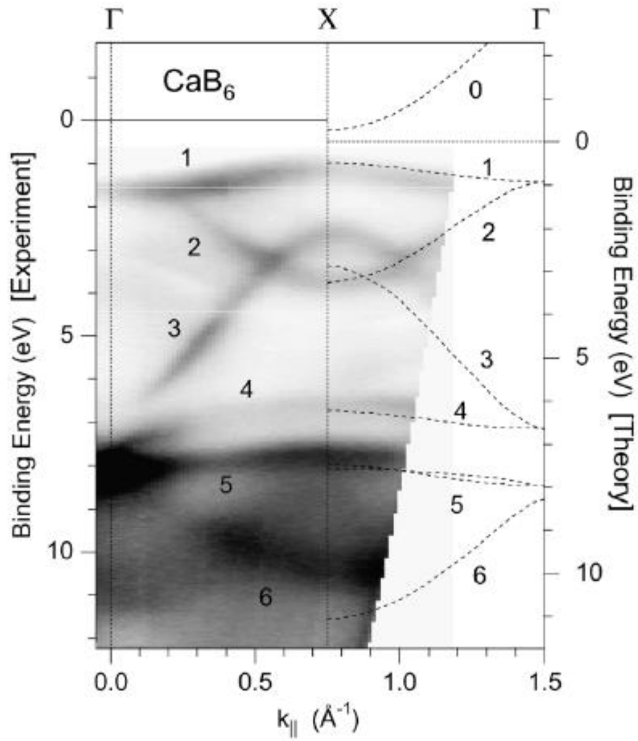


FIG. 1. Comparison of the experimental and theoretical band structures of CaB_6 along Γ-*X*. The reverse gray scale image of ARPES intensities is the sum of two data sets with 30 eV *s*-and *p*-polarized excitation. Dashed lines are from the quasiparticle *GW* calculation [18] giving *X*-point gap between bands 0 and 1.

Photoemission