

THE LAPW METHOD

$$M_{s,t}(E) = K_{s,t} + \sum_{l=0}^{\infty} h_{s,t}^{(l)} z_l(E) - E S_{s,t}$$

mit

$$S_{s,t} = \Omega_0 \delta_{s,t} - 4\pi r_{\text{MT}}^2 \frac{j_1(|\mathbf{k}_s - \mathbf{k}_t| r_{\text{MT}})}{|\mathbf{k}_s - \mathbf{k}_t|},$$

$$\cdot$$

$$K_{s,t} = \frac{\hbar^2}{2m} \mathbf{k}_s \cdot \mathbf{k}_t S_{s,t},$$

$$\cdot$$

$$h_{s,t}^{(l)} = \frac{\hbar^2}{2m} 4\pi r_{\text{MT}}^2 P_l(\cos \vartheta_{s,t}) j_l(k_s r_{\text{MT}}) j_l(k_t r_{\text{MT}}),$$

$$z_l(E) = (2l + 1) \left[\frac{d}{dr} R_l(r; E) / R_l(r; E) \right]_{r=r_{\text{MT}}}$$

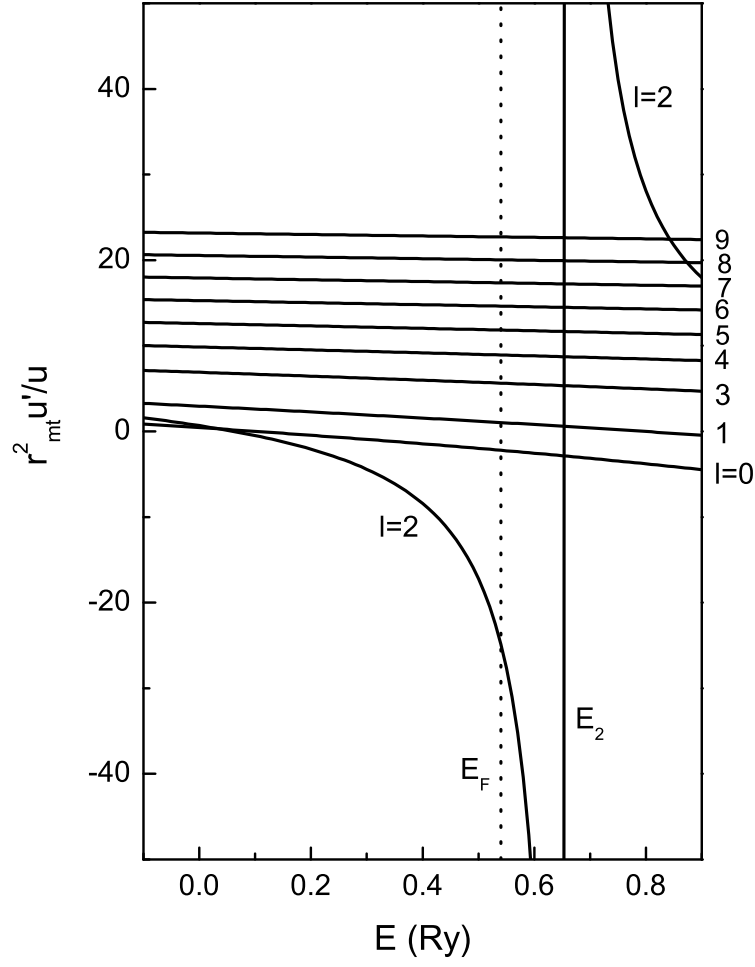
Old Linearization:

An example: Palladium fcc

The following diagram shows the quantities

$$r_{\text{MT}}^2 \frac{R'(r_{\text{MT}})}{R(r_{\text{MT}})}$$

as functions of the energy E for $l = 0, 1, \dots, 9$.



$$z_1(E) \approx a_l - b_l (E - E_0) \quad z_2(E) \approx \frac{1}{\beta_2 (E - E_2)}$$

$$M_{s,t}^{LIN}(E) = \left\{ K_{s,t} + \sum_{l \neq 2} \hat{h}_{s,t}^{(l)} [a_l + b_l E_0] - \hat{h}_{s,t}^{(2)} \beta_2 E_2 \right\} \\ - E \left\{ S_{s,t} + \sum_{l \neq 2} h_{s,t}^{(l)} b_l - \hat{h}_{s,t}^{(2)} \beta_2 \right\} .$$

Modern Linearization (e.g., WIEN code):

APW theory:

$$\phi_{\mathbf{k}_t}^{APW}(\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} A_{\ell m}(\mathbf{k}_t) R_{\ell}(r; E) Y_{\ell m}(\vartheta, \varphi) \quad \text{for } \mathbf{r} \in \text{MTK},$$

$$\phi_{\mathbf{k}_t}^{APW}(\mathbf{r}) = e^{i\mathbf{k}_t \cdot \mathbf{r}} \quad \text{for } \mathbf{r} \in \text{interstitial region}$$

with

$$\left\{ -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} \right) + V_{MT}(r) - E \right\} R_{\ell}(r; E) = 0.$$

LAPW theory:

$$R_{\ell}(r; E) \longrightarrow R_{\ell}(r; E_{\ell}) :$$

The (originally) *free* energy values E are reset by the *parameters* E_s, E_p, E_d etc.

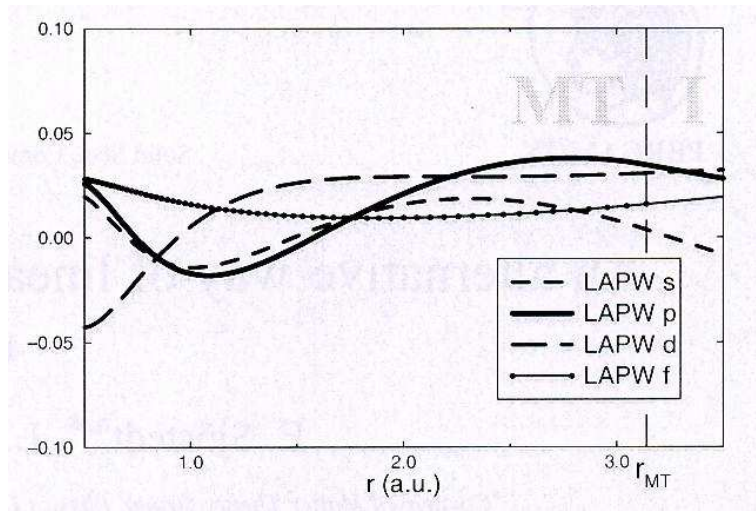
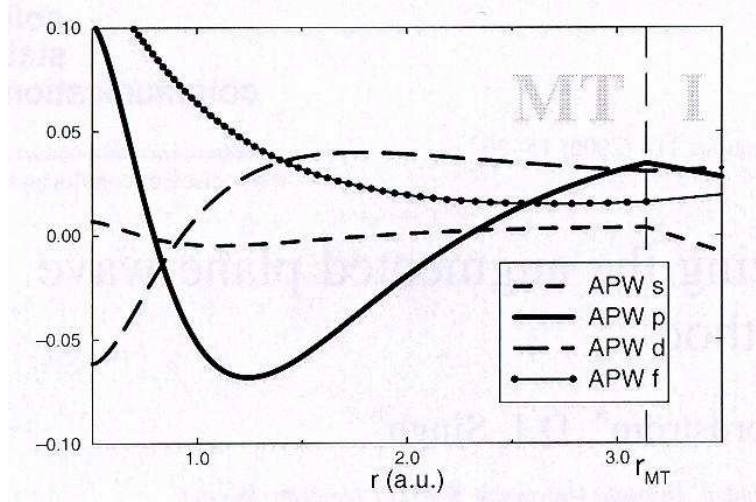
$$\begin{aligned} \phi_{\mathbf{k}_t}^{LAPW}(\mathbf{r}) = & \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} A_{\ell m}(\mathbf{k}_t) R_{\ell}(r; E_{\ell}) Y_{\ell m}(\vartheta, \varphi) + \\ & + \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} B_{\ell m}(\mathbf{k}_t) \dot{R}_{\ell}(r; E_{\ell}) Y_{\ell m}(\vartheta, \varphi) \quad \text{MTK}, \end{aligned}$$

$$\phi_{\mathbf{k}_t}^{LAPW}(\mathbf{r}) = e^{i\mathbf{k}_t \cdot \mathbf{r}} \quad \text{for } \mathbf{r} \in \text{interstitial region}$$

$$\dot{R}_\ell(r; E_\ell) = \left[\frac{\partial}{\partial E} R_\ell(r; E) \right]_{E=E_\ell}$$

means the solution of the differential equation

$$\left\{ -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} \right) + V_{MT}(r) - E \right\} \dot{R}_\ell(r; E) = R_\ell(r, E).$$



APW basis functions (top) and LAPW basis functions (bottom) for Ce (Sjöstedt et al., 2000).

$$M_{s,t}^{APW} = \int_{\Omega_0} d^3r \phi_s^{(APW)*}(\mathbf{r}, E) (\hat{H}_{MT} - E) \phi_t^{(APW)}(\mathbf{r}, E) - \frac{\hbar^2}{2m} \int_{r_{MT}} dS \phi_{a,s}^* \left[\frac{\partial}{\partial r} \phi_{a,t} - \frac{\partial}{\partial r} \phi_{i,t} \right].$$

$$M_{s,t}^{LAPW} = \int_{\Omega_0} d^3r \phi_s^{(LAPW)*}(\mathbf{r}) (\hat{H}_{MT} - E) \phi_t^{(LAPW)}(\mathbf{r})$$

The full-potential LAPW method - relativistic effects

A further important point in bandstructure calculations:
How can we go beyond the muffin-tin approximation?

One can do this by the following two-step procedure:

- The LAPW basis functions are calculated *on the muffin-tin level*, i.e., the differential equations

$$\left\{ -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} \right) + V_{MT}(r) - E \right\} R_\ell(r; E) = 0.$$

and

$$\left\{ -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} \right) + V_{MT}(r) - E \right\} \dot{R}_\ell(r; E) = R_\ell(r, E).$$

are evaluated including a muffin-tin approximation of the real crystal potential.

- However, for the calculation of the LAPW matrix elements, **the muffin-tin Hamiltonian is reset by the real crystal potential (full potential FP):**

$$\hat{H}_{MT} = -\frac{\hbar^2}{2m} \nabla^2 + V_{MT}(|\mathbf{r}|) \quad \longrightarrow \quad \hat{H}_{FP} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}),$$

where the potential $V(\mathbf{r})$ is written in the following form:

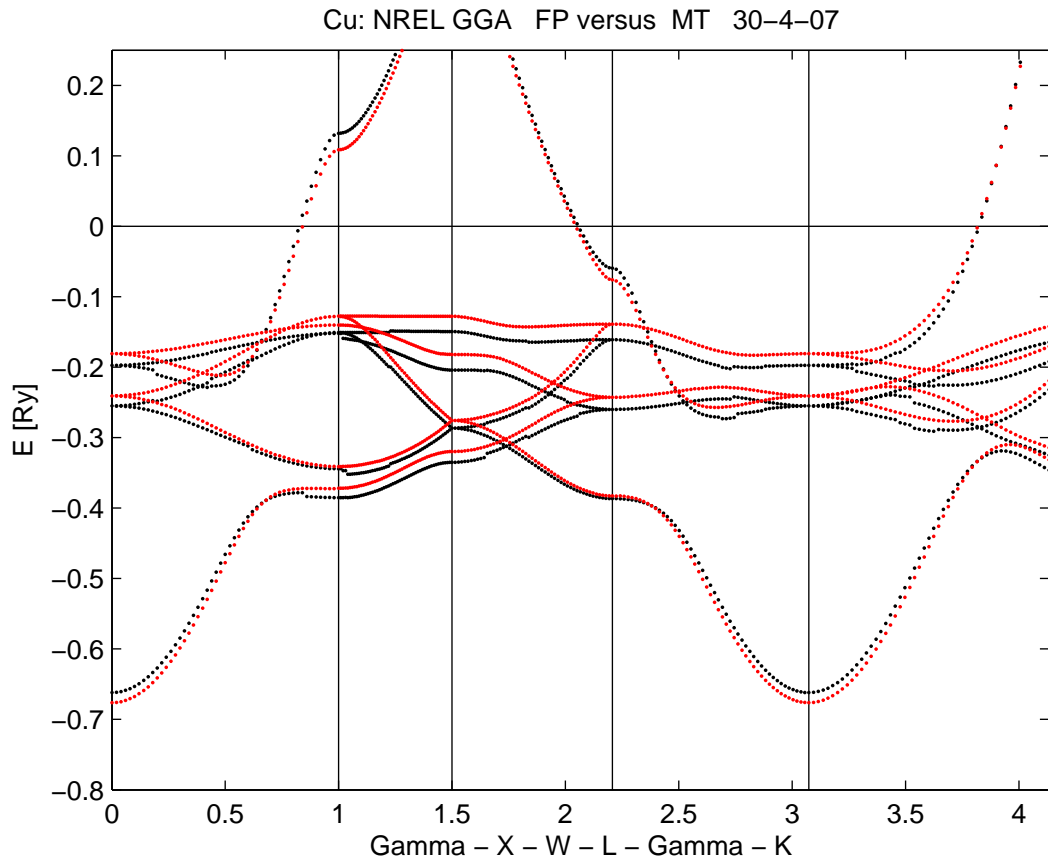
$$V(\mathbf{r}) = \begin{cases} \sum_{l,m} v_{lm}(r) Y_{l,m}(\vartheta, \varphi) & |\mathbf{r}| \leq r_{MT} \\ \cdot & \\ \sum_{\mathbf{K}} v_{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}} & \mathbf{r} \in I \end{cases}$$

Obviously, the *muffin-tin approximation* is given by the first terms in the above expansions ($\ell = m = 0$ and $\mathbf{K} = 0$, respectively).

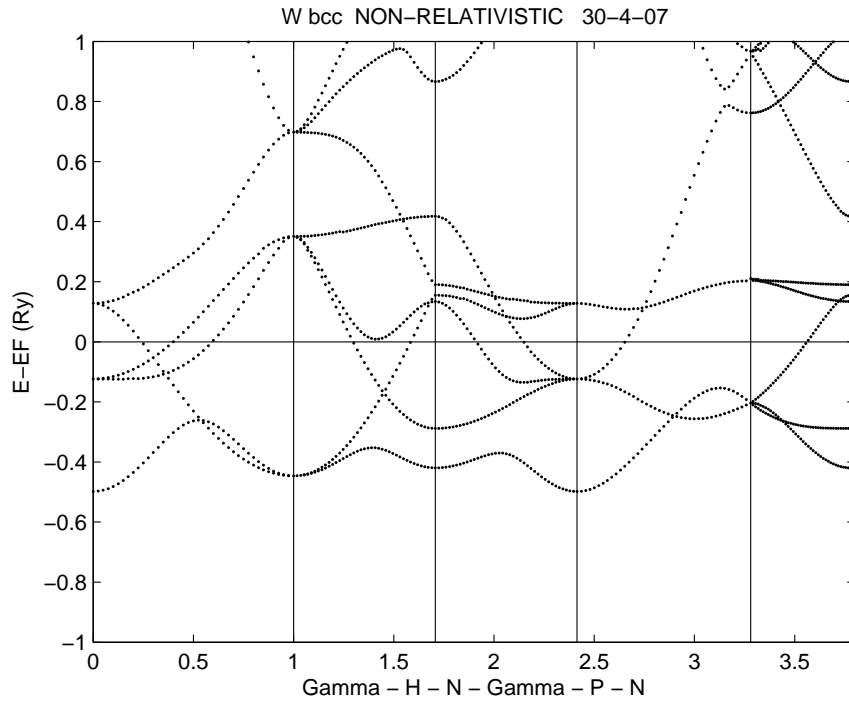
In up-to-date bandstructure programs, the notation *full potential* has often a more extensive meaning, namely, in connection with taking into account **relativistic effects** of the crystal potential: nowadays, all relativistic correction terms - well-known from atomic theory - are included into the bandstructure calculation:

- The **scalar-relativistic** corrections:
mass-velocity correction and Darwin correction,
- the **spin-orbit coupling** correction.

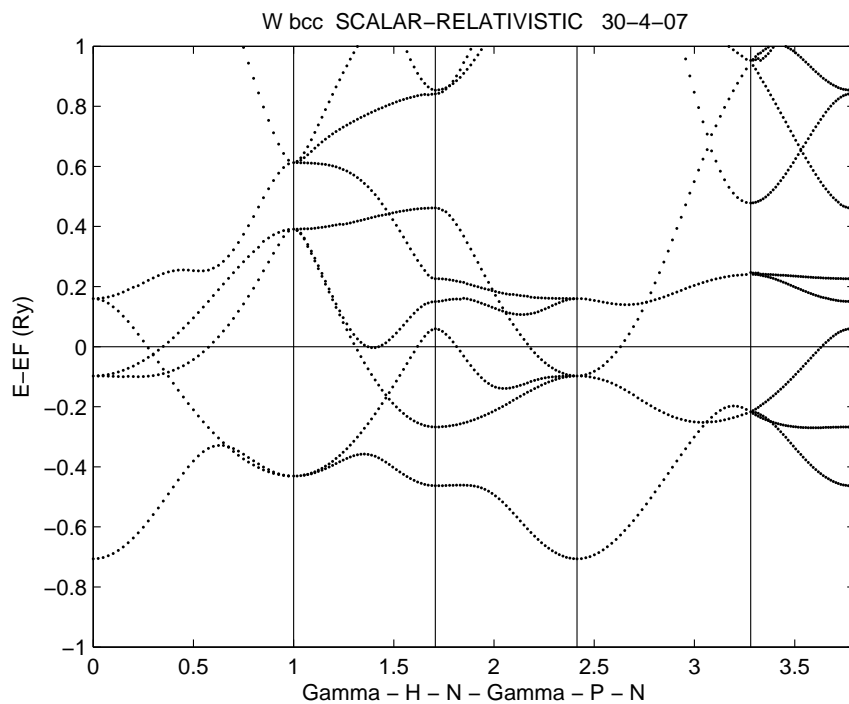
In the following diagrams, some LAPW results are shown that have been obtained by the FP-LAPW program called **WIEN** (Blaha, Schwarz, Sorantin, 1990).



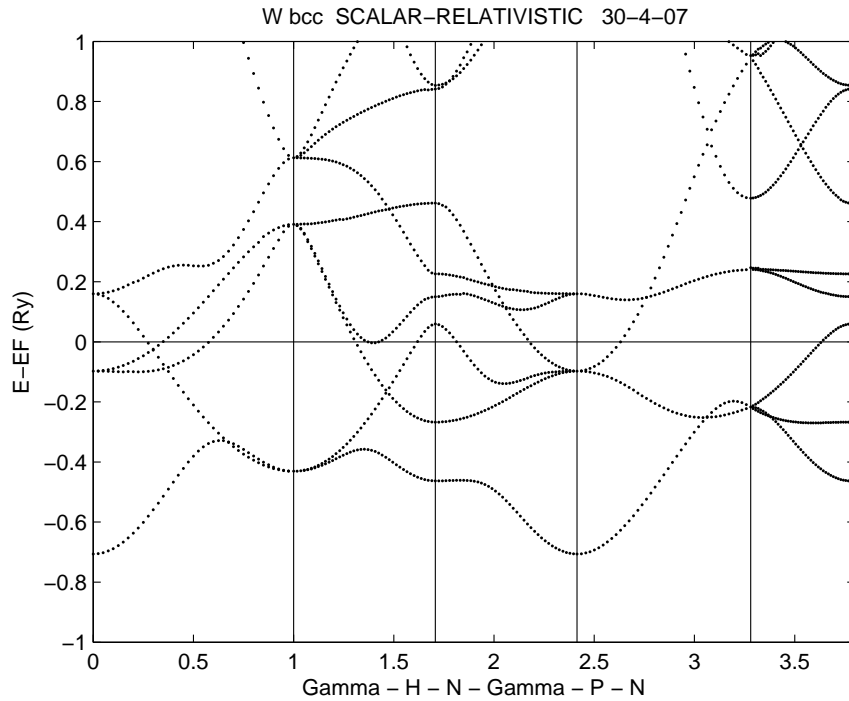
Bandstructure results for fcc copper, calculated by the LAPW program WIEN, using a *muffin-tin potential* (black curves) and a *full potential* (red curves).



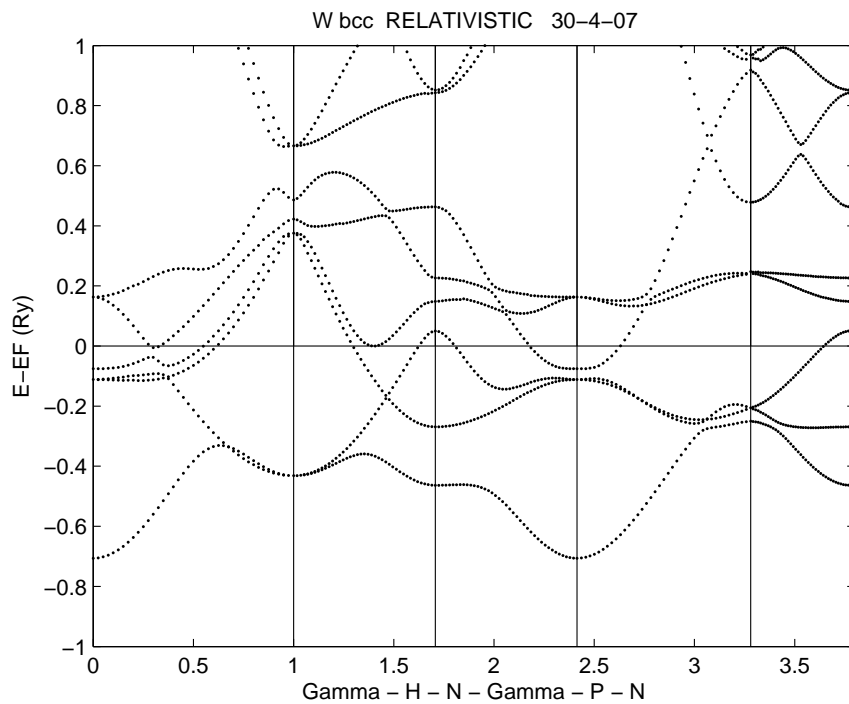
Bandstructure of bcc Tungsten ($Z=74$), *without* relativistic effects.



Bandstructure of bcc Tungsten ($Z=74$), *including* scalar-relativistic effects.



Bandstructure of bcc Tungsten ($Z=74$), including *scalar*-relativistic effects.



Bandstructure of bcc Tungsten ($Z=74$), including *full*-relativistic effects.