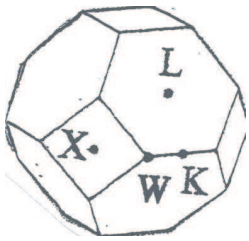
8.511 Theory of Solids I **Problem Set 3** **Due 8:00pm**
October 6, 2015

1. Band Structure of Aluminum. Al is an f.c.c. crystal with $a = 4.05$ Åwhere a is the dimension of the cube.

   (a) Construct the lowest two bands of the free electron band structure and plot it from Γ to X, from X to W, from W to L, and from L to Γ. W is defined in the last problem set and X and L are the points on the zone face in the (100) and (111) directions, respectively. Indicate the degeneracies.



   (b) Use the pseudopotential $V(r) = -\frac{Z}{r}$ for $r > R_c$ and zero for $r < R_c$. Recall the expression for $V(q)$ is

$$V(q) = \frac{1}{\Omega}\int_c d\boldsymbol{r} e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} V(\boldsymbol{r})$$

   where the integration is over the primitive cell in real space and Ω is its volume. By extending the integration over r to infinity, show that

$$V(q) = -\frac{4\pi e^2 Z}{q^2\Omega}\cos(qR_c).$$

   For aluminum use $Z = 3$ and $R_c = 0.6$ Å. Compute the splitting at X, W and L in eV.

   (c) Using this pseudopotential, calculate on a computer the band structure from Γ to X, X to W and from W to L, and L to Γ.

   (d) Estimate the location of the Fermi level. Compare your result with the KKR calculation shown on p.205 of Ashcroft and Mermin.

Figure 11.9
Calculated valence bands for aluminum (three electrons outside of a closed-shell neon configuration)comparedwith *free* electron bands (dashed lines). The bands are computed by the KKR method. (B. Segall, *Phys. Rev.* **124**, 1797 (1961).)