Approximate solution of the Central Equation near the zone boundary:

Let **$k = \frac{1}{2}G + K'$** where **K' is small compared to $\frac{1}{2}G$** .

[recall that at the zone boundary: $k = \frac{1}{2}G$ and $\varepsilon(\pm) = \varepsilon_k \pm U_G$ where $\varepsilon_k = h^2k^2/2m$ is the kinetic energy of the electron].

From the matrix of the Central Equation, using only the 4 inner-most terms, and setting the determinate of these terms equal to 0 gives the condition:

$$\begin{vmatrix} (\varepsilon_{k-G}-\varepsilon) & U_{+G} \\ U_{-G} & (\varepsilon_k-\varepsilon) \end{vmatrix} = 0 \;\Rightarrow\; (\varepsilon_k-\varepsilon)(\varepsilon_{k-G}-\varepsilon) - U_G^2 = 0$$

recall $PE(x) = {}_{n=-\infty}\Sigma^{n=+\infty} U_n \exp[ik_n x]$, where $k_n = n(2\pi/a) = nG$, and $U_G = U_{-G}$.

or $$\varepsilon^2 - \varepsilon(\varepsilon_{k-G}+\varepsilon_k) + \varepsilon_{k-G}\varepsilon_k - U^2 = 0$$ from now on, we'll use U for U_G.

Now we solve for ε using the quadratic formula:

$$\varepsilon = \{ +(\varepsilon_k+\varepsilon_{k-G}) \pm [(\varepsilon_k+\varepsilon_{k-G})^2 - 4(1)(\varepsilon_k\varepsilon_{k-G} - U^2)]^{1/2} \} / 2(1)$$

or $$\varepsilon = +\tfrac{1}{2}(\varepsilon_k+\varepsilon_{k-G}) \pm \tfrac{1}{2}[(\varepsilon_k^2 + 2\varepsilon_k\varepsilon_{k-G} + \varepsilon_{k-G}^2) - 4\varepsilon_k\varepsilon_{k-G} + 4U^2]^{1/2}$$

or $$\varepsilon = +\tfrac{1}{2}(\varepsilon_k + \varepsilon_{k-G}) \pm \tfrac{1}{2}[(\varepsilon_k - \varepsilon_{k-G})^2 + 4U^2]^{1/2} .$$

Recall that $\varepsilon_k = \hbar^2k^2/2m$, and $k = \frac{1}{2}G + K'$, so that:

$$\varepsilon_k = (\hbar^2/2m)(\tfrac{1}{2}G + K')^2 \quad \text{and}$$

$$\varepsilon_{k-G} = (\hbar^2/2m)(\tfrac{1}{2}G + K' - G)^2 = (\hbar^2/2m)(-\tfrac{1}{2}G + K')^2$$

so that $$\varepsilon = \tfrac{1}{2}(\hbar^2/2m)[(\tfrac{1}{2}G + K')^2 + (-\tfrac{1}{2}G + K')^2] \pm \tfrac{1}{2}[(\hbar^2/2m)^2 \{(\tfrac{1}{2}G + K')^2 - (-\tfrac{1}{2}G + K')^2 \}^2 + 4U^2]^{1/2}$$

or $$\varepsilon = \tfrac{1}{2}(\hbar^2/2m)[(\tfrac{1}{4}G^2 + 2(\tfrac{1}{2}G)(K') + K'^2) + (\tfrac{1}{4}G^2 + 2(-\tfrac{1}{2}G)K' + K'^2)] \pm \tfrac{1}{2}[(\hbar^2/2m)^2 \{(\tfrac{1}{4}G^2 + 2(\tfrac{1}{2}G)(K') + K'^2) - (\tfrac{1}{4}G^2 + 2(-\tfrac{1}{2}G)K' + K'^2)\}^2 + 4U^2]^{1/2}$$

or $$\varepsilon = \tfrac{1}{2}(\hbar^2/2m)[\tfrac{1}{2}G^2 + 2K'^2] \pm \tfrac{1}{2}[(\hbar^2/2m)^2 \{4(\tfrac{1}{2}G)K'\}^2 (U^2/U^2) + 4U^2]^{1/2} .$$

Now let $\frac{1}{2}(\frac{1}{2}G^2) = (\frac{1}{2}G)^2$; let $\frac{1}{2}(2K'^2) = K'^2$; cancel ½ in front of √ term with one of the 2^2 in the $[4(\frac{1}{2}G)K']^2$ and the 4 in the $4U^2$; split $(\hbar^2/2m)^2$ factor into two, with one multiplying the $(\frac{1}{2}G)^2$ and the other multiplying the K'^2 in the $[2(\frac{1}{2}G)K']^2$:

so $$\varepsilon = [\hbar^2(\tfrac{1}{2}G)^2/2m] + [\hbar^2K'^2/2m] \pm U[\{4(\hbar^2(\tfrac{1}{2}G)^2/2m)(\hbar^2K'^2/2m)/U^2\} + 1]^{1/2}$$

Now since K' is very small, the first term in the √ is small compared to 1, so we can use the (Taylor series) approximation $(1 + x)^{1/2} \approx 1 + \frac{1}{2}x$:

$$\varepsilon = \hbar^2(\tfrac{1}{2}G)^2/2m + \hbar^2K'^2/2m \pm U[1 + \tfrac{1}{2}4\{\hbar^2(\tfrac{1}{2}G)^2/2m\}\{\hbar^2K'^2/2m\}/U^2] ;$$

or rearranging terms by factoring out the $(\hbar^2K'^2/2m)$ for one part:

$$\varepsilon = \{\hbar^2(\tfrac{1}{2}G)^2/2m \pm U\} + (\hbar^2K'^2/2m)[1 \pm 2\{\hbar^2(\tfrac{1}{2}G)^2/2m\}/U] .$$

But now we recognize the first term: $\{\hbar^2(\frac{1}{2}G)^2/2m \pm U\} = \varepsilon(\text{at edge}) = \varepsilon(\pm)$, and recall that the kinetic energy of the electron at the edge is: $\varepsilon_{edge} = \hbar^2(\frac{1}{2}G)^2/2m$ so that

$$\boldsymbol{\varepsilon = \varepsilon(\pm) + (\hbar^2K'^2/2m)(1 \pm 2\varepsilon_{edge}/U)} \quad . \qquad \text{(where } K' = k - \tfrac{1}{2}G)$$

As k varies from (½G), ε varies as a parabola from the ε at the edge, with ε(+) being the higher and ε(-) being the lower values at the edge (k=½G). Since $U<\varepsilon_{edge}$, then ε for the higher band is parabolic upward since $(1+2\varepsilon_{edge}/U)$ is positive, while the ε for the lower band is parabolic downward since $(1-2\varepsilon_{edge}/U)$ is negative.

See the excel spreadsheet linked from the course web page for this section for a sample calculation and graph.

Remember that we only kept the 1st term, the U_G term, in our approximation. If the higher order terms, U_{nG}, are included, the upward and downward parabolas might be warped somewhat.

We went to a lot of trouble getting this relation between ε (energy) and k (momentum=$\hbar$k). This relation, though, will be key to understanding the weird behaviors of semiconductors.