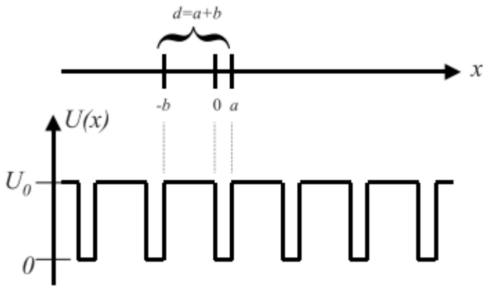
Kronig-Penney Model

Objectives:

- To draw $f(\zeta)$ vs. ζ curves, with a, b, U_0 as parameters.
- To draw E-k diagrams, both extended and folded.

Procedure:



The curves are obtained by solving the following equation:

$$\cos k(a+b) = \frac{1-2\zeta}{2\sqrt{\zeta(1-\zeta)}}\sin\left(\alpha_0 a\sqrt{\zeta}\right)\sinh\left(\alpha_0 b\sqrt{1-\zeta}\right) + \cos\left(\alpha_0 a\sqrt{\zeta}\right)\cosh\left(\alpha_0 b\sqrt{1-\zeta}\right)$$

$$for\, 0 < \zeta < 1$$

$$\cos k(a+b) = \frac{1-2\zeta}{2\sqrt{\zeta(\zeta-1)}}\sin\left(\alpha_0 a\sqrt{\zeta}\right)\sin\left(\alpha_0 b\sqrt{\zeta-1}\right) + \cos\left(\alpha_0 a\sqrt{\zeta}\right)\cos\left(\alpha_0 b\sqrt{\zeta-1}\right)$$

$$for\, 1 < \zeta$$

Where,

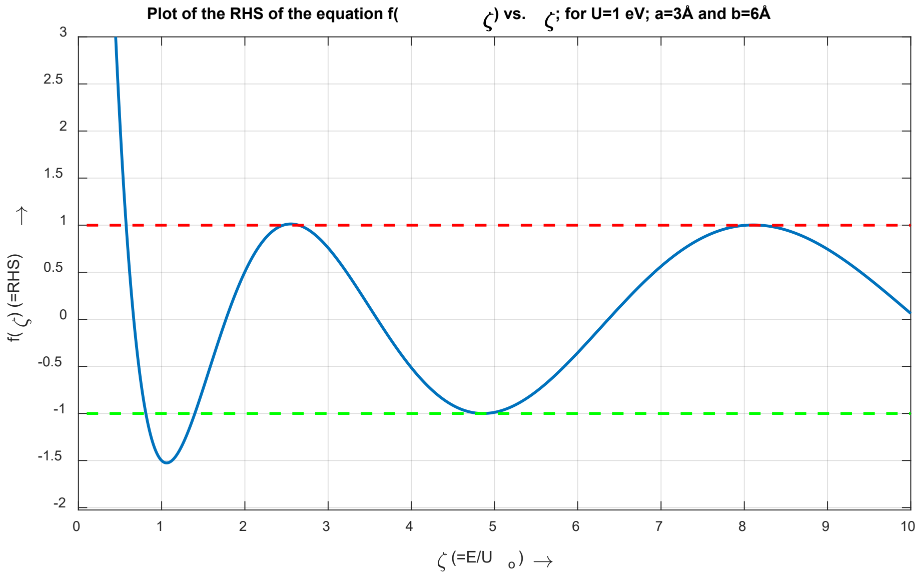
$$\alpha_0 = \sqrt{\frac{2mU_0}{\hbar^2}}$$

$$\zeta = \frac{E}{U_0}$$

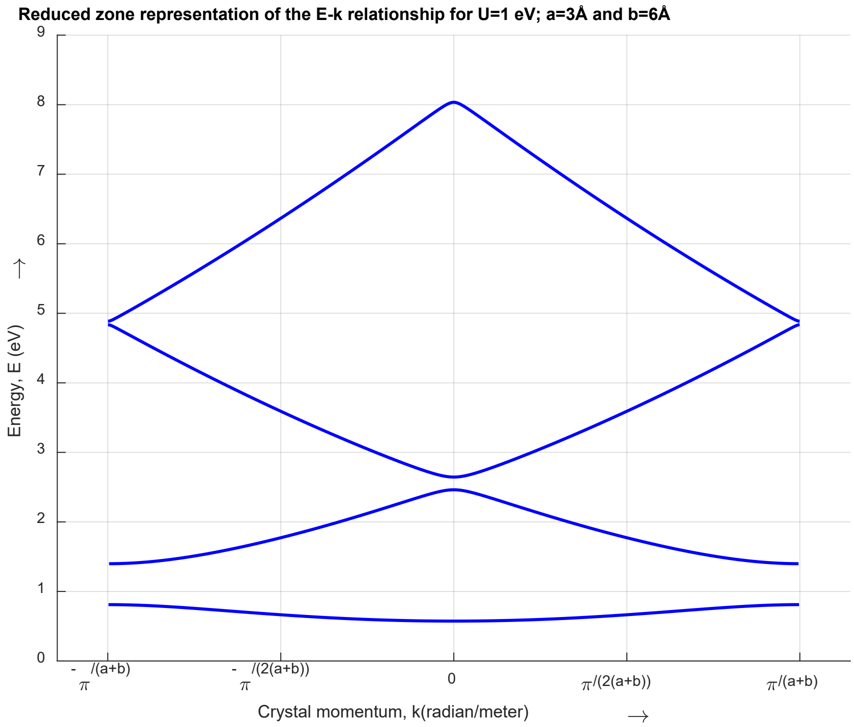
Results:

For U_0=1 eV, a=3 Å, b=6 Å :

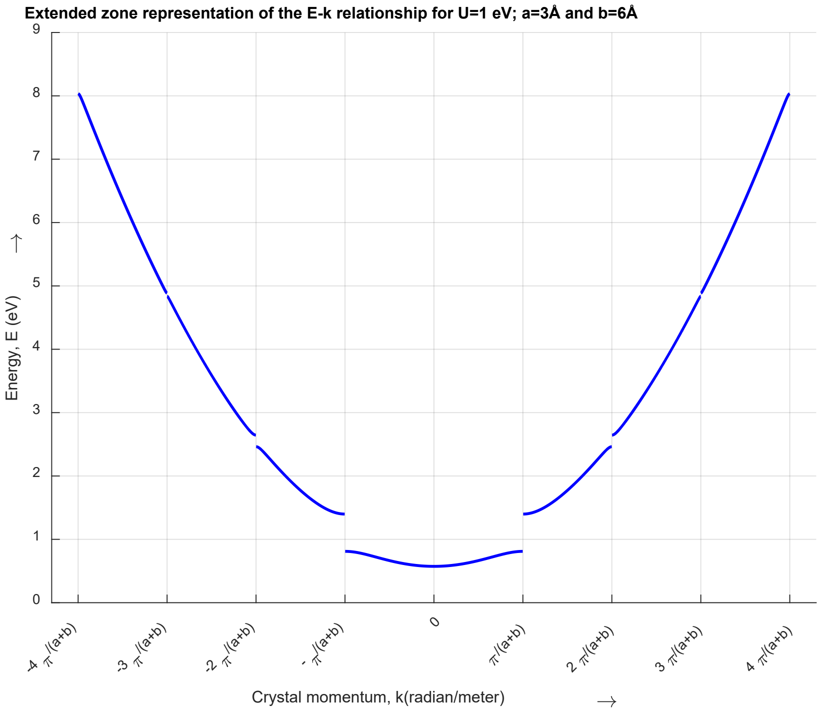
$f(\zeta)$ vs. ζ:



E-k diagram (reduced zone):

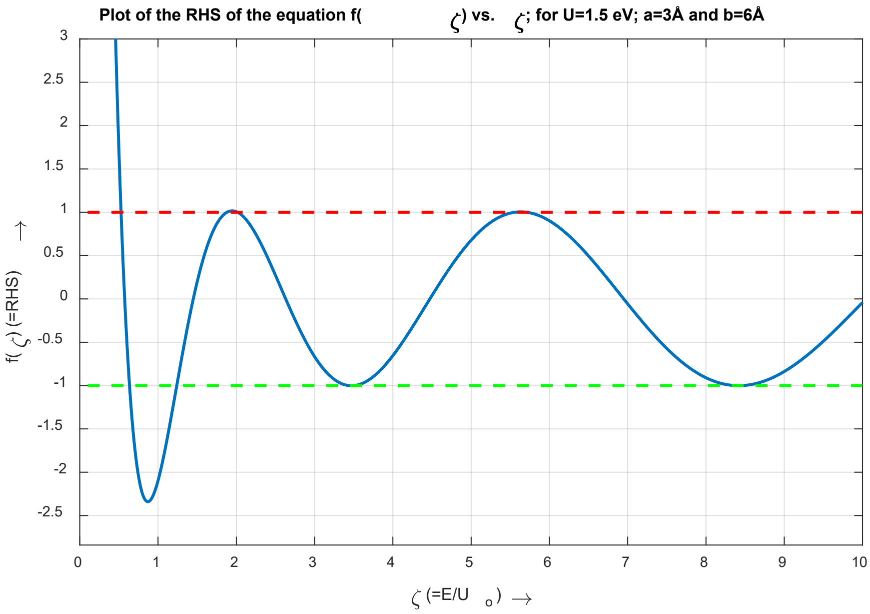


E-k diagram (extended zone):

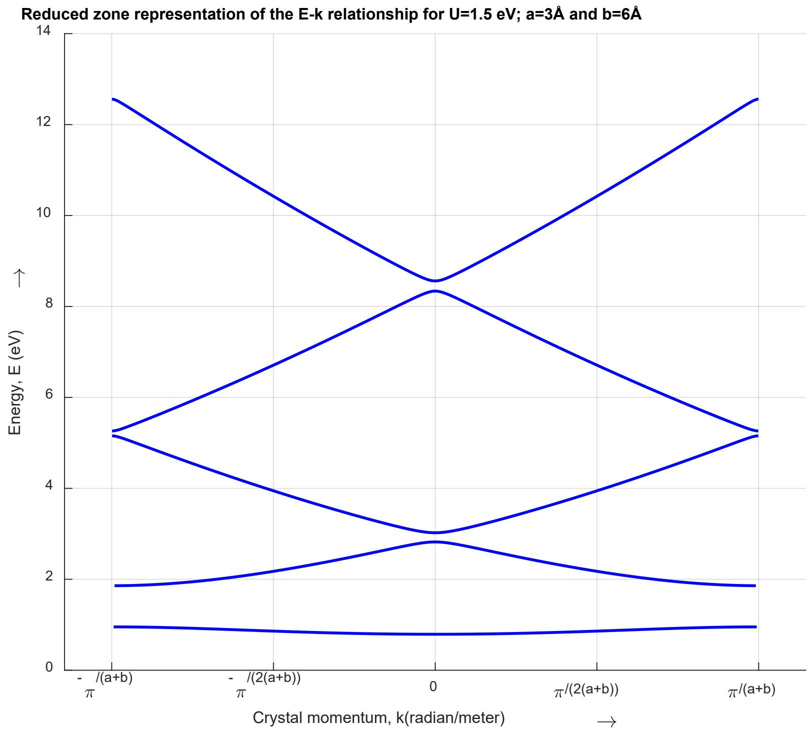


For U_0=1.5 eV, a=3 Å, b=6 Å :

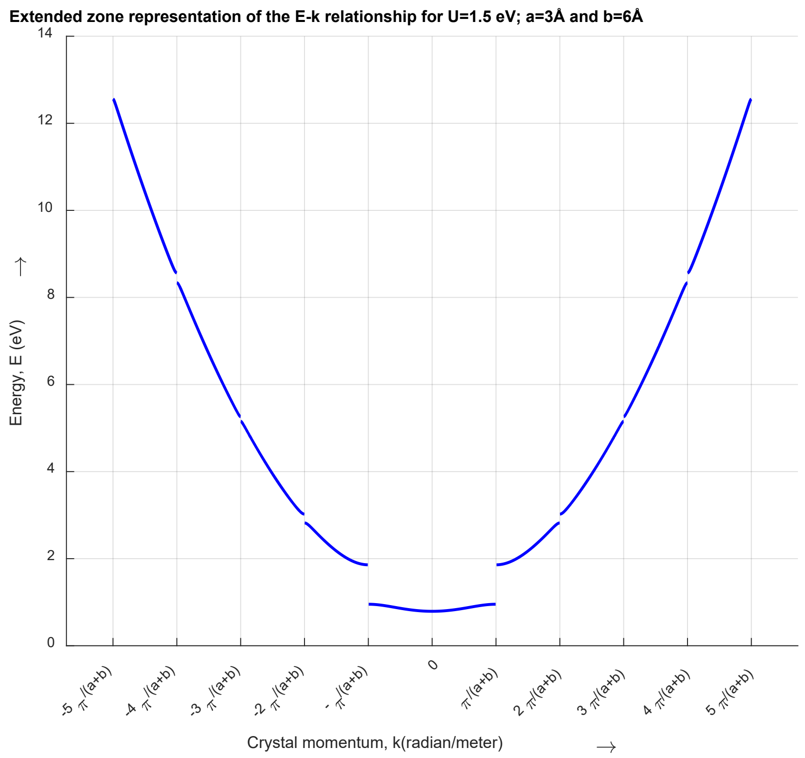
$f(\zeta)$ vs. ζ:



E-k diagram (reduced zone):

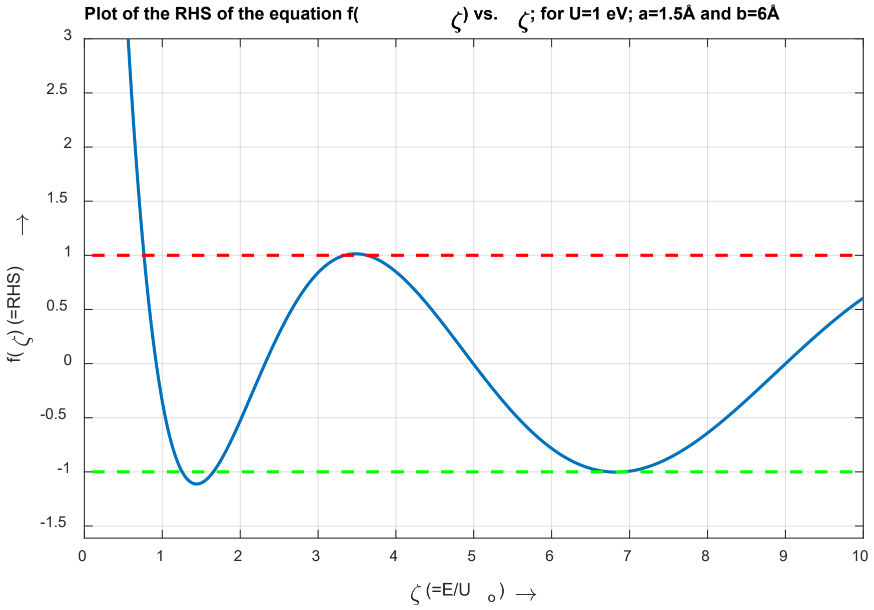


E-k diagram (extended zone):

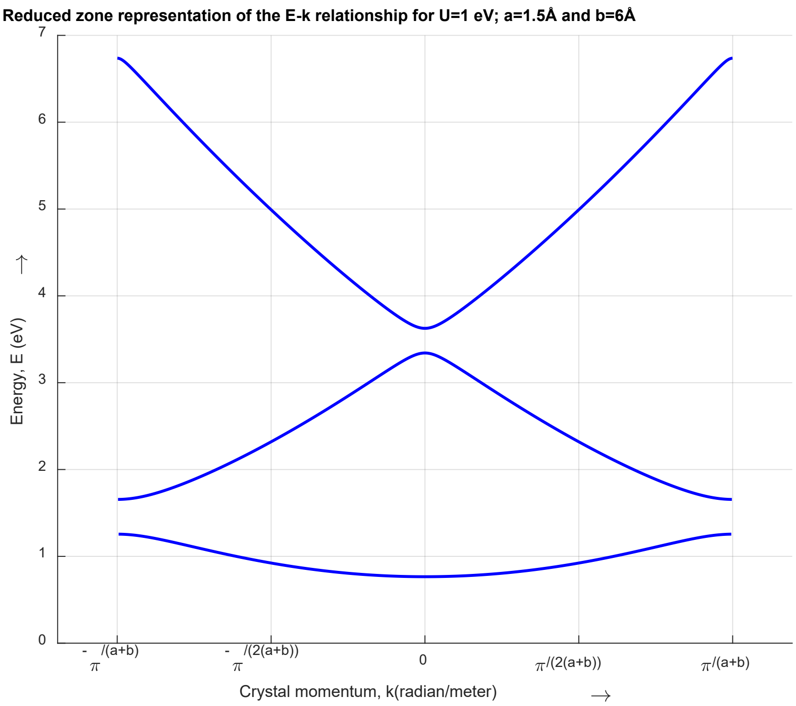


For U_0=1 eV, a=1.5 Å, b=6 Å :

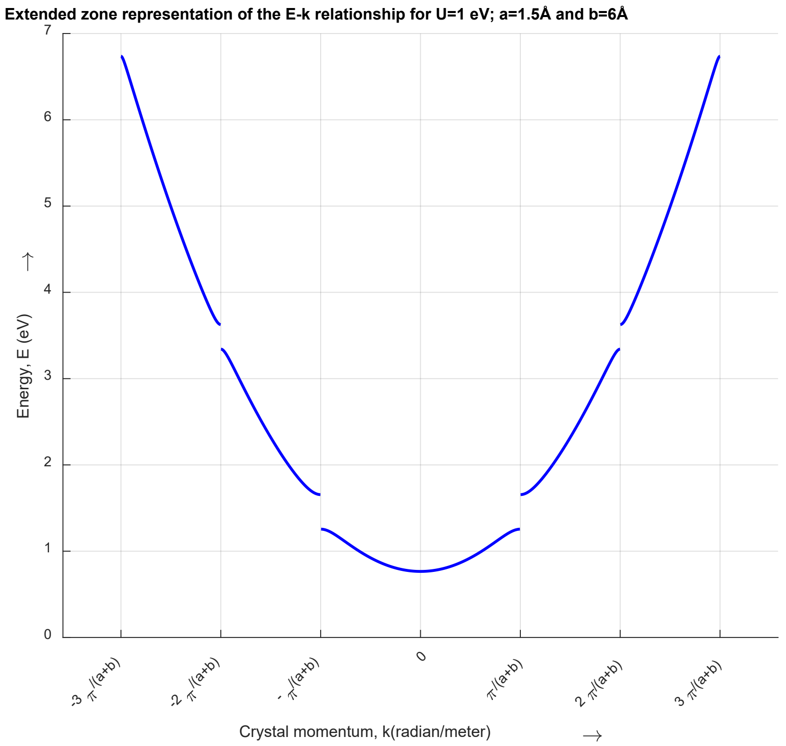
$f(\zeta)$ vs. ζ:



E-k diagram (reduced zone):

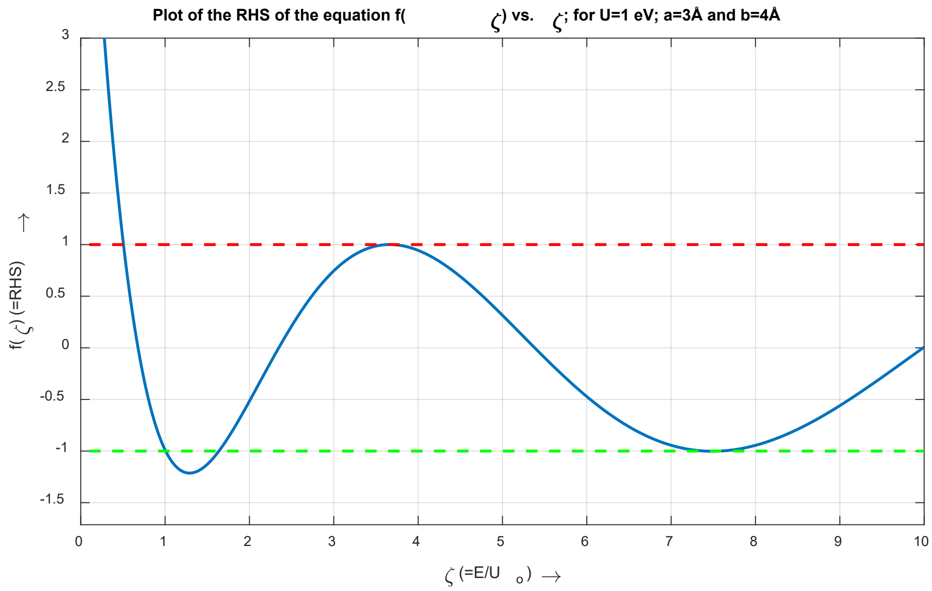


E-k diagram (extended zone):

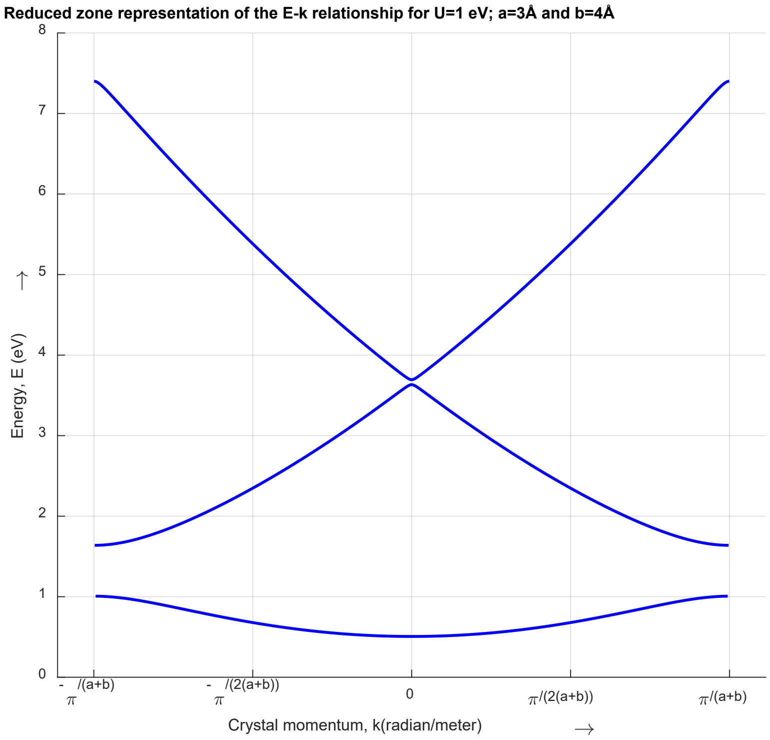


For U_0=1 eV, a=3 Å, b=4 Å :

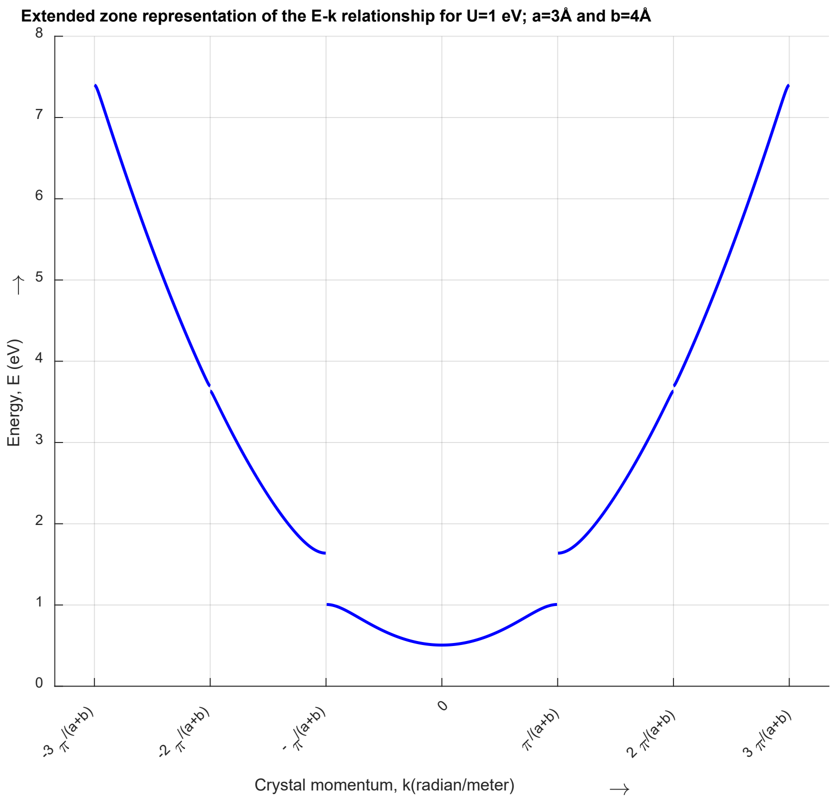
$f(\zeta)$ *vs.* ζ*:*



E-k diagram (reduced zone):



E-k diagram (extended zone):



Conclusions:

General Observations:

- Band width increases and band-gap decreases with higher energy.

- Effective mass decreases for higher energy bands and E-k relationship becomes from parabolic to v-shaped (or inverted v-shaped).

Observations made by varying parameters:

- Increasing height of the potential wells U_0 causes increase in band-gap and decrease in band-width for all bands. Effective masses also increase.
- Decreasing width of the potential wells a causes increase in band-width for lower energy bands. It also increases band-gap for higher energy bands (that are otherwise close together). Effective mass in lower energy bands decreases.
- Decreasing the separation among potential wells b causes increase in band-width for lower energy bands (in this case the first band). However, it decreases band-gap for higher energy bands .Effective mass in lower energy bands decreases.