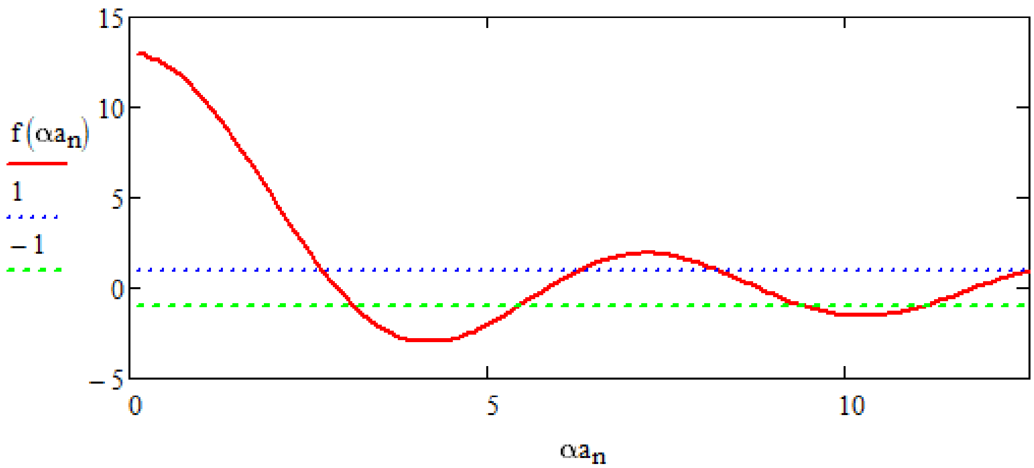
3.9 Using the parameters in Problem 3.5 for a free electron and letting $a = 4.2$ Å, determine the width (in eV) of the allowed energy bands that exist for (a) $0 < ka < \pi$

3.5 (a) Plot the function $f(\alpha a) = 12(\sin \alpha a)/\alpha a + \cos \alpha a$ for $0 \le \alpha a \le 4\pi$. Also, given the function $f(\alpha a) = \cos ka$, indicate the allowed values of αa that will satisfy this equation. (b) Determine the values of αa at (i) $ka = \pi$ and (ii) $ka = 2\pi$.

$$f(aa) := \frac{12 \cdot \sin(aa)}{aa} + \cos(aa) \qquad n := 1..120 \qquad \alpha a_n := \frac{4 \cdot \pi \cdot n}{120}$$

Since -1<= cos(ka) <= 1, plot horizontal lines at +1 & -1



By zooming in on plot & trial-and-error, find αa bands where 1<= f(αa) <= -1.

first band of αa $f(0.859152\pi) = 1$ to $f(\pi) = -1$

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a) Per (3.5), $\alpha^2 = \frac{2mE}{\hbar^2} \rightarrow (\alpha a)^2 = \frac{2mEa^2}{\hbar^2}$

$\hookrightarrow E = \frac{(\alpha a)^2 \hbar^2}{2ma^2}$

For $ka = 0$, $\cos(ka=0) = 1 = f(\alpha a_1 = 0.859\pi)$

$$E_1 = \frac{(0.859152\pi)^2(1.05457 \times 10^{-34})^2}{2(9.1093837 \times 10^{-31})(4.2 \times 10^{-10})^2} = 2.52101 \times 10^{-19}\,J = 1.5735\,eV$$

For $ka = \pi$, $\cos(ka = \pi) = -1 = f(\alpha a_2 = \pi)$

$$E_2 = \frac{\pi^2(1.05457 \times 10^{-34})^2}{2(9.1093837 \times 10^{-31})(4.2 \times 10^{-10})^2} = 3.41534 \times 10^{-19}\,J = 2.1317\,eV$$

$\Delta E = E_2 - E_1 = 2.1317 - 1.5735 \Rightarrow \underline{\underline{\Delta E = 0.5582\,eV}}$