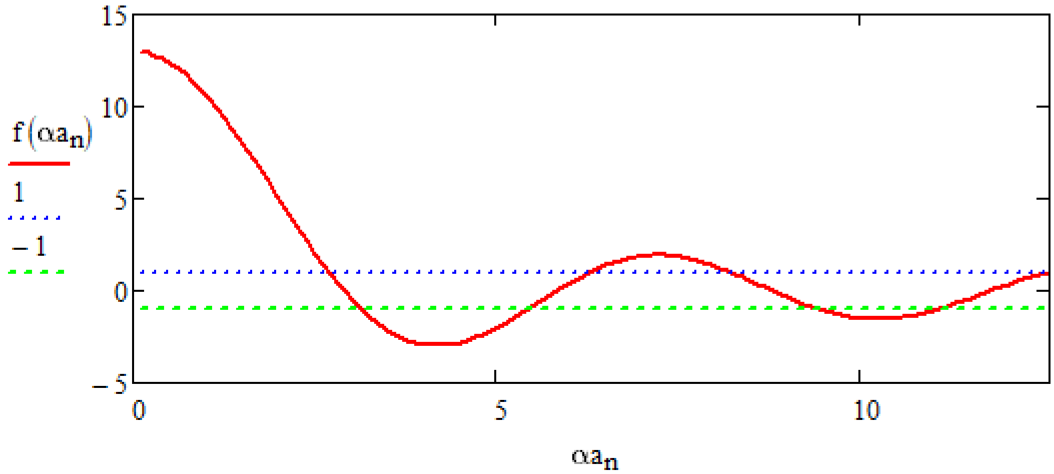
3.9 Using the parameters in Problem 3.5 for a free electron and letting $a = 4$ Å, determine the width (in eV) of the allowed energy bands that exist for (*a*) $0 < ka < \pi$

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*) $ka = 2\pi$.

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

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.

1st band: **0.85915π <= αa <= π** $\quad f(0.859152\pi) = 1$ to $f(\pi) = -1$

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a) Per (3.5), $\alpha^2 = \frac{2mE}{\hbar^2} \Rightarrow (\alpha a)^2 = \frac{2mEa^2}{\hbar^2} \Rightarrow E = \frac{(\alpha a)^2 \hbar^2}{2ma^2}$.

For $ka = 0$, we have $\cos(ka = 0) = 1 = f(\alpha a = 0.859152\pi)$. This yields the first energy

$$E_1 = \frac{(0.859152\pi)^2 (1.0545718 \times 10^{-34})^2}{2(9.1093837 \times 10^{-31})(4 \times 10^{-10})^2} \Rightarrow \mathbf{E_1 = 2.779413 \times 10^{-19}\ J = 1.73477\ eV.}$$

For $ka = \pi$, we have $\cos(ka = \pi) = -1 = f(\alpha a = \pi)$. This yields the second energy

$$E_2 = \frac{\pi^2 (1.0545718 \times 10^{-34})^2}{2(9.1093837 \times 10^{-31})(4 \times 10^{-10})^2} \Rightarrow \mathbf{E_2 = 3.765417 \times 10^{-19}\ J = 2.35019\ eV.}$$

The width of the energy band is then

$$\Delta E = E_2 - E_1 = 3.765417 \times 10^{-19} - 2.779413 \times 10^{-19}\ \text{J} = 2.35019 - 1.73477\ \text{eV}$$

$$\Rightarrow \underline{\mathbf{\Delta E = 0.986004 \times 10^{-19}\ J = 0.61542\ eV}}$$