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 (*b*) $\pi < ka < 2\pi$.

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*) $ka = 2\pi$.

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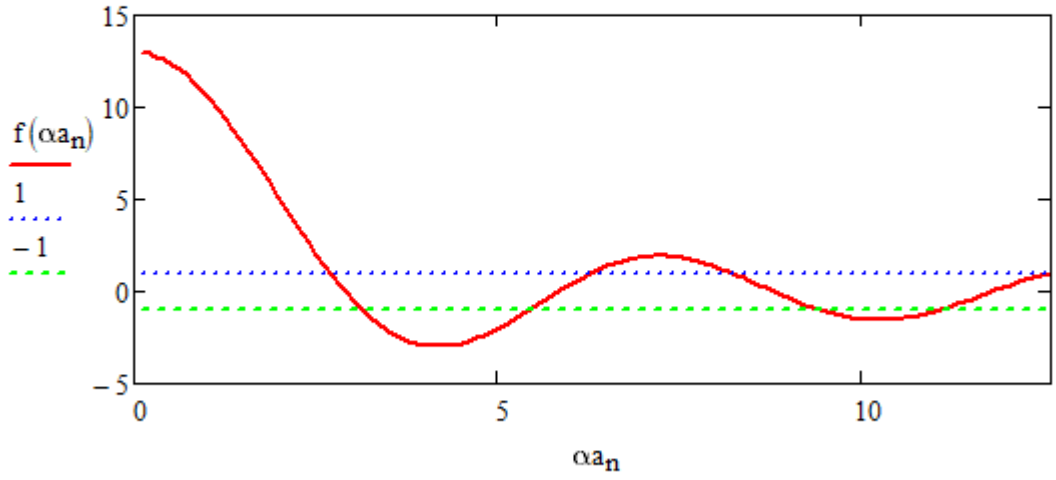
a) $f(aa) := \dfrac{12 \cdot \sin(aa)}{aa} + \cos(aa)$ $\quad n := 1..120$ $\quad \alpha a_n := \dfrac{4 \cdot \pi \cdot n}{120}$

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



second band of αa $\quad f(1.729352\pi) = -1$ $\quad$ to $\quad f(2\pi) = 1$

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b) For $Ka = \pi$, $\cos(Ka = \pi) = -1 = f(\alpha a_1 = 1.729352\pi)$

For $Ka = 2\pi$, $\cos(Ka = 2\pi) = 1 = f(\alpha a_2 = 2\pi)$

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

For $\alpha a_1 = 1.729\pi$, $E_1 = \dfrac{(1.729352\pi)^2(1.054571817\times10^{-34})^2}{2(9.1093837\times10^{-31})(4.2\times10^{-10})^2}$

$= 1.021413\times10^{-18}\,J = 6.37516\ eV$

For $\alpha a_2 = 2\pi$, $E_2 = \dfrac{(2\pi)^2(1.054571817\times10^{-34})^2}{2(9.1093837\times10^{-31})(4.2\times10^{-10})^2}$

$= 1.3661377\times10^{-18}\,J = 8.52676\ eV$

$\Delta E = E_2 - E_1 = 8.52676 - 6.37516 \Rightarrow \underline{\Delta E = 2.1516\ eV}$