

Problem 1

restart :

$$Y0 := (n, m, l) \rightarrow \left(\frac{2}{a}\right)^{\frac{3}{2}} \cdot \sin\left(\frac{n \cdot \text{Pi} \cdot x}{a}\right) \cdot \sin\left(\frac{m \cdot \text{Pi} \cdot y}{a}\right) \cdot \sin\left(\frac{l \cdot \text{Pi} \cdot z}{a}\right)$$

$$(n, m, l) \rightarrow 2 \sqrt{2} \left(\frac{1}{a}\right)^{3/2} \sin\left(\frac{n \pi x}{a}\right) \sin\left(\frac{m \pi y}{a}\right) \sin\left(\frac{l \pi z}{a}\right) \quad (1)$$

$$Y0(1, 1, 1) := \left(\frac{2}{a}\right)^{\frac{3}{2}} \cdot \sin\left(\frac{\text{Pi} \cdot x}{a}\right) \cdot \sin\left(\frac{\text{Pi} \cdot y}{a}\right) \cdot \sin\left(\frac{\text{Pi} \cdot z}{a}\right)$$

$$2 \sqrt{2} \left(\frac{1}{a}\right)^{3/2} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{a}\right) \sin\left(\frac{\pi z}{a}\right) \quad (2)$$

$$E0 := (n, m, l) \rightarrow \frac{\pi^2 \cdot h^2}{2 \cdot mm \cdot a^2} \cdot (n^2 + m^2 + l^2)$$

$$(n, m, l) \rightarrow \frac{1}{2} \frac{\pi^2 h^2 (n^2 + m^2 + l^2)}{mm a^2} \quad (3)$$

$$Hp := V0 \cdot \tan\left(\frac{\text{Pi} \cdot x}{2 \cdot a}\right) \cdot \tan\left(\frac{\text{Pi} \cdot y}{2 \cdot a}\right)$$

$$V0 \tan\left(\frac{1}{2} \frac{\pi x}{a}\right) \tan\left(\frac{1}{2} \frac{\pi y}{a}\right) \quad (4)$$

1)

assume($n :: \text{integer}, m :: \text{integer}, l :: \text{integer}$)

$$E1 := \text{int}(\text{int}(\text{int}(Y0(1, 1, 1) \cdot Y0(1, 1, 1) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$\frac{16 V0}{\pi^2} \quad (5)$$

b)

$$Waa := \text{int}(\text{int}(\text{int}(Y0(2, 1, 1) \cdot Y0(2, 1, 1) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$\frac{64}{3} \frac{V0}{\pi^2} \quad (6)$$

$$Wbb := \text{int}(\text{int}(\text{int}(Y0(1, 2, 1) \cdot Y0(1, 2, 1) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$\frac{64}{3} \frac{V0}{\pi^2} \quad (7)$$

$$Wcc := \text{int}(\text{int}(\text{int}(Y0(1, 1, 2) \cdot Y0(1, 1, 2) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$\frac{16 V0}{\pi^2} \quad (8)$$

$$Wab := \text{int}(\text{int}(\text{int}(Y0(2, 1, 1) \cdot Y0(1, 2, 1) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$\frac{64}{9} \frac{V0}{\pi^2} \quad (9)$$

$$Wac := \text{int}(\text{int}(\text{int}(Y0(2, 1, 1) \cdot Y0(1, 1, 2) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$0 \quad (10)$$

$$Wba := \text{int}(\text{int}(\text{int}(Y0(1, 2, 1) \cdot Y0(2, 1, 1) \cdot Hp, x=0..a), y=0..a), z=0..a)$$

$$\frac{64}{9} \frac{V0}{\pi^2} \quad (11)$$

$$Wca := \text{int}(\text{int}(\text{int}(Y0(1, 1, 2) \cdot Y0(2, 1, 1) \cdot Hp, x=0..a), y=0..a), z=0..a) \quad (12)$$

$$Wbc := \text{int}(\text{int}(\text{int}(Y0(1, 2, 1) \cdot Y0(1, 1, 2) \cdot Hp, x=0..a), y=0..a), z=0..a) \quad (13)$$

$$Wcb := \text{int}(\text{int}(\text{int}(Y0(1, 1, 2) \cdot Y0(1, 2, 1) \cdot Hp, x=0..a), y=0..a), z=0..a) \quad (14)$$

$$W := \langle \langle Waa, Wab, Wac \rangle | \langle Wba, Wbb, Wbc \rangle | \langle Wca, Wcb, Wcc \rangle \rangle$$

$$\begin{bmatrix} \frac{64}{3} \frac{V0}{\pi^2} & \frac{64}{9} \frac{V0}{\pi^2} & 0 \\ \frac{64}{9} \frac{V0}{\pi^2} & \frac{64}{3} \frac{V0}{\pi^2} & 0 \\ 0 & 0 & \frac{16 V0}{\pi^2} \end{bmatrix} \quad (15)$$

with(LinearAlgebra) :
Eigenvalues(W)

$$\begin{bmatrix} \frac{16 V0}{\pi^2} \\ \frac{256}{9} \frac{V0}{\pi^2} \\ \frac{128}{9} \frac{V0}{\pi^2} \end{bmatrix} \quad (16)$$

$$Ellone := \frac{256}{9} \cdot \frac{V0}{\pi^2}$$

$$\frac{256}{9} \frac{V0}{\pi^2} \quad (17)$$

$$Elltwo := \frac{16 V0}{\pi^2}$$

$$\frac{16 V0}{\pi^2} \quad (18)$$

$$Ellthree := \frac{128}{9} \frac{V0}{\pi^2}$$

$$\frac{128}{9} \frac{V0}{\pi^2} \quad (19)$$

c)
Eigenvectors(W, output='list')

$$\left[\left[\frac{128}{9} \frac{V0}{\pi^2}, 1, \left\{ \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix} \right\}, \left[\frac{16 V0}{\pi^2}, 1, \left\{ \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}, \left[\frac{256}{9} \frac{V0}{\pi^2}, 1, \left\{ \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \right\} \right] \right] \quad (20)$$

$$Normalize \left(\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, Euclidean \right)$$

$$\begin{bmatrix} \frac{1}{2} \sqrt{2} \\ \frac{1}{2} \sqrt{2} \\ 0 \end{bmatrix} \quad (21)$$

d)

$$V0 := 1 \cdot 1.6 \cdot 10^{-19} ;$$

$$a := 1 \cdot 10^{-10} ;$$

$$h := 1.054 \cdot 10^{-34} ;$$

$$mm := 9.1 \cdot 10^{-31} ;$$

$$Eground := evalf \left(\frac{E0(1, 1, 1)}{1.6 \cdot 10^{-19}} \right)$$

$$112.9564023 \quad (22)$$

$$FOD := evalf \left(\frac{EI}{1.6 \cdot 10^{-19}} \right)$$

$$1.621138938$$

$$CorrectedEnergy := Eground + FOD$$

$$114.5775412 \quad (24)$$

Problem 2

restart :

$$Y := n \rightarrow \text{sqrt} \left(\frac{2}{a} \right) \sin \left(\frac{n \cdot \text{Pi} \cdot x}{a} \right)$$

$$n \rightarrow \sqrt{\frac{2}{a}} \sin \left(\frac{n \pi x}{a} \right) \quad (25)$$

$$E0 := n \rightarrow \frac{n^2 \cdot \pi^2 \cdot h^2}{2 \cdot mm \cdot a^2}$$

$$n \rightarrow \frac{1}{2} \frac{n^2 \pi^2 h^2}{mm a^2} \quad (26)$$

$$Hp := V0 \cdot \sin \left(\frac{\text{Pi} \cdot x}{2 \cdot a} \right)$$

$$V0 \sin \left(\frac{1}{2} \frac{\pi x}{a} \right) \quad (27)$$

a)

assume($n :: integer$)

$EI := n \rightarrow int(Y(n) \cdot Y(n) \cdot Hp, x=0 ..a)$

$$n \rightarrow \int_0^a Y(n) Y(n) Hp \, dx \quad (28)$$

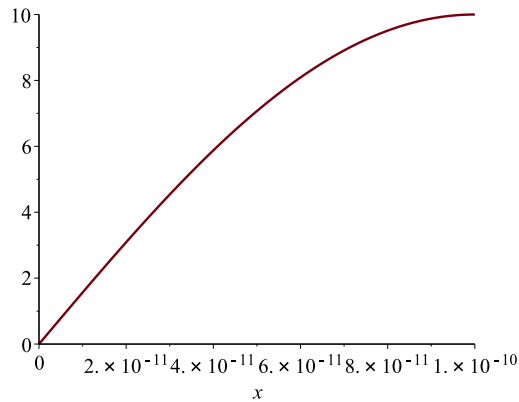
$EI(n)$

$$\frac{32 \, n^2 \, V0}{\pi (16 \, n^2 - 1)} \quad (29)$$

$V0 := 10 :$

$a := 1 \cdot 10^{-10} :$

plot($Hp, x=0 ..a$)



b)

$V0 := 10 \cdot 1.6 \cdot 10^{-19} :$

$a := 1 \cdot 10^{-10} :$

$h := 1.054 \cdot 10^{-34} :$

$mm := 9.1 \cdot 10^{-31} :$

$Egr := evalf\left(\frac{E0(1)}{1.6 \cdot 10^{-19}}\right)$

$$37.65213408 \quad (30)$$

$FOC := evalf\left(\frac{EI(1)}{1.6 \cdot 10^{-19}}\right)$

$$6.790610906 \quad (31)$$

$CorrectedEnergy := Egr + FOC$

$$44.44274499 \quad (32)$$

c)

$unassign('V0','a','h','mm')$
 $assume(m :: integer)$
 $br := n \rightarrow int(Y(m) \cdot Hp \cdot Y(n), x = 0 .. a)$

$$n \rightarrow \int_0^a Y(m) Hp Y(n) dx \quad (33)$$

$$br(n) - \frac{32 n \sim m \sim V0}{\pi (16 m \sim^4 - 32 m \sim^2 n \sim^2 + 16 n \sim^4 - 8 m \sim^2 - 8 n \sim^2 + 1)} \quad (34)$$

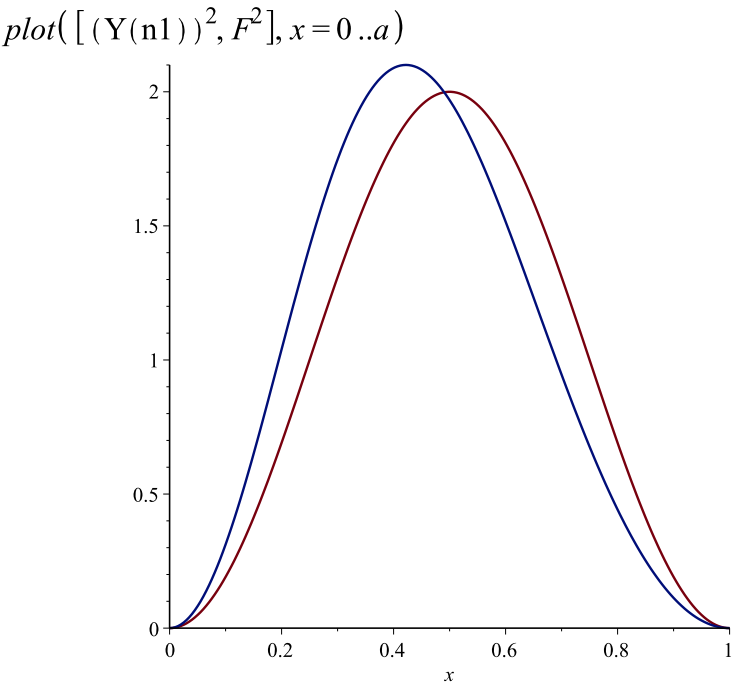
$$g := \frac{br(n)}{E0(n) - E0(m)} \cdot Y(m) - \frac{32 n \sim m \sim V0 \sqrt{2} \sqrt{\frac{1}{a}} \sin\left(\frac{m \sim \pi x}{a}\right)}{\pi (16 m \sim^4 - 32 m \sim^2 n \sim^2 + 16 n \sim^4 - 8 m \sim^2 - 8 n \sim^2 + 1) \left(\frac{1}{2} \frac{n \sim^2 \pi^2 h^2}{mm a^2} - \frac{1}{2} \frac{m \sim^2 \pi^2 h^2}{mm a^2}\right)} \quad (35)$$

$$f := piecewise(m \neq n, g) \left\{ \begin{array}{ll} - \frac{32 n \sim m \sim V0 \sqrt{2} \sqrt{\frac{1}{a}} \sin\left(\frac{m \sim \pi x}{a}\right)}{\pi (16 m \sim^4 - 32 m \sim^2 n \sim^2 + 16 n \sim^4 - 8 m \sim^2 - 8 n \sim^2 + 1) \left(\frac{1}{2} \frac{n \sim^2 \pi^2 h^2}{mm a^2} - \frac{1}{2} \frac{m \sim^2 \pi^2 h^2}{mm a^2}\right)} & m \sim \neq n \sim \\ 0 & otherwise \end{array} \right.$$

$$fp := evalf(sum(f, m = 1 .. 3)) \left(\left\{ \begin{array}{ll} - \frac{14.40506105 n \sim V0 \sqrt{\frac{1}{a}} \sin\left(\frac{3.141592654 x}{a}\right)}{(16. n \sim^4 - 40. n \sim^2 + 9.) \left(\frac{4.934802202 n \sim^2 h^2}{mm a^2} - \frac{4.934802202 h^2}{mm a^2}\right)} & 1. \neq n \sim \\ 0 & otherwise \end{array} \right\} + \left\{ \begin{array}{ll} - \frac{28.81012210 n \sim V0 \sqrt{\frac{1}{a}} \sin\left(\frac{6.283185308 x}{a}\right)}{(16. n \sim^4 - 136. n \sim^2 + 225.) \left(\frac{4.934802202 n \sim^2 h^2}{mm a^2} - \frac{19.73920881 h^2}{mm a^2}\right)} & 2. \neq n \sim \\ 0 & otherwise \end{array} \right\} \right) \quad (37)$$

$$\begin{aligned} &\text{d)} \\ &nI := 1 : \\ &mm := 1 : \\ &h := 1 : \\ &a := 1 : \\ &V0 := 10 : \\ &ff := \text{piecewise}\left(m \neq nI, \frac{br(nI)}{E0(nI) - E0(m)} \cdot Y(m)\right) \\ &\quad \left\{ \begin{array}{ll} -\frac{320 \, m\sim \sqrt{2} \sin(m\sim \pi x)}{\pi (16 \, m\sim^4 - 40 \, m\sim^2 + 9) \left(\frac{1}{2} \pi^2 - \frac{1}{2} \, m\sim^2 \pi^2\right)} & m\sim \neq 1 \\ 0 & \text{otherwise} \end{array} \right. \end{aligned} \tag{38}$$

$$F := fp2 + Y(nI) \\ 0.1853381379 \sin(6.283185308 x) + 0.01158363362 \sin(9.424777962 x) \\ + 0.002246522883 \sin(12.56637062 x) + 0.0006750369241 \sin(15.70796327 x) \\ + 0.0002592141788 \sin(18.84955592 x) + 0.0001167416798 \sin(21.99114858 x) \\ + 0.00005885151636 \sin(25.13274123 x) + 0.00003227637850 \sin(28.27433389 x) \\ + 0.00001889994350 \sin(31.41592654 x) + \sqrt{2} \sin(\pi x) \quad (40)$$



e)

$unassign('V0','a','h','mm')$

$fe := n2 \rightarrow piecewise\left(m \neq n2, \frac{abs(br(n2))^2}{E0(n2) - E0(m)}\right)$

$n2 \rightarrow piecewise\left(m \neq n2, \frac{|br(n2)|^2}{E0(n2) - E0(m)}\right)$ (41)

$E2 := evalf(sum(fe(n2), m = 1..3))$

$$\left\{ \begin{array}{ll} \frac{6.484555750 \left| \frac{V0 \left(-3. \sin(3.141592654 n2) + 4. \sin(3.141592654 n2) n2^2 + 4. n2 \right)}{16. n2^4 - 40. n2^2 + 9.} \right|^2}{\frac{4.934802202 n2^2 h^2}{mm a^2} - \frac{4.934802202 h^2}{mm a^2}} & 1. \neq n2 \\ 0 & otherwise \end{array} \right.$$

$$\begin{aligned}
& \left. \right) + \left\{ \left[\frac{25.93822300 \left| \frac{V0 (15. \sin(3.141592654 n2) - 4. \sin(3.141592654 n2) n2^2 + 4. n2)}{16. n2^4 - 136. n2^2 + 225.} \right|^2}{\frac{4.934802202 n2^2 h^2}{mm a^2} - \frac{19.73920881 h^2}{mm a^2}} \right] \right. \\
& \left. \right) + \left\{ \left[\frac{58.36100175 \left| \frac{V0 (-35. \sin(3.141592654 n2) + 4. \sin(3.141592654 n2) n2^2 + 4. n2)}{16. n2^4 - 296. n2^2 + 1225.} \right|^2}{\frac{4.934802202 n2^2 h^2}{mm a^2} - \frac{44.41321982 h^2}{mm a^2}} \right] \right. \\
& \left. \right)
\end{aligned}$$

2. $\neq n$
otherwi
3. \neq
otherw

$$E2n1 := evalf(\text{sum}(fe(1), m = 1 .. 10)) \\
- \frac{0.002571379916 |V0|^2 mm a^2}{h^2} \quad (43)$$

$$E2n2 := evalf(\text{sum}(fe(2), m = 1 .. 10)) \\
\frac{0.0007995258445 |V0|^2 mm a^2}{h^2} \quad (44)$$

$$E2n3 := evalf(\text{sum}(fe(3), m = 1 .. 10)) \\
\frac{0.0004561125807 |V0|^2 mm a^2}{h^2} \quad (45)$$

For "enough" I wanted to get to 4 sig figs that are somewhat stable if we increse summation by a lot.
Bellow I calculate the actual value.

$$h := 1.054 \cdot 10^{-34} :$$

$$mm := 9.1 \cdot 10^{-31} :$$

$$V0 := 10 \cdot 1.6 \cdot 10^{-19} :$$

$$a := 1 \cdot 10^{-10} :$$

$$E2n1 := evalf(\text{sum}(fe(1), m = 1 .. 600)) \\
-5.392206644 \cdot 10^{-21}$$

$$E2n2 := evalf(\text{sum}(fe(2), m = 1 .. 800)) \\
1.676604326 \cdot 10^{-21} \quad (47)$$

$$E2n3 := evalf(\text{sum}(fe(3), m = 1 .. 1100)) \\
9.564502783 \cdot 10^{-22} \quad (48)$$

f)

$$SOC := \frac{E2nI}{1.6 \cdot 10^{-19}} \quad -0.03370129152 \quad (49)$$

$$E2Cor := evalf(SOC + FOC + Egr) \quad 44.40904369 \quad (50)$$

Extra Credit

restart :

$$E := (n, j) \rightarrow -\frac{13.6}{n^2} \cdot \left(1 + \frac{\left(\frac{1}{137} \right)}{n^2} \cdot \left(\frac{n}{\left(j + \frac{1}{2} \right)} - \frac{3}{4} \right) \right) \\ (n, j) \rightarrow \frac{(-1) \cdot 13.6 \left(1 + \frac{1}{137} \frac{\frac{n}{j + \frac{1}{2}} - \frac{3}{4}}{n^2} \right)}{n^2} \quad (51)$$

$$En := n \rightarrow -\frac{13.6}{n^2} \\ n \rightarrow \frac{(-1) \cdot 13.6}{n^2} \quad (52)$$

$$ss := seq\left(E(3, j), j = \frac{1}{2} \dots \frac{5}{2}, 1\right) \\ -1.513868613, -1.512030279, -1.511417500 \quad (53)$$

with(plots) :

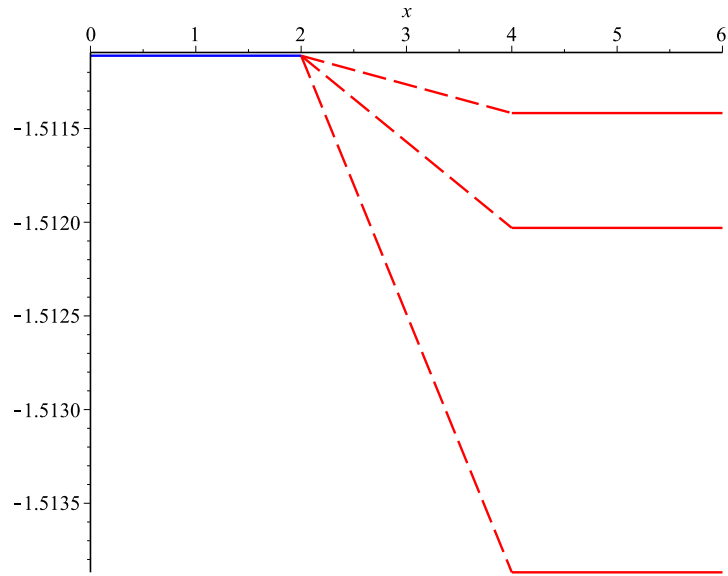
$$jpl := plot([ss], x = 4 .. 6, color = red) \\ PLOT(...) \quad (55)$$

$$qq := seq\left((x - 2) \cdot \frac{(E(3, j) - En(3))}{2} + En(3), j = \frac{1}{2} \dots \frac{5}{2}, 1\right) \\ -0.0013787510 x - 1.508353609, -0.0004595840 x - 1.510191943, -0.0001531945 x \\ - 1.510804722 \quad (56)$$

$$tran := plot([qq], x = 2 .. 4, linestyle = dash, color = red) \\ PLOT(...) \quad (57)$$

$$n30 := plot(En(3), x = 0 .. 2, color = blue) \\ PLOT(...) \quad (58)$$

display(jpl, tran, n30)



$$ss := seq\left(E(3,j) - En(3) + 1, j = \frac{1}{2} \dots \frac{5}{2}, 1\right)$$

(59)

with(plots) :
jpl := plot([ss], x = 6 .. 8, color = red)

PLOT(...)

PLOT(...) (61)

$$qq := seq\left((x-4) \cdot \frac{(E(3,j) - En(3))}{2} + 1, j = \frac{1}{2} \dots \frac{5}{2}, 1\right)$$

(62)

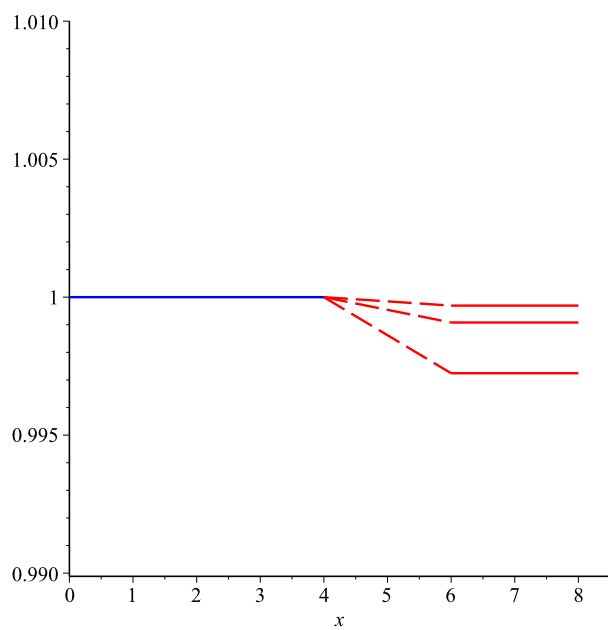
tran := plot([qq], x = 4 .. 6, linestyle = dash, color = red)

PLOT(...) (63)

n30 := plot(1, x = 0 .. 4, color = blue)

PLOT(...) (64)

display(jpl, tran, n30, view = [0 .. 8.5, 0.99 .. 1.01])



Here I shifted it so it is the way you had it - just in case. I didn't scale it the way you did though.