Question 1

In[ ]:=

$$\hbar c = 197;$$

$$\text{mcsq} = 0.511;$$

$$a = 10;$$

$$b = 5;$$

$$\text{psi}[\text{x\_}] := \left(a^2 - x^2\right) e^{-c\,x^2}$$

$$H[\text{psi\_}] := -\frac{\hbar c^2}{\text{mcsq}} \,\text{D}[\text{psi}, \{x, 2\}] + b\left(a^2 - x^2\right)\text{psi}$$

$$\text{int} = \frac{\text{Integrate}[\text{psi}[x] \times H[\text{psi}[x]], \{x, -a, a\}]}{\text{Integrate}[\text{psi}[x] \times \text{psi}[x], \{x, -a, a\}]};$$

$$\text{Minimize}[\text{int}, c]$$

Out[ ]= {2308.24, {c → 0.00208365}}

Question 2

In[ ]:=

$$\$\text{Assumptions} = \text{Element}[m, \text{Integers}];$$

$$\text{en0} = \frac{\hbar c^2\, \pi^2}{8\, \text{mcsq}\, a^2}$$

$$\text{en1} = \text{NIntegrate}\left[b\, \text{Sin}\left[\frac{\pi\, x}{2\, a}\right]^2 \left(2\, a\, x - x^2\right), \{x, 0, 2\, a\}\right]$$

$$\text{ans} = \frac{\text{Integrate}\left[b\, \text{Sin}\left[\frac{\pi x}{2 a}\right] \text{Sin}\left[\frac{m \pi x}{2 a}\right]\left(2\, a\, x - x^2\right), \{x, 0, 2\, a\}\right]^2}{\text{en0} - \frac{\hbar c^2\, \pi^2\, m}{8\, \text{mcsq}\, a^2}};$$

$$\text{en2} = \text{Sum}[\text{ans} \;/.\; m \to n, \{n, 2, 100\,001\}] \;//\; \text{N}$$

$$\text{en0} + \text{en1} + \text{en2}$$

Out[ ]= 936.961

Out[ ]= 4346.55

Out[ ]= −313.966

Out[ ]= 4969.54

Question 3

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e = 250;
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$$k = \sqrt{\frac{2\,\text{mcsq}\,e}{\hbar c^2}};$$

$$\text{int3[x\_]} = \text{Integrate}\left[\left(2\left(e - b\left(a^2 - x^2\right)\right)\right)^{1/2}, x\right];$$

$$\text{psi[x\_]} = A\, e^{-i\,k\,a}\, e^{i\sqrt{\frac{\text{mcsq}}{\hbar c^2}}\,(\text{int3[x]}-\text{int3[-a]})}; \text{(* psi at -a < x < a *)}$$

$$\left(\frac{\text{psi[a]}}{A}\ //\ \text{Expand}\right)\text{Conjugate}\left[\frac{\text{psi[a]}}{A}\ //\ \text{Expand}\right]\ /.$$

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{Conjugate[A] → A, Conjugate[B] → B} // Expand
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Out[ ]= 0.164894 + 0. i

Question 4

In[ ]:=
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H0 = α IdentityMatrix[2];
H1 = {{γ, -ⅈ β}, {ⅈ β, -γ}};
diags = Eigenvectors[H1];
en10 = diags[[1]].H0.diags[[1]];
en11 = diags[[1]].H1.diags[[1]];
en12 = diags[[2]].H1.diags[[1]] / (diags[[1]].H0.diags[[1]] - diags[[2]].H0.diags[[2]]);
en20 = diags[[2]].H0.diags[[2]];
en21 = diags[[2]].H1.diags[[2]];
en22 = diags[[1]].H1.diags[[2]] / (diags[[2]].H0.diags[[2]] - diags[[1]].H0.diags[[1]]);
en1 = en10 + en11 + en12 // Simplify
en2 = en20 + en21 + en22 // Simplify
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Out[ ]=
$$-\frac{\beta^2}{2\,\alpha\,\gamma}-\frac{2\,\gamma\left(\beta^2+\gamma\left(\gamma-\sqrt{\beta^2+\gamma^2}\right)\right)}{\beta^2}+\frac{2\,\alpha\,\gamma\left(\beta^2+\gamma\left(\gamma-\sqrt{\beta^2+\gamma^2}\right)\right)}{\beta^2\sqrt{\beta^2+\gamma^2}}$$

Out[ ]=
$$-\frac{\beta^2}{2\,\alpha\,\gamma}-\frac{2\,\gamma\left(\beta^2+\gamma\left(\gamma+\sqrt{\beta^2+\gamma^2}\right)\right)}{\beta^2}-\frac{2\,\alpha\,\gamma\left(\beta^2+\gamma\left(\gamma+\sqrt{\beta^2+\gamma^2}\right)\right)}{\beta^2\sqrt{\beta^2+\gamma^2}}$$

Question 5

In[ ]:= $\$\text{Assumptions} = \text{Re}\left[\frac{m\,\omega^2}{\hbar}\right] \geq 0 \;\&\&\; \text{Element}[m \,|\, \hbar \,|\, \omega \,|\, \lambda \,|\, \alpha \,|\, t, \text{Reals}] \;\&\&\; m\,\omega^2\,\hbar > 0;$

$$\omega f = \left(\frac{5}{2} - \frac{3}{2}\right) \hbar\,\omega;$$

$$\text{psi}[n\_, x\_] := \left(\frac{m\,\omega}{\pi\,\hbar\,2^{2\,n}\,(n!)^2}\right)^{1/4} e^{-\frac{m\,\omega^2\,x^2}{2\,\hbar}}\ \text{HermiteH}\left[n, \left(\frac{m\,\omega}{\hbar}\right)^{1/2} x\right];$$

$$\text{int} = \text{Integrate}[\text{psi}[1, x]\,\lambda\,x\,\text{Sin}[\alpha\,t]\,\text{psi}[2, x], \{x, -\text{Infinity}, \text{Infinity}\}];$$

$$\text{dft} = -\frac{i}{\hbar}\,\text{Integrate}\left[\text{int}\,e^{i\,\omega f\,t}, \{t, 0, t\}\right] \text{ // FullSimplify};$$

$$\text{dft}\ \frac{-i\,\lambda\,(-3+\omega)\,\sqrt{\frac{\hbar}{m}}\left(\alpha + e^{-i\,t\,\omega\,\hbar}\,(-\alpha\,\text{Cos}[t\,\alpha] - i\,\omega\,\hbar\,\text{Sin}[t\,\alpha])\right)}{2\,\hbar\,(\alpha - \omega\,\hbar)\,(\alpha + \omega\,\hbar)\,\text{Abs}[\omega]^3} \text{ // TrigToExp // Expand // FullSimplify}$$

Out[ ]=
$$\frac{1}{8\,m\,\omega^6\,\hbar\,\left(\alpha^2 - \omega^2\,\hbar^2\right)^2} \lambda^2\,(-3+\omega)^2 \left(3\,\alpha^2 + \omega^2\,\hbar^2 + (\alpha - \omega\,\hbar)\,(\alpha + \omega\,\hbar)\,\text{Cos}[2\,t\,\alpha] - 4\,\alpha\,(\alpha\,\text{Cos}[t\,\alpha]\,\text{Cos}[t\,\omega\,\hbar] + \omega\,\hbar\,\text{Sin}[t\,\alpha]\,\text{Sin}[t\,\omega\,\hbar])\right)$$