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(*H-Atom-M5*)
(*Jared Frazier*)
(*Description:

Reproducing radial distribution functions, spherical harmonics, and probability density functions
for the hydrogen atom from Quantum Chemistry 2nd Edition (McQuarrie).

*)
(*Date: 10/25/2020*)

Clear["Global`*"]

(*----------------------------*)
(*Question 1: Radial Functions*)
(*----------------------------*)

Print["(*----------------------------*)
(*Question 1: Radial Functions*)
(*----------------------------*)"]

(*Part a -- table form*)
Print["(a) Radial Wave Functions R_nl(r) through n = 2 where  0 <= l <= n-1 for n ∈ ℤ⁺:"]
tableEle = {{"R_10(r) = 2(Z/a_0)^(3/2) e^(-ρ)"}, {"R_20(r) = (Z/(2a_0))^(3/2) (2-ρ) e^(-ρ/2)"}, {"R_21(r) = 1/√3 (Z/(2a_0))^(3/2) ρ e^(-ρ/2)
Grid[tableEle, Frame→All]
Print["where Z is the nuclear charge and ρ = Zr/a_0 and SubscriptBox[a,0\]is the Bohr radius."]
a0 = 1;
Print["Z = 1, ρ = -r/a_0, and a_0 = 5.29E-11m = 1 bohrs \n"]

(*Part b -- plot radial distribution functions pg328 MQ2e*)
Print["(b) Plot the corresponding radial distributions (r^2 R_nl^2(r)), also in table form:"]

(*Radial functions of r to plot for part b*)
R1s = r^2*(2/a0^(3/2)*Exp[-r/a0])^2;
R2s = r^2*(1/(2*a0^(3/2))*(2-(r/a0))*Exp[-r/(2*a0)])^2;
R2p = r^2*(1/(Sqrt[3]*(2*a0)^(3/2))*(r/a0)*Exp[-r/(2*a0)])^2;

(*Plots for each radial dist functions for table -- range for r from pg 329 in MQ2e*)
r1 = Plot[R1s, {r,0,5}, PlotRange→All, PlotStyle→{Orange}, PlotLabel→"Probability density for 1s
          AxesLabel→{"r/a_0","r^2[R_10(r)]^2/a_0"}, ImageSize→250];
r2 = Plot[R2s, {r,0,15}, PlotRange→All, PlotStyle→{Red}, PlotLabel→"Probability density for 2s H
          AxesLabel→{"r/a_0","r^2[R_20(r)]^2/a_0"}, ImageSize→250];
r3 = Plot[R2p, {r,0,15}, PlotRange→All, PlotStyle→{Blue}, PlotLabel→"Probability density for 2p
          AxesLabel→{"r/a_0","r^2[R_21(r)]^2/a_0"}, ImageSize→250];
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radialDistTable = {r1,r2,r3};
TableForm[radialDistTable, TableDirections→Row]

(*Part c -- max probability radius for 1s state*)
R1sFunc[r_] := r^2*((2/a0^(3/2))*Exp[-r/a0])^2;
R1sDerivative = D[R1s, {r, 1}];          (*First derivative*)
critPt = NSolve[R1sDerivative == 0, r]; (*Critical points*)
Print["\n(c) Maximum probability radius for 1s state is when r = ", r/.critPt[[2]]]
Print["Therefore r^2[R_10(1)]^2/a_0 = ", R1sFunc[r/.critPt[[2]]]]

(*Part d -- 1s wave function is orthogonal to that of of the 2s*)
Print["\n(d) Show that 1s radial function is orthogonal to that of 2s"]
R10 = 2(1/a0)^(3/2) Exp[-r/a0];
R20 = (1/(2*a0))^(3/2)*(2-(r/a0))*Exp[-r/(2*a0)];
orthogonalRadFuncs = Integrate[(r^2)*R10*R20, {r, 0, Infinity}];
Print["From Mathematica calculations, <R_10 | R_20> = ", orthogonalRadFuncs]

(*--------------------------------*)
(*Question 2: Spherical Harmonics*)
(*--------------------------------*)

(*Pg MQ2e Pg 323*)

Print["\n(*--------------------------------*)
(*Question 2: Spherical Harmonics*)
(*--------------------------------*)"]

(*Spherical Harmonic Elements of Table*)
shR1 = SphericalHarmonicY[0, 0, θ, φ];
shR2 = SphericalHarmonicY[1, 0, θ, φ];
shR3 = SphericalHarmonicY[1, 1, θ, φ];
shR4 = SphericalHarmonicY[1, -1, θ, φ];
shR5 = SphericalHarmonicY[2, 0, θ, φ];
shR6 = SphericalHarmonicY[2, 1, θ, φ];
shR7 = SphericalHarmonicY[2, -1, θ, φ];
shR8 = SphericalHarmonicY[2, 2, θ, φ];
shR9 = SphericalHarmonicY[2, -2, θ, φ];

(*Print grid -- part 1*)
Print["Part 1 -- Table of Y_ℓ^m_ℓ(θ, φ) for 0 ≤ ℓ ≤ 2 and -ℓ ≤ m_ℓ ≤ +ℓ"]
Grid[
    {
        {"Y_ℓ^m_ℓ(θ, φ) = ", "Definition"},
        {"Y_0^0(θ, φ) = ",  shR1},
        {"Y_1^0(θ, φ) = ", shR2},
        {"Y_1^1(θ, φ) = ", shR3},
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        {"Y₁⁻¹(θ, φ) = ", shR4},
        {"Y₂⁰(θ, φ) = ", shR5},
        {"Y₂¹(θ, φ) = ", shR6},
        {"Y₂⁻¹(θ, φ) = ", shR7},
        {"Y₂²(θ, φ) = ", shR8},
        {"Y₂⁻²(θ, φ) = ", shR9}
    },
    Frame→All
]

(*Print spherical plot*)
Print["Part 2 -- Visualizing the Spherical Harmonics"]
Print["---------------"]
Print["Y₀⁰(θ, φ) plot"]
Print["---------------"]
SphericalPlot3D[shR1, {θ, 0, Pi}, {φ, 0, 2*Pi}]
Print["----------------"]
Print["Y₁^mℓ(θ, φ) plots"]
Print["----------------"]
Table[
    SphericalPlot3D[
        {Abs[SphericalHarmonicY[1, m, θ, φ]]},
        {θ, 0, Pi},
        {φ, 0, 2*Pi}
    ],
    {m, 0, 1}
]
Print["----------------"]
Print["Y₂^mℓ(θ, φ) plots"]
Print["----------------"]
Table[
    SphericalPlot3D[
        {Abs[SphericalHarmonicY[2, m, θ, φ]]},
        {θ, 0, Pi},
        {φ, 0, 2*Pi}
    ],
    {m, 0, 2}
]

(*------------------*)
(*Question 3: Energy*)
(*------------------*)
Print["\n(*------------------*)
(*Question 3: Energy*)
(*------------------*)"]

Print["(a) For ψ_nℓmℓ(r, θ, ϕ) = R_nℓ(r)Yℓ^mℓ(θ, ϕ) then for 1s function n = 1, ℓ = 0, mℓ = 0"]
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Print["ψ1s(r, θ, ϕ) = ψ100(r, θ, ϕ) = R10(r)Y0^0(θ, ϕ) = 1/√π (1/a0)^3/2 (-r/a0)"]

Print["\tExplanation: For the 1s function to satisfy the radial Schrodinger equation, lim_(r→∞) ψ1s(r, θ
This is because the number of radial nodes -- radial sections in the spherical coordinate plane
where Rnℓ(r) = 0 -- that is predicted from n - ℓ - 1 should also be described by ψ1s(r, θ, ϕ). Sin
quantum number, is 1 and ℓ, the angular quantum number, is 0, n - ℓ - 1 predicts that number of ra
 lim_(r→∞) ψ1s(r, θ, ϕ) = 0 predicts the same thing. Therefore, ψ1s(r, θ, ϕ satisfies the radial Schrodi
Print["The energy of the electron in the 1s state is En = -13.6 eV/n^2, or simply E1 = -13.6 eV]"]

 Print["\n(b) Deriving the energy for two trial functions ϕ1 and ϕ2"]
 phi1 = Exp[-α*r];
 phi2 = Exp[-α*r^2];
 Print["Part 1 --> ϵ[ϕ1] for ϕ1 = e^-αr"]
 Print["To get ϵ[ϕ1] = < ϕ1 | Ĥϕ1 > / < ϕ1 | ϕ1 >, I will first get < ϕ1 | ϕ1 >"]
 Print["(1) < ϕ1 | ϕ1 > = ∫_0^∞ r^2 ϕ1^2 dr, or ",
 Normal[Assuming[Element[α, PositiveReals], Integrate[r^2 * phi1^2, {r, 0, Infinity}]]]
 ]
 Print["(2) Then < ϕ | Ĥϕ > for Ĥ = -ħ^2/(2me r^2) d/dr (r^2 d/dr) - e^2/(4πϵ0 r)."]
 Print["(3) Substituting Ĥ into < ϕ | Ĥϕ > =>
< ϕ | -ħ^2/(2me r^2) d/dr (r^2 d/dr) - e^2/(4πϵ0 r) | ϕ >"]
Print["(4) This is equivalent to:
- < ϕ | -ħ^2/(2me r^2) d/dr (r^2 d/dr) | ϕ > - < ϕ | e^2/(4πϵ0 r) | ϕ >"]
lhsIntegration = Assuming[
    Element[α, PositiveReals],
    Integrate[
        Exp[-α*r]*(-2*α*r*Exp[-α*r]+α^2*r^2*Exp[-α*r]),
        {r, 0, Infinity}]
];
Print["(5) The left side of the equation is -∫_0^∞ r^2 e^-αr (-ħ^2/(2me r^2) d/dr (r^2 d/dr) e^-αr) dr.
Integrating using mathematica, this is: ħ^2/(2me)*", lhsIntegration]
rhsIntegration = Assuming[
    Element[α, PositiveReals],
    Integrate[
        r*Exp[-2*α*r],
        {r, 0, Infinity}]
];
Print["(6) The right side of the equation is -∫_0^∞ r^2 e^-αr ((e^2/(4πϵ0 r)) e^-αr) dr, or
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$\frac{-1e^2}{4\pi\epsilon_0}\int_0^\infty (re^{-\alpha r} * e^{-\alpha r})\,dr$, or $\frac{-1}{4\pi\epsilon_0}\int_0^\infty re^{-2\alpha r}dr$.

Integrating using mathematica: $\frac{-1}{4\pi\epsilon_0}$ * ", rhsIntegration]

Print["(7) Combining the results from step 1 (the denominator), step 5 and 6 (the numerator),

$\epsilon[\phi_1] = \frac{\left[\frac{\hbar}{2m_e} * \frac{1}{4\alpha}\right] - \left[\frac{1e^2}{4\pi\epsilon_0} * \frac{1}{4\alpha^2}\right]}{\left[\frac{1}{4\alpha^3}\right]}$"]

Print["\nPart 2 --> $\epsilon[\phi_2]$ for $\phi_1 = e^{-\alpha r^2}$"]

Print["(1) Separating the numerator out and denominator out as before,

the denominator is < $\phi_2$ | $\phi_2$ > = $\int_0^\infty r^2 {\phi_2}^2 dr$, or ",

```
Normal[Assuming[Element[α, PositiveReals], Integrate[r^2 * phi2^2, {r, 0, Infinity}]]]]
lhsIntegrationPhi2 = Assuming[
    Element[α, PositiveReals],
    Integrate[
        Exp[-α*r^2]*(3*α*r^2*Exp[-α*r^2]-2*α^2r^4*Exp[-α*r^2]),
        {r, 0, Infinity}
    ]
];
```

Print["(2) The left side of the numerator is $\int_0^\infty r^2 e^{-\alpha r^2}\left(\frac{-\hbar^2}{2m_e r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)e^{-\alpha r^2}\right)dr$,

so the result is $-\frac{\hbar}{m_e}$*", lhsIntegrationPhi2]

```
rhsIntegrationPhi2 = Assuming[
    Element[α, PositiveReals],
    Integrate[
        r*Exp[-2*α*r^2],
        {r, 0, Infinity}]
];
```

Print["(3) The right side of the numerator is $-\int_0^\infty r^2 e^{-\alpha r^2}\left(\left(\frac{e^2}{4\pi\epsilon_0 r}\right)e^{-\alpha r^2}\right)dr$,

so the result is $-\frac{e^2}{4\pi\epsilon_0}$* ", rhsIntegrationPhi2]

Print["(4) Putting the results of step 1, 2, and 3 together:

$\epsilon[\phi_2] = \frac{-\left[\frac{\hbar}{m_e} * \frac{3\sqrt{\frac{\pi}{2}}}{16\sqrt{\alpha}}\right] - \left[\frac{e^2}{4\pi\epsilon_0} * \frac{1}{4\alpha}\right]}{\left[\frac{\sqrt{\frac{\pi}{2}}}{8\alpha^{3/2}}\right]}$"]

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(*-----------------------------*)
(*Question 1: Radial Functions*)
(*-----------------------------*)
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(a) Radial Wave Functions $R_{nl}(r)$ through n = 2 where 0 <= l <= n-1 for n ∈ $\mathbb{Z}^+$:

Out[559]=

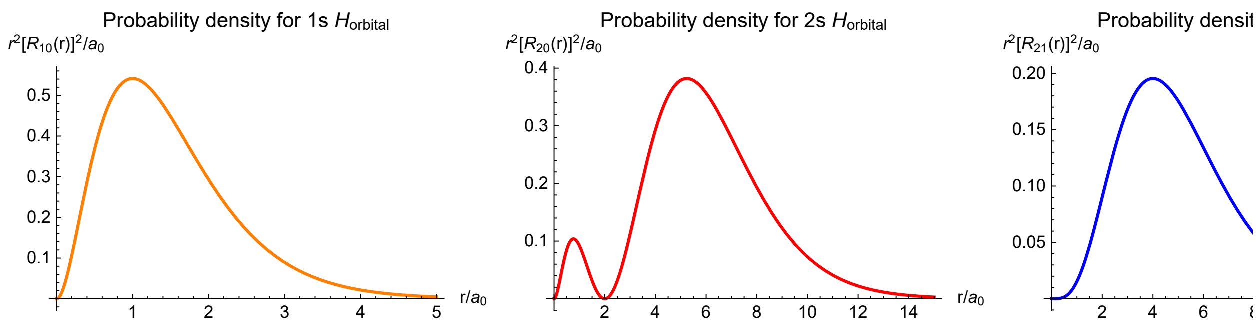
| |
|---|
| $R_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\rho}$ |
| $R_{20}(r) = \left(\frac{Z}{2\,a_0}\right)^{3/2} (2-\rho)\, e^{-\rho/2}$ |
| $R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2\,a_0}\right)^{3/2} \rho e^{-\rho/2}$ |

where Z is the nuclear charge and $\rho = Zr/a_0$ and SubscriptBox[a,0\]is the Bohr radius.

$Z = 1$, $\rho = -r/a_0$, and $a_0 = 5.29E-11m = 1$ bohrs

(b) Plot the corresponding radial distributions $(r^2 R_{nl}{}^2(r))$, also in table form:

Out[571]//TableForm=




(c) Maximum probability radius for 1s state is when $r = 1$.

Therefore $r^2[R_{10}(1)]^2/a_0 = 0.541341$

(d) Show that 1s radial function is orthogonal to that of 2s

From Mathematica calculations, $\langle R_{10} \mid R_{20} \rangle = 0$

(*--------------------------------*)
(*Question 2: Spherical Harmonics*)
(*--------------------------------*)

Part 1 -- Table of $Y_\ell^{m_\ell}(\theta, \varphi)$ for $0 \le \ell \le 2$ and $-\ell \le m_\ell \le +\ell$

Out[591]=

| $Y_{\ell}^{m_\ell}(\theta,\ \varphi)$ = | Definition |
|---|---|
| $Y_0^0(\theta,\ \varphi)$ = | $\frac{1}{2\sqrt{\pi}}$ |
| $Y_1^0(\theta,\ \varphi)$ = | $\frac{1}{2}\sqrt{\frac{3}{\pi}}\ \mathrm{Cos}[\theta]$ |
| $Y_1^1(\theta,\ \varphi)$ = | $-\frac{1}{2}\ e^{i\varphi}\sqrt{\frac{3}{2\pi}}\ \mathrm{Sin}[\theta]$ |
| $Y_1^{-1}(\theta,\ \varphi)$ = | $\frac{1}{2}\ e^{-i\varphi}\sqrt{\frac{3}{2\pi}}\ \mathrm{Sin}[\theta]$ |
| $Y_2^0(\theta,\ \varphi)$ = | $\frac{1}{4}\sqrt{\frac{5}{\pi}}\ \left(-1+3\,\mathrm{Cos}[\theta]^2\right)$ |
| $Y_2^1(\theta,\ \varphi)$ = | $-\frac{1}{2}\ e^{i\varphi}\sqrt{\frac{15}{2\pi}}\ \mathrm{Cos}[\theta]\ \mathrm{Sin}[\theta]$ |
| $Y_2^{-1}(\theta,\ \varphi)$ = | $\frac{1}{2}\ e^{-i\varphi}\sqrt{\frac{15}{2\pi}}\ \mathrm{Cos}[\theta]\ \mathrm{Sin}[\theta]$ |
| $Y_2^2(\theta,\ \varphi)$ = | $\frac{1}{4}\ e^{2i\varphi}\sqrt{\frac{15}{2\pi}}\ \mathrm{Sin}[\theta]^2$ |
| $Y_2^{-2}(\theta,\ \varphi)$ = | $\frac{1}{4}\ e^{-2i\varphi}\sqrt{\frac{15}{2\pi}}\ \mathrm{Sin}[\theta]^2$ |

Part 2 -- Visualizing the Spherical Harmonics

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$Y_0^0(\theta,\ \varphi)$ plot

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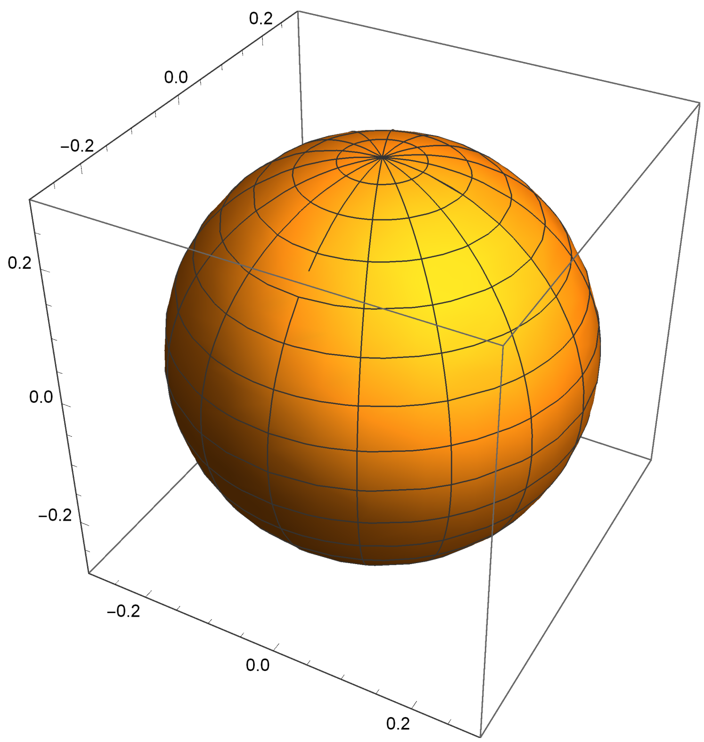
Out[596]=

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$Y_1^{m_\ell}(\Theta, \varphi)$ plots

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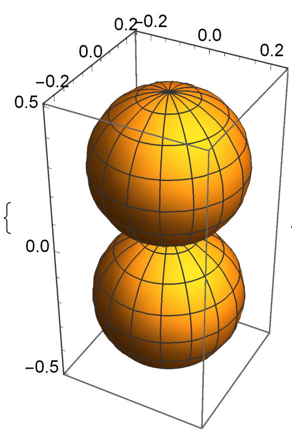
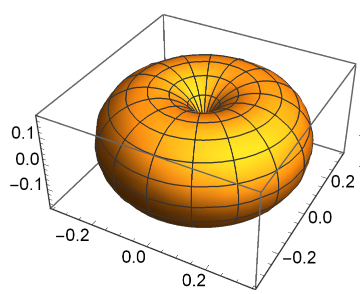
Out[600]= {




,




}

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$Y_2^{m_\ell}(\Theta, \varphi)$ plots

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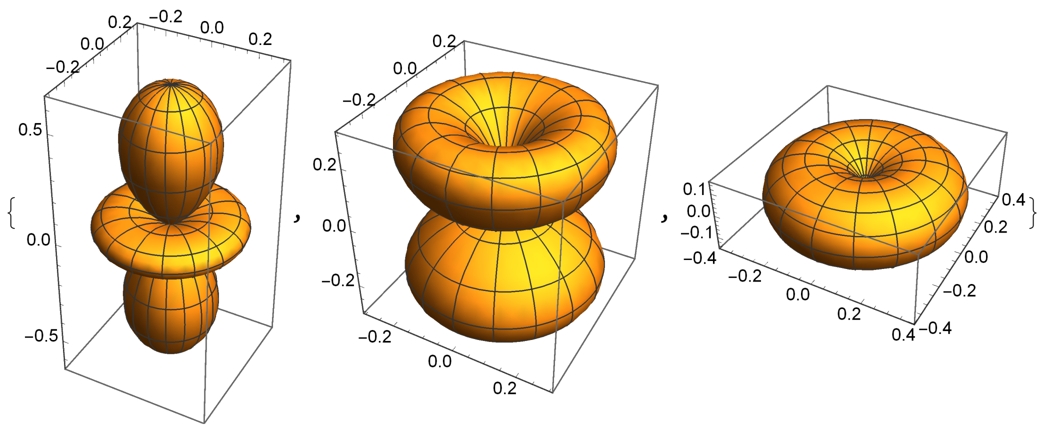
Out[604]=

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(*------------------*)
(*Question 3: Energy*)
(*------------------*)
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(a) For $\psi_{n\ell m_\ell}(r, \theta, \phi) = R_{n\ell}(r) Y_\ell^{m_\ell}(\theta, \phi)$ then for 1s function $n = 1$, $\ell = 0$, $m_\ell = 0$

$$\psi_{1s}(r, \theta, \phi) = \psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0(\theta, \phi) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} (-r/a_0)$$

Explanation: For the 1s function to satisfy the radial Schrodinger equation, $\lim_{r \to \infty} \psi_{1s}(r, \theta, \phi) = 0$.
This is because the number of radial nodes -- radial sections in the spherical coordinate plane where $R_{n\ell}(r) = 0$ -- that is predicted from $n - \ell - 1$ should also be described by $\psi_{1s}(r, \theta, \phi)$. Since $n$, the principle quantum number, is 1 and $\ell$, the angular quantum number, is 0, $n - \ell - 1$ predicts that number of radial nodes is 0. $\lim_{r \to \infty} \psi_{1s}(r, \theta, \phi) = 0$ predicts the same thing. Therefore, $\psi_{1s}(r, \theta, \phi$ satisfies the radial Schrodinger equation.

The energy of the electron in the 1s state is $E_n = -\frac{13.6 \text{ eV}}{n^2}$, or simply $E_1 = -13.6$ eV]

(b) Deriving the energy for two trial functions $\phi_1$ and $\phi_2$

Part 1 --> $\epsilon[\phi_1]$ for $\phi_1 = e^{-\alpha r}$

To get $\epsilon[\phi_1] = \frac{\langle \phi_1 \mid \hat{H} \phi_1 \rangle}{\langle \phi_1 \mid \phi_1 \rangle}$, I will first get $\langle \phi_1 \mid \phi_1 \rangle$

(1) $\langle \phi_1 \mid \phi_1 \rangle = \int_0^\infty r^2 \phi_1{}^2 dr$, or $\frac{1}{4 \alpha^3}$

(2) Then $\langle \phi \mid \hat{H} \phi \rangle$ for $\hat{H} = \frac{-\hbar^2}{2 m_e r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr}\right) - \frac{e^2}{4 \pi \epsilon_0 r}$.

(3) Substituting $\hat{H}$ into $\langle \phi \mid \hat{H} \phi \rangle$ =>

$$\langle \phi \mid \frac{-\hbar^2}{2 m_e r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr}\right) - \frac{e^2}{4 \pi \epsilon_0 r} \mid \phi \rangle$$

(4) This is equivalent to:

$$- \langle \phi \mid \frac{-\hbar^2}{2 m_e r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr}\right) \mid \phi \rangle - \langle \phi \mid \frac{e^2}{4 \pi \epsilon_0 r} \mid \phi \rangle$$

(5) The left side of the equation is $-\int_0^\infty r^2 e^{-\alpha r}\left(\frac{-\hbar^2}{2 m_e r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)e^{-\alpha r}\right)dr$.

Integrating using mathematica, this is: $\frac{\hbar^2}{2 m_e}$*ConditionalExpression$\left[-\frac{1}{4\alpha}, \mathrm{Re}[\alpha] > 0\right]$

(6) The right side of the equation is $-\int_0^\infty r^2 e^{-\alpha r}\left(\left(\frac{e^2}{4\pi\epsilon_0 r}\right)e^{-\alpha r}\right)dr$, or

$\frac{-1\, e^2}{4\pi\epsilon_0}\int_0^\infty (r e^{-\alpha r} * e^{-\alpha r})\,dr$, or $\frac{-1}{4\pi\epsilon_0}\int_0^\infty r e^{-2\alpha r}dr$.

Integrating using mathematica: $\frac{-1}{4\pi\epsilon_0}$ * ConditionalExpression$\left[\frac{1}{4\alpha^2}, \mathrm{Re}[\alpha] > 0\right]$

(7) Combining the results from step 1 (the denominator), step 5 and 6 (the numerator),

$$\epsilon[\phi_1] = \frac{\left[\frac{\hbar}{2 m_e} * \frac{1}{4\alpha}\right] - \left[\frac{1 e^2}{4\pi\epsilon_0} * \frac{1}{4\alpha^2}\right]}{\left[\frac{1}{4\alpha^3}\right]}$$

Part 2 --> $\epsilon[\phi_2]$ for $\phi_1 = e^{-\alpha r^2}$

(1) Separating the numerator out and denominator out as before,

the denominator is $<\phi_2 \mid \phi_2> = \int_0^\infty r^2 \phi_2{}^2 dr$, or $\frac{\sqrt{\frac{\pi}{2}}}{8\alpha^{3/2}}$

(2) The left side of the numerator is $\int_0^\infty r^2 e^{-\alpha r^2}\left(\frac{-\hbar^2}{2 m_e r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)e^{-\alpha r^2}\right)dr$,

so the result is $-\frac{\hbar}{m_e}$*ConditionalExpression$\left[\frac{3\sqrt{\frac{\pi}{2}}}{16\sqrt{\alpha}}, \mathrm{Re}[\alpha] > 0\right]$

(3) The right side of the numerator is $-\int_0^\infty r^2 e^{-\alpha r^2}\left(\left(\frac{e^2}{4\pi\epsilon_0 r}\right)e^{-\alpha r^2}\right)dr$,

so the result is $-\frac{e^2}{4\pi\epsilon_0}$* ConditionalExpression$\left[\frac{1}{4\alpha}, \mathrm{Re}[\alpha] > 0\right]$

(4) Putting the results of step 1, 2, and 3 together:

$$\epsilon[\phi_2] = \frac{-\left[\frac{\hbar}{m_e} * \frac{3\sqrt{\frac{\pi}{2}}}{16\sqrt{\alpha}}\right] - \left[\frac{e^2}{4\pi\epsilon_0} * \frac{1}{4\alpha}\right]}{\left[\frac{\sqrt{\frac{\pi}{2}}}{8\alpha^{3/2}}\right]}$$