PHYS 606 – Spring 2017 – Homework VIII – Solution

Problem [1]

Preparations

- Define useful quantities in terms of energy e and potential energy v

```
In[1]:= ϵ = κ / k - k / κ;
ϵp = kp / k + k / kp;
κ = Sqrt[2 * m * (v - e)] / hb;
k = Sqrt[2 * m * e] / hb;
kp = Sqrt[2 * m * (e - v)] / hb; (* for barrier, v → -v for well *)
β2 = a ^ 2 / hb ^ 2 * 2 * m * v;
(* for well only *)
```

- Replacement list with numerical values uses here: hbar (eV s), electron mass (eV s^2/m^2), potential energy level (eV), potential barrier/well width (m)

```
In[7]:= rep = {hb → 4.13 * 10 ^ (-15) / (2 * π),
  m → N[511 * 10 ^ 3 / (3 * 10 ^ 8) ^ 2], v → 1, a → 0.1 * 10 ^ (-8) / 2}
```

Out[7]= $\{hb \to 6.5731 \times 10^{-16},\ m \to 5.67778 \times 10^{-12},\ v \to 1,\ a \to 5. \times 10^{-10}\}$

Discuss Bound States in the Well

- This is β squared with the given numbers

```
In[8]:= β2num = β2 /. rep
```

Out[8]= 6.57065

- This is the number of bound states in the well: look how often β fits into multiples of $\pi/2$

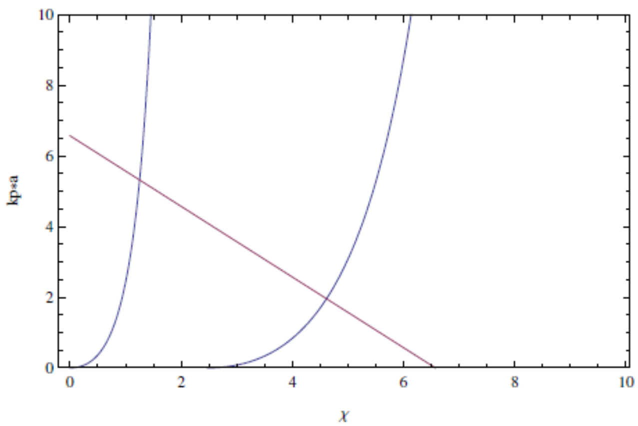
```
In[9]:= Nbound = Quotient[Sqrt[β2 /. rep], π / 2] + 1
```

Out[9]= 2

- For a graphical solution one would proceed like this. Two bound states (intersection points) are confirmed.

In[28]:=
```
f = Piecewise[
    {{χ * Tan[Sqrt[χ]] ^2, Tan[Sqrt[χ]] > 0}, {χ * Cot[Sqrt[χ]] ^2, Tan[Sqrt[χ]] < 0}}];
Plot[{f, β2num - χ}, {χ, 0, (2 * π / 2) ^2}, PlotRange → {0, 10},
 Frame → True, FrameLabel → {"χ", "kp*a"}]
```

Out[29]=



- Numerical Solutions

In[36]:=
```
sol1 =
 NSolve[χ * Tan[Sqrt[χ]] ^2 == β2num - χ && 0 ≤  χ ≤ β2num && Tan[Sqrt[χ]] > 0, χ, Reals]
```

Solve::ratnz :
 Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result. ≫

Out[36]= {{χ → 1.25223}}

In[37]:=
```
sol2 =
 NSolve[χ * Cot[Sqrt[χ]] ^2 == β2num - χ && 0 < χ < β2num && Tan[Sqrt[χ]] < 0, χ, Reals]
```

Solve::ratnz :
 Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result. ≫

Out[37]= {{χ → 4.61399}}

- Check both solutions for χ: Results are good enough

In[38]:=
```
sol = Join[sol1, sol2];
(f - β2num + χ) /. sol
```

Out[39]= $\{-8.88178\times10^{-16},\ 6.66134\times10^{-16}\}$

- 2 bound state energies (in eV):

In[40]:=
```
elist = Sort[(-hb^2 / (2 * m * a^2) * (β2num - χ) /. sol) /. rep]
```

Out[40]= {-0.80942, -0.297788}

- Corresponding wave vectors needed for the wave functions (need v -> v for well!)

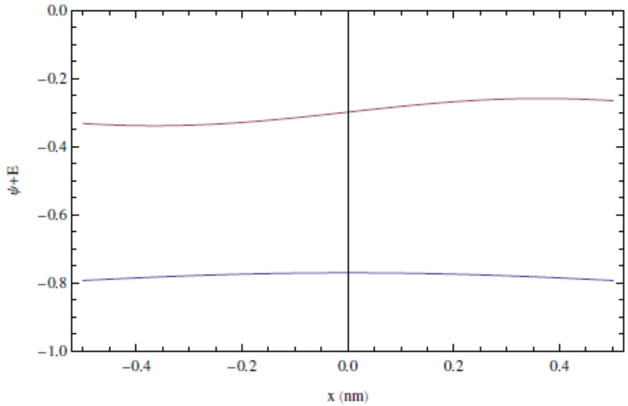
In[41]:=
```
kplist = ((kp /. (v → -v)) /. e → elist) /. rep
```

Out[41]= $\{2.23806\times10^{9},\ 4.29604\times10^{9}\}$

- Wave functions are alternatingly even and odd (Cos and Sin); normalization is arbitrary and offset depicts the energy of the state (first states only)

In[46]:=
```
wflist = {Cos[kplist[[1]] * x / 10^9] * 0.04 + elist[[1]],
   Sin[kplist[[2]] * x / 10^9] * 0.04 + elist[[2]]};
Plot[wflist, {x, -10^9 * a /. rep, 10^9 * a /. rep}, Frame → True,
 PlotRange → {-1.0, 0}, FrameLabel → {"x (nm)", "ψ+E"}]
```

Out[47]=



Transmission Coefficients and Phase Shifts

- Transmission coefficient and phase shift for scattering solution (barrier) for subthreshold energy

In[50]:=
```
t1 = 1 / (Cosh[2 * κ * a]^2 + ϵ^2 / 4 * Sinh[2 * κ * a]^2);
s1 = 2 * k * a - ArcTan[Cosh[2 * κ * a], -ϵ / 2 * Sinh[2 * κ * a]];
```

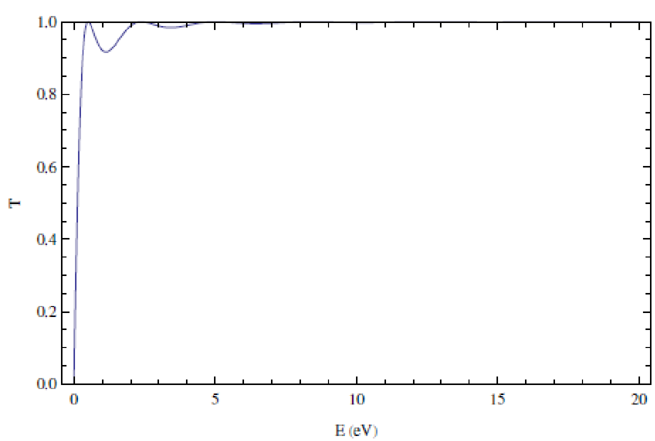
- Transmission coefficient and phase shift for scattering solution (barrier and well) for above threshold energy

In[52]:=
```
t2 = 1 / (Cos[2 * kp * a]^2 + ϵp^2 / 4 * Sin[2 * kp * a]^2);
s2 = 2 * k * a - ArcTan[Cos[2 * kp * a], ϵp / 2 * Sin[2 * kp * a]];
```

- T for the potential well for E>0. Remember that there are also 2 bound states for E<0. There are several sharp resonances followed by severl more that are less very well defined, then the transmission coefficient is almost flat.

In[54]:=
```
Plot[(t2 /. {v → -v}) /. rep, {e, 0, 20},
 PlotRange → {0, 1}, Frame → True, FrameLabel → {"E (eV)", "T"}]
```

Out[54]=

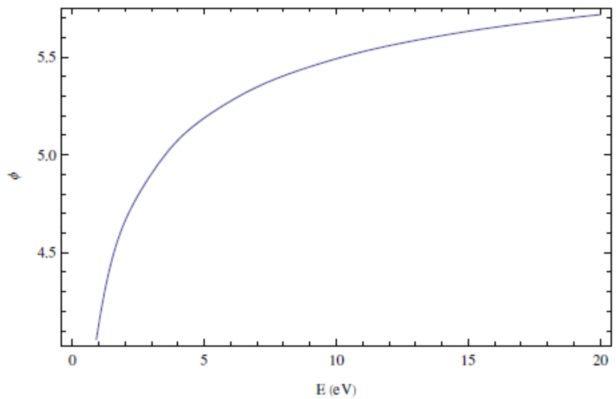


- Phase shift for the potential well for E>0. s20 is the phase shift at zero energy. Because of the periodicity of the phase shift there are several ways of plotting this quantity. Here the Mod function folds the function back into the interval (s20,s20+2π)

In[55]:=
```
s20 = Re[Limit[(s2 /. {v → -v}) /. rep, e → 0]];
```

In[56]:=
```
Plot[Mod[((s2 /. {v → -v}) /. rep) - s20, 2 * π] + s20,
 {e, 0, 20}, Frame → True, FrameLabel → {"E (eV)", "ϕ"}]
```

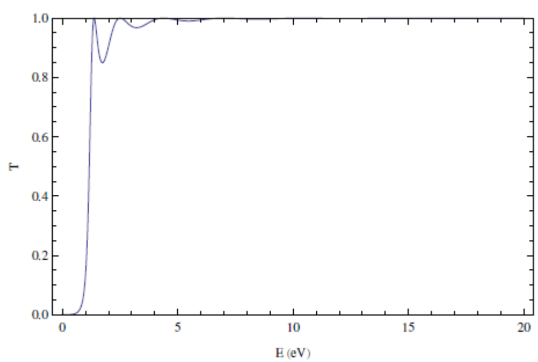
Out[56]=



- T for the potential barrier. There are again several well defined resonances (sharp peaks) above the barrier threshold and maybe two more that are identifyable but not very well defined anymore. Below the threshold of 5 eV the transmission dies off very quickly.

In[57]:=
```
Plot[t1 /. rep, {e, 0, 20}, Frame → True,
 FrameLabel → {"E (eV)", "T"}, PlotRange → {0, 1}]
```

Out[57]=

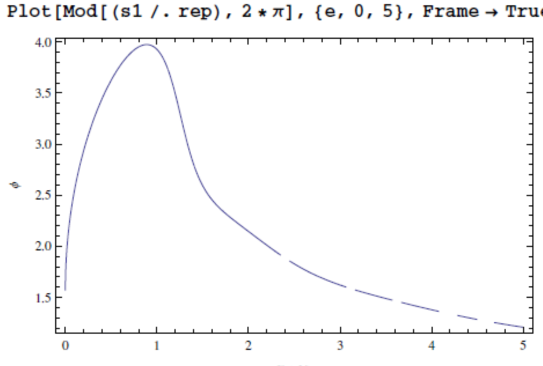


- Phase shift for the potential barrier. Because of the periodicity of the phase shift there are several ways of plotting this quantity. Here the Mod function folds the function back into the interval (0,2π)

In[60]:=
```
s10 = Re[Limit[s1 /. rep, e → 0]];
```

In[65]:=
```
Plot[Mod[(s1 /. rep), 2 * π], {e, 0, 5}, Frame → True, FrameLabel → {"E (eV)", "ϕ"}]
```

Out[65]=



Problem [2]

(a) $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + b|x|\psi = E\psi$

symmetric pot. energy $\Rightarrow$ H commutes with parity operator $\Rightarrow$ energy eigenfcts. can be chosen even or odd

Thus it is sufficient to solve $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + bx\psi = E\psi$ for $x>0$

Substitution: define $z = \left(\frac{2mb}{\hbar^2}\right)^{1/3}\left(x - \frac{E}{b}\right) \Rightarrow \frac{d^2}{dx^2} = \left(\frac{2mb}{\hbar^2}\right)^{2/3}\frac{d^2}{dz^2}$

$\Rightarrow \frac{d^2\psi}{dz^2} - z\psi = 0$

$\Rightarrow$ Physical solution (regular) Airy fct. $Ai(z)$

(b) From (a) for eigenvalue E_n the eigenfct. is (for $x>0$)

$\psi_n(x) = C_n\, Ai\left(\left(\frac{2mb}{\hbar^2}\right)^{1/3}\left(x - \frac{E_n}{b}\right)\right)$ and C_n determined by $\int_{\mathbb{R}} |\psi_n|^2 dx = 1$

$\psi_n(x) = \psi_n(-x)$ for $x<0$ for even eigenfcts.

$\psi_n(x) = -\psi_n(-x)$ for $x<0$ for odd eigenfcts.

Even eigenfcts. require $\frac{d}{dx}\psi_n(0) = 0$

Odd eigenfcts. require $\psi_n(0) = 0$

$\Rightarrow$ "odd eigenvalues" given by zeros of $Ai\left(-\left(\frac{2mb}{\hbar^2}\right)^{1/3}\frac{E_n}{b}\right)$, "even eigenvalues" given by zeros of $\frac{d}{dx}Ai\left(-\left(\frac{2mb}{\hbar^2}\right)^{1/3}\frac{E_n}{b}\right)$

Smallest zeros (absolute value) of Ai and Ai' are $-2.33811 =: -a_1$ and $-1.01879 =: -a_0$ resp.

$$\Rightarrow \quad E_0 = a_0 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \qquad (\text{even})$$

$$E_1 = a_1 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \qquad (\text{odd})$$

Problem [3]

(a) Trial fct. $\psi(x) = \left(\frac{2\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2 x^2}$ (i.e. $\int_{\mathbb{R}} |\psi|^2 dx = 1$ for all $\alpha \in \mathbb{R}$)

$$\langle H \rangle = \int_{\mathbb{R}} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + b|x|\psi(x)\, dx$$

$$= -\frac{\hbar^2}{2m}\left(\frac{2\alpha^2}{\pi}\right)^{1/2} \int_{\mathbb{R}} \left(-2\alpha^2 + 4\alpha^4 x^2\right) e^{-2\alpha^2 x^2} dx + 2b \int_0^\infty x e^{-2\alpha^2 x^2} dx \left(\frac{2\alpha^2}{\pi}\right)^{1/2}$$

$$= -\frac{\hbar^2}{2m}\left(-2\alpha^2 + 4\alpha^4 \frac{1}{4\alpha^2}\right) + 2b \frac{1}{4\alpha^2}\sqrt{\frac{2}{\pi}}\,\alpha = \frac{\hbar^2 \alpha^2}{2m} + \frac{b}{\sqrt{2\pi}\,\alpha}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 \Rightarrow \frac{\hbar^2 \alpha}{m} - \frac{b}{\sqrt{2\pi}\,\alpha^2} = 0 \Rightarrow \alpha = \left(\frac{bm}{\sqrt{2\pi}\,\hbar^2}\right)^{1/3}$$

$$\Rightarrow \langle H \rangle = \frac{(\hbar b)^{2/3}}{m^{1/3}} \frac{1}{2(2\pi)^{1/3}} + \frac{(\hbar^2 b)^{2/3}}{m^{1/3}} \frac{1}{(2\pi)^{1/3}} = \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \frac{3}{2\pi^{1/3}}$$

$$\approx 1.024 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \quad \text{vs} \quad E_0 = 1.019 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3}$$

(b) Odd trial fct. $\psi(x) = 2\alpha^{3/2}\left(\frac{2}{\pi}\right)^{1/4} x\, e^{-\alpha^2 x^2}$ ($\int_{\mathbb{R}} |\psi|^2 dx = 1$ with this prefactor)

$$\langle H \rangle = -\frac{\hbar^2}{2m} 4\alpha^3 \left(\frac{2}{\pi}\right)^{1/2} \int \left(-6\alpha^2 x^2 + 4\alpha^4 x^4\right) e^{-2\alpha^2 x^2} + 2b\, 4\alpha^3 \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty x^3 e^{-2\alpha^2 x^2} dx$$

$$= \frac{3\hbar^2 \alpha^2}{2m} + \frac{2b}{\sqrt{2\pi}\,\alpha}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 \Rightarrow \frac{3\hbar^2 \alpha}{m} - \frac{2b}{\sqrt{2\pi}\,\alpha^2} = 0 \Rightarrow \alpha = \left(\frac{\frac{2}{3} bm}{\sqrt{2\pi}\,\hbar^2}\right)^{1/3}$$

$$\Rightarrow \langle H \rangle = \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \left(\frac{3}{2}\left(\frac{2^2}{3^2 \pi}\right)^{1/3} + \frac{2\, 3^{1/3}}{(2\pi)^{1/3}}\right) = \left(\frac{\hbar^2 b}{2m}\right)^{1/3} 3\left(\frac{3}{2\pi}\right)^{1/3}$$

$$\approx 2.3448 \left(\frac{\hbar^2 b}{2m}\right)^{1/3} \quad \text{vs} \quad E_0 = 2.3381 \left(\frac{\hbar^2 b}{2m}\right)^{1/3}.$$

(c) Trial function $\varphi(x) = \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\frac{16\alpha^5}{3}}\, x^2 e^{-\alpha^2 x^2}$ ($\int |\psi|^2 dx = 1$ w/ this prefactor)

$$\langle H \rangle = -\frac{\hbar^2}{2m} \frac{16\alpha^5}{3} \sqrt{\frac{2}{\pi}} \int_{-\infty}^{+\infty} \left(2 + \overset{10}{8}(-\alpha^2) x^2 + 4\alpha^4 x^4\right) x^2 e^{-2\alpha^2 x^2}\, dx$$

$$+ \frac{16\alpha^5}{3} \sqrt{\frac{2}{\pi}}\, b\, 2 \int_0^{\infty} x^5 e^{-2\alpha^2 x^2}\, dx$$

$$= \frac{7\hbar^2 \alpha^2}{6m} + \frac{4b}{3\alpha} \sqrt{\frac{2}{\pi}}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 \Rightarrow \frac{7\hbar^2 \alpha}{3m} - \frac{4b}{3\alpha^2} \sqrt{\frac{2}{\pi}} = 0 \Rightarrow \alpha = \left(\frac{4bm}{7\hbar^2} \sqrt{\frac{2}{\pi}}\right)^{1/3}$$

$$\Rightarrow \underset{\text{at extr.}}{\langle H \rangle} = \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \left[\frac{7}{6} \left(\frac{4^2}{7^2} \frac{4/\pi}{\sqrt[3]{\ldots}}\right)^{1/3} + \frac{4}{3} \left(\frac{7}{4}\right)^{1/3} \left(\frac{4}{\pi}\right)^{1/3}\right] =$$

$$= \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} 2 \left(\frac{7}{\pi}\right)^{1/3} \approx 2.6122 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3}$$

Not a good approximation of the ground state energy!

Second excited state given by the second zero of Ai' (it's even in parity) at $-a_2 = -3.2482$

$$\Rightarrow E_2 = a_2 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3}$$

Our trial fct. is a better approx. for the second excited state energy but it is not ideal.

Problem [4]

(a) (i) $[L_j, L_k] = \varepsilon_{jlm}\varepsilon_{kno}[r_l p_m, r_n p_o] = \varepsilon_{jlm}\varepsilon_{kno}\Big(r_l r_n \underbrace{[p_m, p_o]}_{=0} + r_l [p_m, r_n] p_o$

$\qquad + \underbrace{[r_l, r_n]}_{=0} p_o p_m + r_n [r_l, p_o] p_m\Big)$

$= i\hbar\, \varepsilon_{jlm}\varepsilon_{kno}\left(-\delta_{mn} r_l p_o + \delta_{lo} r_n p_m\right)$

$= i\hbar\left[(\delta_{jk}\delta_{lo} - \delta_{jo}\delta_{kl}) r_l p_o - (\delta_{jk}\delta_{mn} - \delta_{jn}\delta_{km}) r_n p_m\right]$

$= i\hbar\left(-r_k p_j + r_j p_k\right) = i\hbar\, \varepsilon_{jkl} L_l$

(ii) $[L_j, L^2] = \underbrace{[L_j, L_j^2]}_{=0} + \sum_{i\neq j} [L_j, L_i^2] = \sum_{i \neq j}\left(L_i [L_j, L_i] + [L_j, L_i] L_i\right)$

$= \sum_{i\neq j} (i\hbar)\, \varepsilon_{jik}\left(L_i L_k + L_k L_i\right) = 0$

symmetric in i,k

antisymmetric in i,k

(b) Spherical coordinates:
$$\begin{pmatrix} r = \sqrt{x^2+y^2+z^2} \\ \phi = \arctan \frac{y}{x} \\ \theta = \arccos \frac{z}{\sqrt{x^2+y^2+z^2}} \end{pmatrix}$$

Unit vectors:
$$\hat{r} = \sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z}$$
$$\hat{\theta} = \cos\theta\cos\phi\,\hat{x} + \cos\theta\sin\phi\,\hat{y} - \sin\theta\,\hat{z}$$
$$\hat{\phi} = -\sin\phi\,\hat{x} + \cos\phi\,\hat{y}$$

Jacobi matrix:
$$J = \frac{\partial(r,\theta,\phi)}{\partial(x,y,z)} = \begin{pmatrix} \frac{x}{r} & \frac{y}{r} & \frac{z}{r} \\ \frac{1}{r^2}\frac{xz}{\sqrt{x^2+y^2}} & \frac{1}{r^2}\frac{yz}{\sqrt{x^2+y^2}} & -\frac{1}{r^2}\sqrt{x^2+y^2} \\ \frac{-y/x^2}{1+y^2/x^2} & \frac{1/x}{1+y^2/x^2} & 0 \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \frac{1}{r}\cos\theta\cos\phi & \frac{1}{r}\cos\theta\sin\phi & -\frac{1}{r}\sin\theta \\ -\frac{1}{r}\frac{\sin\phi}{\sin\theta} & \frac{1}{r}\frac{\cos\phi}{\sin\theta} & 0 \end{pmatrix}$$

$$\frac{\partial}{\partial x} = J_{11}\frac{\partial}{\partial r} + J_{21}\frac{\partial}{\partial\theta} + J_{31}\frac{\partial}{\partial\phi} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial}{\partial\theta} - \frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi}$$

$\frac{\partial}{\partial y}$, $\frac{\partial}{\partial z}$ similarly

$$\Rightarrow \nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}$$

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r}\frac{\partial}{\partial r}$$
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \qquad \text{(standard form)}$$

(c) $L_x = (-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = -i\hbar\Big[r\sin\theta\sin\phi\left(\cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}\right)$

$\qquad - r\cos\theta\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\sin\phi\frac{\partial}{\partial\theta} + \frac{1}{r}\frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\phi}\right)\Big]$

$$= -i\hbar\left[-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]$$

Similarly $L_y = -i\hbar\left[\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right]$

$L_z = -i\hbar\frac{\partial}{\partial\phi}$

$$L^2 = -\hbar^2\left[\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\theta^2} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + \cot\theta\frac{\partial}{\partial\theta}\right] = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]$$