CSE 389D: Mathematical Modeling **Spring 2025**

Problem Set 2

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Problem 2.1

Part a

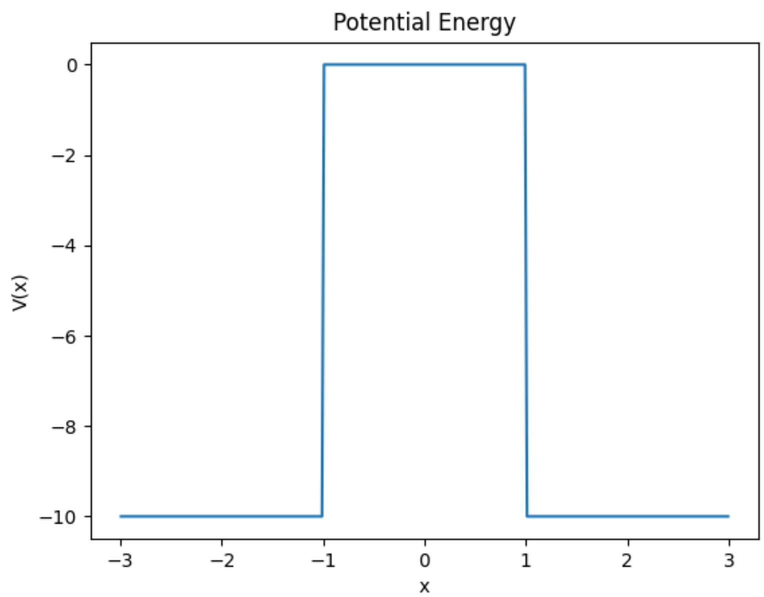

Figure 2.1. Sketch of $V(x)$ for $a = 1$,$b = 3$, and $V_0 = 10$

The time-independent Schrodinger's equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) = E\phi(x)$$

Part b

If we consider the bounded state where $-V_0 < E < 0$, and $0 < x < a$, then we get that $V(x) = 0$ and

$$-\frac{\hbar^2}{2m}\phi''(x) = E\phi(x) \implies \phi''(x) = \frac{2m|E|}{\hbar^2}\phi(x)$$

solving the differential equation above gives the general solution,

$$\phi(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

where

$$\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}$$

however since it is symmetric we get that

$$\phi(x) = Ae^{\kappa x} + Ae^{-\kappa x} = 2A\cosh(\kappa x)$$

now if we consider the case where $a \leq x \leq b$, we have that $V(x) - V_0$ and get

$$-\frac{\hbar^2}{2m}\phi''(x) - V_0\phi(x) = E\phi(x) \implies \phi''(x) = -\frac{2m(E+V_0)}{\hbar^2}\phi(x)$$

solving the above differential equation yields the following general solution

$$\phi(x) = C\cos(\xi(b-x)) + D\sin(\xi(b-x))$$

where

$$\xi = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

then since $V(b) = \infty$ we require that $\phi(b) = 0$ and hence

$$\phi(x) = D\sin(\xi(b-x))$$

now $x = a$ we have that

$$2A\cosh(\kappa a) = D\sin(\xi(b-a))$$

taking the derivatives

$$2A\kappa\sinh(\kappa a) = -D\xi\cos(\xi(b-a))$$

then dividing both equations yields

$$\frac{\kappa\sinh(\kappa a)}{\cosh(\kappa a)} = -\frac{\xi\cos(\xi(b-a))}{\sin(\xi(b-a))} \implies \kappa\tanh(\kappa a) = -\xi\cot(\xi(b-a)) = -\xi\frac{1+\tan(\xi a)\tan(\xi b)}{\tan(\xi b)-\tan(\xi a)}$$

thus

$$\kappa\tanh(\kappa a) + \xi\frac{1+\tan(\xi a)\tan(\xi b)}{\tan(\xi b)-\tan(\xi a)} = 0$$

letting $v = \xi b$ and $a = \gamma b$ then we get that

$$\kappa\tanh(\kappa a) + (v/b)\frac{1+\tan(\gamma v)\tan(v)}{\tan(v)-\tan(\gamma v)} = 0$$

note that if we define

$$S = \frac{b\sqrt{2mV_0}}{\hbar}$$

then we have that

$$\begin{aligned}\kappa = \sqrt{\frac{2m|E|}{\hbar^2}} = \sqrt{\frac{2m(V_0-(E+V_0)}{\hbar^2}} &= \sqrt{\frac{2mV_0}{\hbar^2} - \xi^2} \\ &= \sqrt{\frac{2mV_0}{\hbar^2} - \frac{v^2}{b^2}} \\ &= \frac{1}{b}\sqrt{S^2 - v^2}\end{aligned}$$

therefore we have that

$$\sqrt{S^2 - v^2}\tanh(\gamma\sqrt{S^2 - v^2}) - v\frac{1 + \tan(\gamma v)\tan(v)}{\tan(\gamma v) - \tan(v)} = 0$$

and hence our eigenvalues are given by

$$E + V_0 = \frac{\hbar^2\xi^2}{2m} = \frac{\hbar^2 v^2}{2mb^2} \implies \frac{E}{V_0} = -1 + \frac{v^2}{S^2}$$

Part c

Solving for v from the equation below we get

$$\begin{aligned} v_1 &= 9.87725 \\ v_2 &= 6.84406 \\ v_3 &= 3.46525 \end{aligned}$$

plugging these values into the equation

$$\frac{E}{V_0} = -1 + \frac{v^2}{S^2}$$

yields

$$\begin{aligned} \frac{E}{V_0} &= -1 + \frac{(9.87725)^2}{S^2} \approx -0.0244 \\ \frac{E}{V_0} &= -1 + \frac{(6.84406)^2}{S^2} \approx -0.5316 \\ \frac{E}{V_0} &= -1 + \frac{(3.46525)^2}{S^2} \approx -0.8799 \end{aligned}$$

as the eigenvalues of the even bounded state problem.

Part d

Part e

To show the odd parity of the wave function we will get a similar result as in part b. However we notice that since the wave is odd we we get that in the case $|x| < a$ the wave function is given by

$$\phi(x) = Ae^{\kappa x} - Ae^{-\kappa x} = 2A\sinh(\kappa x)$$

and in the case $a < x < b$ we have that

$$\phi(x) = D\sin(\xi(b - x))$$

as before. Then we have that

$$\begin{aligned} 2A\sinh(\kappa a) &= D\sin(\xi(b - a)) \\ 2A\kappa\cosh(\kappa a) &= -D\xi\cos(\xi(b - a)) \end{aligned}$$

then dividing the two equations yields

$$\frac{\kappa \cosh(\kappa a)}{\sinh(\kappa a)} = -\frac{\xi \cos(\xi(b-a))}{\sin(\xi(b-a))} \implies \kappa \coth(\kappa a) = -\xi \cot(\xi(b-a))$$

then by doing similar algebra and subsitutions as in part b we get that

$$\frac{\sqrt{S^2 - v^2}}{\tanh(\gamma\sqrt{S^2 - v^2})} - v\frac{\tan(\gamma v)\tan(v) + 1}{\tan(\gamma v) - \tan(v)} = 0$$

and hence the eigenvalues are given by

$$\frac{E}{V_0} = -1 + \frac{v^2}{S^2}$$

as desired.

Part f

Solving for v from the equation below, using $S = 10$ and $\gamma = 0.2$ we get that

$$v_1 = 6.96192$$
$$v_2 = 3.49913$$

plugging these values into the equation gives the following eigenvalues

$$\frac{E}{V_0} = -1 + \frac{(6.96192)^2}{S^2} \approx -0.5153$$
$$\frac{E}{V_0} = -1 + \frac{(3.49913)^2}{S^2} \approx -0.8775$$

Part g

The parity of the ground-state wavefunction is even.

Part h

Part i

Here we assume that the wavefunction is given in the form

$$\psi(x,t) = c_1(t)\psi_1(x) + c_2(t)\psi_2(x)$$

then we get that from the time-dependent Schrodinger's equation, that

$$i\hbar\frac{d\psi}{dt} = \hat{H}\psi$$

$$i\hbar\frac{d}{dt}(c_1(t)\psi_1(x) + c_2(t)\psi_2(x)) = \hat{H}(c_1(t)\psi_1(x) + c_2(t)\psi_2(x))$$

which gives us

$$i\hbar \left(\frac{dc_1}{dt}\psi_1(x) + \frac{dc_2}{dt}\psi_2(x) \right) = \hat{H}(c_1(t)\psi_1(x) + c_2(t)\psi_2(x))$$

next we can multiply by $\psi_1^*(x)$ and $\psi_2^*(x)$ separately and integrate over all space to get the following

$$\begin{aligned} i\hbar\dot{c}_1(t) &= \hat{H}c_1(t) = E_1c_1(t) \\ i\hbar\dot{c}_2(t) &= \hat{H}c_2(t) = E_2c_2(t) \end{aligned}$$

solving the above differential equations gives us that

$$c_1(t) = c_1(0)e^{-iE_1t/\hbar} \quad c_2(t) = c_2(0)e^{-iE_2t/\hbar}$$

using the boundary conditions we get that

$$c_1(0) = \frac{1}{\sqrt{2}} \quad c_2(0) = \frac{1}{\sqrt{2}}$$

and thus the full solution is given by

$$\psi(x,t) = \frac{1}{\sqrt{2}} \left(e^{-iE_1t/\hbar}\psi_1(x) + e^{-iE_2t/\hbar}\psi_2(x) \right)$$

Part j

If we suppose that the wavefunction is normalized at $t = 0$ then we have that

$$\int_{-\infty}^{\infty} |\psi(x,0)|^2 \, dx = 1$$

and thus for $t > 0$ we have that

$$\begin{aligned} \int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\, dx = \frac{1}{2}\int_{-\infty}^{\infty} &\psi_1^*(x)\psi_1(x) + \psi_2^*(x)\psi_2(x) + \psi_1^*(x)\psi_2(x)e^{i(E_1-E_2)t/\hbar} \\ &+ \psi_2^*(x)\psi_1(x)e^{i(E_2-E_1)t/\hbar}\, dx \end{aligned}$$

and since ψ_1 and ψ_2 are orthogonal we get that

$$\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\, dx = \frac{1}{2}\int_{-\infty}^{\infty} |\psi_1(x)|^2 + |\psi_2(x)|^2 \, dx = 1$$

and hence the wavefunction is normalized for all time.

Part k

If we consider the probability density of ψ we get that

$$\begin{aligned}|\psi(x,t)|^2 &= \frac{1}{2}(|\psi_1(x)|^2 + |\psi_2(x)|^2 + \psi_1^*(x)\psi_2(x)e^{i(E_1-E_2)t/\hbar} + \psi_2^*(x)\psi_1(x)e^{i(E_2-E_1)t/\hbar}) \\ &= \frac{1}{2}(|\psi_1(x)|^2 + |\psi_2(x)|^2 + 2\,\mathrm{Re}\left(\psi_1^*(x)\psi_2(x)e^{i(E_2-E_1)t/\hbar}\right)\end{aligned}$$

Then we see that when $t = \pi\hbar/(E_2 - E_1)$ we have that

$$|\psi(x,t)|^2 = \frac{1}{2}|\psi_1(x) + \psi_2(x)|^2$$

and for $t = -\pi\hbar/(E_2 - E_1)$ we have that

$$|\psi(x,t)|^2 = \frac{1}{2}|\psi_1(x) - \psi_2(x)|^2$$

and hence has a period

$$T = \frac{2\pi\hbar}{E_2 - E_1}$$

Part l

Problem 2.2

Part a

Recall that the expectation value of the electron distance from the nucleus in state ψ_{nlm} is given by

$$r_{nlm} = \int r|\psi_{nlm}|^2\,d\mathbf{r} = n^2\left\{1 + \frac{1}{2}\left[1 - \frac{l(l+1)}{n^2}\right]\right\}a_0$$

where a_0 is the Bohr radius. For s-states we have that $l = 0$ and hence $m = 0$ and thus $r_{n00} = \frac{3}{2}n^2 a_0$. So we have that the expectation value of the electron distance from the nucleus are

$$\begin{aligned}r_{100} &= \frac{3}{2}a_0 \\ r_{200} &= 6a_0 \\ r_{300} &= \frac{27}{2}a_0\end{aligned}$$

for the $1s-, 2s-, 3s-$states respectively.

Part b

Recall that $a_0 = 0.0529177\text{nm}$ and hence we get that the expectation values in part a are

$$\begin{aligned}r_{100} &= 0.07937655\text{nm} \\ r_{200} &= 0.3175062\text{nm} \\ r_{300} &= 0.71438895\text{nm}\end{aligned}$$

Part c

To show that the $1s$-state and $2s$-state are orthogonal we check to see if their inner product is 0. First notice that

$$\begin{aligned}\psi_{100} &= R_{10}(r)Y_{00}(\theta,\phi)\\ \psi_{200} &= R_{20}(r)Y_{00}(\theta,\phi)\end{aligned}$$

then we have that

$$\begin{aligned}\int_0^\infty\int_0^\pi\int_0^{2\pi} r^2\sin(\theta)\psi_{100}^*\psi_{200}\,drd\theta d\phi &= \int_0^\infty\int_0^\pi\int_0^{2\pi} R_{10}^*R_{20}r^2|Y_{00}|^2\sin(\theta)\,drd\theta d\phi\\ &= \int_0^\infty R_{10}^*R_{20}\,dr\end{aligned}$$

and note that

$$\begin{aligned}R_{10} &= 2a_0^{-3/2}e^{-r/a_0}\\ R_{20} &= \frac{1}{\sqrt{2}}a_0^{-3/2}\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}\end{aligned}$$

and hence our integral becomes

$$\int_0^\infty R_{10}^*R_{20}\,dr = \frac{2a_0^{-3}}{\sqrt{2}}\int_0^\infty r^2\left(1-\frac{r}{2a_0}e^{\frac{-3r}{2a_0}}\right)\,dr$$

using Mathematica to evaluate the integral, we get that

$$\int_0^\infty r^2\left(1-\frac{r}{2a_0}\right)e^{\frac{-3r}{2a_0}}\,dr = 0$$

and hence

$$\int_0^\infty\int_0^\pi\int_0^{2\pi} r^2\sin(\theta)\psi_{100}^*\psi_{200}\,drd\theta d\phi = 0$$

thus ψ_{100} and ψ_{200} are orthogonal.

Part d

To show that the $2s$-state and the $2p$-states are orthogonal we aim to show that their inner product is zero. First recall that

$$\begin{aligned}\psi_{200} &= R_{20}(r)Y_{00}(\theta,\phi)\\ \psi_{21m} &= R_{21}(r)Y_{1m}(\theta,\phi)\end{aligned}$$

then we have that

$$\int_0^\infty\int_0^\pi\int_0^{2\pi} r^2\sin(\theta)\psi_{21m}^*\psi_{200}\,drd\theta d\phi = \int_0^\infty\int_0^\pi\int_0^{2\pi} R_{20}^*R_{21}r^2Y_{00}^*Y_{1m}\sin(\theta)\,drd\theta d\phi$$

and since

$$\int_0^\pi \int_0^{2\pi} Y_{00}^* Y_{1m} \sin(\theta)\, d\theta d\phi = \delta_{01}\delta_{m0} = 0$$

and hence our above integral becomes

$$\delta_{01}\delta_{m0} \int_0^\infty R_{20}^* R_{21} r^2 \, dr = 0$$

thus ψ_{200} and ψ_{21m} are orthogonal for all m.

Problem 2.3

Part a

We consider

$$\left[\frac{-\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0} + e\varepsilon x\right] |\psi\rangle = E\,|\psi\rangle$$

and assume that $\psi = c_1\psi_{1s} + c_2\psi_{2x}$. Then we have that $\langle\psi_{1s}|\psi\rangle = c_1$ and $\langle\psi_{2x}|\psi\rangle = c_2$ since the ψ_{1s} and ψ_{2x} are orthonormal. Then we have that

$$\langle\psi_{1s}|\, H\,|\psi\rangle = c_1\,\langle\psi_{1s}|\, H\,|\psi_{1s}\rangle + c_2\,\langle\psi_{1s}|\, H\,|\psi_{2x}\rangle = \langle\psi_{1s}|\, E\,|\psi\rangle = c_1 E$$

and

$$\langle\psi_{2x}|\, H\,|\psi\rangle = c_1\,\langle\psi_{2x}|\, H\,|\psi_{1s}\rangle + c_2\,\langle\psi_{2x}|\, H\,|\psi_{2x}\rangle = \langle\psi_{2x}|\, E\,|\psi\rangle = c_2 E$$

where

$$H = \frac{-\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0} + e\varepsilon x$$

Note that

$$(\langle\psi_{1s}|\, H\,|\psi_{2x}\rangle)^* = \langle\psi_{2x}|\, H\,|\psi_{1s}\rangle$$

and hence by letting

$$\begin{aligned} h_{11} &= \langle\psi_{1s}|\, H\,|\psi_{1s}\rangle \\ h_{22} &= \langle\psi_{2x}|\, H\,|\psi_{2x}\rangle \\ h_{12} &= \langle\psi_{1s}|\, H\,|\psi_{2x}\rangle = e\varepsilon\,\langle\psi_{1s}|x|\psi_{2x}\rangle \end{aligned}$$

we get that

$$\begin{pmatrix} h_{11} & h_{12} \\ h_{12}^* & h_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Part b

Recall that

$$\begin{cases} \psi_{1s} &= R_{10}(r)Y_{00}(\theta,\phi) \\ \psi_{2p_x} &= \frac{R_{21}(r)}{\sqrt{2}}\left(Y_{1,-1}(\theta,\phi) - Y_{1,1}(\theta,\phi)\right) \end{cases}$$

Note that

$$\begin{aligned} R_{10}(r) &= 2a_0^{-3/2}e^{-r/a_0} \\ R_{21}(r) &= \frac{1}{\sqrt{6}}a_0^{-3/2}\left(\frac{r}{2a_0}\right)e^{-r/2a_0} \\ Y_{1,-1} &= \sqrt{\frac{3}{8\pi}}e^{-i\phi}\sin(\theta) \\ Y_{1,1} &= -\sqrt{\frac{3}{8\pi}}e^{i\phi}\sin(\theta) \\ Y_{0,0} &= \sqrt{\frac{1}{4\pi}} \end{aligned}$$

and so we have that

$$\begin{cases} \psi_{1s} &= \frac{2}{\sqrt{4\pi}}a_0^{-3/2}e^{-r/a_0} \\ \psi_{2px} &= \frac{1}{\sqrt{32\pi}}a^{-3/2}\left(\frac{r}{a_0}\right)e^{-r/2a_0}\sin(\theta)\cos(\phi) \end{cases}$$

so then we have that

$$\begin{aligned} \langle\psi_{1s}|\, x\,|\psi_{2p_x}\rangle &= \int_0^\infty\int_0^\pi\int_0^{2\pi} r\sin(\theta)\cos(\phi)\psi_{1s}^*\psi_{2p_x}r^2\sin\theta\, drd\theta d\phi \\ &= \left(\frac{2}{\sqrt{4\pi}}\right)\left(\frac{1}{\sqrt{32\pi}}\right)a_0^{-4}\int_0^\infty r^4e^{-3r/2a_0}\,dr\int_0^\pi\sin^3(\theta)\,d\theta\int_0^{2\pi}\cos^2(\phi)\,d\phi \\ &= \frac{128\sqrt{6}}{243}a_0 \end{aligned}$$

and hence $e\varepsilon\langle\psi_{1s}|x|\psi_{2p_x}\rangle = \frac{128\sqrt{6}}{243}e\varepsilon a_0$

Part c

We compute the eigenvalues of the matrix above by

$$\det\left(\begin{bmatrix} h_{11}-E & h_{12} \\ h_{12}^* & h_{22}-E \end{bmatrix}\right) = 0 \implies (h_{11}-E)(h_{22}-E)-|h_{12}|^2 = E^2-E(h_{11}+h_{22})+h_{11}h_{22}-|h_{12}|^2 = 0$$

solving the above equation gives us the eigenvalues of the matrix as

$$E = \frac{h_{11}+h_{22}}{2} \pm \sqrt{\left(\frac{h_{11}+h_{22}}{2}\right)^2 - (h_{11}h_{22}-|h_{12}|^2)}$$

we take the $(-)$ term to get the lower energy eigenvalue. Then we get that

$$\begin{aligned} c_1 h_1 1 + c_2 h_{12} = E c_1 \\ c_1 h_{12}^* + c_2 h_{22} = E c_2 \end{aligned}$$

Letting $c_1 = 1$ we get that

$$c_2 = \frac{E - h_{11}}{h_{12}}$$

and hence we have

$$\psi = \psi_{1s} + \frac{E - h_{11}}{h_{12}} \psi_{2p_x}$$

then normalizing the wavefunction gives us that

$$\psi = \frac{1}{\sqrt{1 + \frac{(E-h_{11})^2}{h_{12}^2}}} \left(\psi_{1s} + \frac{E - h_{11}}{h_{12}} \psi_{2p_x} \right)$$

Part d

Part e

Computing the dipole moment μ we get that

$$\begin{aligned} \mu = -e \langle \psi | x | \psi \rangle &= -e \left[\langle \psi_{1s} | x | \psi_{1s} \rangle + M^2 \langle \psi_{2p_x} | x | \psi_{2p_x} \rangle + M \langle \psi_{1s} | x | \psi_{2p_x} \rangle + M \langle \psi_{2p_x} | x | \psi_{1s} \rangle \right] \\ &= -2eM \langle \psi_{1s} | x | \psi_{2p_x} \rangle \end{aligned}$$

where

$$M = \frac{h_{12}}{h_{11} - h_{22}}$$

and get

$$\mu = \frac{-2e^2 \varepsilon}{h_{11} - h_{22}} \left(\frac{128\sqrt{6}}{243} a_0 \right)^2$$

Part f

We have that

$$\alpha = \frac{2e^2}{h_{22} - h_{11}} \left(\frac{128\sqrt{6}}{243} \right)^2$$

and

$$\frac{\alpha}{4\pi\epsilon_0} \approx \frac{4}{3} \frac{2e^2}{4\pi\epsilon_0 E_{ha}} \left(\frac{128\sqrt{6}}{243} \right)^2 (a_0)^2 \approx a_0^3 \frac{8}{3} \left(\frac{128\sqrt{6}}{243} \right)^2 = 4.439 a_0^3$$

which is close to experimental value of $4.61 a_0^3$.

Problem 2.4

Let $\hat{P}$ be the parity operator, that is $\hat{P}f(r) = f(-r)$. Then if f is an eigenfunction of $\hat{P}$ with eigenvalue p then we have that

$$\hat{P}f(r) = f(-r) = \lambda f(r)$$

and

$$\hat{P}^2 f(r) = f(-(-r)) = f(r) = \lambda^2 f(r) \implies \lambda^2 = 1$$

and hence $\lambda = \pm 1$. In the case $\lambda = 1$ we have that

$$f(r) = f(-r)$$

which implies that f is an even function. Similarly for the case $\lambda = -1$ we have that

$$-f(r) = f(-r)$$

which implies that f is an odd function. Thus our eigenvalues are ± 1 and the eigenfunctions are even and odd functions respectively.

Problem 2.5

Part a

If an operator $\hat{A}$ has eigenstates $|a\rangle$ with eigenvalues α then we have that

$$\hat{A}|a\rangle = \alpha |a\rangle$$

additionally recall that the Taylor Expansion of e^x is given by

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

and so

$$e^{\hat{A}}|a\rangle = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}|a\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}|a\rangle = e^{\alpha}|a\rangle$$

Part b

Recall that z component of the angular momentum operator is given by $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$. Additionally recall that a wavefunction is given by

$$\psi(r, \theta, \psi) = \sum_{lm} R_{lm}(r) Y_{lm}(\theta, \psi)$$

and hence we have that

$$\hat{L}_z \psi(r, \theta, \psi) = \sum_{lm} R_{lm}(r) \hat{L}_z Y_{lm}(\theta, \psi)$$

and since $Y_{lm}(\theta, \psi)$ are eigenfunctions of $\hat{L}_z$ we have that

$$\hat{L}_z Y_{lm}(\theta, \psi) = m\hbar Y_{lm}(\theta, \psi)$$

and hence

$$\hat{L}_z \psi(r, \theta, \psi) = \sum_{lm} R_{lm}(r) m\hbar Y_{lm}(\theta, \psi)$$

and thus

$$e^{i\hat{L}_z \phi_0/\hbar} \psi(r, \theta, \psi) = \sum_{lm} R_{lm}(r) e^{im\phi_0} Y_{lm}(\theta, \psi)$$

However note that

$$e^{im\phi_0} Y_{lm}(\theta, \psi) = (-1)^{(m+|m|)/2} \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos(\theta)) e^{im\phi + \phi_0} = Y_{lm}(\theta, \psi + \phi_0) \quad (2.1)$$

and hence

$$e^{i\hat{L}_z \phi_0/\hbar} \psi(r, \theta, \psi) = \sum_{lm} R_{lm}(r) Y_{lm}(\theta, \psi + \phi_0) = \psi(r, \theta, \psi + \phi_0)$$

and hence the operator $e^{i\hat{L}_z \phi_0/\hbar}$ is the operator that rotates the wavefunction by an angle ϕ_0 about the z-axis.