Student handout

1 1-D Particle-in-a-Box

Hamiltonian:

$$\hat{H} \doteq -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{1}$$

Eigenstates:

$$|n\rangle \doteq \sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L} \tag{2}$$

$$n = \{1, 2, 3, \dots\} \tag{3}$$

Eigenvalue Equations:

$$\hat{H}\,|n\rangle = \frac{\pi^2\hbar^2}{2\mu L^2}\,n^2\,|n\rangle \tag{4}$$

$$\tag{5}$$

2 Particle-on-a-Ring

Hamiltonian:

$$\hat{H} \doteq -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial \phi^2} \tag{6}$$

Eigenstates:

$$|m\rangle \doteq \frac{1}{\sqrt{2\pi r_0}}\,e^{im\phi} \tag{7}$$

$$m = \{\cdots -2, -1, 0, 1, 2, \dots\} \tag{8}$$

Eigenvalue Equations:

$$\hat{H}\,|m\rangle = \frac{\hbar^2}{2I}\,m^2\,|m\rangle \tag{9}$$

$$\hat{L}^2\,|m\rangle = \hbar^2\,m^2\,|m\rangle \tag{10}$$

$$\hat{L}_z\,|m\rangle = \hbar\,m\,|m\rangle \tag{11}$$

3 2-D Particle-in-a-Box

Hamiltonian:

$$\hat{H} \doteq -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right) \tag{12}$$

Eigenstates:

$$|mn\rangle \doteq \sqrt{\frac{2}{L_x}}\sqrt{\frac{2}{L_y}}\,\sin\frac{m\pi x}{L_x}\sin\frac{n\pi y}{L_y} \tag{13}$$

$$m = \{1,2,3,\dots\} \tag{14}$$

$$n = \{1,2,3,\dots\} \tag{15}$$

Eigenvalue Equations:

$$\hat{H}\,|mn\rangle = \frac{\pi^2\hbar^2}{2\mu}\,\left(\frac{m^2}{L_x^2}+\frac{n^2}{L_y^2}\right)|mn\rangle \tag{16}$$

$$\tag{17}$$

4 Particle-on-a-Sphere

Hamiltonian:

$$\hat{H} \doteq -\frac{\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{18}$$

Eigenstates:

$$|\ell m\rangle \doteq Y_\ell^m(\theta,\phi) \tag{19}$$

$$= (-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{im\phi} \tag{20}$$

$$\ell = \{0,1,2,\dots\} \tag{21}$$

$$m = \{-\ell,\dots,0,\dots,\ell\} \tag{22}$$

Eigenvalue Equations:

$$\hat{H}\,|\ell m\rangle = \frac{\hbar^2}{2I}\,\ell(\ell+1)\,|\ell m\rangle \tag{23}$$

$$\hat{L}^2\,|\ell m\rangle = \hbar^2\,\ell(\ell+1)\,|\ell m\rangle \tag{24}$$

$$\hat{L}_z\,|\ell m\rangle = \hbar\,m\,|\ell m\rangle \tag{25}$$

5 Hydrogen Atom

Hamiltonian:

$$\hat{H} \doteq -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{ke^2}{r} \tag{26}$$

$$\doteq -\frac{\hbar^2}{2\mu r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] - \frac{ke^2}{r} \tag{27}$$

Eigenstates:

$$|n\ell m\rangle \doteq R_{n\ell}(r)\, Y_\ell^m(\theta,\phi) \tag{28}$$

$$= -\sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\left(\frac{2\rho}{n}\right)^\ell e^{-\frac{\rho}{n}}\, L_{n+\ell}^{2\ell+1}(\tfrac{2\rho}{n})(-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, e^{im\phi} \tag{29}$$

$$\rho = \frac{Zr}{a_0} \tag{30}$$

$$n = \{1, 2, 3, \dots\} \tag{31}$$

$$\ell = \{0, 1, 2, \dots, n-1\} \tag{32}$$

$$m = \{-\ell, \dots, 0, \dots, \ell\} \tag{33}$$

Eigenvalue Equations:

$$\hat{H}\,|n\ell m\rangle = -\frac{1}{2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 \frac{\mu}{\hbar^2}\,\frac{1}{n^2}\;|n\ell m\rangle \tag{34}$$

$$= -13.6\text{eV}\,\frac{1}{n^2}\;|n\ell m\rangle \tag{35}$$

$$\hat{L}^2\,|n\ell m\rangle = \hbar^2\,\ell(\ell+1)\,|n\ell m\rangle \tag{36}$$

$$\hat{L}_z\,|n\ell m\rangle = \hbar\, m\,|n\ell m\rangle \tag{37}$$