4.1

(a) Work out all of the canonical commutation relations for components of the operators $\hat{r}$ and $\hat{p}$: $[x, y]$, $[x, p_y]$ $[x, p_x]$, $[p_y, p_z]$, and so on.

Answer: $[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij}$,

$$[r_i, r_j] = [p_i, p_j] = 0$$

where the indices stand for x, y, or z, and $r_x = x$, $r_y = y$, and $r_z = z$

(b) Confirm the 3D version of Ehrenfest's theorem,

$$\frac{d}{dt}\langle r \rangle = \frac{1}{m}\langle p \rangle, \quad \text{and} \quad \frac{d}{dt}\langle p \rangle = \langle -\nabla V \rangle$$

(Each of these, of course, stands for 3 eqns — one for each component.)

Hint: First check that the "generalized" Ehrenfest theorem, eqn 3.73, is valid in 3D.

(c) Formulate Heisenberg's uncertainty principle in 3D.

Answer: $\sigma_x \sigma_{p_x} \geq \frac{\hbar}{2}$, $\sigma_y \sigma_{p_y} \geq \frac{\hbar}{2}$, $\sigma_z \sigma_{p_z} \geq \frac{\hbar}{2}$, but there is no restriction on, say, $\sigma_x \sigma_{p_y}$.

(a) $[x,y] = \hat{x}\hat{y} - \hat{y}\hat{x} = xy - yx = 0 = [y,x]$

$[x,z] = \hat{x}\hat{z} - \hat{z}\hat{x} = xz - zx = 0 = [z,x]$

$[y,z] = \hat{y}\hat{z} - \hat{z}\hat{y} = yz - zy = 0 = [z,y]$

$\Rightarrow \boxed{[r_i, r_j] = 0}$

$$[p_x, p_y]f = -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial f}{\partial y}\right) + i\hbar\frac{\partial}{\partial y}\left(-i\hbar\frac{\partial f}{\partial x}\right)$$

$$= -\hbar^2\left(\frac{\partial^2 f}{\partial x\partial y} - \frac{\partial^2 f}{\partial y\partial x}\right) = 0$$

$\boxed{[p_i, p_j] = 0}$ following the same logic

$$[x, p_x]f = i\hbar\left(x\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}(xf)\right) = i\hbar f$$

$\Rightarrow \boxed{[r_i, p_i] = i\hbar}$ ——— (1)

$$[x, p_y]f = i\hbar\left(x\frac{\partial f}{\partial y} - \frac{\partial}{\partial y}(xf)\right) = i\hbar\left(x\frac{\partial f}{\partial y} - x\frac{\partial f}{\partial y}\right) = 0$$

$\Rightarrow \boxed{[r_i, p_j] = 0}$ ——— (2)

Combining (1), (2) : $[r_i, p_j] = i\hbar\delta_{ij}$

$[p_i, r_j] = -i\hbar\delta_{ij}$

(b) $$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\langle \underbrace{[H,x]}\rangle$$

$$= \left[\frac{p^2}{2m}+V, x\right] = \frac{1}{2m}\left[P_x^2+\cancel{P_y^2}+\cancel{P_z^2}, x\right] = \frac{1}{2m}[P_x^2, x]$$

$$= \frac{1}{2m}\left(P_x[P_x,x]+[P_x,x]P_x\right) = \frac{1}{\cancel{2}m}\left(-\cancel{2}i\hbar P_x\right) = \frac{\hbar}{im}P_x$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = \frac{\cancel{i}}{\cancel{\hbar}}\left\langle \frac{\cancel{\hbar}}{\cancel{i}m}P_x\right\rangle \Rightarrow \frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle p\rangle$$

By the same reasoning, we can prove the same in y, z:

$$\frac{d\langle \vec{r}\rangle}{dt} = \frac{1}{m}\langle \vec{p}\rangle$$

$$\frac{d\langle P_x\rangle}{dt} = \frac{i}{\hbar}\langle \underbrace{[H,P_x]}\rangle$$

$$= \left[\cancel{\frac{p^2}{2m}}+V, P_x\right] = [V,P_x] = i\hbar\frac{\partial V}{\partial x}$$

$[p^2, p]=0$

Note: $f\hat{p} - \hat{p}f = f\left(-i\hbar\frac{\partial}{\partial x}\right) + i\hbar\frac{\partial f}{\partial x}$

$$[f,\hat{p}]g = f\left(-i\hbar\frac{dg}{dx}\right) + i\hbar\frac{d}{dx}(fg)$$

$f=f(x)$, $g=g(x)$

$$= \cancel{-i\hbar f\frac{dg}{dx}} + i\hbar g\frac{df}{dx} + \cancel{i\hbar f\frac{dg}{dx}}$$

$$= i\hbar g\frac{df}{dx}$$

$\rightarrow = [f,\hat{p}]$

$$\frac{d\langle P_x\rangle}{dt} = \frac{i}{\hbar}\left\langle i\hbar\frac{\partial V}{\partial x}\right\rangle = \left\langle -\frac{\partial V}{\partial x}\right\rangle$$

By the same reasoning, we can prove the same in y, z:

$$\frac{d\langle \vec{p}\rangle}{dt} = \langle -\nabla V\rangle$$

(c) $\sigma_x^2 \sigma_{p_x}^2 \geqslant \left(\frac{1}{2i} \langle \underbrace{[x, p_x]}_{= i\hbar} \rangle \right)^2 \Rightarrow \sigma_x \sigma_{p_x} \geqslant \frac{\hbar}{2}$

By the same reasoning, we can prove the same in y, z:

$$\sigma_{r_i} \sigma_{p_j} \geqslant \frac{\hbar}{2} \delta_{ij}$$

4.4 Use eqn 4.27, 4.28, and 4.32, to construct Y_0^0 and Y_2^1.

Check that they are normalized and orthogonal.

$$\text{eqn } (4.27) \rightarrow P_\ell^m(x) \equiv (-1)^m (1-x^2)^{m/2} \left(\frac{d}{dx}\right)^m P_\ell(x)$$

$$\text{eqn } (4.28) \rightarrow P_\ell(x) \equiv \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

$$\text{eqn } (4.32) \rightarrow Y_\ell^m(\theta, \phi) = \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\, e^{im\phi} P_\ell^m(\cos\theta)$$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} (1) \underbrace{P_0^0(\cos\theta)}_{} \longrightarrow Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$= (-1)^0 (1-x^2)^0 \left(\frac{d}{dx}\right)^0 \underbrace{P_0(x)}_{}, \quad x = \cos\theta$$

$$= (1) \left(\frac{d}{dx}\right)^0 (x^2-1)^0$$

$$Y_2^1 = \underbrace{\sqrt{\frac{(2(2)+1)(2-1)!}{4\pi(2+1)!}}}_{\sqrt{\frac{5}{24\pi}}}\, e^{i\phi}\, \underbrace{P_2^1(\cos\theta)}_{}$$

$$= -\sqrt{1-x^2}\, \frac{d}{dx} \underbrace{P_2(x)}_{} = -\frac{1}{\cancel{2}}\sqrt{1-x^2}\,(\cancel{6}^{\,3} x)$$

$$= \frac{1}{8} \frac{d^2}{dx^2} (x^2-1)^2$$

$$= \frac{1}{2}(3x^2-1)$$

$$\Rightarrow P_2^1(\cos\theta) = -3\sin\theta\cos\theta$$

$$\Rightarrow Y_2^1 = -\sqrt{\frac{15}{8\pi}}\, e^{i\phi} \sin\theta\cos\theta$$

Normalized?

$$Y_0^0: \quad \iint |Y_0^0|^2 \sin\theta \, d\theta \, d\phi = \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta = \frac{4\pi}{4\pi} = 1 \quad ✓$$

$$Y_2^1: \quad \iint |Y_2^1|^2 \sin\theta \, d\theta \, d\phi = \frac{15}{8\pi} \int_0^{2\pi} d\phi \int_0^{\pi} \sin^3\theta \cos^2\theta \, d\theta$$

$$= \frac{15}{4} \left(-\frac{\cos^3\theta}{3} + \frac{\cos^5\theta}{5} \right)_0^{\pi} = \frac{\cancel{15}}{\cancel{4}} \left(\frac{\cancel{4}}{\cancel{15}} \right) = 1 \quad ✓$$

Orthogonal?

$$\iint Y_0^{0*} Y_2^1 \sin\theta \, d\theta \, d\phi = -\frac{1}{\sqrt{4\pi}} \sqrt{\frac{15}{8\pi}} \underbrace{\int_0^{2\pi} e^{i\phi} \, d\phi}_{=0} \underbrace{\int_0^{\pi} \sin^2\theta \cos\theta \, d\theta}_{=0} = 0 \quad ✓$$

4.10

(a) Check that $Arj_1(kr)$ satisfies the radial equation with $V(r)=0$ and $l=1$.

(b) Determine graphically the allowed energies for the infinite spherical well, when $l=1$. Show that for large N,

$$E_{N1} \approx \left(\frac{\hbar^2\pi^2}{2ma^2}\right)\left(N+\frac{1}{2}\right)^2.$$

Hint: First show that $j_1(x)=0 \Rightarrow x=\tan x$. Plot x and $\tan x$ on the same graph, and locate the points of intersection

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(a) $$j_l(x) \equiv (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin x}{x}$$

$$j_1(kr) = -\cancel{kr}\left(\frac{1}{\cancel{kr}}\cdot\frac{d}{d(kr)}\right)\frac{\sin kr}{kr} = \frac{\sin kr}{k^2r^2} - \frac{\cos kr}{kr}$$

$$Arj_1(kr) = \frac{A}{k}\left(\frac{\sin kr}{kr} - \cos kr\right) \equiv u$$

Radial eqn: $$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\cancel{V}^{\,0} + \frac{\hbar^2}{2m}\cdot\frac{l(l+1)}{r^2}\right]u = Eu$$

$l=1 \Rightarrow \frac{2}{r^2}$

$$\frac{du}{dr} = \frac{A}{k}\left(\frac{\cos kr}{r} - \frac{\sin kr}{kr^2} + k\sin kr\right)$$

$$\frac{d^2u}{dr^2} = A\left(k\cos kr + \frac{2\sin kr}{k^2r^3} - \frac{2\cos kr}{kr^2} - \frac{\sin kr}{r}\right)$$

$$= Ak\left(\cos kr + \frac{2\sin kr}{k^3r^3} - \frac{2\cos kr}{k^2r^2} - \frac{\sin kr}{kr}\right)$$

$$= Ak\left[\left(1-\frac{2}{k^2r^2}\right)\cos kr + \left(\frac{2}{k^3r^3} - \frac{1}{kr}\right)\sin kr\right]$$

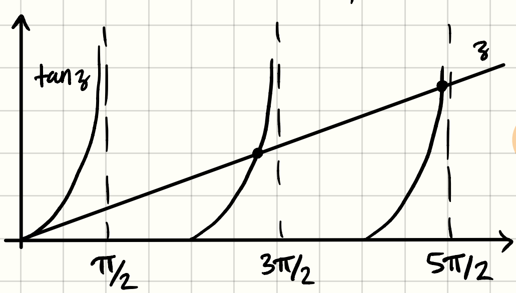
$$\Rightarrow \frac{d^2u}{dr^2} - \frac{2}{r^2}u = -\overset{\overset{k^2}{\equiv}}{\frac{2mE}{\hbar^2}}u$$

$$\Rightarrow Ak\left[\left(1-\cancel{\frac{2}{k^2r^2}}\right)\cos kr + \left(\cancel{\frac{2}{k^3r^3}} - \frac{1}{kr}\right)\sin kr - \frac{2}{k^2r^2}\left(\cancel{\frac{\sin kr}{kr}} - \cancel{\cos kr}\right)\right]$$

$$= Ak\left(\cos kr - \frac{\sin kr}{kr}\right) = -k^2u \checkmark$$

(b) From B.C. $\longrightarrow j_1(x) = 0 \Rightarrow \frac{\sin x}{x^2} - \frac{\cos x}{x} = 0$

$$\Rightarrow \tan x = x \xrightarrow[\text{transcendental eqn}]{} z = \tan z, \quad z = ka \text{ for B.C.}$$



$z \approx (N+\frac{1}{2})\pi$, $N = 1,2,3,\ldots$

$$E = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2 z^2}{2ma^2} \approx \frac{\hbar^2(N+\frac{1}{2})^2\pi^2}{2ma^2}$$

as $N \to \infty$, $z = (N+\frac{1}{2})\pi$ becomes a better and better approximation.

4.13

(a) Normalize R_{20} (eqn 4.82), and construct ψ_{200}.

(b) " R_{21} (eqn 4.83), " " ψ_{211}, ψ_{210}, and ψ_{21-1}.

(a) eqn (4.82) $\longrightarrow$ $R_{20}(r) = \frac{c_0}{2a}\left(1 - \frac{r}{2a}\right)e^{-r/2a}$

$$\int_0^\infty |R|^2 r^2 dr = 1 \rightarrow \frac{c_0^2}{4a^2}\int_0^\infty \left(1 - \frac{r}{2a}\right)^2 e^{-r/a} r^2 dr$$

$u = \frac{r}{a}$

$du = \frac{dr}{a}$

$$= a\frac{c_0^2}{4}\int_0^\infty u^2\left(1 - u + \frac{u^2}{4}\right)e^{-u}du = \frac{c_0^2 a}{4}\int_0 e^{-u}\left(u^2 - u^3 + \frac{u^4}{4}\right)du$$

$$= \frac{c_0^2 a}{4}\left(-\frac{e^{-u}}{4}(u^4 + 4u^2 + 8u + 8)\right)\Bigg|_0^\infty = \frac{c_0^2 a}{2} = 1$$

$$\Rightarrow \boxed{c_0 = \sqrt{\frac{2}{a}}}$$

$$\int_0^\infty x^n e^{-x/a} dx = n!\, a^{n+1}$$

$$\psi_{200} = R_{20}Y_0^0 = \frac{1}{2a}\sqrt{\frac{2}{a}}\left(1 - \frac{r}{2a}\right)e^{-r/2a} \cdot \frac{1}{\sqrt{4\pi}}$$

$$\boxed{= \frac{1}{2a}\cdot\frac{1}{\sqrt{2\pi a}}\left(1 - \frac{r}{2a}\right)e^{-r/2a}}$$

(b) eqn (4.83) $\longrightarrow R_{21}(r) = \frac{c_0}{4a^2} r e^{-r/2a}$

$$\int_0^\infty |R|^2 r^2 dr = 1 \rightarrow \frac{c_0^2}{16a^4} \int_0^\infty r^4 e^{-r/a} dr$$

$u = \frac{r}{a}$
$du = \frac{dr}{a}$

$$= \frac{c_0^2}{16\cancel{a^4}} \cancel{a^5} \int_0^\infty u^4 e^{-u} du = \frac{3c_0^2 a}{2} = 1$$

$$\Rightarrow c_0 = \sqrt{\frac{2}{3a}}$$

$Y_1^{\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \, e^{\pm i\phi}, \quad Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$

$$\psi_{211} = R_{21} Y_1^1$$

$$= -\frac{1}{8a^2} \cdot \frac{1}{\sqrt{\pi a}} r e^{-r/2a + i\phi} \sin\theta$$

$$\psi_{210} = R_{21} Y_1^0 = \frac{1}{4a^2} \cdot \frac{1}{\sqrt{2\pi a}} r e^{-r/2a} \cos\theta$$

$$\psi_{21-1} = R_{21} Y_1^{-1} = \frac{1}{8a^2} \cdot \frac{1}{\sqrt{\pi a}} r e^{-r/2a - i\phi} \sin\theta$$

4.15

(a) Find $\langle r\rangle$ and $\langle r^2\rangle$ for an electron in the ground state of hydrogen. Express your answers in terms of the Bohr radius.

(b) Find $\langle x\rangle$ and $\langle x^2\rangle$ for an electron in the ground state of hydrogen. Hint: This requires no new integration. Note that $r^2 = x^2+y^2+z^2$, and exploit the symmetry of the ground state.

(c) Find $\langle x^2\rangle$ in the state $n=2$, $l=1$, $m=1$. Hint: this state is <u>not</u> symmetrical in x, y, and z. Use $x = r\sin\theta\cos\phi$.

(a) $\psi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \longrightarrow \langle r\rangle = \frac{1}{\pi a^3}\int r e^{-2r/a} \cdot r^2 \underbrace{\sin\theta\, dr\, d\theta\, d\phi}_{=4\pi}$

$$= \frac{4}{a^3}\int_0^\infty r^3 e^{-2r/a}\, dr = \frac{3a}{2}$$

$$\int_0^\infty x^n e^{-x/a}\, dx = n!\, a^{n+1}$$

$$\langle r^2\rangle = \frac{4}{a^3}\int_0^\infty r^4 e^{-2r/a}\, dr = 3a^2$$

where a is the Bohr radius.

(b) $\langle x\rangle = \frac{1}{\pi a^3}\int \underbrace{r\sin\theta\cos\phi}_{=x} \cdot e^{-2r/a} \cdot r^2 \sin\theta\, dr\, d\theta\, d\phi$

$$= \frac{1}{\pi a^3}\underbrace{\cancel{\int_0^{2\pi}\cos\phi\, d\phi}}_{0}\int_0^\pi \sin^2\theta\, d\theta \int_0^\infty r^3 e^{-2r/a}\, dr = 0$$

$$\langle x^2 \rangle = \frac{1}{3}\langle r^2 \rangle = a^2$$

$\uparrow$ by symmetry of ground state

(c) $$\psi_{211} = -\frac{1}{8a^2}\cdot\frac{1}{\sqrt{\pi a}}\, r e^{-r/2a + i\phi} \sin\theta$$

$$\langle x^2 \rangle = \frac{1}{64\pi a^5}\int r^6 e^{-r/a} \sin^5\theta \cos^2\phi \, dr\, d\theta\, d\phi$$

$$= \frac{1}{64\pi \cancel{a^5}}\cdot 720 a^{\cancel{7}\,2}\cdot\frac{16\pi}{15} = 12a^2$$