Problem 21.1 (Griffiths 4.1)

a. let r_i $i=1,2,3$ refer to the Cartesian components x, y, z, & p_i $i=1,2,3$ the momenta p_x, p_y & p_z.

$$[r_i, p_j] f(\vec{r}) = r_i \frac{\hbar}{i}\frac{\partial}{\partial x_j} f - \frac{\hbar}{i}\frac{\partial}{\partial x_j}(r_i f) = \frac{\hbar}{i}\left(r_i \frac{\partial f}{\partial x_j} - \delta_{ij} f - r_i \frac{\partial f}{\partial x_j}\right) = i\hbar \delta_{ij} f$$

so

$$\boxed{[r_i, p_j] = i\hbar \delta_{ij}}$$

For positions only: $[r_i, r_j] f(\vec{r}) = r_i r_j f - r_j r_i f = r_i r_j f - r_i r_j f = \emptyset$

so

$$\boxed{[r_i, r_j] = \emptyset.}$$

For momenta: $[p_i, p_j] f(\vec{r}) = -\hbar^2\left[\frac{\partial^2 f}{\partial r_i \partial r_j} - \frac{\partial^2 f}{\partial r_j \partial r_i}\right] = -\hbar^2\left[\frac{\partial^2 f}{\partial r_j \partial r_i} - \frac{\partial^2 f}{\partial r_j \partial r_i}\right] = \emptyset.$

so

$$\boxed{[p_i, p_j] = \emptyset.}$$

b. Equation (3.71) clearly holds for the individual Cartesian vector components, so we expect:

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

& we need to compute: $[H, r_j]$ for $H = \frac{1}{2m}\sum_{k=1}^{3} p_k p_k + V(\vec{r})$.

then

$$[H, r_j] = \frac{1}{2m}\left[\sum_{k=1}^{3} p_k p_k, r_j\right] = \frac{1}{2m}\left(\sum_{k=1}^{3} p_k p_k r_j - \sum_{k=1}^{3} r_j p_k p_k\right)$$

now using $r_j p_k - p_k r_j = i\hbar \delta_{jk}$, we have:

$$= \frac{1}{2m}\left(\sum_{k=1}^{3} p_k (r_j p_k - i\hbar \delta_{jk}) - \sum_{k=1}^{3} (i\hbar \delta_{jk} + p_k r_j) p_k\right)$$

$$= \frac{1}{2m}(-2i\hbar\, p_j) = -\frac{i\hbar}{m} p_j$$

Then $\frac{d}{dt}\langle r_j \rangle = \frac{i}{\hbar}\langle -\frac{i\hbar}{m} p_j \rangle = \frac{1}{m}\langle p_j \rangle$ or $\frac{d}{dt}\langle \vec{r} \rangle = \frac{1}{m}\langle \vec{p} \rangle$.

For $\frac{d}{dt}\langle \vec{p} \rangle$, we need $[H, \vec{p}] = [V(\vec{r}), \vec{p}]$, or using a test function:

$$[V(\vec{r}), \vec{p}] f(\vec{r}) = V \cdot \frac{\hbar}{i}\nabla f - \frac{\hbar}{i}\nabla(Vf) = \left(-\frac{\hbar}{i}\nabla V\right) f$$

& then:

$$[H, \vec{p}] = -\frac{\hbar}{i}\nabla V, \text{ so that } \frac{d}{dt}\langle \vec{p} \rangle = \frac{i}{\hbar}\langle [H, \vec{p}] \rangle = -\langle \nabla V \rangle.$$

c. Using: $\sigma_A \sigma_B \geq \left|\frac{1}{2i}\langle [A, B] \rangle\right|$ we have:

$$\sigma_{r_i} \sigma_{p_j} \geq \left|\frac{1}{2i}\langle [r_i, p_j] \rangle\right| = \left|\frac{1}{2i} i\hbar \delta_{ij}\right| = \frac{\hbar}{2}\delta_{ij}.$$

Problem 21.2 (Griffiths 4.2)

For $V(x,y,z) = \begin{cases} 0 & \text{if } 0 \le x \le a,\ 0 \le y \le a,\ 0 \le z \le a \\ \infty & \text{else} \end{cases}$

we know that outside the box, we must have $\psi(x,y,z) = 0$ – then continuity demands:

$$\psi(0,y,z) = \psi(a,y,z) = 0$$
$$\psi(x,0,z) = \psi(x,a,z) = 0.$$
$$\psi(x,y,0) = \psi(x,y,a) = 0.$$

The time-independent Schrödinger eqn. is:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right] = E\psi$$

take $\psi(x,y,z) = X(x)\cdot Y(y)\cdot Z(z)$, then:

$$\underbrace{-\frac{\hbar^2}{2m}\frac{X''}{X}}_{\equiv \alpha^2} \underbrace{- \frac{\hbar^2}{2m}\frac{Y''}{Y}}_{\equiv \beta^2} \underbrace{- \frac{\hbar^2}{2m}\frac{Z''}{Z}}_{\equiv \gamma^2} = E$$

w/: $\frac{X''}{X} = -\frac{2m\alpha^2}{\hbar^2} \Rightarrow X(x) = A\sin\left(\sqrt{\frac{2m\alpha^2}{\hbar^2}}\,x\right) + B\cos\left(\sqrt{\frac{2m\alpha^2}{\hbar^2}}\,x\right)$

when we impose the boundary conditions:

$$X(0) = \boxed{B = 0}$$

$$X(a) = A\sin\Big(\underbrace{\sqrt{\tfrac{2m\alpha^2}{\hbar^2}}\,a}_{=p\pi}\Big) = 0 \Rightarrow \alpha^2 = \frac{p^2\pi^2\hbar^2}{2ma^2} \text{ w/ } p \in \mathbb{Z}^+$$

& sim. for $Y(y)$ & $Z(z)$:

$$\boxed{\psi(x,y,z) = A\sin\left(\frac{p\pi x}{a}\right)\sin\left(\frac{q\pi y}{a}\right)\sin\left(\frac{r\pi z}{a}\right)} \text{ w/ } p,q,r \in \mathbb{Z}^+$$

&

$$\boxed{E = \frac{\pi^2\hbar^2}{2ma^2}(p^2+q^2+r^2)}$$

Energy (in units of $\frac{\pi^2\hbar^2}{2ma^2}$)	Ways of Obtaining (p,q,r)	Degeneracy
3	(1,1,1)	1
6	(1,1,2), (1,2,1), (2,1,1)	3
9	(1,2,2), (2,1,2), (2,2,1)	3
11	(1,1,3), (1,3,1), (3,1,1)	3
12	(2,2,2)	1
14	(1,2,3), (3,1,2), (2,3,1), (1,3,2), (2,1,3), (3,2,1).	6
17		
18		
19		
21		
22		
24		
26		
27	(1,1,5) or (3,3,3)	4 ?!

E_{14}

(1,1,5), (1,5,1), (5,1,1)

we expect 1,3,6, this one is strange

Problem 21.3

a. We have: $\dot{z}(t) = -\alpha z(t)$ w/ $z(0) = A$

Let $z(t) = t^p \sum_{j=0}^{\infty} c_j t^j = \sum_{j=0}^{\infty} c_j t^{j+p}$

then the derivative is:

$$\boxed{\dot{z} = \sum_{j=0}^{\infty} c_j (j+p) t^{j+p-1} = t^p \sum_{j=0}^{\infty} c_j (j+p) t^{j-1} = t^p \sum_{k=-1}^{\infty} c_{k+1}(k+p+1) t^k}$$

so the ODE reads:

b.
$$\boxed{\begin{aligned} \dot{z} + \alpha z &= t^p \left[\sum_{j=0}^{\infty} \alpha c_j t^j + \sum_{j=-1}^{\infty} c_{j+1} (j+p+1) t^j \right] \\ &\overset{!}{=} t^p \left[c_0 p t^{-1} + \sum_{j=0}^{\infty} (\alpha c_j + c_{j+1}(j+p+1)) t^j \right] \end{aligned}}$$

c. For this to be zero, we must have $\boxed{p = 0}$ and

$$\boxed{c_{j+1} = \frac{-c_j \alpha}{j+p+1} = -\frac{c_j}{j+1}\alpha}$$

Then:

$$c_0 = A$$
$$c_1 = -\frac{A}{1}\alpha$$
$$c_2 = -\left(-\frac{A}{1}\right) \cdot \frac{1}{2} \alpha^2$$
$$c_3 = -\left(+\frac{A}{1}\right) \cdot \frac{1}{2} \frac{1}{3} \alpha^3$$

or

$$c_n = (-1)^n \cdot \frac{A}{n!} \alpha^n$$

And we can compare this series:

$$z(t) = A \sum_{n=0}^{\infty} (-1)^n \cdot \frac{\alpha^n}{n!} t^n$$

w/ the expansion for: $w(t) = Ae^{-\alpha t} = A - \alpha A + \frac{1}{2}\alpha^2 A - \frac{1}{6}\alpha^3 A + \cdots$

they are the same, so we conclude that

$$z(t) = Ae^{-\alpha t}. \checkmark$$