Assignment (14)

① $[l_y,[l_y,l_z]] = [l_y, i\hbar l_x] = i\hbar[l_y,l_x] = i\hbar(-i\hbar l_z) = \hbar^2 l_z$

② a) $[H,p_x]$: i) $\left[\frac{p_x^2}{2m}+V, p_x\right]f = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V, \frac{\hbar}{i}\frac{d}{dx}\right]f = \left[\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right) - \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\right]f$

$f=f(x)$

$= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\left(\frac{\hbar}{i}\frac{df}{dx}\right) - \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2}+Vf\right)$

$= \left(-\frac{\hbar^2}{2m}\right)\left(\frac{\hbar}{i}\right)\left(\frac{d^3f}{dx^3}\right) + \left(\frac{\hbar}{i}\right)\left(V\frac{df}{dx}\right) - \left(\frac{\hbar}{i}\right)\left(-\frac{\hbar^2}{2m}\right)\left(\frac{d^3f}{dx^3}\right) - \left(\frac{\hbar}{i}\right)\left(V\frac{df}{dx}\right) = 0$

ii) $\left[\frac{p_x^2}{2m}+\frac{kx^2}{2}, p_x\right]f = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}, \frac{\hbar}{i}\frac{d}{dx}\right]f = \left[\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right) - \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}\right)\right]f$

$= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}\right)\left(\frac{\hbar}{i}\frac{df}{dx}\right) - \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2}+\frac{kx^2}{2}f\right)$

$= \left(-\frac{\hbar^2}{2m}\right)\left(\frac{\hbar}{i}\right)\left(\frac{d^3f}{dx^3}\right) + \left(\frac{\hbar}{i}\right)\left(\frac{kx^2}{2}\right)\left(\frac{df}{dx}\right) - \frac{\hbar}{i}\left[-\frac{\hbar^2}{2m}\frac{d^3f}{dx^3}\right] - \frac{\hbar}{i}\left(\frac{k}{2}\right)\left(\frac{d(x^2f)}{dx}\right)$

$= \left(\frac{\hbar}{i}\right)\left(\frac{kx^2}{2}\right)\left(\frac{df}{dx}\right) - \left(\frac{\hbar}{i}\right)\left(\frac{k}{2}\right)\left(x^2\frac{df}{dx}+2xf\right) = \left(\frac{\hbar}{i}\right)\left(\frac{kx^2}{2}\right)\left(\frac{df}{dx}\right) - \left(\frac{\hbar}{i}\right)\left(\frac{kx^2}{2}\right)\left(\frac{df}{dx}\right) - \frac{\hbar k}{i}xf = -\frac{\hbar k x}{i}$

b) $[H,x]$: i) $\left[\frac{p_x^2}{2m}+V, x\right]f(x) = \left[\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)x - x\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V\right)\right]f(x)$

$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(xf(x)) + \cancel{Vxf(x)} + x\frac{\hbar^2}{2m}\frac{d^2f}{dx^2} - \cancel{Vxf(x)}$

$= -\frac{\hbar^2}{2m}\frac{d}{dx}\left(f(x)+x\frac{df}{dx}\right) + x\frac{\hbar^2}{2m}\frac{d^2f}{dx^2}$

$= -\frac{\hbar^2}{2m}\left(\frac{df}{dx}+\frac{df}{dx}+x\frac{d^2f}{dx^2}\right) + x\frac{\hbar^2}{2m}\frac{d^2f}{dx^2} = -\frac{\hbar^2}{m}\frac{df}{dx}$

ii) $\left[\frac{p_x^2}{2m}+\frac{kx^2}{2}, x\right]f(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}, x\right]f(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}\right)(xf(x)) - x\left(-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2}+\frac{kx^2}{2}f(x)\right)$

$= -\frac{\hbar^2}{2m}\frac{d}{dx}\left(f(x)+x\frac{df}{dx}\right) + \cancel{\frac{kx^3}{2}f(x)} + \frac{x\hbar^2}{2m}\frac{d^2f}{dx^2} - \cancel{\frac{kx^3}{2}f(x)}$

$= -\frac{\hbar^2}{2m}\frac{df}{dx} - \frac{\hbar^2}{2m}\frac{df}{dx} - \cancel{\frac{\hbar^2}{2m}x\frac{d^2f}{dx^2}} + \cancel{\frac{\hbar^2}{2m}x\frac{d^2f}{dx^2}} = -\frac{\hbar^2}{m}\frac{df}{dx}$

③ $\langle x\rangle = \int_0^a \psi_n^*(x)\, x\, \psi_n(x)\,dx = \frac{2}{a}\int_0^a x\sin^2(n\pi x/a)\,dx = \frac{2}{a}\int_0^a x\left(\frac{1}{2}\right)\left(1-\cos\left(\frac{2n\pi x}{a}\right)\right)dx$

$dv = \cos(2n\pi x/a)\,dx$
$v = \left(\frac{a}{2n\pi}\right)\sin(2n\pi x/a)$
$u = x$
$du = dx$

$= \frac{2}{a}\left(\frac{1}{2}\right)\left[\int_0^a x\,dx - \int_0^a x\cos\left(\frac{2n\pi x}{a}\right)\right]dx = \frac{1}{a}\left[\frac{x^2}{2}\Big|_0^a - \frac{ax}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)\Big|_0^a + \int_0^a \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)dx\right]$

$= \frac{1}{a}\left[\frac{a^2}{2} - \frac{a^2}{2n\pi}\sin(2n\pi) + \left(\frac{a}{2n\pi}\right)^2\left(-\cos\left(\frac{2n\pi x}{a}\right)\right)\Big|_0^a\right] = \frac{1}{a}\left[\frac{a^2}{2} - 0 + \frac{a^2}{4n^2\pi^2}\left(-\cos(2n\pi)+\cos(0)\right)\right] = \frac{a}{2}$

$\langle x^2\rangle = \langle\psi_n|x^2|\psi_n\rangle = \frac{2}{a}\int_0^a x^2\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\int_0^a x^2\left(\frac{1}{2}\right)\left(1-\cos\left(\frac{2n\pi x}{a}\right)\right)dx = \frac{2}{a}\left(\frac{1}{2}\right)\left[\int_0^a x^2\,dx - \int_0^a x^2\cos\left(\frac{2n\pi x}{a}\right)dx\right]$

$u = x^2$
$du = 2x\,dx$

$= \frac{1}{a}\left[\frac{x^3}{3}\Big|_0^a - \left(\frac{a}{2n\pi}\right)(x^2)\sin\left(\frac{2n\pi x}{a}\right)\Big|_0^a + \left(\frac{a}{n\pi}\right)\int_0^a x\sin\left(\frac{2n\pi x}{a}\right)dx\right]$

$u = x$
$du = dx$
$dv = \sin(2n\pi x/a)\,dx$
$v = \left(\frac{a}{2n\pi}\right)(-\cos(2n\pi x/a))$

$= \frac{1}{a}\left[\frac{a^3}{3} - 0 + \left(\frac{a}{n\pi}\right)\left(\frac{a}{2n\pi}\right)\left(-x\cos\left(\frac{2n\pi x}{a}\right)\right)\Big|_0^a + \frac{a}{2n\pi}\int_0^a \cos\left(\frac{2n\pi x}{a}\right)dx\right]$

$= \frac{1}{a}\left[\frac{a^3}{3} - \frac{a^3}{2n^2\pi^2}(\cos 2n\pi) + \left(\frac{a}{2n\pi}\right)^2\sin\left(\frac{2n\pi x}{a}\right)\Big|_0^a\right] = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}$

$\langle p_x\rangle = \langle\psi_n|-i\hbar\frac{d}{dx}|\psi_n\rangle = \frac{2}{a}\int_0^a(-i\hbar)\sin\left(\frac{n\pi x}{a}\right)\frac{d}{dx}\sin\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\int_0^a(-i\hbar)\,u\,du$

$u = \sin(n\pi x/a)$
$du = d\sin(n\pi x/a)/dx \cdot dx$

$= -\frac{2i\hbar}{a}\frac{u^2}{2}\Big|_0^a = \frac{-i\hbar}{a}\sin^2\left(\frac{n\pi x}{a}\right)\Big|_0^a = 0$

$\langle p_x^2\rangle = -\langle\psi_n|\hbar^2\frac{d^2}{dx^2}|\psi_n\rangle = \frac{-2}{a}\int_0^a\hbar^2\sin\left(\frac{n\pi x}{a}\right)\frac{d^2}{dx^2}\sin\left(\frac{n\pi x}{a}\right)dx = \frac{-2\hbar^2}{a}\int_0^a\sin\left(\frac{n\pi x}{a}\right)\left(\frac{n\pi}{a}\right)^2\left(-\sin\left(\frac{n\pi x}{a}\right)\right)dx$

$= \frac{2\hbar^2}{a}\left(\frac{n^2\pi^2}{a^2}\right)\int_0^a\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{2\hbar^2n^2\pi^2}{a^3}\left(\frac{1}{2}\right)\int_0^a 1-\cos\left(\frac{2n\pi x}{a}\right)dx$

$= \frac{n^2\hbar^2\pi^2}{a^3}\left[x\Big|_0^a - \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)\Big|_0^a\right] = \left(\frac{n^2\hbar^2\pi^2}{a^3}\right)(a) = \frac{n^2\hbar^2\pi^2}{a^2}$

$\sigma_x\sigma_{p_x} = \left(\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}\right)^{1/2}\left(\frac{n^2\pi^2\hbar^2}{a^2} - 0\right)^{1/2} = \left[\left(\frac{a^2}{12n^2\pi^2}\right)\left(4n^2\pi^2 - 6 - 3n^2\pi^2\right)\right]^{1/2}\left[\frac{n\pi\hbar}{a}\right] = \left(\frac{n\pi\hbar}{a}\right)\left(\frac{a}{n\pi}\right)\left(\frac{1}{12}\right)^{1/2}(n^2\pi^2-6)^{1/2}$

$= \hbar\left(\frac{n^2\pi^2-6}{12}\right)^{1/2}$ → smallest $\sigma_x\sigma_{p_x}$ is when $n=1$

$\sigma_x\sigma_{p_x}(n=1) = \hbar\left(\frac{\pi^2-6}{12}\right)^{1/2} \approx 1.136\times\frac{\hbar}{2} \geq \frac{\hbar}{2}$, so $\sigma_x\sigma_{p_x}(n) \geq \frac{\hbar}{2}$

④ a) $\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{k_e}{2}(r-r_e)^2$

$\hat{H}\psi_0(r) = \left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{k_e}{2}(r-r_e)^2\right)\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{\alpha}{2}(r-r_e)^2} = \left(\frac{\alpha}{\pi}\right)^{1/4}\left[-\frac{\hbar^2}{2\mu}\frac{d}{dr}\left\{-\alpha(r-r_e)e^{-\frac{\alpha}{2}(r-r_e)^2}\right\} + \frac{k_e}{2}(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2}\right]$

$= \left(\frac{\alpha}{\pi}\right)^{1/4}\left[-\frac{\hbar^2}{2\mu}(-\alpha)\left\{e^{-\frac{\alpha}{2}(r-r_e)^2} - \alpha(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2}\right\} + \frac{k_e}{2}(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2}\right]$

$= \left(\frac{\alpha}{\pi}\right)^{1/4}\left[\frac{\hbar^2}{2\mu}\left\{\sqrt{\frac{k_e\mu}{\hbar^2}}e^{-\frac{\alpha}{2}(r-r_e)^2} + \left(\frac{k_e\mu}{\hbar^2}\right)(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2}\right\} + \frac{k_e}{2}(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2}\right]$

$= \left(\frac{\alpha}{\pi}\right)^{1/4}\left[\frac{\hbar}{2}\sqrt{\frac{k_e}{\mu}}e^{-\frac{\alpha}{2}(r-r_e)^2} - \frac{k_e}{2}(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2} + \frac{k_e}{2}(r-r_e)^2e^{-\frac{\alpha}{2}(r-r_e)^2}\right]$

$= \frac{\hbar}{2}\sqrt{\frac{k_e}{\mu}}\psi_0(r) = E_0\psi(r)$

$E_0 = \frac{\hbar}{2}\sqrt{\frac{k_e}{\mu}}$

b) $\sigma_r^2 = \langle\psi_0|r^2|\psi_0\rangle - \langle\psi_0|r|\psi_0\rangle^2 = \langle\psi_0|(r-\langle r\rangle)^2|\psi_0\rangle$

$\langle r\rangle = r_e$

$\sigma_r^2 = \langle\psi_0(r)|(r-r_e)^2|\psi_0(r)\rangle$

$E_0 = \frac{\hbar}{2}\sqrt{\frac{k_e}{\mu}}$ → $\frac{\partial E}{\partial k_e} = \langle\psi_0|\frac{\partial\hat{H}}{\partial k_e}|\psi_0\rangle = \langle\psi_0|\frac{\partial}{\partial k_e}\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{k_e}{2}(r-r_e)^2\right]|\psi_0\rangle$

$\frac{1}{2}k_e^{-1/2}\left(\frac{\hbar}{2}\right)\left(\frac{1}{\mu}\right)^{1/2} = \langle\psi_0|\frac{1}{2}(r-r_e)^2|\psi_0\rangle = \frac{1}{2}\sigma_r^2$

$\sigma_r^2 = \frac{\hbar}{2}\left(\frac{1}{k_e\mu}\right)^{1/2}$

$\hbar\omega = \Delta E = \hbar\sqrt{\frac{k_e}{\mu}}\left(1+v+\frac{1}{2}\right) - \hbar\sqrt{\frac{k_e}{\mu}}\left(v+\frac{1}{2}\right) = \hbar\sqrt{\frac{k_e}{\mu}}$

$k_e = (2\pi\omega)^2\mu = (2\pi)^2(6.42\times10^{13}\text{ Hz})^2\left(\frac{12\cdot16}{12+16}\right)(1.661\times10^{-27}\text{ kg/u}) = 1853\text{ kg/s}^2$

$\sigma_r^2 = \frac{\hbar}{2}\left(\frac{1}{k_e\mu}\right)^{1/2} = \frac{1.0546\times10^{-34}\text{ J}\cdot\text{s}}{2}\left(\frac{1}{(1.139\times10^{-26}\text{ kg})(1853\text{ kg/s}^2)}\right)^{1/2} = 1.148\times10^{-23}\text{ m}^2$

$\sigma_r = 3.39\times10^{-12}\text{ m}$

c) $\sigma_r\sigma_p \geq \frac{1}{2}\hbar$

$\sigma_p \geq \frac{1}{2}\hbar/\sigma_r$

$\sigma_p^2 \geq \frac{\hbar^2}{4\sigma_r^2}$

$\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2 = \langle p^2\rangle \geq \frac{\hbar^2}{4\sigma_r^2}$

$T = \langle\psi_0|-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}|\psi_0\rangle = \langle\psi_0|\frac{p^2}{2\mu}|\psi_0\rangle = \frac{1}{2\mu}\langle\psi_0|p^2|\psi_0\rangle = \frac{\langle p^2\rangle}{2\mu}$

$T \geq \left(\frac{\hbar^2}{4\sigma_r^2}\right)\left(\frac{1}{2\mu}\right)$

$T \geq \left[\frac{(1.0546\times10^{-34}\text{ J}\cdot\text{s})}{(8)(1.139\times10^{-26}\text{ kg})(3.39\times10^{-12}\text{ m})^2}\right]$

$T \geq 1.06\times10^{-20}\text{ J}$