HW #3

(1)

$$a = \frac{1}{\sqrt{2}}(Q + iP) \qquad a^{\dagger} = \frac{1}{\sqrt{2}}(Q - iP)$$

where $Q = \sqrt{\frac{m\omega}{\hbar}}\, x$ and $P = -i\frac{\partial}{\partial Q}$

$$= \frac{1}{\sqrt{m\hbar\omega}}\, p_x$$

since from the chain rule,

$$\frac{\partial}{\partial Q} = \frac{\partial x}{\partial Q}\frac{\partial}{\partial x}$$

$$= \left(\frac{\hbar}{\sqrt{mk}}\right)^{1/2}\frac{\partial}{\partial x}$$

so $P = -i\left(\frac{\hbar}{\sqrt{mk}}\right)^{1/2}\frac{\partial}{\partial x}$

$$= \frac{1}{\hbar}\left(\frac{\hbar}{\sqrt{mk}}\right)^{1/2} p_x \qquad \text{since } p_x = -i\hbar\frac{\partial}{\partial x}$$

$$= \frac{1}{\sqrt{m\hbar\omega}}\, p_x$$

so $\hat{a} = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\, x + \frac{i}{\sqrt{m\hbar\omega}}\, p_x\right]$

$$\hat{a}^{\dagger} = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\, x - \frac{i}{\sqrt{m\hbar\omega}}\, p_x\right]$$

<u>Add</u>:

$$a + a^{\dagger} = \frac{2}{\sqrt{2}}\sqrt{\frac{m\omega}{\hbar}}\, x$$

or $x = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^{\dagger}\right)$

<u>subtract</u>:

$$a - a^{+} = \frac{2i}{\sqrt{2}} \cdot \frac{1}{\sqrt{m\hbar\omega}}\, p_x$$

or

$$p_x = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}\,\left(a - a^{+}\right)$$

$$= i\sqrt{\frac{m\hbar\omega}{2}}\,\left(a^{+} - a\right)$$

(2) $\left[a^{\dagger}, a\right] = ?$

(a) $$= \frac{1}{2}\left[(Q - iP), (Q + iP)\right]$$

$$= \frac{1}{2}\left\{\underbrace{[Q,Q]}_{0} + \underbrace{[P,P]}_{0} + i[Q,P] - i[P,Q]\right\}$$

what is $[Q,P]$?

$$\left[Q, -i\frac{d}{dQ}\right]f = -i\left(Q\frac{df}{dQ} - \frac{d}{dQ}Qf\right)$$

$$= -i\left(Q\frac{df}{dQ} - Q\frac{df}{dQ} - \frac{dQ}{dQ}f\right)$$

$$= if$$

so $[Q,P] = i$

$$\therefore \left[a^{\dagger}, a\right] = \left\{i(i) - i(-i)\right\}\frac{1}{2}$$

$$= -1$$

(b) $[H, a^\dagger] = (a^\dagger a + \frac{1}{2})a^\dagger - a^\dagger(a^\dagger a + 1/2)$

$= a^\dagger(a a^\dagger - a^\dagger a)$

$= a^\dagger [a, a^\dagger]$

$= a^\dagger$

(3) $x^3 = \left(\frac{\hbar}{2m\omega}\right)^{3/2} (a+a^\dagger)(a+a^\dagger)(a+a^\dagger)$

$= \left(\quad \right)(a+a^\dagger)(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)$

$= \left(\quad \right)(aaa + aaa^\dagger + aa^\dagger a + aa^\dagger a^\dagger + a^\dagger aa + a^\dagger aa^\dagger + a^\dagger a^\dagger a + a^\dagger a^\dagger a^\dagger)$

$\langle v' | x^3 | v \rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} \times \Big\{$

$\sqrt{v}\sqrt{v-1}\sqrt{v-2}\,\delta_{v',v-3} + \sqrt{v+1}\sqrt{v+1}\sqrt{v}\,\delta_{v',v-1} +$

$\sqrt{v}\sqrt{v}\sqrt{v}\,\delta_{v',v-1} + \sqrt{v+1}\sqrt{v+2}\sqrt{v+2}\,\delta_{v',v+1} +$

$\sqrt{v}\sqrt{v-1}\sqrt{v-1}\,\delta_{v',v-1} + \sqrt{v+1}\sqrt{v+1}\sqrt{v+1}\,\delta_{v',v+1} +$

$\sqrt{v}\sqrt{v}\sqrt{v+1}\,\delta_{v',v+1} + \sqrt{v+1}\sqrt{v+2}\sqrt{v+3}\,\delta_{v',v+3} \Big\}$

$= \left(\frac{\hbar}{2m\omega}\right)^{3/2} \Big\{ \sqrt{v(v-1)(v-2)}\,\delta_{v',v-3} + 3v\sqrt{v}\,\delta_{v',v-1}$

$+ 3(v+1)\sqrt{v+1}\,\delta_{v',v+1} +$

$\sqrt{(v+1)(v+2)(v+3)}\,\delta_{v',v+3} \Big\}$

(4) Single-walled nanotube as electron on a cylindrical surface of length L and radius a.

a) Kinetic energy:

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dz^2} - \frac{\hbar^2}{2ma^2}\frac{d^2}{d\phi^2}$$

particle in a box for translation along z

particle on a ring

b) Obviously $\hat{H}$ is separable ~~into~~ in z and ϕ, so ψ is the product of particle in a box and particle on a ring wavefunctions:

$$\psi_{nk} = A \sin\left(\frac{n\pi}{L} z\right) e^{ik\phi}$$

$$n = 1, 2, 3, \ldots$$
$$k = 0, \pm 1, \pm 2, \ldots$$

c) the energy then is a sum: $E = E_{box} + E_{ring}$

$$E_{n,k} = \frac{h^2 n^2}{8mL^2} + \frac{\hbar^2 k^2}{2ma^2}$$

for $a = 5.5$ Å and $L = 120$ Å

lowest level is $n=1$, $k=0$

$$E_{1,0} = \frac{h^2}{8mL^2} = \frac{(6.62607\times10^{-34})^2}{8(9.10938\times10^{-31})(120\times10^{-10})^2}$$

$$= 4.1838\times10^{-22}\ \text{J}$$

$$= 0.00261\ \text{eV}$$

since $l >> a$, the translation energy levels will be more closely spaced than the rotational ones

$\therefore$ 2nd state is $E_{2,0} = \frac{4h^2}{8mL^2}$

$$= 0.0104\ \text{eV}$$

$$\Delta E = 0.00783\ \text{eV}$$

(5) Convert ∇^2 from cartesians to plane polar via the chain rule

---

$$\left(\frac{\partial f}{\partial x}\right)_y = \underbrace{\left(\frac{\partial r}{\partial x}\right)_y}_{\text{coef.}}\left(\frac{\partial f}{\partial r}\right)_\phi + \underbrace{\left(\frac{\partial \phi}{\partial x}\right)_y}_{\text{coef.}}\left(\frac{\partial f}{\partial \phi}\right)_r$$

$$\left(\frac{\partial r}{\partial x}\right)_y = \frac{1}{2}\left(x^2+y^2\right)^{-1/2}(2x) = \frac{x}{\sqrt{x^2+y^2}} = \frac{x}{r} = \cos\phi$$

$$\left(\frac{\partial \phi}{\partial x}\right)_y = \frac{1}{1+(y/x)^2}\left(-yx^{-2}\right) = \frac{-y}{\left(1+y^2/x^2\right)x^2}$$

$$= \frac{-y}{x^2+y^2} = \frac{-y}{r^2} = \frac{-\sin\phi}{r}$$

so $\left(\frac{\partial f}{\partial x}\right)_y = \cos\phi\left(\frac{\partial f}{\partial r}\right)_\phi - \frac{\sin\phi}{r}\left(\frac{\partial f}{\partial \phi}\right)_r$

apply again to get $\left(\frac{\partial^2 f}{\partial x^2}\right)$

let $g = \left(\frac{\partial f}{\partial x}\right)_y$

then $\left(\frac{\partial^2 f}{\partial x^2}\right) = \left(\frac{\partial g}{\partial x}\right)_y = \left(\frac{\partial r}{\partial x}\right)_y\left(\frac{\partial g}{\partial r}\right)_\phi + \left(\frac{\partial \phi}{\partial x}\right)_y\left(\frac{\partial g}{\partial \phi}\right)_r$

do the same for $\left(\frac{\partial^2 f}{\partial y^2}\right)$

One obtains

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}$$

(6) Show that $[l_y, l_z] = i\hbar l_x$

$$l_y = z p_x - x p_z$$

$$l_z = x p_y - y p_x$$

$$[l_y, l_z] = [z p_x - x p_z,\ x p_y - y p_x]$$

$$= \underbrace{[z p_x, x p_y]} - \underbrace{[z p_x, y p_x]}_{=0} - \underbrace{[x p_z, x p_y]}_{=0} + [x p_z, y p_x]$$

$$= [z p_x, x p_y] + [x p_z, y p_x]$$

$$= z \underbrace{[p_x, x]}_{-i\hbar} p_y + p_z \underbrace{[x, p_x]}_{i\hbar} y$$

$$= i\hbar (y p_z - z p_y) = i\hbar l_z \quad ✓$$

Show that $[l^2, l_x] = 0$

$$[l^2, l_x] = [l_x^2 + l_y^2 + l_z^2, l_x] = [l_y^2, l_x] + [l_z^2, l_x]$$

$$= [l_y l_y, l_x] + [l_z l_z, l_x]$$

$$= l_y [l_y, l_x] + [l_y, l_x] l_y + l_z [l_z, l_x] + [l_z, l_x] l_z$$

$$= l_y(-i\hbar l_z) + (-i\hbar l_z) l_y + l_z (i\hbar l_y) + (i\hbar l_y) l_z$$

$$= i\hbar(-l_y l_z - l_z l_y + l_z l_y + l_y l_z)$$

$$= 0 \quad ✓$$