Physics 522: Problem Set #4 Solutions

<u>Problem 1</u> Cohen-Tannoudji et al. vol I, Prob 5 p 767

Given $\psi(x,y,z) = N(x+y+z)\,e^{-r^2/\alpha^2}$

We want to decompose this wave function ~~as~~ in terms of the spherical harmonics.

Let us use the "spherical bases"

Recall:
$$Y_{1,\pm 1}(\vec{e}_r) = \mp\sqrt{\frac{3}{8\pi}}\left(\frac{x \pm iy}{r}\right) \Rightarrow \frac{x}{r} = \sqrt{\frac{8\pi}{3}}\left(\frac{-Y_{1,1}+Y_{1,-1}}{2}\right), \quad \frac{y}{r} = -\sqrt{\frac{8\pi}{3}}\left(\frac{Y_{1,1}+Y_{1,-1}}{2i}\right)$$
$$Y_{1,0}(\vec{e}_r) = \sqrt{\frac{3}{4\pi}}\,\frac{z}{r}$$

$$\Rightarrow \psi(x,y,z) = \tilde{\psi}(r,\vec{e}_r) = Nr\left(\frac{x}{r}+\frac{y}{r}+\frac{z}{r}\right)e^{-r^2/\alpha^2}$$
$$= \underbrace{N\sqrt{\frac{4\pi}{3}}}_{\text{new constant } N'}\, r\,e^{-\frac{r^2}{\alpha}}\Bigg(\underbrace{\left(\frac{-1+i}{\sqrt{2}}\right)}_{e^{i3\pi/4}}Y_{1,1}(\theta,\phi) + \underbrace{\left(\frac{1+i}{\sqrt{2}}\right)}_{e^{i\pi/4}}Y_{1,-1}(\theta,\phi) + Y_{1,0}(\theta,\phi)\Bigg)$$

$$\Rightarrow \boxed{\psi(x,y,z) = N' f(r)\left(e^{i3\pi/4}\,Y_{1,1}(\theta,\phi) + e^{i\pi/4}\,Y_{1,-1}(\theta,\phi) + Y_{1,0}(\theta,\phi)\right) \quad \text{where } f(r) = \cancel{N}\, r\,e^{-\frac{r^2}{\alpha}}}$$

From the form of the wave function we immediately see that its is an <u>equally weighted</u> superposition of $l=1$, $m_z = 1, 0, -1$

$\Rightarrow$ $\boxed{\text{Probability of measuring } l=0 = 0}$

$\boxed{\text{Probability of measuring } l=1 \;\; m_z = 1, 0, -1 : \frac{1}{3}}$

<u>Note:</u> We can think of the state as the "spinor"

$$|\psi\rangle = N' \; |f(r)\rangle \otimes \left(e^{i\pi/4} |l=1, m=1\rangle + e^{i3\pi/4} |l=1, m=-1\rangle + |l=1, m=0\rangle \right)$$

$$= N' \begin{pmatrix} e^{i\pi/4} f(r) \; Y_{1,1}(\theta,\phi) \\ f(r) \; Y_{1,0}(\theta,\phi) \\ e^{i3\pi/4} f(r) \; Y_{1,-1}(\theta,\phi) \end{pmatrix} \begin{array}{l} : m=1 \\ : m=0 \\ : m=-1 \end{array}$$

We find the normalization constant by setting $\langle\psi|\psi\rangle = 1$

$$\Rightarrow \langle\psi|\psi\rangle = N'^2 \langle f(r)| f(r)\rangle \left\{ \langle \overset{l}{1}, \overset{m}{1} | 1\,1\rangle + \langle 1,-1| 1\,-1\rangle + \langle 1\,0|1\,0\rangle \right\}$$

$$= 3N'^2 \int_0^\infty dr\, r^2 f(r) = 3N'^2 \underbrace{\int_0^\infty dr\, r^3 e^{-r^2/\alpha}}_{=6\alpha^4} = 1$$

$$\Rightarrow N' = \frac{1}{\sqrt{3}} \sqrt{6}\,\alpha^2$$

Set $\langle r|f(r)\rangle = \sqrt{6}\,\alpha^2\, r\, e^{-r^2/\alpha} \quad \Rightarrow \langle f(r)|f(r)\rangle = 1$

$$\Rightarrow \boxed{|\psi\rangle = |f'(r)\rangle \otimes \left\{ \frac{e^{i\pi/4} |l=1, m=1\rangle + e^{i3\pi/4} |l=1, m=-1\rangle + |l=1, m=0\rangle}{\sqrt{3}} \right\}}$$

Normalized state vector ~~with~~ written such that radial and angular parts are separately normalized

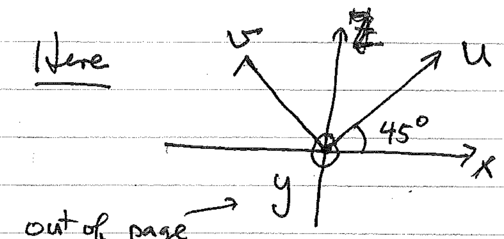
Problem 2 : Cohen-Tannoudji et al. Vol I, Prob 6 p. 768

System with angular momentum $l = 1$

Hamiltonian: $$\hat{H} = \frac{\omega_0}{\hbar}\left(\hat{L}_u^2 - \hat{L}_v^2\right) = \hbar\omega_0\left(\hat{l}_u^{\,2} - \hat{l}_v^{\,2}\right)$$

(Coupling of an electric quadrapole to a gradient field : Interaction energy
$$W = -\frac{1}{6}\sum_{ij}{}' Q_{ij}\,\frac{\partial E_i}{\partial x_j} \qquad \text{(see e.g. Jackson)}$$
)

Here



$$\left.\begin{aligned} \hat{l}_u &\equiv \frac{\hat{L}_u}{\hbar} = \frac{\hat{l}_x + \hat{l}_z}{\sqrt{2}} \\ \hat{l}_v &\equiv \frac{\hat{L}_v}{\hbar} = \frac{\hat{l}_x - \hat{l}_z}{\sqrt{2}} \end{aligned}\right\}$$ rotation transform about y-axis by $45°$ ("passive" rotation)

$$\Rightarrow \hat{l}_u^{\,2} = \left(\hat{l}_x^{\,2} + \hat{l}_z^{\,2} + \hat{l}_x\hat{l}_z + \hat{l}_z\hat{l}_x\right)/2$$
$$\hat{l}_v^{\,2} = \left(\hat{l}_x^{\,2} + \hat{l}_z^{\,2} - \hat{l}_x\hat{l}_z - \hat{l}_z\hat{l}_x\right)/2$$

$$\Rightarrow \hat{H} = \hbar\omega_0\left\{\hat{l}_x\hat{l}_z + \hat{l}_z\hat{l}_x\right\} = \frac{\hbar\omega_0}{2}\left\{\hat{l}_+\hat{l}_z + \hat{l}_z\hat{l}_+ + \hat{l}_-\hat{l}_z + \hat{l}_z\hat{l}_-\right\}$$

use $\hat{l}_x = \dfrac{\hat{l}_+ + \hat{l}_-}{2}$

(a) Now using properties of the eigenstates $\{|{+1}\rangle, |0\rangle, |{-1}\rangle\}$

$$\hat{l}_z|m\rangle = m|m\rangle \qquad \hat{l}_\pm|m\rangle = \sqrt{2 \mp m(m\pm 1)}\;|m\pm 1\rangle$$

$$\Rightarrow \boxed{\hat{H} \doteq \frac{\hbar\omega_0}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}}$$

In ordered basis $\{|1\rangle, |0\rangle, |{-1}\rangle\}$

Finding the stationary states:

$\hat{H}|E_n\rangle = E_n |E_n\rangle$

Secular equation $\det\{\hat{H} - E_n \mathbb{1}\} = 0$

$$\Rightarrow \det\begin{bmatrix} -\tilde{E}_n & 1 & 0 \\ 1 & -\tilde{E}_n & -1 \\ 0 & -1 & -\tilde{E}_n \end{bmatrix} = 0$$ where $\tilde{E}_n = E_n / \left(\frac{\hbar\omega_0}{\sqrt{2}}\right)$

$$\Rightarrow -\tilde{E}_n(\tilde{E}_n^2 - 1) - 1(-\tilde{E}_n) = 0$$

$$\Rightarrow -\tilde{E}_n^3 + 2\tilde{E}_n = 0 \Rightarrow \tilde{E}_n = 0 \text{ or } -\tilde{E}_n^2 + 2 = 0$$

$\Rightarrow$ Eigenvalues $\tilde{E}_n = 0$, $\tilde{E}_n = \pm\sqrt{2}$

Or with units $E_n = 0, \pm\hbar\omega_0$

$$\Rightarrow \boxed{E_1 = \hbar\omega_0, \quad E_0 = 0, \quad E_2 = -\hbar\omega_0}$$

The eigenvectors: $|E_n\rangle = \sum_{m=1}^{-1} c_m^{(n)} |m\rangle$

$$\hat{H}|E_1\rangle = \hbar\omega_0 |E_1\rangle \Rightarrow \frac{\hbar\omega_0}{\sqrt{2}}\begin{bmatrix} -\sqrt{2} & 1 & 0 \\ 1 & -\sqrt{2} & -1 \\ 0 & -1 & -\sqrt{2} \end{bmatrix}\begin{bmatrix} c_1^{(1)} \\ c_0^{(1)} \\ c_{-1}^{(1)} \end{bmatrix} = 0$$

$$\Rightarrow -\sqrt{2}c_1^{(1)} + c_0^{(1)} = 0 \Rightarrow c_0^{(1)} = +\sqrt{2}\, c_1^{(1)}$$

$$-c_0^{(1)} - \sqrt{2}\, c_{-1}^{(1)} = 0 \Rightarrow c_0^{(1)} = -\sqrt{2}\, c_{-1}^{(1)} \quad \Rightarrow c_1^{(1)} = -c_{-1}^{(1)}$$

$\Rightarrow$ Unnormalized $|E_1\rangle = N\begin{bmatrix} 1 \\ \sqrt{2} \\ -1 \end{bmatrix}$

(Next page)

Normalization : $\langle E_1 | E_1 \rangle = 4N^2 = 1 \Rightarrow N = \frac{1}{2}$

$\Rightarrow$ Up to an overall arbitrary phase

$$|E_1\rangle = \frac{1}{2}|1\rangle + \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{2}|-1\rangle$$

Proceding along the same lines for the other eigenvalues, we find

$$\boxed{\begin{aligned} E_1 &= +\hbar\omega_0, & |E_1\rangle &= \tfrac{1}{2}|1\rangle + \tfrac{1}{\sqrt{2}}|0\rangle - \tfrac{1}{2}|-1\rangle \\ E_2 &= 0, & |E_2\rangle &= \tfrac{1}{\sqrt{2}}|1\rangle + \tfrac{1}{\sqrt{2}}|-1\rangle \\ E_3 &= -\hbar\omega_0, & |E_3\rangle &= \tfrac{1}{2}|1\rangle - \tfrac{1}{\sqrt{2}}|0\rangle - \tfrac{1}{2}|-1\rangle \end{aligned}}$$

__Checks__: Note $\langle E_i | E_j \rangle = \delta_{ij}$ (orthonormal)

In position representation: $\langle \vec{x} | \pm 1 \rangle = \mp C \left(\frac{x \pm iy}{\sqrt{2}} \right)$

(spherical basis, with normalization constant) $\langle \vec{x} | 0 \rangle = C\, z$

$\sqrt{3/4\pi}$

$$\Rightarrow \langle \vec{x} | E_1 \rangle = -C \left(\frac{x - z}{\sqrt{2}} \right)$$

$$\langle \vec{x} | E_2 \rangle = -iC\,(y)$$

$$\langle \vec{x} | E_3 \rangle = -C \left(\frac{x + z}{\sqrt{2}} \right)$$

These are expected given the symmetry of the problem

(b) At time $t=0$: $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle)$

For $t>0$ $\quad |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$

There are many ways to procede. Here's one.

Decompose $|\psi(0)\rangle$ into stationary states

$$|\psi(0)\rangle = \sum_n c_n |E_n\rangle \qquad c_n = \langle E_n|\psi(0)\rangle$$

Then $|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |E_n\rangle$

Here $c_1 = \langle E_1|\psi(0)\rangle = \frac{1}{\sqrt{2}}$, $\quad c_2 = \langle E_2|\psi(0)\rangle = 0$

$c_3 = \langle E_3|\psi(0)\rangle = \frac{1}{\sqrt{2}}$

$$\Rightarrow |\psi(0)\rangle = \frac{1}{\sqrt{2}}(|E_1\rangle + |E_3\rangle)$$

$$\therefore \boxed{|\psi(t)\rangle = \frac{1}{\sqrt{2}}(e^{-iE_1 t/\hbar}|E_1\rangle + e^{-iE_3 t/\hbar}|E_3\rangle)}$$

or in the original basis, substituting for $|E_1\rangle$ and $|E_3\rangle$

$$\Rightarrow \boxed{|\psi(t)\rangle = \frac{1}{\sqrt{2}} \cos\omega_0 t\,|1\rangle - i\sin\omega_0 t\,|0\rangle - \frac{1}{\sqrt{2}}\cos\omega_0 t\,|-1\rangle}$$

Probability of finding:

$m=1$: $\quad P_1(t) = |\langle 1|\psi(t)\rangle|^2 = \frac{1}{2}\cos^2\omega_0 t$

$m=0$: $\quad P_0(t) = |\langle 0|\psi(t)\rangle|^2 = \sin^2\omega_0 t$

$m=-1$: $\quad P_{-1}(t) = |\langle -1|\psi(t)\rangle|^2 = \frac{1}{2}\cos^2\omega_0 t$

To better understand the time evolution of the state, let us consider the position representation:

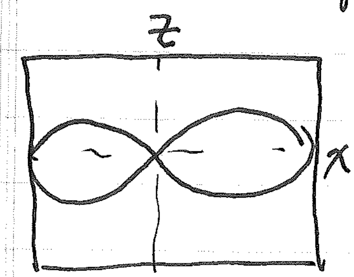
$$\langle \vec{e}_r | \psi(t) \rangle = \frac{c}{r}\left(\frac{\cos\omega_0 t}{\sqrt{2}} \left(-\frac{x-iy}{\sqrt{2}}\right) - i \sin\omega_0 t \, z - \cos\omega_0 t/\sqrt{2} \left(\frac{x-iy}{\sqrt{2}}\right)\right)$$

$$= -\frac{c}{r}\left(x\cos\omega_0 t + i z \sin\omega_0 t \right)$$

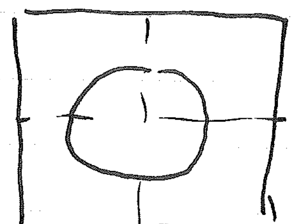
$$\Rightarrow |\langle \vec{e}_r | \psi(t) \rangle|^2 = \left(\frac{c}{r}\right)^2 \left[x^2 \cos^2\omega_0 t + z^2 \sin^2\omega_0 t \right]$$

$$= \left(\frac{c}{r}\right)^2 \left(\frac{x^2+z^2}{2} + \left(\frac{x^2-z^2}{2}\right)\cos 2\omega_0 t \right)$$

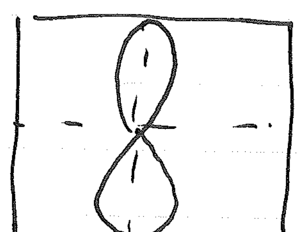
Below is a polar plot in the x-z plane



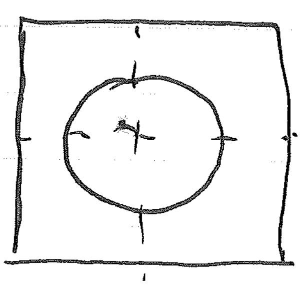
$\omega_0 t = 0$



$\omega_0 t = \pi/4$



$\omega_0 t = \pi/2$



$\omega_0 t = 3\pi/4$

A movie of the quadrapolar motion can be seen at the web site

(C) Using matrix representation in basis $\{|1\rangle, |0\rangle, |-1\rangle\}$

$$\hat{L}_x = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad \hat{L}_y = \frac{\hbar}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}$$

$$\Rightarrow \langle \hat{L}_x \rangle_t = \frac{\hbar}{\sqrt{2}}\left[\frac{\cos\omega_0 t}{\sqrt{2}},\ i\sin\omega_0 t,\ -\frac{\cos\omega_0 t}{\sqrt{2}}\right]\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}\begin{bmatrix} \frac{\cos\omega_0 t}{\sqrt{2}} \\ -i\sin\omega_0 t \\ \frac{\cos\omega_0 t}{\sqrt{2}} \end{bmatrix}$$

$$\Rightarrow \langle \hat{L}_x \rangle_t = 0$$

Proceding along similar lines:

$$\boxed{\begin{aligned} \langle \hat{L}_x \rangle_t &= \langle \hat{L}_z \rangle_t = 0 \\ \langle \hat{L}_y \rangle_t &= \frac{\hbar}{2}\sin 2\omega_0 t \end{aligned}}$$

This makes sense physically since the rotation is in x-z plane.

Note: Oscillation frequency is $2\omega_0$.

This is expected classically for a quadrapole, given "driving field" at frequency ω_0

The angular momentum vector thus oscillates along the y-axis as the wave function executes quadrapolar motion in the x-z plane along symmetry axes

$\vec{e}_x \pm \vec{e}_z$

(d) At time t a measurement of $\hat{L}_z^2$ is performed

The possible values:

$m^2 = 1$: Probability $\cos^2\omega_0 t$ (sum of $P_{m=1}$ and $P_{m=-1}$)

$m^2 = 0$: " $\sin^2\omega_0 t$

(i) $\Rightarrow$ when $\omega_0 t = \frac{n}{2}\pi$ (n odd integer), $\langle \hat{L}_z^2 \rangle = 0$
$\Rightarrow$ uncertainty in $\Delta L_z = 0$ $\Rightarrow$ system is in an eigenstate of $\hat{L}_z$

This is clear from the solution to $|\psi(t)\rangle$ found in part (b): $|\psi(t = \frac{n\pi}{2})\rangle = \pm i\,|0\rangle$

(ii) Suppose a measurement yields $+\hbar^2$ for $\hat{L}_z^2$
$\Rightarrow$ $m = 1$ or $m = -1$

$\Rightarrow$ Von Neumann measurement with projection operator

$$\hat{\mathbb{P}} = |1\rangle\langle 1| + |-1\rangle\langle -1|$$

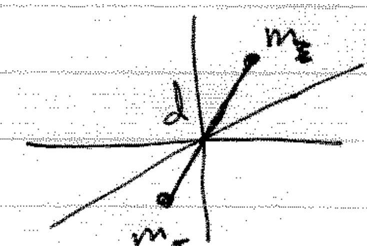
After measurement $|\psi\rangle \Rightarrow \dfrac{\hat{\mathbb{P}}|\psi\rangle}{\|\hat{\mathbb{P}}|\psi\rangle\|}$

$$\hat{\mathbb{P}}|\psi\rangle = \frac{\cos\omega_0 t}{\sqrt{2}}\left(|1\rangle - |-1\rangle\right) \Rightarrow \boxed{|\psi\rangle_{after} = \frac{|1\rangle - |-1\rangle}{\sqrt{2}}}$$

This is equivalent to setting

$\boxed{|\psi(t)\rangle \Rightarrow |\psi(0)\rangle, \text{ so the evolution is as in (b)}}$

Problem # 3. Rigid Rotator



Point masses fixed to a rigid (massless) rod of length d

(a) There is no external potential on these masses. Thus the Hamiltonian is just ~~kinetic~~ kinetic energy. Furthermore, the motion of the center of mass is fixed — only relative motion has dynamics. This motion is all angular since the rod is rigid

$$\Rightarrow \boxed{\hat{H} = \frac{\hat{L}^2}{2I} \quad \text{where } I = \mu d^2 = \text{moment of inertia}, \quad \mu = \frac{m}{2} = \text{reduced mass}}$$

(b) Energy levels: $\hat{H}|\psi\rangle = E|\psi\rangle$

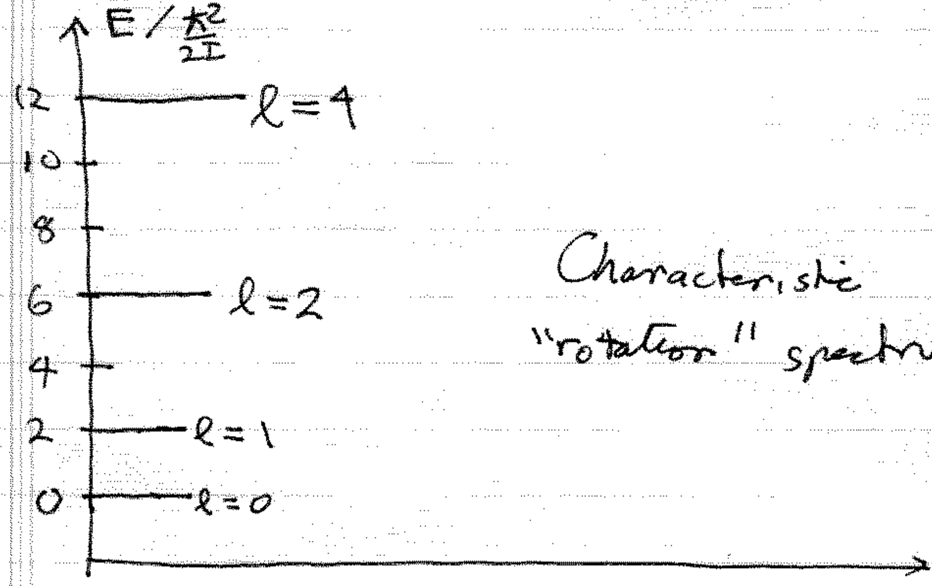
$$\Rightarrow \frac{1}{2I}\hat{L}^2|\psi\rangle = E|\psi\rangle$$

$\Rightarrow$ Stationary states are eigenstates of $\hat{L}^2$

$$\Rightarrow \boxed{E_\ell = \frac{\hbar^2}{2I}\ell(\ell+1)}$$

$$|\psi\rangle \doteq Y_\ell^m(\theta,\phi) \quad , \boxed{2\ell+1 \text{ degeneracy}}$$

Energy level diagram



Characteristic "rotation" spectrum

(c) Example N_2 molecule, with $d = 100\,pm = 10^{-10}\,m$
$= 1\,Å$

Nitrogen mass $= 14$ amu (atomic mass units)

1 amu = mass proton, $M_p c^2 = 932$ MeV

$$\Rightarrow \frac{\hbar^2}{2I} = \frac{\hbar^2}{M_N d^2} = \frac{(\hbar c)^2}{(M_N c^2)\, d^2}$$

<u>Aside:</u> Useful units $\hbar c = 1974$ eV Å ≈ 2 MeV Å

$$\Rightarrow E_c = \frac{\hbar^2}{2I} = \frac{(2\text{ MeV Å})^2}{(14 \times 932\text{ MeV})\,(1\text{ Å})^2} = 3 \times 10^{-4}\text{ MeV} = 0.3\text{ eV}$$

Characteristic ~~wavelength~~ frequency

$$\boxed{\nu = \frac{E_c}{h} = 7.26 \times 10^{13}\text{ Hz} = \text{infrared}}$$

Now the characteristic frequencies set the scale. Generally the energy of the photon will depend on the initial + final state l

$$\Delta E = E_{l_{final}} - E_{l_{initial}} = \left(\frac{\hbar^2}{2I}\right)\left(l_f(l_f+1) - l_i(l_i+1)\right)$$

for $l \leftrightarrow l+1$ transition

$$\Delta E_{l\leftrightarrow l+1} = \frac{\hbar^2}{2I}\left((l+1)(l+2) - l(l+1)\right) = 2(l+1)\underbrace{\boxed{\frac{\hbar^2}{2I}}}_{0.3\,eV}$$

(d) Given the spectrum, we can find the moment of inertia of the molecule by inverting the expression above

$$I = \left(\frac{\Delta E_{l\to l+1}}{\hbar^2/2}\right)$$