1D SHO $\hat{H}(x)=\frac{1}{2m}\left(\hat{p}^2+m^2\omega^2x^2\right)$ Define $x_0\equiv\sqrt{\frac{\hbar}{m\omega}}$, $\xi\equiv\frac{x}{x_0}$ $\rightarrow$ $\hat{H}(\xi)=\frac{\hbar\omega}{2}\left(\xi^2-\frac{d^2}{d\xi^2}\right)$

$$E_n=\left(n+\tfrac{1}{2}\right)\hbar\omega\,,\quad \psi_n(x)=\left(\frac{1}{\pi x_0^2}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\frac{x}{x_0}\right)e^{-\frac{x^2}{2x_0^2}}\quad\text{where}\quad \begin{array}{l} H_0(\xi)=1,\quad H_2(\xi)=4\xi^2-2,\\ H_1(\xi)=2\xi,\ H_3(\xi)=8\xi^3-12\xi,\end{array}$$

$$\hat{a}_\pm=\frac{1}{\sqrt{2}}\left(\xi\mp\frac{d}{d\xi}\right)\ \rightarrow\ \begin{array}{l}\hat{a}_+\psi_n=\sqrt{n+1}\,\psi_{n+1}\\ \hat{a}_-\psi_n=\sqrt{n}\,\psi_{n-1}\end{array},\quad \begin{array}{l}\hat{H}=\hbar\omega\left(\hat{a}_+\hat{a}_-+\tfrac{1}{2}\right)\\ \left[\hat{a}_-,\hat{a}_+\right]=1\end{array}\quad H_n(\xi)=(-1)^n e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2}$$

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for −8/15 read $-\sqrt{8/15}$.

Notation:

		J J ... / M M ...
m_1	m_2	Coefficients
m_1	m_2	
.	.	

$$Y_1^0=\sqrt{\frac{3}{4\pi}}\cos\theta$$
$$Y_1^1=-\sqrt{\frac{3}{8\pi}}\sin\theta\,e^{i\phi}$$
$$Y_2^0=\sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta-\frac{1}{2}\right)$$
$$Y_2^1=-\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\,e^{i\phi}$$
$$Y_2^2=\frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\,e^{2i\phi}$$
$$Y_\ell^{-m}=(-1)^m Y_\ell^{m*}$$

$$\langle j_1j_2m_1m_2|j_1j_2JM\rangle=(-1)^{J-j_1-j_2}\langle j_2j_1m_2m_1|j_2j_1JM\rangle$$

1/2×1/2

m_1 m_2	J=1, M=+1
+1/2 +1/2	1

m_1 m_2	J=1, M=0	J=0, M=0
+1/2 −1/2	1/2	1/2
−1/2 +1/2	1/2	−1/2

m_1 m_2	J=1, M=−1
−1/2 −1/2	1

1×1/2

m_1 m_2	J=3/2, M=+3/2
+1 +1/2	1

m_1 m_2	J=3/2, M=+1/2	J=1/2, M=+1/2
+1 −1/2	1/3	2/3
0 +1/2	2/3	−1/3

m_1 m_2	J=3/2, M=−1/2	J=1/2, M=−1/2
0 −1/2	2/3	1/3
−1 +1/2	1/3	−2/3

m_1 m_2	J=3/2, M=−3/2
−1 −1/2	1

2×1/2

m_1 m_2	J=5/2, M=+5/2
+2 +1/2	1

m_1 m_2	J=5/2, M=+3/2	J=3/2, M=+3/2
+2 −1/2	1/5	4/5
+1 +1/2	4/5	−1/5

m_1 m_2	J=5/2, M=+1/2	J=3/2, M=+1/2
+1 −1/2	2/5	3/5
0 +1/2	3/5	−2/5

m_1 m_2	J=5/2, M=−1/2	J=3/2, M=−1/2
0 −1/2	3/5	2/5
−1 +1/2	2/5	−3/5

m_1 m_2	J=5/2, M=−3/2	J=3/2, M=−3/2
−1 −1/2	4/5	1/5
−2 +1/2	1/5	−4/5

m_1 m_2	J=5/2, M=−5/2
−2 −1/2	1

3/2×1/2

m_1 m_2	J=2, M=+2
+3/2 +1/2	1

m_1 m_2	J=2, M=+1	J=1, M=+1
+3/2 −1/2	1/4	3/4
+1/2 +1/2	3/4	−1/4

m_1 m_2	J=2, M=0	J=1, M=0
+1/2 −1/2	1/2	1/2
−1/2 +1/2	1/2	−1/2

m_1 m_2	J=2, M=−1	J=1, M=−1
−1/2 −1/2	3/4	1/4
−3/2 +1/2	1/4	−3/4

m_1 m_2	J=2, M=−2
−3/2 −1/2	1

2×1

m_1 m_2	J=3, M=+3
+2 +1	1

m_1 m_2	J=3, M=+2	J=2, M=+2
+2 0	1/3	2/3
+1 +1	2/3	−1/3

m_1 m_2	J=3, M=+1	J=2, M=+1	J=1, M=+1
+2 −1	1/15	1/3	3/5
+1 0	8/15	1/6	−3/10
0 +1	2/5	−1/2	1/10

m_1 m_2	J=3, M=0	J=2, M=0	J=1, M=0
+1 −1	1/5	1/2	3/10
0 0	3/5	0	−2/5
−1 +1	1/5	−1/2	3/10

m_1 m_2	J=3, M=−1	J=2, M=−1	J=1, M=−1
0 −1	2/5	1/2	1/10
−1 0	8/15	−1/6	−3/10
−2 +1	1/15	−1/3	3/5

m_1 m_2	J=3, M=−2	J=2, M=−2
−1 −1	2/3	1/3
−2 0	1/3	−2/3

m_1 m_2	J=3, M=−3
−2 −1	1

1×1

m_1 m_2	J=2, M=+2
+1 +1	1

m_1 m_2	J=2, M=+1	J=1, M=+1
+1 0	1/2	1/2
0 +1	1/2	−1/2

m_1 m_2	J=2, M=0	J=1, M=0	J=0, M=0
+1 −1	1/6	1/2	1/3
0 0	2/3	0	−1/3
−1 +1	1/6	−1/2	1/3

m_1 m_2	J=2, M=−1	J=1, M=−1
0 −1	1/2	1/2
−1 0	1/2	−1/2

m_1 m_2	J=2, M=−2
−1 −1	1

3/2×1

m_1 m_2	J=5/2, M=+5/2
+3/2 +1	1

m_1 m_2	J=5/2, M=+3/2	J=3/2, M=+3/2
+3/2 0	2/5	3/5
+1/2 +1	3/5	−2/5

m_1 m_2	J=5/2, M=+1/2	J=3/2, M=+1/2	J=1/2, M=+1/2
+3/2 −1	1/10	2/5	1/2
+1/2 0	3/5	1/15	−1/3
−1/2 +1	3/10	−8/15	1/6

m_1 m_2	J=5/2, M=−1/2	J=3/2, M=−1/2	J=1/2, M=−1/2
+1/2 −1	3/10	8/15	1/6
−1/2 0	3/5	−1/15	−1/3
−3/2 +1	1/10	−2/5	1/2

m_1 m_2	J=5/2, M=−3/2	J=3/2, M=−3/2
−1/2 −1	3/5	2/5
−3/2 0	2/5	−3/5

m_1 m_2	J=5/2, M=−5/2
−3/2 −1	1

3/2×3/2

m_1 m_2	J=3, M=+3
+3/2 +3/2	1

m_1 m_2	J=3, M=+2	J=2, M=+2
+3/2 +1/2	1/2	1/2
+1/2 +3/2	1/2	−1/2

m_1 m_2	J=3, M=+1	J=2, M=+1	J=1, M=+1
+3/2 −1/2	1/5	1/2	3/10
+1/2 +1/2	3/5	0	−2/5
−1/2 +3/2	1/5	−1/2	3/10

m_1 m_2	J=3, M=0	J=2, M=0	J=1, M=0	J=0, M=0
+3/2 −3/2	1/20	1/4	9/20	1/4
+1/2 −1/2	9/20	1/4	−1/20	−1/4
−1/2 +1/2	9/20	−1/4	−1/20	1/4
−3/2 +3/2	1/20	−1/4	9/20	−1/4

m_1 m_2	J=3, M=−1	J=2, M=−1	J=1, M=−1
+1/2 −3/2	1/5	1/2	3/10
−1/2 −1/2	3/5	0	−2/5
−3/2 +1/2	1/5	−1/2	3/10

m_1 m_2	J=3, M=−2	J=2, M=−2
−1/2 −3/2	1/2	1/2
−3/2 −1/2	1/2	−1/2

m_1 m_2	J=3, M=−3
−3/2 −3/2	1

2×3/2

m_1 m_2	J=7/2, M=+7/2
+2 +3/2	1

m_1 m_2	J=7/2, M=+5/2	J=5/2, M=+5/2
+2 +1/2	3/7	4/7
+1 +3/2	4/7	−3/7

m_1 m_2	J=7/2, M=+3/2	J=5/2, M=+3/2	J=3/2, M=+3/2
+2 −1/2	1/7	16/35	2/5
+1 +1/2	4/7	1/35	−2/5
0 +3/2	2/7	−18/35	1/5

m_1 m_2	J=7/2, M=+1/2	J=5/2, M=+1/2	J=3/2, M=+1/2	J=1/2, M=+1/2
+2 −3/2	1/35	6/35	2/5	2/5
+1 −1/2	12/35	5/14	0	−3/10
0 +1/2	18/35	−3/35	−1/5	1/5
−1 +3/2	4/35	−27/70	2/5	−1/10

m_1 m_2	J=7/2, M=−1/2	J=5/2, M=−1/2	J=3/2, M=−1/2	J=1/2, M=−1/2
+1 −3/2	4/35	27/70	2/5	1/10
0 −1/2	18/35	3/35	−1/5	−1/5
−1 +1/2	12/35	−5/14	0	3/10
−2 +3/2	1/35	−6/35	2/5	−2/5

m_1 m_2	J=7/2, M=−3/2	J=5/2, M=−3/2	J=3/2, M=−3/2
0 −3/2	2/7	18/35	1/5
−1 −1/2	4/7	−1/35	−2/5
−2 +1/2	1/7	−16/35	2/5

m_1 m_2	J=7/2, M=−5/2	J=5/2, M=−5/2
−1 −3/2	4/7	3/7
−2 −1/2	3/7	−4/7

m_1 m_2	J=7/2, M=−7/2
−2 −3/2	1

2×2

m_1 m_2	J=4, M=+4
+2 +2	1

m_1 m_2	J=4, M=+3	J=3, M=+3
+2 +1	1/2	1/2
+1 +2	1/2	−1/2

m_1 m_2	J=4, M=+2	J=3, M=+2	J=2, M=+2
+2 0	3/14	1/2	2/7
+1 +1	4/7	0	−3/7
0 +2	3/14	−1/2	2/7

m_1 m_2	J=4, M=+1	J=3, M=+1	J=2, M=+1	J=1, M=+1
+2 −1	1/14	3/10	3/7	1/5
+1 0	3/7	1/5	−1/14	−3/10
0 +1	3/7	−1/5	−1/14	3/10
−1 +2	1/14	−3/10	3/7	−1/5

m_1 m_2	J=4, M=0	J=3, M=0	J=2, M=0	J=1, M=0	J=0, M=0
+2 −2	1/70	1/10	2/7	2/5	1/5
+1 −1	8/35	2/5	1/14	−1/10	−1/5
0 0	18/35	0	−2/7	0	1/5
−1 +1	8/35	−2/5	1/14	1/10	−1/5
−2 +2	1/70	−1/10	2/7	−2/5	1/5

m_1 m_2	J=4, M=−1	J=3, M=−1	J=2, M=−1	J=1, M=−1
+1 −2	1/14	3/10	3/7	1/5
0 −1	3/7	1/5	−1/14	−3/10
−1 0	3/7	−1/5	−1/14	3/10
−2 +1	1/14	−3/10	3/7	−1/5

m_1 m_2	J=4, M=−2	J=3, M=−2	J=2, M=−2
0 −2	3/14	1/2	2/7
−1 −1	4/7	0	−3/7
−2 0	3/14	−1/2	2/7

m_1 m_2	J=4, M=−3	J=3, M=−3
−1 −2	1/2	1/2
−2 −1	1/2	−1/2

m_1 m_2	J=4, M=−4
−2 −2	1

Atomic Structure

Bohr magneton: $\mu_B=\frac{e\hbar}{2m_e}$

gyromag. ratio γ: $\vec{\mu}_J=\gamma\vec{J}$, $\gamma_{\text{classical}}=\frac{e}{2m}$

g factor: $\vec{\mu}_L=\frac{e}{2m}\vec{L}$, $\vec{\mu}_S=g\frac{e}{2m}\vec{S}$, $g_{\text{spin-1/2 point particle}}=2$

Hund rules: 1. Max S 2. Max L 3. Min J for ≤ 1/2-filled shells

$l=$ 0 1 2 3 4... / s p d f g...

term symbol: $^{2S+1}L_J$

Perturbation Theory – Time-Independent

$H = H_0 + H'$

- H_0 solvable w eigen-* $\{E_n^{(0)}\},\{|n^{(0)}\rangle\}$
- $H' \ll H_0$

Expansions for eigen-* of H: $E_n = E_n^{(0)} + E_n^{(1)} + \cdots$ & $|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle + \cdots$

For a **non-degenerate** eigenvalue $E_n^{(0)}$ of H_0: $|n^{(1)}\rangle = \sum_{m\neq n} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle$ with $H'_{mn} \equiv \langle m^{(0)}|H'|n^{(0)}\rangle$

$$E_n^{(j)} = \langle n^{(0)}|H'|n^{(j-1)}\rangle \quad \rightarrow \quad E_n^{(1)} = H'_{nn}, \quad E_n^{(2)} = \sum_{m\neq n} \frac{|H'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$$

For a **degenerate** eigenvalue $E_D^{(0)}$ of H_0:

- Let $\{ |\alpha_1^{(0)}\rangle, ..., |\alpha_n^{(0)}\rangle \}$ = degen. subspace D sharing e-value $E_D^{(0)}$
- Find $\{ |\beta_1^{(0)}\rangle, ..., |\beta_n^{(0)}\rangle \}$ = e-vectors of H' within subspace D

  = linear combinations of $|\alpha_i^{(0)}\rangle$ states that diagonalize $\mathbf{H'}$

$\Rightarrow$ 1st order energy correction is $E_{\beta i}^{(1)} = \langle \beta_i^{(0)}|H'|\beta_i^{(0)}\rangle$

Generators of Transformations

$$f(q+\Delta) = U(\Delta) f(q)$$

for q = position, angle, time:

$$U_{\hat{a}}(\Delta) = \exp\left(\Delta \hat{a}\cdot\vec{\nabla}\right) = \exp\left(-\frac{\Delta}{i\hbar}\hat{a}\cdot\vec{\mathbf{p}}\right)$$

$$U_{\hat{z}}(\Delta) = \exp\left(\Delta\frac{\partial}{\partial\phi}\right) = \exp\left(-\frac{\Delta}{i\hbar}\hat{z}\cdot\vec{\mathbf{L}}\right)$$

$$U(\Delta) = \exp\left(\Delta\frac{\partial}{\partial t}\right) = \exp\left(-\frac{\Delta}{i\hbar}\cdot(-\mathbf{H})\right)$$

Variational Principle

$E_{gs} \le \langle\psi|H|\psi\rangle \ \forall\ \psi$

Sudden / Adiabatic Approx

ψ / n unchanged by ΔH

Perturbation Theory – Time Dependent

- $H(t) = H^{(0)} + H'(t)$
- $\{ E_n^{(0)}, |n^{(0)}\rangle \}$ = the eigen-* of $H^{(0)}$
- $\omega_{fn} \equiv \left(E_f^{(0)} - E_n^{(0)}\right)/\hbar$
- $H'_{fn} \equiv \langle f^{(0)}|H'|n^{(0)}\rangle$

$$|\psi(t)\rangle = \sum_n c_n(t)\, e^{-i\omega_n t}|n^{(0)}\rangle \quad \text{where} \quad i\hbar\dot{c}_f(t) = \sum_n H'_{fn}\, e^{i\omega_{fn}t} c_n(t)$$

To 1st order in $H' \ll H^{(0)}$, with $|\psi(t_0)\rangle = |i^{(0)}\rangle$: $c_f(t) \approx \delta_{fi} + \frac{1}{i\hbar}\int_{t_0}^{t} H'_{fi}(t')\, e^{i\omega_{fi}t'}\, dt' \ \rightarrow\ P_{i\to f} = |c_f(t)|^2$

relevant math for analyzing time- & frequency-dependence: $\frac{\sin(x)}{x} \xrightarrow[x\to 0]{} 1$, $\quad \frac{\sin^2(ax)}{a x^2} \xrightarrow[a\to\infty]{} \pi\delta(x)$

Fermi's Golden Rule: $W_{i\to f} \equiv \frac{P_{i\to f}}{t} = \frac{2\pi}{\hbar}|V_{fi}|^2\, n(E_f)$ at resonance

$E_f = E_i \pm \hbar\omega$ for $H' = V(r)\left(e^{i\omega t} + e^{-i\omega t}\right)$

$E_f = E_i$ for $H' = V(r)\,\Theta(t)$

E1 radiation: when $\lambda \gg r$ and F_B negligible, $H' = V(\vec{r})\cos(\omega t)$, $V(\vec{r}) \approx -q\vec{E}_0\cdot\vec{r}$ $\rightarrow$ E1 selection rules:

For the electron making the transition

(a) $\Delta l = \pm 1$
(b) $\Delta m_l = 0, \pm 1$

For the atom as a whole

(a) $\Delta S = 0$
(b) $\Delta L = 0, \pm 1$ ($L = 0 \leftrightarrow L' = 0$ forbidden)
(c) $\Delta M_L = 0, \pm 1$
(d) $\Delta J = 0, \pm 1$ ($J = 0 \leftrightarrow J' = 0$ forbidden)
(e) $\Delta M_J = 0, \pm 1$

spontaneous emission rate = Einstein's $A_{i\to f} = \frac{\omega_{if}^3 q^2 |\vec{r}_{fi}|^2}{3\pi\varepsilon_0\hbar c^3}$ with $\vec{r}_{fi} \equiv \langle f^{(0)}|\vec{r}|i^{(0)}\rangle$

lifetime $\tau_i = \frac{1}{\sum_f A_{i\to f}}$