Phys 137B 28Aug19

"concurrent enrollment" (?)

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Friday October 11th Midterm
Friday ~~Decemb~~ November 15th
Friday December 20th 3pm Final

HW 40%
Midterms 18% each, might shift between the two
Final 24%

Three Parts

I Combining Degrees of Freedom
II Sobering Realization Time
Approximation Methods
III Scattering Theory
IV Special Topics

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Review: The Elements of Dirac Notation and the Postulates of Quantum Mechanics

Postulate I: A given quantum system is described by a Hilbert Space. The state of a quantum system is given by a normalized Vector or ket in the Hilbert space.

Ket: $|\text{ket}\rangle$ $\quad |\uparrow\rangle \quad |\downarrow\rangle$

spin up $\quad$ spin down

$$\mathcal{H}_{1/2} = \{ |\alpha\rangle = a|\uparrow\rangle + b|\downarrow\rangle \mid a,b \in \mathbb{C} \} \qquad |\alpha\rangle \doteq \chi_\alpha = \begin{bmatrix} a \\ b \end{bmatrix}$$

normalized $\langle \alpha | \alpha \rangle = 1 = |a|^2 + |b|^2$

$$\mathcal{H}_{1/2} = \mathbb{C}^2$$

SHO $\quad \{|n\rangle\} \quad n = 0, 1, 2, \ldots$

$$\mathcal{H}_{SHO} = \{ |\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle \mid c_n \in \mathbb{C} \}$$

normalized $\langle \alpha | \alpha \rangle = 1 = \sum_{n=0}^{\infty} |c_n|^2$

$$|\alpha\rangle \doteq \vec{\Psi}_\alpha = \begin{bmatrix} c_0 \\ c_1 \\ \vdots \end{bmatrix}$$

Dual Hilbert Space $\mathcal{H}^*$

$$\langle \beta | : \mathcal{H} \to \mathbb{C}$$

$$\underbrace{\langle \beta | \alpha \rangle}_{\text{bracket}} = \text{a number}$$

ket basis: $|e_i\rangle$

Dual bra basis: $\langle e^i|$

$$\langle e^i | e_j \rangle = \delta^i_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$$|\alpha\rangle = \sum_i c^i |e_i\rangle \qquad \langle\beta| = \sum_i c_i \langle e^i|$$

$$c^i = \langle e^i|\alpha\rangle \qquad c_i = \langle\beta|e_i\rangle$$

$$|\alpha\rangle = \frac{i}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle$$

$$\langle\uparrow|\alpha\rangle = \frac{i}{\sqrt{2}}\langle\uparrow|\uparrow\rangle - \frac{1}{\sqrt{2}}\langle\uparrow|\downarrow\rangle = \frac{i}{\sqrt{2}}$$

$$|\alpha\rangle \doteq \vec{\Psi}_\alpha = \begin{bmatrix} \langle e^1|\alpha\rangle \\ \langle e^2|\alpha\rangle \\ \vdots \end{bmatrix} \qquad \langle\beta| \doteq \vec{\Psi}_\beta = \begin{bmatrix} \langle\beta|e_1\rangle & \langle\beta|e_2\rangle & \cdots \end{bmatrix}$$

$$|\alpha\rangle \Rightarrow \langle\alpha|$$

$$c^i \qquad c_i \qquad c_i = (c^i)^*$$

Spin $\frac{1}{2}$ system

$$\underset{\text{spin in}}{|\otimes\rangle} = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle) \doteq \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

$$\langle\otimes| = \frac{1}{\sqrt{2}}(\langle\uparrow| - i\langle\downarrow|) \doteq \frac{1}{\sqrt{2}}[1 \ -i]$$

$$\langle\otimes|\otimes\rangle = \frac{1}{2}[1 \ -i]\begin{bmatrix} 1 \\ i \end{bmatrix} = 1$$

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$$

Positive ~~Defit~~ Definiteness $\langle\alpha|\alpha\rangle \geq 0 \qquad \langle\alpha|\alpha\rangle = 0$ iff $|\alpha\rangle = 0$

Operators: $\mathcal{H}\to$ $\mathcal{H} \to \mathcal{H}$

$\hat{A}$

$$\underbrace{|\alpha\rangle\langle\beta|}_{\text{Outer product}}$$

Operator basis $|e_i\rangle\langle e^j|$

$$\hat{A} = \sum_{ij} A^i_j \, |e_i\rangle\langle e^j| \;, \quad A^i_j \in \mathbb{C} \;, \quad \langle e^i|\hat{A}|e_j\rangle = A^i_j$$

$$\hat{A} \doteq \overset{\leftrightarrow}{A} = \begin{bmatrix} A^1_1 & A^1_2 & \cdots & A^1_N \\ \vdots & & \ddots & \vdots \\ A^N_1 & \cdots & \cdots & A^N_N \end{bmatrix}$$

$$\hat{\mathbb{1}} = \sum_i |e_i\rangle\langle e^i|$$

Resolution of the identity

Commutator

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$|x\rangle$

Positron eigenket

$$\hat{\mathbb{1}} = \int_{-\infty}^{\infty} |x\rangle\langle x| \, dx$$

$$\mathbb{1}|\alpha\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\alpha\rangle \, dx$$

$\langle x|\alpha\rangle = \psi_\alpha(x)$ the wave function

$$1 = \int_{-\infty}^{\infty} |\psi_\alpha(x)|^2 dx$$

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$$\hat{A}|\psi\rangle = \lambda|\psi\rangle$$

$\hat{A} \doteq \overleftrightarrow{A}$ λ an eigenvalue $\Rightarrow \det(\overleftrightarrow{A} - \lambda \overleftrightarrow{\mathbb{1}}) = 0$

$\pm\prod_r (\lambda - \lambda_r)^{N_r} = 0$ N_r multiplicity of root

Indicates Degeneracy

$\hat{A}^\dagger = \hat{A}$

Hermitian

$U^\dagger U = \mathbb{1}$ or $\hat{U}^\dagger = \hat{U}^{-1}$

Unitary

Spin $\frac{1}{2}$ System

$\{|\uparrow\rangle, |\downarrow\rangle\}$ $\mathcal{H}_{1/2} = \mathbb{C}^2$

$$\hat{A} = a|\uparrow\rangle\langle\uparrow| + \overset{c}{\cancel{a}}|\downarrow\rangle\langle\uparrow| + b|\uparrow\rangle\langle\downarrow| + d|\downarrow\rangle\langle\downarrow|$$

$$\doteq \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$\hat{A}^\dagger \doteq \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$$

$$\hat{A} \doteq \begin{bmatrix} a & z \\ z^* & d \end{bmatrix}$$ the most general Hermitian Operator

$$= a\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + b_x\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + b_y\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + b_z\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$= a\overleftrightarrow{\mathbb{1}} + \vec{b}\cdot\vec{\sigma}$$

$a = \frac{1}{2}\operatorname{tr}\overleftrightarrow{A}$ $b = \frac{1}{2}\operatorname{tr}(\vec{\sigma}\overleftrightarrow{A})$

Hydrogen

Energy E   Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2\mu} - \frac{e^2}{4\pi\varepsilon_0 \hat{r}}$

Eigenvalues $E_n = \frac{E_1}{n^2}$ $E_1 = -13.6 eV$

-Magnitude of Orbital Angular Momentum $\hat{L}^2$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$\hat{L}_a = \sum_c \varepsilon_{abc} \hat{x}_a \hat{P}_b$$

$\hat{L}^2 |\alpha\rangle = \hbar^2 l(l+1) |\alpha\rangle$ $l = 0, 1, \dots, n-1$

z component L_z operator $\hat{L}_z$ eigenvalues $\hbar m$ $m = -l, \dots, l$

$\hat{L}_z |\alpha\rangle = \hbar m |\alpha\rangle$

λ_r

$$\hat{P}_r = \sum_{\mu_r = 1}^{N_r} |\lambda_r \mu_r\rangle\langle\lambda_r \mu_r|$$

Hydrogen energy E_2:

$|200\rangle\langle 200| + |21{-1}\rangle\langle 21{-1}|$

$+ |210\rangle\langle 210| + |211\rangle\langle 211|$

$$\hat{A} = \sum_r \lambda_r \hat{P}_r$$

Hydrogen

$$|\alpha\rangle = \frac{1}{\sqrt{3}}|200\rangle - \frac{i}{\sqrt{6}}|21{-1}\rangle - \frac{1}{\sqrt{2}}|31{+1}\rangle$$

$$P(E_2) = \left|\frac{1}{\sqrt{3}}\right|^2 + \left|\frac{-i}{\sqrt{6}}\right|^2 = \frac{1}{3} + \frac{1}{6} = \frac{1}{2}$$

after $\sqrt{\frac{2}{3}}|200\rangle - \frac{i}{\sqrt{3}}|21{-1}\rangle$

$$\frac{d\langle \hat{A}\rangle}{dt} = \left\langle \frac{i}{\hbar}[\hat{H},\hat{A}]\right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t}\right\rangle$$

Angular Momentum

$$\vec{J}$$

$$\Downarrow$$

$$\vec{\hat{J}} = \begin{bmatrix}\hat{J}_x\\ \hat{J}_y\\ \hat{J}_z\end{bmatrix} = \hat{J}_x \check{x} + \hat{J}_y \check{y} + \hat{J}_z \check{z}$$

$$\hat{J}^2 = \sum_a \hat{J}_a^2 \qquad [\hat{J}_a, \hat{J}_b] = \sum_c \varepsilon_{abc} i\hbar \hat{J}_c$$

$$[\hat{J}^2, \hat{J}_a] = 0$$

Orbittal Angular Momentum $\vec{L}$

$$\vec{L} = \vec{X} \times \vec{p}$$

$$\mathcal{H}_{3D} = \mathcal{H}_{radial} \otimes \mathcal{H}_{angular}$$

$$\psi(\vec{x}) =^{ish} R(r)\, Y(\theta,\phi)$$

$$\psi(\vec{x}) = \sum_n a_n R_n(r)\, Y_n(\theta,\phi)$$

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Angular Momentum Commutation Relations

$$[\hat{J}_a, \hat{J}_b] = \sum_c i\hbar\,\varepsilon_{abc}\hat{J}_c \qquad [\hat{J}_a, \hat{J}^2] = 0$$

$$\hat{J}_a = \begin{cases} \hat{J}_1 = \hat{J}_x & a=1 \\ \hat{J}_2 = \hat{J}_y & a=2 \\ \hat{J}_3 = \hat{J}_z & a=3 \end{cases} \qquad \varepsilon_{abc} = \begin{cases} 1 & \text{even permutation} \\ -1 & \text{odd permutation} \\ 0 & \text{else} \end{cases}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Orbital Angular Momentum

$$\hat{\vec{L}} = \hat{\vec{X}} \times \hat{\vec{p}} \Rightarrow \hat{L}_a = \sum_{bc} \varepsilon_{abc}\hat{X}_b p_c$$

$$\hat{L}^2\psi(\vec{r}) = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big)\psi$$

$$\hat{L}_z\psi(\vec{r}) = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\psi$$

Eigenfunctions: Spherical Harmonics $Y_\ell^m(\theta,\phi)$

$$\hat{L}^2 Y_\ell^m(\theta,\phi) = \hbar^2 \ell(\ell+1) Y_\ell^m(\theta,\phi)$$

$$\hat{L}_z Y_\ell^m(\theta,\phi) = \hbar m\, Y_\ell^m(\theta,\phi)$$

$\ell = 0, 1, 2, 3, \ldots$

$m = -\ell, \ldots, \ell$

A ladder operator $\hat{R}$ for an operator $\hat{A}$

$$[\hat{A}, \hat{R}] = r\hat{R}$$

"ladder step"

$$\hat{A}|a\rangle = a|a\rangle$$

$$|b\rangle \equiv \hat{R}|a\rangle$$

$$\hat{A}|b\rangle = (a+r)|b\rangle$$

$$\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$$

$$[\hat{J}^2, \hat{J}_{\pm}] = 0$$

Doesn't change magnitude of angular momentum

$$[\hat{J}_z, \hat{J}_{\pm}] = \pm\hbar \hat{J}_{\cancel{z}\pm}$$

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$$

$$\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$$

$$|j, m_j\rangle$$

$$\hat{J}^2|j, m_j\rangle = \hbar^2 j(j+1)|j, m_j\rangle$$

, $j = 0, 1, 2, 3, \ldots, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$

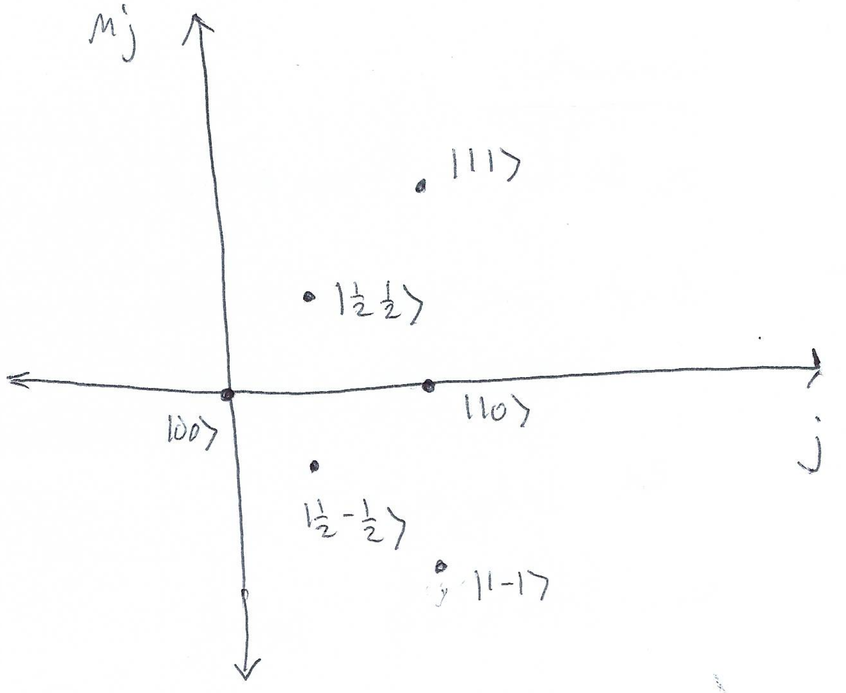
~~$m_j = -j, \ldots, j$~~

$$\hat{J}_z|jm_j\rangle = \hbar m_j|jm_j\rangle$$

$m_j = -j, \ldots, j$

$$\hat{J}_{\pm}|jm_j\rangle = \hbar\sqrt{j(j+1) - m_j(m_j \pm 1)}\,|j, m_j \pm 1\rangle$$

$(2j+1)$ possible m_j values



Spin $\frac{1}{2}$ System

$$\mathcal{H}_{\text{spin }\frac{1}{2}}$$

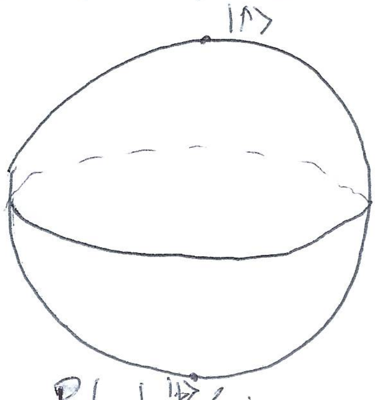
$$|\tfrac{1}{2}\tfrac{1}{2}\rangle \equiv |\uparrow\rangle \doteq \begin{bmatrix}1\\0\end{bmatrix} \qquad |\tfrac{1}{2}-\tfrac{1}{2}\rangle \equiv |\downarrow\rangle \doteq \begin{bmatrix}0\\1\end{bmatrix} \qquad \chi = \begin{bmatrix}a\\b\end{bmatrix} \doteq a|\uparrow\rangle + b|\downarrow\rangle$$

$$\hat{S}_a \doteq \frac{\hbar}{2}\sigma_a \qquad \hat{S}^2 = \frac{3}{4}\hbar^2\hat{\mathbb{1}}$$

$$\langle\vec{S}\rangle = \begin{bmatrix}\langle S_x\rangle\\ \langle S_y\rangle\\ \langle S_z\rangle\end{bmatrix}$$

Spin Polarization vector

spin $\frac{1}{2}$: $|\langle\vec{S}\rangle| = \frac{\hbar}{2}$



Bloch Sphere

System 1	System 2	Combined
$\mathcal{H}_1$ N_1	$\mathcal{H}_2$ N_2	$\mathcal{H}_1 \otimes \mathcal{H}_2$ tensor product space
$\|\alpha\rangle_1$	$\|\beta\rangle_2$	Simple or separable state $\|\alpha\rangle_1 \otimes \|\beta\rangle_2 = \|\alpha, \beta\rangle$
$\{\|e_i\rangle_1\}$	$\{\|f_j\rangle_2\}$	ex. $\|n l m_\ell m_s\rangle$
$\|nlm\rangle$	$\|\uparrow\rangle, \|\downarrow\rangle$	basis: $\{\|e_i f_j\rangle\}$ $N_1 \times N_2$
$\mathcal{H}_{space}$	$\mathcal{H}_{spin}$	

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Angular Momentum 1

Symbols $\vec{L}$

Hilbert $\mathcal{H}_L$

Basis $|l\, m_l\rangle$

$$[\hat{L}_a, \hat{L}_b] = \sum_c i\hbar \varepsilon_{abc} \hat{L}_c$$

$$[\hat{L}^2, \hat{L}_a] = 0$$

Angular Momentum 2

Symbols S

Hilbert $\mathcal{H}_S$

Basis $|s\, m_s\rangle$

$$[\hat{S}_a, \hat{S}_b] = \sum_c i\hbar \varepsilon_{abc} \hat{S}_c$$

$$[\hat{S}^2, \hat{S}_a] = 0$$

Total Angular Momentum

$$\vec{J} = \vec{L} + \vec{S}$$

$$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$$

$$\mathcal{H}_J = \mathcal{H}_L \otimes \mathcal{H}_S$$

$$[\hat{J}_a, \hat{J}_b] = \sum_c i\hbar \varepsilon_{abc} \hat{J}_c$$

$$[\hat{J}^2, \hat{J}_a] = 0$$

$$[\hat{J}_a, \hat{J}_b] = [\hat{L}_a + \hat{S}_a, \hat{L}_b + \hat{S}_b] = [\hat{L}_a, \hat{L}_b] + [\hat{L}_a, \hat{S}_b] + [\hat{S}_a, \hat{L}_b] + [\hat{S}_a, \hat{S}_b]$$

$$= \sum_c i\hbar \varepsilon_{abc} \hat{L}_c + \sum_c i\hbar \varepsilon_{abc} \hat{S}_c = \sum_c i\hbar \varepsilon_{abc} (\hat{L}_c + \hat{S}_c) = \sum_c i\hbar \varepsilon_{abc} \hat{J}_c$$

Uncoupled Basis of $\mathcal{H}_J$

$$|l,m_l\rangle \otimes |s,m_s\rangle = |l,s,m_l,m_s\rangle$$

$$\{\hat{L}^2, \hat{L}_z, \hat{S}^2, \hat{S}_z\}$$

$$\hat{L}^2|l s m_l m_s\rangle = \hbar l(l+1)|l s m_l m_s\rangle$$

$$\hat{S}^2|l s m_l m_s\rangle = \hbar s(s+1)|l s m_l m_s\rangle$$

$$\hat{L}_z|l s m_l m_s\rangle = \hbar m_l|l s m_l m_s\rangle$$

$$\hat{S}_z|l s m_l m_s\rangle = \hbar m_s|l s m_l m_s\rangle$$

$$\boxed{\begin{matrix}\hat{L}^2 & \hat{S}^2 \\ \hat{L}_z & \hat{S}_z\end{matrix}}\ \begin{matrix}\hat{J}^2 \\ \hat{J}_z\end{matrix} \qquad \begin{matrix}\boxed{\hat{L}^2 \ \ \hat{S}^2 \ \ \hat{J}^2} \\ \hat{L}_z \ \ \hat{S}_z \ \ \boxed{\hat{J}_z}\end{matrix}$$

coupled basis

uncoupled basis

CSCO's

$$\hat{J}^2 = (\hat{\vec{L}} + \hat{\vec{S}})\cdot(\hat{\vec{L}} + \hat{\vec{S}}) = \hat{L}^2 + \hat{S}^2 + 2\hat{\vec{L}}\cdot\hat{\vec{S}}$$

$$\hat{\vec{L}}\cdot\hat{\vec{S}} = \frac{\hat{J}^2 - \hat{L}^2 - \hat{S}^2}{2}$$

Coupled Basis of $\mathcal{H}_J$

$$\{\hat{L}^2, \hat{S}^2, \hat{J}^2, \hat{J}_z\}, \quad |l,s;j,m_j\rangle$$

$$\hat{L}^2|l,s;j,m_j\rangle = \hbar l(l+1)|l,s;j,m_j\rangle$$

$$\hat{S}^2|l,s;j,m_j\rangle = \hbar s(s+1)|l,s;j,m_j\rangle$$

$$\hat{J}^2|l,s;j,m_j\rangle = \hbar j(j+1)|l,s;j,m_j\rangle$$

$$\hat{J}_z|l,s;j,m_j\rangle = \hbar m_j|l,s;j,m_j\rangle$$

$$|l,s;j,m_j\rangle = \sum C_{l's'm_lm_s} |l's'm_lm_s\rangle$$

$C_{l's'm_lm_s} = 0$ if $l \neq l'$ or $s \neq s'$ or $m_j \neq m_l + m_s$, $\hat{J}_z = \hat{L}_z + \hat{S}_z$

$$|l,s;j,m_j\rangle = \sum_{m_l=-l}^{l} C^{lsj}_{m_lm_sm_j} |l,s,m_l,m_s\rangle$$

$$\boxed{C^{lsj}_{m_lm_sm_j} = \langle l s m_l m_s | l s j m_j\rangle = \langle l s m_l m_s | j m_j\rangle}$$

Clebsch Gordan Coefficients

$$\langle j m_j | l s m_l m_s\rangle = \langle l s m_l m_s | j m_j\rangle$$

$|2,1;3 0\rangle$

$l=2, s=1, j=3, m_j=0$

m_l	m_s
~~2~~	~~-2~~
1	-1
0	0
-1	1
~~-2~~	~~2~~

$$= C^{213}_{1-10}|2,1,1,-1\rangle + C^{213}_{000}|2,1,0,0\rangle + C^{213}_{-110}|2,1,-1,1\rangle$$

$$|l,s,m_e,m_s\rangle = \sum_{j=|l-s|}^{l+s} C^{l s j}_{m_e m_s m_j} |l,s;j,m_j\rangle$$

j is an integer if $l+s$ is.

j is a half integer if $l+s$ is.

} $l+s+j$ is always an integer

$$|l-s| \leq j \leq l+s$$

$$\underset{l\ \ s\ \ m_e\ \ m_s}{\left|\tfrac{3}{2},1,\tfrac{1}{2},0\right\rangle} = C^{\frac{3}{2}\,1\,\frac{1}{2}}_{\frac{1}{2}\,0\,\frac{1}{2}} \left|\tfrac{3}{2},1;\tfrac{1}{2},\overset{\frac{1}{2}}{\cancel{0}}\right\rangle + C^{\frac{3}{2}\,1\,\frac{3}{2}}_{\frac{1}{2}\,0\,\frac{1}{2}} \left|\tfrac{3}{2},1;\tfrac{3}{2},\overset{\frac{1}{2}}{\cancel{0}}\right\rangle$$

$$+ C^{\frac{3}{2}\,1\,\frac{5}{2}}_{\frac{1}{2}\,0\,\frac{1}{2}} \left|\tfrac{3}{2},1;\tfrac{5}{2},\overset{\frac{1}{2}}{\cancel{0}}\right\rangle$$

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$$\vec{L}+\vec{S}=\vec{J} \qquad C^{lsj}_{m_l m_s m_j} = \langle l s m_l m_s | j m_j \rangle$$

$$= \langle j m_j | l s m_l m_s \rangle$$

$$|l s j m_j\rangle = \sum_{m_l}{}' |l s m_l m_s\rangle\langle l s m_l m_s | j m_j\rangle$$

$$|l s m_l m_s\rangle = \sum_{j}{}' |l s j m_j\rangle\langle j m_j | l s m_l m_s\rangle$$

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

$l \times s$	j m_j
$m_l \; m_s$	coefficient

$$\left\langle 1, \tfrac{3}{2}, 1, \tfrac{1}{2} \middle| \tfrac{5}{2}, \tfrac{3}{2} \right\rangle = (-1)^0 \left\langle \tfrac{3}{2}, 1, \tfrac{1}{2}, 1 \middle| \tfrac{5}{2}, \tfrac{3}{2} \right\rangle = \sqrt{\tfrac{3}{5}}$$

$$\langle s\, l\, m_s\, m_l | j\, m_j \rangle = \langle l\, s\, m_l\, m_s | j\, m_j \rangle (-1)^{j-l-s}$$

$$\left|\tfrac{3}{2}, 1; \tfrac{1}{2}, 0\right\rangle = \sqrt{\tfrac{3}{5}}\left|\tfrac{3}{2}, 1; \tfrac{5}{2}, \tfrac{1}{2}\right\rangle + \frac{1}{\sqrt{15}}\left|\tfrac{3}{2}, 1; \tfrac{3}{2}, \tfrac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left|\tfrac{3}{2}, 1; \tfrac{1}{2}, \tfrac{1}{2}\right\rangle$$

$l \quad s \quad m_l \quad m_s$

uncoupled

$|\uparrow\uparrow\rangle$

$|\uparrow\downarrow\rangle$

$|\downarrow\uparrow\rangle$

$|\downarrow\downarrow\rangle$

get jumbled under rotations

Coupled

$\boxed{|00\rangle}$ invariant under rotation

$|11\rangle$

$|10\rangle$

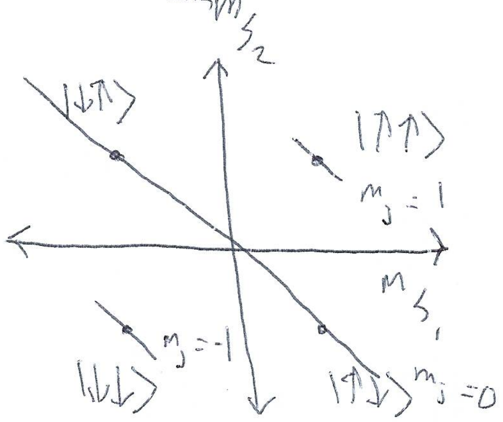
$|1\ -1\rangle$

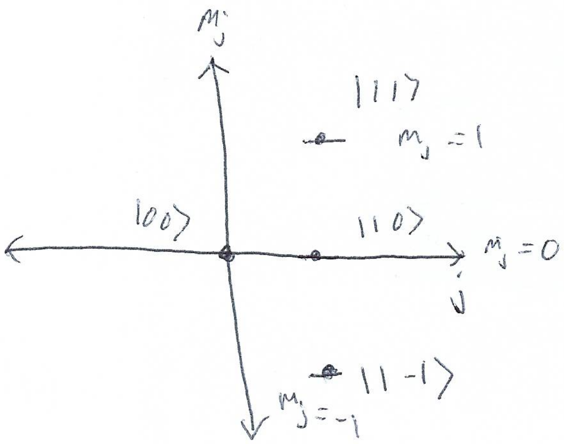
jumbled up amongst each other under rotation

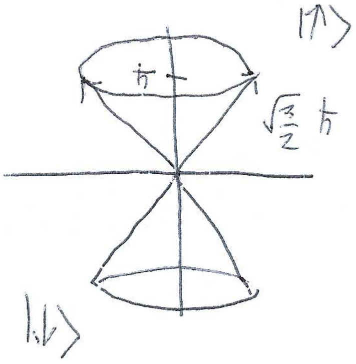
$$\mathcal{H}_{1/2} \otimes \mathcal{H}_{1/2} = \mathcal{H}_0 \oplus \mathcal{H}_1$$

$$2 \times 2 = 1 + 3$$

$= 4$ dimensions







$|00\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

$|11\rangle = |\uparrow\uparrow\rangle$

$|10\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$

$|1 -1\rangle = |\downarrow\downarrow\rangle$

$|11\rangle$ stretch state $j = l+s$, $m_j = +j$

$|11\rangle = |\uparrow\uparrow\rangle$

~~$\hat{J}_-|11\rangle = |10\rangle$~~

$\hat{J}_-|11\rangle = \hat{J}_-|\uparrow\uparrow\rangle$

$\hbar\sqrt{j(j+1) - m_j(m_j-1)}\ |10\rangle = \hat{S}_{1-}|\uparrow\uparrow\rangle + \hat{S}_{2-}|\uparrow\uparrow\rangle = \hbar|\downarrow\uparrow\rangle + \hbar|\uparrow\downarrow\rangle$

$= \hbar\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)$

$\sqrt{2}\hbar\,|10\rangle = \hbar\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)$

$|10\rangle = \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)$

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Two spin $\frac{1}{2}$ system

$$\vec{S}_1 + \vec{S}_2 = \vec{J}$$

$$S_1 = S_2 = \frac{1}{2}$$

Uncoupled

$$|\uparrow\uparrow\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}, m_{s_1} = \tfrac{1}{2}, m_{s_2} = \tfrac{1}{2}\rangle \doteq \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$

$$|\uparrow\downarrow\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}, m_{s_1} = \tfrac{1}{2}, m_{s_2} = -\tfrac{1}{2}\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$|\downarrow\uparrow\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}, m_{s_1} = -\tfrac{1}{2}, m_{s_2} = \tfrac{1}{2}\rangle = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$$

$$|\downarrow\downarrow\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}, m_{s_1} = -\tfrac{1}{2}, m_{s_2} = -\tfrac{1}{2}\rangle \doteq \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

Coupled

Singlet $|00\rangle = |s_1 = \frac{1}{2}, s_2 = \frac{1}{2}; j = 0, m_j = 0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \doteq \begin{bmatrix}0\\ \frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\\ 0\end{bmatrix}$

Triplets

$$\begin{cases} |11\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}; j = 1, m_j = 1\rangle = |\uparrow\uparrow\rangle \doteq \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \\ |10\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}; j = 1, m_j = 0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \doteq \begin{bmatrix}0\\ \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\\ 0\end{bmatrix} \\ |1\,{-1}\rangle = |s_1 = \tfrac{1}{2}, s_2 = \tfrac{1}{2}; j = 1, m_j = -1\rangle = |\downarrow\downarrow\rangle \doteq \begin{bmatrix}0\\0\\0\\1\end{bmatrix} \end{cases}$$

$$\hat{H}_{\text{spin spin}} = A\, \hat{\vec{S}}_e \cdot \hat{\vec{S}}_p$$

$$\vec{S}_e |\uparrow\rangle_e = \frac{\hbar}{2}\begin{bmatrix}|\downarrow\rangle\\ i|\downarrow\rangle\\ |\uparrow\rangle\end{bmatrix} \qquad \hat{\vec{S}}|\downarrow\rangle_e = \frac{\hbar}{2}\begin{bmatrix}|\uparrow\rangle\\ -i|\uparrow\rangle\\ -|\downarrow\rangle\end{bmatrix}$$

$$\hat{H}|\uparrow\downarrow\rangle = A\left(\hat{\vec{S}}_e|\uparrow\rangle\right)\cdot\otimes\left(\hat{\vec{S}}_p|\downarrow\rangle\right)$$

$$= A\frac{\hbar^2}{4}\left(|\downarrow\uparrow\rangle + |\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle\right)$$

$$\hat{H} \doteq \begin{array}{c|cccc} & |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ \hline \langle\uparrow\uparrow| & 1 & 0 & 1 & 0 \\ \langle\uparrow\downarrow| & 0 & -1 & 2 & 0 \\ \langle\downarrow\uparrow| & 0 & 2 & -1 & 0 \\ \langle\downarrow\downarrow| & 0 & 0 & 0 & 1 \end{array} \frac{A\hbar^3}{4}$$

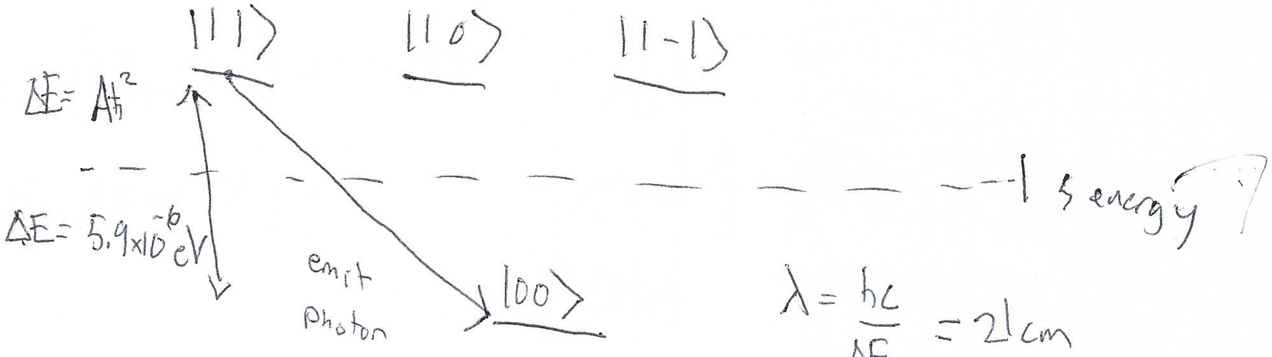
$$\hat{\vec{S}}_e \cdot \hat{\vec{S}}_p = \frac{\hat{J}^2 - \hat{S}_e^2 - \hat{S}_p^2}{2}$$

$$\hat{H}_{spinspin} |j m_j\rangle = \hat{H}_{spinspin} |s_e, s_p, j, m_j\rangle$$

$$A \frac{\hat{J}^2 - \hat{S}_e^2 - \hat{S}_p^2}{2} |s_e, s_p, j, m_j\rangle = \cancel{A\hbar^2}$$

$$= A\hbar^2 \frac{j(j+1) - \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}+1)}{2} = A\hbar^2\left(j(j+1) - \frac{3}{2}\right) |s_e, s_p, j, m_j\rangle$$

$$\hat{H}_{ss} \doteq \left[\begin{array}{c|ccc} -3 & 0 & 0 & 0 \\ \hline 0 & & & \\ 0 & & +\hat{1} & \\ 0 & & & \end{array}\right]$$



$$\lambda = \frac{hc}{\Delta E} = 21\,\text{cm}$$

$$|\text{post transition}\rangle = \sum c \left|\begin{array}{c}\text{electrons final}\\ \text{spin state}\end{array}\right\rangle \otimes \left|\begin{array}{c}\text{photon spin}\\ \text{state}\end{array}\right\rangle = \left|\begin{array}{c}\text{coupled state with}\\ \text{some } j\ m_j \text{ quantum}\\ \text{numbers as initial electron}\end{array}\right\rangle$$

$$= \widetilde{\left|\begin{array}{c}\text{initial electron}\\ \text{spin state}\end{array}\right\rangle}$$

Multiple Particles

Two particle System

A, B

$\vec{r}_A \quad \vec{r}_B$

$\mathcal{H}_A$ - Hilbert space for particle A with basis $|\hat{e}_i\rangle_A$ and state $|\alpha\rangle_A$

$\mathcal{H}_B$ - Hilbert space for particle B with basis $|f_j\rangle_B$ and state $|\beta\rangle_B$

$|\vec{r}_A\rangle_A \quad |\vec{r}_B\rangle_B$

$$\psi_\alpha(\vec{r}_A) = \langle \vec{r}_A | \alpha \rangle$$

$$\psi_\beta(\vec{r}_B) = \langle \vec{r}_B | \beta \rangle$$

$|\vec{r}_A, \vec{r}_B\rangle$

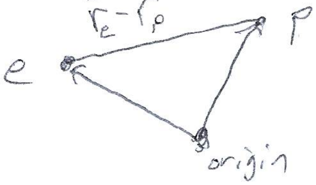
$$\psi_{state}(\vec{r}_A, \vec{r}_B) = \langle \vec{r}_A \vec{r}_B | state \rangle$$

$$|state\rangle = |\alpha, \beta\rangle = |\alpha\rangle \otimes |\beta\rangle$$

$$\psi_{state} = \psi_{\alpha\beta} = \langle \vec{r}_A, \vec{r}_B | \alpha, \beta \rangle = \langle \vec{r}_A | \alpha \rangle \langle \vec{r}_B | \beta \rangle = \psi_\alpha(\vec{r}_A)\psi_\beta(\vec{r}_B)$$

Hydrogen

$$\hat{H} = \frac{\hat{p}_e^2}{2m_e} + \frac{\hat{p}_p^2}{2m_p} + V(\hat{\vec{r}}_e, \hat{\vec{r}}_p)$$



$$-\frac{\hbar^2}{2m_e}\nabla_e^2\psi(\vec{r}_e, \vec{r}_p) - \frac{\hbar^2}{2m_p}\nabla_p^2\psi(\vec{r}_e, \vec{r}_p) - \frac{e^2\psi(\vec{r}_e, \vec{r}_p)}{4\pi\epsilon_0|\vec{r}_e - \vec{r}_p|} = E\psi(\vec{r}_e, \vec{r}_p)$$

$$V(\hat{\vec{r}}_e, \hat{\vec{r}}_p) = \frac{-e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_e - \vec{r}_p|}$$

$$\hat{\vec{r}} \equiv \hat{\vec{r}}_e - \hat{\vec{r}}_p$$

$$\hat{\vec{R}} \equiv \frac{m_e\vec{r}_e + m_p\vec{r}_p}{m_e + m_p}$$

$$M = m_e + m_p$$

$$\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_p}$$

$$\hat{H} = \frac{\hat{P}_R^2}{2M} + \frac{\hat{p}_r^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}}$$

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Systems of Identical Particles

$$\mathcal{H}_{3D} = L^2(\mathbb{R}^3)$$

Let $\mathcal{H}_1 = \mathcal{H}_2$ = some common Hilbert space and consider $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$

eg) $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$

$|\uparrow\uparrow\rangle$
$|\uparrow\downarrow\rangle$
$|\downarrow\uparrow\rangle$
$|\downarrow\downarrow\rangle$

Exchange Operator

(an example of a Permutation Operator)

$$\hat{P}_{1\leftrightarrow 2} |\alpha, \beta\rangle = |\beta, \alpha\rangle$$

particle 1 in $|\alpha\rangle_1 \in \mathcal{H}_1$
particle 2 in $|\beta\rangle_2 \in \mathcal{H}_2$

$$\hat{P}_{1\leftrightarrow 2} |\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$$

$$\hat{P}_{1\leftrightarrow 2} |\uparrow\downarrow\rangle = |\downarrow\uparrow\rangle$$

$$\hat{P}_{1\leftrightarrow 2} |\downarrow\uparrow\rangle = |\uparrow\downarrow\rangle$$

$$\hat{P}_{1\leftrightarrow 2} |\downarrow\downarrow\rangle = |\downarrow\downarrow\rangle$$

Property 1 $\hat{P}_{1\leftrightarrow 2}$ is unitary

$$\hat{P}_{1\leftrightarrow 2}\Psi_\alpha(\vec{r}_1,\vec{r}_2) = \Psi_\alpha(\vec{r}_2,\vec{r}_1)$$

$$\hat{P}^2_{1\leftrightarrow 2} = \hat{\mathbb{1}}$$

$\hat{P}_{1\leftrightarrow 2}$ is Hermitian

Eigenvalues of $\hat{P}_{1\leftrightarrow 2}$ $\lambda = \pm 1$

+1) "symmetric"

-1) "anti-symmetric"

$$\hat{P}_{1\leftrightarrow 2}|11\rangle = \hat{P}_{1\leftrightarrow 2}|\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle = +|11\rangle$$

$$\hat{P}_{1\leftrightarrow 2}|10\rangle = \hat{P}_{1\leftrightarrow 2}\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\right) = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) = +|10\rangle$$

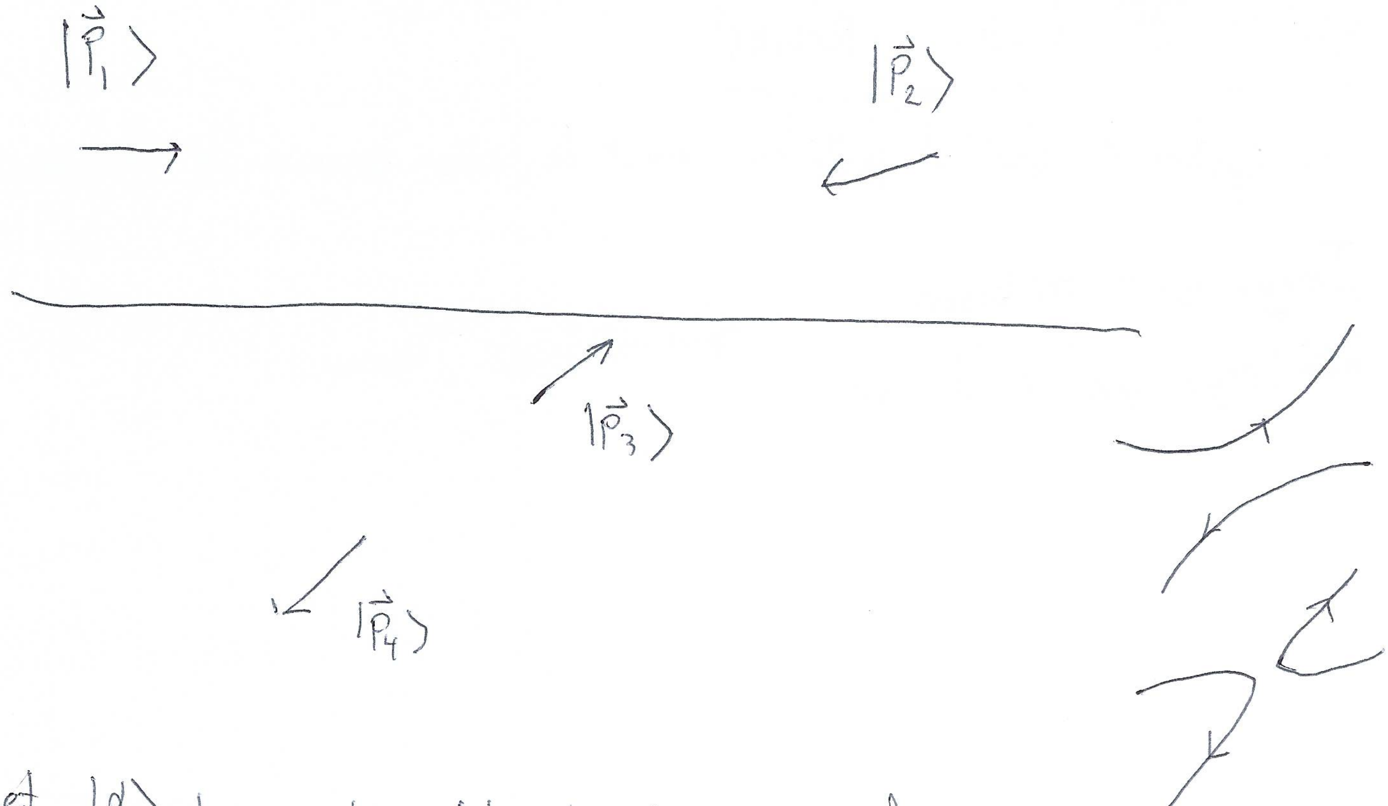
$$\hat{P}_{1\leftrightarrow 2}|1-1\rangle = \hat{P}_{1\leftrightarrow 2}|\downarrow\downarrow\rangle = |\downarrow\downarrow\rangle = +|1-1\rangle$$

$$\hat{P}_{1\leftrightarrow 2}|00\rangle = \hat{P}_{1\leftrightarrow 2}\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right) = \left(\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)\right) = -|00\rangle$$

Two particle Exchange Projectors

$$\hat{P}_{sym} = \frac{1}{2}(\hat{\mathbb{1}} + \hat{P}_{1\leftrightarrow 2}) \qquad |\alpha,\beta\rangle \Rightarrow \frac{1}{2}(|\alpha\beta\rangle + |\beta\alpha\rangle)$$

$$\hat{P}_{antisym} = \frac{1}{2}(\hat{\mathbb{1}} - \hat{P}_{1\leftrightarrow 2}) \qquad \Rightarrow \frac{1}{2}(|\alpha\beta\rangle - |\beta\alpha\rangle)$$



Let $|\alpha\rangle$ be a two particle state for a pair of identical/indistinguishable particles

$$\hat{P}_{1\leftrightarrow 2}|\alpha\rangle = \underbrace{e^{i\phi}}_{\text{Can only be } \pm 1}|\alpha\rangle$$

⇒ Any physical state for a pair of identical particles must be an eigenstate of $\hat{P}_{1\leftrightarrow 2}$

If I have a multiparticle system and I add the requirement that all physical states must be completely symmetric under exchange of any pair of particles $(\lambda = 1)$ then the behavior of the system is said to obey Bose-Einstein statistics

If The ~~antsym~~ antisymmetric condition, the system obeys Fermi-Dirac statistics

Postulate VII (Identical Particles)

A system of identical particles must be either bosonic or fermionic

Integer spin ⇒ boson
Half integer spin ⇒ fermion

Spin statistics Theorem

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$\mathcal{H}_{one}$ - one particle Hilbert Space

$\mathcal{H}_{two} = \mathcal{H}_{one} \otimes \mathcal{H}_{one}$

Define $\mathcal{H}_S$ = states symmetric under exchange +1 eigenspace of $\hat{P}_{A\leftrightarrow B}$

$\mathcal{H}_{AS}$ = states antisymmetric under exchange -1 eigenspace of $\hat{P}_{A\leftrightarrow B}$

Bosons (s = integer): the state space is $\mathcal{H}_S$

Fermions (s = half integer): the state space is $\mathcal{H}_{AS}$

Our "Good" observables/operators have to keep us in $\mathcal{H}_S$ for bosons or $\mathcal{H}_{AS}$ for fermions

$\Rightarrow$ any "good" Operator $\hat{A}$ must commute with the exchange operator

$$[\hat{A}, \hat{P}_{A\leftrightarrow B}] = 0$$

$$\hat{P}^{\dagger}_{A\leftrightarrow B}\hat{A}\hat{P}^{\dagger}_{A\leftrightarrow B} = \hat{A}$$

$\hat{A}$ is invariant under exchange

$$\hat{P}^{\dagger}_{A\leftrightarrow B}\,\hat{X}_A\,\hat{P}_{A\leftrightarrow B} = \hat{X}_B$$

$\vec{J} = \vec{S}_A + \vec{S}_B$ is a good operator

$$\mathcal{H}_{one} = \mathcal{H}^{space} \otimes \mathcal{H}^{spin}$$

$$\mathcal{H}_{two} = \left(\mathcal{H}^{space}_{A} \otimes \mathcal{H}^{spin}_{A}\right) \otimes \left(\mathcal{H}^{space}_{B} \otimes \mathcal{H}^{spin}_{B}\right)$$

$$= \underbrace{\mathcal{H}^{space}_{two}}_{\psi(x_A, x_B)} \otimes \underbrace{\mathcal{H}^{spin}_{two}}_{\chi_{A,B}} \leftarrow |\uparrow\downarrow\rangle$$

$$\hat{P}^{space}_{A\leftrightarrow B}$$

$$\hat{P}^{spin}_{A\leftrightarrow B}$$

$L_1 \; S_1$

$L_2 \; S_2$

$\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 \qquad \hat{\vec{L}}_1 \cdot \hat{\vec{S}}_1 + \hat{\vec{L}}_2 \cdot \hat{\vec{S}}_2$

$\hat{\vec{L}}_1 \cdot \hat{\vec{L}}_2 \qquad \hat{\vec{L}}_1 \cdot \hat{\vec{S}}_2 + \hat{\vec{L}}_2 \cdot \hat{\vec{S}}_1$

2 spin $\frac{1}{2}$ particles in a SHO

A: $|0, \uparrow\rangle$ B: $|1, \downarrow\rangle$

$|state\rangle = |0, 1, \uparrow, \downarrow\rangle \qquad \hat{P}_{A\leftrightarrow B} = \hat{P}^{space}_{A\leftrightarrow B}\,\hat{P}^{spin}_{A\leftrightarrow B}$

$\hat{P}^{space}_{A\leftrightarrow B}|state\rangle = |1, 0, \uparrow, \downarrow\rangle$

$\hat{P}^{spin}_{A\leftrightarrow B}|state\rangle = |0, 1, \downarrow, \uparrow\rangle$

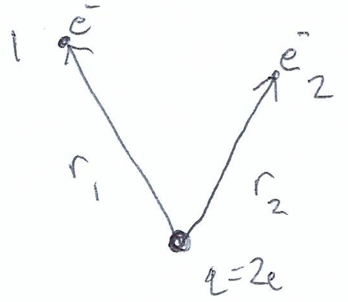
$\hat{H}$ must commute with exchange $\hat{P}_{A\leftrightarrow B}$

but often also commutes separately with $P^{space}_{A\leftrightarrow B}$ and $P^{spin}_{A\leftrightarrow B}$

Helium 2 identical electrons in a hydrogen like potential

$q = 2e$

$$\hat{H} = \frac{\hat{P}_1^2}{2m_e} + \frac{-2e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}_1} + \frac{\hat{P}_2^2}{2m_e} - \frac{2e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}_2} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}$$



$\hat{H}$, $P^{space}_{A\leftrightarrow B}$, $P^{spin}_{A\leftrightarrow B}$

~~Bosons~~	$\hat{P}_{A\leftrightarrow B}$	$P^{space}_{A\leftrightarrow B}$	$P^{spin}_{A\leftrightarrow B}$
		+1	+1
Bosons	+1 (sym)	-1	-1
		+1	-1
Fermions	-1 (antisym)	-1	+1

Spin States

Use coupled basis $|j, m_j\rangle$

Spin	symmetric	antisymmetric
$s=0$	$j=0$	N/A
$s=\frac{1}{2}$	$j=1$	$j=0$
$s=1$	$j=2$ $j=0$	$j=1$
$s=\frac{3}{2}$	$j=3$ $j=1$	$j=2$ $j=0$

2 spin 0 (bosons): $\begin{pmatrix}\text{space}\\ \text{sym}\end{pmatrix} \otimes (j=0)$

2 spin ½ (fermions) : $\begin{pmatrix}\text{space}\\ \text{sym}\end{pmatrix} \otimes (j=0)$ or $\begin{pmatrix}\text{space}\\ \text{antisym}\end{pmatrix} \otimes (j=1)$

$\psi_a(x) = \langle x|a\rangle \quad \psi_b(x) = \langle x|b\rangle \quad \langle a|b\rangle = 0$

$\psi_D(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$

$\psi_{\substack{S\\ AS}}(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\psi_a(x_1)\psi_b(x_2) \pm \psi_a(x_2)\psi_b(x_1)\right)$

$\langle r^2\rangle \equiv \langle (x_1 - x_2)^2\rangle$

$$\langle r^2\rangle_D = \langle x^2\rangle_a + \langle x^2\rangle_b - 2\langle x\rangle_a \langle x\rangle_b$$

$$\langle r^2\rangle_S = \langle r^2\rangle_D - 2|\langle a|x|b\rangle|^2$$

Exchange Interaction

$$\langle r^2\rangle_{AS} = \langle r^2\rangle_D + 2|\langle a|x|b\rangle|^2$$

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Helium (Z=2)

ion) $$\hat{H}_{He^+} = \frac{\hat{p}^2}{2m_e} + V(\hat{\vec{r}}) \qquad V = -\frac{2e^2}{4\pi\epsilon_0|\vec{r}|}$$

State $|n\,l\,m_e\rangle \otimes |s=\tfrac{1}{2}, m_s\rangle$

$$E_n = \frac{Z^2E_1}{n^2} = \frac{4E_1}{n^2} = \frac{-54.4\,eV}{n^2}$$

atom) 2 electron system

all states must be antisymmetric under exchange of the 2 electrons

$$\hat{H}_{He} = \hat{H}_{He^+,1} + \hat{H}_{He^+,2} + \boxed{\hat{H}_{interact}}$$ → ignore due to lack of tools

~~States: (Spatially~~

States: (Spatially symmetric under exchange) x (Spin antisymmetric)

$$\frac{1}{\sqrt{2}}\left(|n\,l\,m_e\rangle|n'l'm_e'\rangle + |n'l'm_e'\rangle|n\,l\,m_e\rangle\right)|00\rangle$$ "spin singlets"

~~(Spatially antisymmetric) & (spin symmetric)~~

$$\frac{1}{\sqrt{2}}\left(|n\,l\,m_e\rangle|n'l'm_e'\rangle - |n'l'm_e'\rangle|n\,l\,m_e\rangle\right)|1\,m_j\rangle$$ "spin triplets"

$$E_{nn'} = 4E_1\left(\frac{1}{n^2} + \frac{1}{n'^2}\right)$$

if $n = n' = 1$ (two electrons each in a 1s state) $1s^2$

$$\underbrace{|100\rangle|100\rangle}_{\text{space}} \ \underbrace{|00\rangle}_{\text{spin}} \qquad E_{\text{ground}} = -108\,eV$$

$n' = 1, n \neq 1$ $\quad E = 4E_1\left(1 + \frac{1}{n^2}\right) \leq -54.4\,eV$

$n' = 1$ + unbound electron $\quad E = 4E_1 + KE_2 \geq -54.4\,eV$

$n = 2, n' = 2$ $\quad E = 2E_1 =$ ~~27.2~~ $-27.2\,eV$

Helium spatial states

$$\frac{1}{\sqrt{2}}\left(|100\rangle|nlm\rangle \pm |nlm\rangle|100\rangle\right)$$

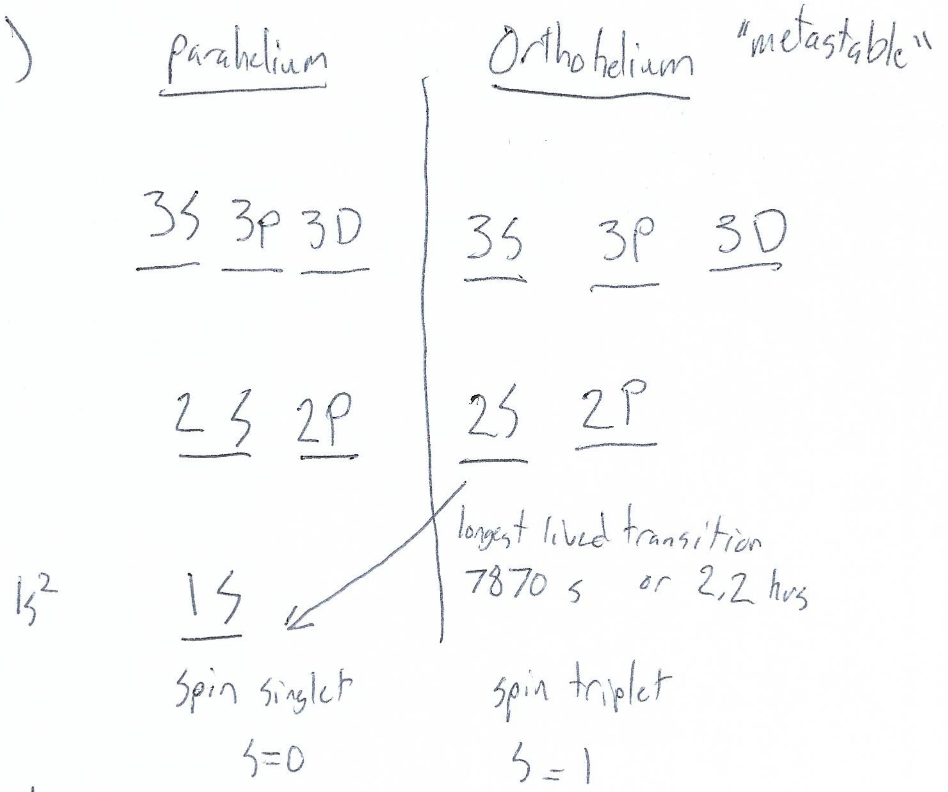
total spin S singlet $S = 0$
triplet $S = 1$

total orbital L since $l' = 0$, $L = l$

total total J

~~1S (n=1, l=0)~~

1S (n=1, l=0)



Russel-Sanders Notation

$$^{2S+1}L_J$$

the total spin multiplet

$|L-S| \leq J \leq L+S$

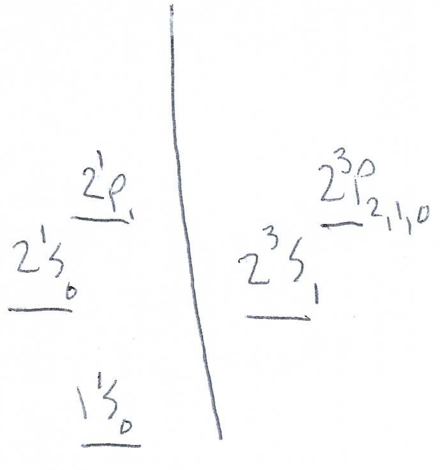
a letter in spectroscopic notation

L = 0 1 2 3 4 5, ...

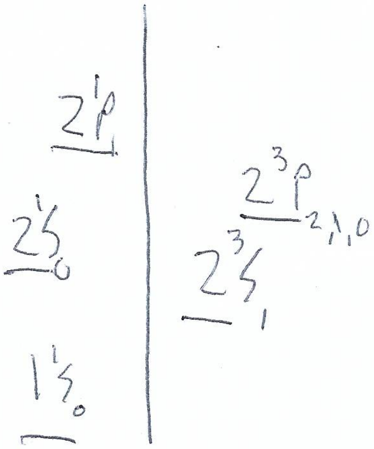
~~[illegible]~~ Letter = S P D F G H I K

$2^1S_0, 2^1P_1$ | $2^3S_1, 2^3P_{2,1,0}$

1^1S_0



Interaction $\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}$



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Even More Identical Particles

N identical particles

$\mathcal{H}_{one}$ - one-particle Hilbert space

$$\mathcal{H}_{enn} \equiv \mathcal{H}_{one} \otimes \mathcal{H}_{one} \otimes \cdots \otimes \mathcal{H}_{one} = \mathcal{H}_{one}^{N}$$

eg. $\mathcal{H}_{three} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$

$\hat{P}_{i \leftrightarrow j}$ exchanges the ith and jth one-particle states

$\frac{N(N-1)}{2}$ different exchanges

Permutations

A permutation, σ, is a shuffling of objects

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{bmatrix}$$

for set of n, there are $n!$ permutations

Permutations of $\{x, y, z\}$

$$\begin{bmatrix} x & y & z \\ x & y & z \end{bmatrix} \begin{bmatrix} x & y & z \\ x & z & y \end{bmatrix} \begin{bmatrix} x & y & z \\ z & y & x \end{bmatrix} \begin{bmatrix} x & y & z \\ y & x & z \end{bmatrix} \begin{bmatrix} x & y & z \\ y & z & x \end{bmatrix} \begin{bmatrix} x & y & z \\ z & x & y \end{bmatrix}$$

Under any permutation, boson states are symmetric and fermion states ~~are ant~~ have eigenvalue $\mathrm{sgn}(\sigma)$

Let $|\alpha_i\rangle_j$ be the state "particle j is in a state i"

$$|\text{fermion}\rangle = \frac{1}{\sqrt{N!}} \sum_{\sigma} \mathrm{sgn}(\sigma) |\alpha_{\sigma(1)} \cdots \alpha_{\sigma(N)}\rangle$$

$|\alpha\rangle_1 \; |\beta\rangle_2 \; |\gamma\rangle_3$.

$$|\text{fermion}\rangle = \frac{1}{\sqrt{6}}\left(|\alpha\beta\gamma\rangle - |\alpha\gamma\beta\rangle - |\gamma\beta\alpha\rangle - |\beta\alpha\gamma\rangle + |\beta\gamma\alpha\rangle + |\gamma\alpha\beta\rangle \right)$$

The "Slater Determinant"

$|\alpha\rangle_1 , |\beta\rangle_2 , |\gamma\rangle_3$

$$|\text{fermion}\rangle = \frac{1}{\sqrt{N!}} \det\left(\begin{bmatrix} |\alpha\rangle_1 & |\beta\rangle_1 & |\gamma\rangle_1 \\ |\alpha\rangle_2 & |\beta\rangle_2 & |\gamma\rangle_2 \\ |\alpha\rangle_3 & |\beta\rangle_3 & |\gamma\rangle_3 \end{bmatrix} \right) = \frac{1}{\sqrt{6}}\Big(|\alpha\beta\gamma\rangle - |\alpha\gamma\beta\rangle - |\beta\alpha\gamma\rangle + |\beta\gamma\alpha\rangle + |\gamma\alpha\beta\rangle - |\gamma\beta\alpha\rangle \Big)$$

Lithium ($Z = 3$) 3 electron system

	Spatial state	Spin state
$1s^3$	$\|100\rangle\|100\rangle\|100\rangle$	totally antisymmetric spin state does not exis } forbidden
$1s^2 2s$	$\|100\rangle\|100\rangle\|200\rangle$	$\frac{1}{\sqrt{2}}(\|\uparrow\downarrow\uparrow\rangle - \|\downarrow\uparrow\uparrow\rangle)$
	$\|100\rangle\|200\rangle\|100\rangle$	$\frac{1}{\sqrt{2}}(\|\uparrow\uparrow\downarrow\rangle - \|\downarrow\uparrow\uparrow\rangle)$
	$\|200\rangle\|100\rangle\|100\rangle$	$\frac{1}{\sqrt{2}}(\|\uparrow\uparrow\downarrow\rangle - \|\uparrow\downarrow\uparrow\rangle)$

~~$\Rightarrow \frac{1}{\sqrt{6}}$~~

$$\Rightarrow \; 1s^2 2s = \frac{1}{\sqrt{6}}\Big(|100\rangle|100\rangle|200\rangle\big(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle\big) + - |100\rangle|200\rangle|100\rangle\big(|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle\big)$$
$$+ |200\rangle|100\rangle|100\rangle\big(|\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle\big)\Big)$$

$${}^{2s+1}L_J \qquad s=\frac{1}{2} \quad L=0 \qquad \boxed{{}^2S_{1/2}}$$

Periodic Table

$$\hat{H}_i = \frac{\hat{p}_i^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0|\hat{r}_i|} \qquad i = 1, \ldots, Z$$

$$\hat{H}_{ij} = \frac{e^2}{4\pi\epsilon_0|\hat{\vec{r}}_i - \hat{r}_j|}$$

$$\hat{H}_Z = \sum_{i=1}^{Z} \hat{H}_i + \sum_{i<j} \hat{H}_{ij}$$

Hund's Rules for the ground state (not perfect, are exceptions)

1) For a given configuration ~~of~~, states with the highest total spin S have the lowest energy. Helium $1s\,2p$ $\quad {}^1P_1 \quad \underbrace{{}^3P_0 \quad {}^3P_1 \quad {}^3P_2}_{\text{less energy}}$ than ${}^1P_1$

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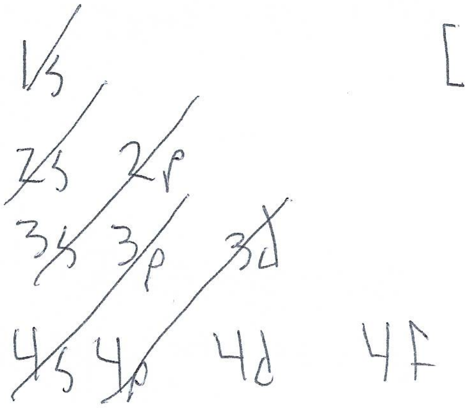
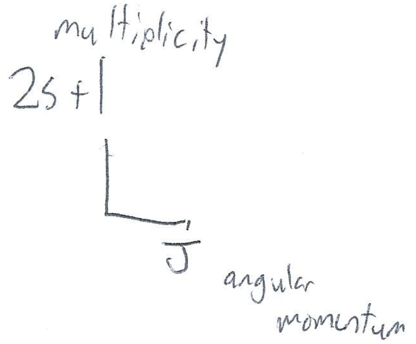
Molybdenum

$Z = 42$

$[1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6] 5s^1 4d^5$

$[Kr] 5s^1 4d^5$





$L = 0 \; 1 \; 2 \; 3 \; 4$

$\;\;\;\;\; S \; P \; D \; F \; G$

For any filled subshell (ns^2, np^6, nd^{10}, etc.)

$S = L = J = 0$

Silicon $(Z = 14)$

$1s^2 2s^2 2p^6 3s^2 3p^2$

$3p^2$ 2 electrons in p subshell

total spin: 0, 1

total orbital: 0, 1, 2

$\cancel{^1S}$

$^1S_0 \qquad \cancel{^3S_1}$

$\cancel{^1P_1} \qquad {^3P_{0,1,2}}$

$^1D_2 \qquad \cancel{^3D_{1,2,3}}$

crossed out due to symmetry

Hund's first Rule (S)

for a given configuration the lowest energy goes with the highest S.

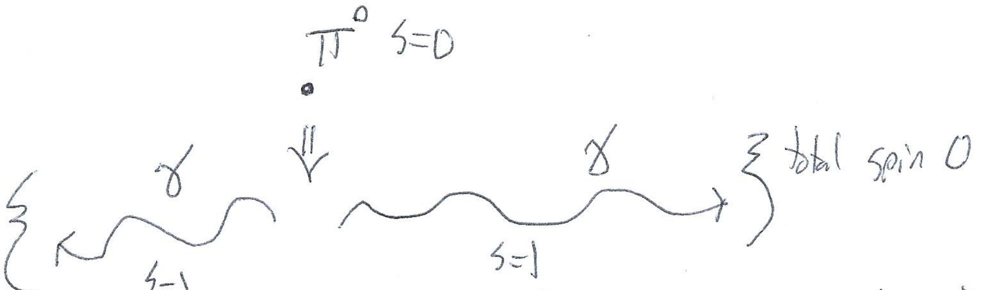
Hund's Second Rule (L)

Given a configuration and an S value, the lowest energy goes to the largest L

Hund's Third Rule (J)

Given a configuration with all but possibly one subshell filled the lowest energy state is $J \begin{cases} L+S & \text{the subshell is more than half full} \\ |L-S| & \text{the subshell is less than half full or exactly half full} \end{cases}$

EPR Experiment

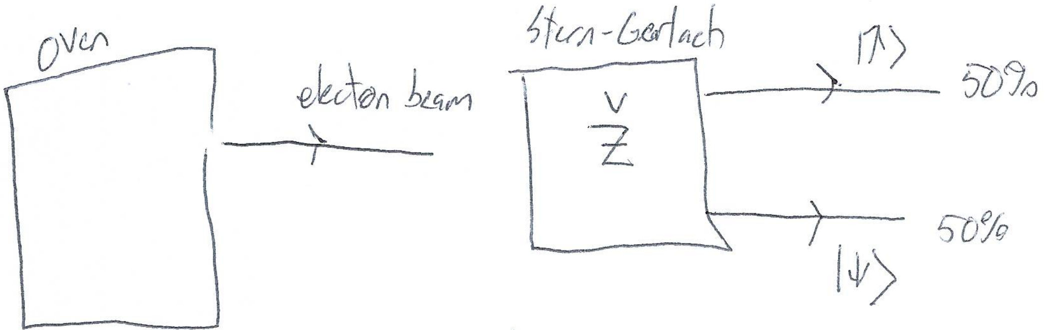


$\frac{1}{\sqrt{3}}(|1,-1\rangle - |0,0\rangle + |-1,1\rangle)$

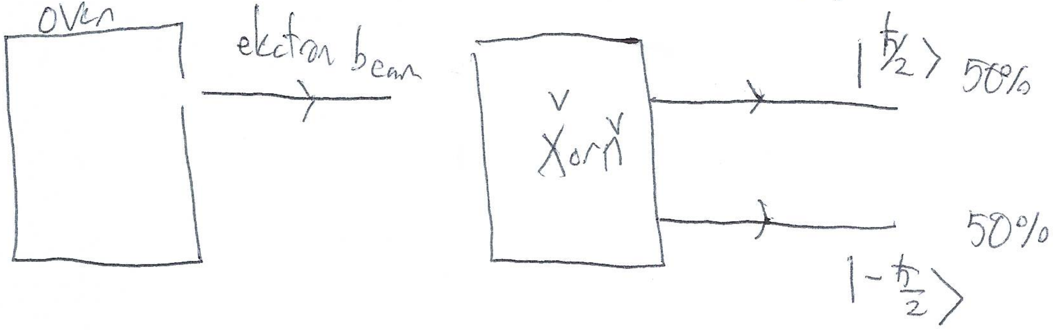
$|m_{s_1}, m_{s_2}\rangle$

↳ doesn't occur

$\frac{1}{\sqrt{2}}(|1,-1\rangle + |-1,1\rangle)$



$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + e^{i\phi}|\downarrow\rangle\right)$$



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The Density Operator

Pure State $|\alpha\rangle$

$\Rightarrow$ density operator $\hat{\rho} \equiv |\alpha\rangle\langle\alpha|$

Spin $\frac{1}{2}$ Basis $\{|\uparrow\rangle, |\downarrow\rangle\}$

$$|\uparrow\rangle : \hat{\rho}_{\uparrow} \doteq \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$|\downarrow\rangle : \hat{\rho}_{\downarrow} \doteq \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$|\rightarrow\rangle \text{ or } |\leftarrow\rangle : \hat{\rho}_{\rightarrow} \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$$\hat{\rho}_{\leftarrow} \doteq \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

The Trace

$$\text{Tr}\hat{A} \equiv \sum_i \langle e_i|\hat{A}|e_i\rangle = \sum_i \hat{A}^i_i = \text{Tr}\hat{A} = \underbrace{\sum_i \lambda_i}$$

sum of the eigenvalues

- Linear $\text{Tr}(a\hat{A}_1 + b\hat{A}_2) = a\text{Tr}\hat{A}_1 + b\text{Tr}\hat{A}_2$
- Cyclic $\text{Tr}(\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{B}\hat{C}\hat{A}) = \text{Tr}(\hat{C}\hat{A}\hat{B})$
- Trace of an outerproduct $|\alpha\rangle\langle\beta|$ is the inner product $\langle\beta|\alpha\rangle$

Density Operator

- Hermitian $\hat{\rho}_\alpha^\dagger = \hat{\rho}_\alpha$
- Normalization $Tr\,\hat{\rho}_\alpha = 1$
- (Pure states only) Idempotent $\hat{\rho}_\alpha^2 = \hat{\rho}_\alpha \Rightarrow Tr\,\hat{\rho}_\alpha^2 = 1$

Expectation Value

$$\langle A \rangle = \langle \alpha | \hat{A} | \alpha \rangle = Tr(\hat{A}|\alpha\rangle\langle\alpha|) = Tr(\hat{A}\hat{\rho}_\alpha)$$

$$\langle S_z \rangle = Tr\left(\frac{\hbar}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\rho\right)$$

$$|\uparrow\rangle: \frac{\hbar}{2} Tr\left(\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\right) = \frac{\hbar}{2} Tr\left(\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\right) = \frac{\hbar}{2}$$

$$|\leftarrow\rangle: \frac{\hbar}{2} Tr\left(\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}\frac{1}{2} & -\frac{1}{2}\\-\frac{1}{2} & \frac{1}{2}\end{bmatrix}\right) = \frac{\hbar}{2} Tr\left(\begin{bmatrix}1/2 & -1/2\\\frac{1}{2} & -\frac{1}{2}\end{bmatrix}\right) = 0$$

Probability of measuring $\hat{A}$ and find result λ
- projection operator $\hat{P}_\lambda$ for the λ eigenspace
- Probability$(\lambda) = \langle \hat{P}_\lambda \rangle = Tr(\hat{\rho}_\alpha \hat{P}_\lambda)$

$$i\hbar \frac{d\hat{\rho}_\alpha}{dt} = [\hat{H}, \rho_\alpha] \qquad |\alpha\rangle \mapsto \hat{U}(t)|\alpha\rangle$$

$$e^{-i\hat{H}t/\hbar}|\alpha\rangle$$

$$\hat{\rho}_\alpha(t) = \hat{U}(t)\,\hat{\rho}_\alpha(0)\,U^\dagger(t)$$

Now for Mixed States

$\langle A \rangle$ for a mixed state

Want it to look like
$\langle A \rangle = Tr(\hat{\rho}\hat{A})$

P_α for $|\alpha\rangle$

P_β for $|\beta\rangle$

$0 \leq P \leq 1$

$P_\alpha + P_\beta = 1$

operator $\hat{A}$
eigenvalues λ_i
eigenbasis $\{|\lambda_i\rangle\}$

$|\alpha\rangle = \sum_i c_{\alpha i} |\lambda_i\rangle$ $\quad |\beta\rangle = \sum_i c_{\beta i} |\lambda_i\rangle$

Probability of measuring λ_i just for $|\alpha\rangle$ is $|c_{\alpha i}|^2$

Probability of measuring λ_i for mixed state

$$P_\alpha |c_{\alpha i}|^2 + P_\beta |c_{\beta i}|^2$$

$$|c_{\alpha i}|^2 = |\langle \lambda_i | \alpha \rangle|^2 = \langle \alpha | \lambda_i \rangle \langle \lambda_i | \alpha \rangle$$

$$\text{Prob}(\lambda_i) = P_\alpha \langle \alpha | \lambda_i \rangle \langle \lambda_i | \alpha \rangle + P_\beta \langle \beta | \lambda_i \rangle \langle \lambda_i | \beta \rangle$$

$$\langle A \rangle = \sum_i \lambda_i \,\text{Prob}(\lambda_i) = \sum_i \lambda_i \left(P_\alpha \langle \alpha | \lambda_i \rangle \langle \lambda_i | \alpha \rangle + P_\beta \langle \beta | \lambda_i \rangle \langle \lambda_i | \beta \rangle \right)$$

$$= P_\alpha \left(\sum_i \lambda_i \langle \alpha | \lambda_i \rangle \langle \lambda_i | \alpha \rangle \right) + P_\beta \left(\sum_i \lambda_i \langle \beta | \lambda_i \rangle \langle \lambda_i | \beta \rangle \right)$$

$$= P_\alpha \langle \alpha | \left(\sum_i \lambda_i | \lambda_i \rangle \langle \lambda_i | \right) | \alpha \rangle + P_\beta \langle \beta | \left(\sum_i \lambda_i | \lambda_i \rangle \langle \lambda_i | \right) | \beta \rangle$$

$$\langle A \rangle = P_\alpha \langle A \rangle_\alpha + P_\beta \langle A \rangle_\beta$$

$$\langle A \rangle = \sum_k P_k \langle A \rangle_k$$ k labels the state within the mixed state

$$= \sum_k P_k \mathrm{Tr}(\hat{\rho}_k \hat{A}) = \mathrm{Tr}\Big(\underbrace{\big(\sum_k P_k \hat{\rho}_k\big)}_{\text{mixed state density operator}} \hat{A} \Big)$$

$$\boxed{\begin{gathered} \hat{\rho} = \sum_k P_k |\alpha_k\rangle\langle\alpha_k| \\ 0 \le P_k \le 1 \\ \sum_k P_k = 1 \end{gathered}}$$

Hermitian $\hat{\rho}^\dagger = \hat{\rho}$

Normalized $\mathrm{Tr}\hat{\rho} = \sum_k P_k = 1$

Expectation $\langle A \rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$

$\mathrm{Prob}(\lambda) = \mathrm{Tr}(\hat{\rho}\hat{P}_\lambda)$

Time evolution: $i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}]$

$$\mathrm{Tr}(\hat{\rho}^2) = \sum_k P_k^2 \le 1$$

Equality for a pure state

$$S \equiv -k_B \mathrm{Tr}(\hat{\rho} \ln \hat{\rho})$$

entropy

If $|\alpha_k\rangle$ are all orthogonal

$$S = -k_B \sum_k P_k \ln P_k$$

Pure state $S = 0$ maximally mixed $S = k_B \ln N$

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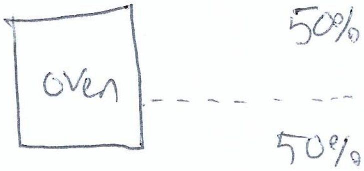
Density Operator

$$\hat{\rho} = \sum_k P_k |a_k\rangle\langle a_k| \qquad 0 \le P_k \le 1$$

$$\mathrm{Tr}\,\hat{\rho} = 1 \qquad \mathrm{Tr}\,\hat{\rho}^2 \le 1$$

Note: Starting with $\hat{\rho}$ we can find the relevant mixtures by solving for the eigenvalues (P_k) and eigenkets $|a_k\rangle$

Degeneracy in eigenvalues means there is more than one way to make the mixture



50% $|\uparrow\rangle$ $\qquad |\uparrow\rangle \doteq \begin{bmatrix}1\\0\end{bmatrix}$

50% $|\downarrow\rangle$ $\qquad |\downarrow\rangle \doteq \begin{bmatrix}0\\1\end{bmatrix}$

$$\hat{\rho} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| \doteq \frac{1}{2}\begin{bmatrix}1&0\\0&1\end{bmatrix}$$

$$\hat{\rho}^2 = \frac{1}{4}\begin{bmatrix}1&0\\0&1\end{bmatrix}, \quad \mathrm{Tr}\,\hat{\rho}^2 = \frac{1}{2} \le 1$$

50% $|\rightarrow\rangle \doteq \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$

50% $|\leftarrow\rangle \doteq \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$

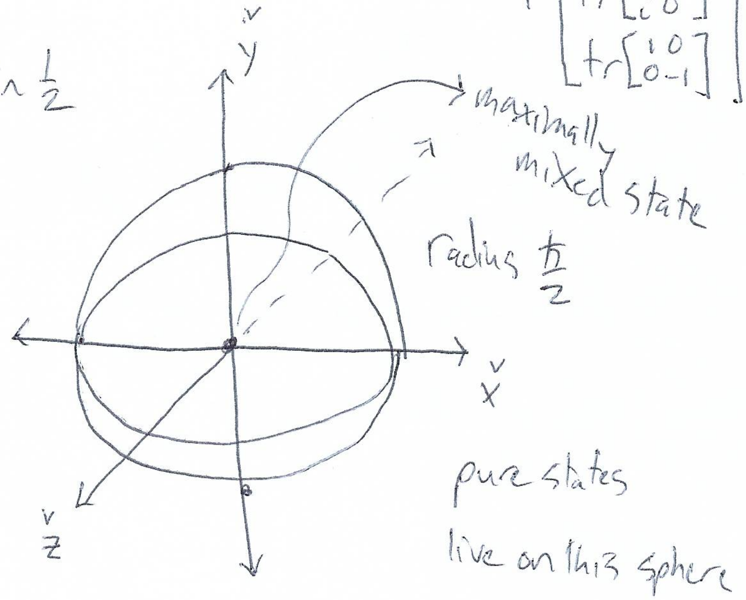
$$\hat{\rho} = \frac{1}{2}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\end{bmatrix} + \frac{1}{4}\begin{bmatrix}1\\-1\end{bmatrix}\begin{bmatrix}1&-1\end{bmatrix}$$

$$= \frac{1}{4}\left(\begin{bmatrix}1&1\\1&1\end{bmatrix} + \begin{bmatrix}1&-1\\-1&1\end{bmatrix}\right) = \frac{1}{4}\begin{bmatrix}2&0\\0&2\end{bmatrix} = \begin{bmatrix}1/2&0\\0&\frac{1}{2}\end{bmatrix}$$

$$\langle \vec{S} \rangle = \begin{bmatrix} \langle S_x \rangle \\ \langle S_y \rangle \\ \langle S_z \rangle \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} \mathrm{tr}\rho\sigma_x \\ \mathrm{tr}\rho\sigma_y \\ \mathrm{tr}\rho\sigma_z \end{bmatrix}$$

For $\hat{\rho} = \frac{1}{2}\hat{1}$ $\langle \vec{S} \rangle = \frac{\hbar}{4} \begin{bmatrix} \mathrm{tr}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \mathrm{tr}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ \mathrm{tr}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{bmatrix} = \frac{\hbar}{4} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \vec{0}$

Spin $\frac{1}{2}$



Any spin $\frac{1}{2}$ mixed state gives a vector in this $\frac{\hbar}{2}$ radius ball.

Bloch Sphere

Hilbert Space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$

If we have a pure state

$$|\alpha\rangle \in \mathcal{H}$$

$$|\alpha\rangle = \sum_k c_k |a_k, b_k\rangle$$

Let $|e_i\rangle$ be a basis for $\mathcal{H}_A$ $|f_I\rangle$ a basis for $\mathcal{H}_B$

$$|\alpha\rangle = \sum_{i,I} C_{iI} |e_i, f_I\rangle$$

$$\hat{\rho} = \sum_{\substack{i,j \\ I,J}} (c_{iI} c^*_{jJ}) |e_i, f_I\rangle\langle e_j, f_J|$$

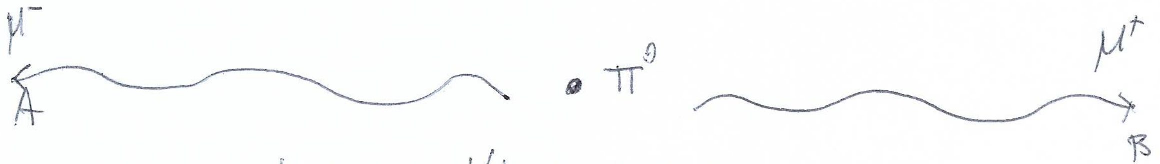
$$\rho^{iI}_{jJ} \equiv \langle e_i f_I | \hat{\rho} | e_j, f_J \rangle$$

Reduced Density operator Ignoring H_B states

$$\left[\hat{\rho}^{red}_A\right]^i_j = \sum_I \langle e_i, f_I | \hat{\rho} | e_j, f_I \rangle \quad \text{"Partial Trace"}$$

$$= \sum_I \rho^{iI}_{jI}$$

EPR Experiment



$$|00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$ pure muon state after the decay

$$\hat{\rho} = \frac{1}{2}(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|)$$

$$\hat{\rho} \doteq \left[\begin{array}{cc|cc} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ \hline 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

$$\rho^{red}_A = \begin{bmatrix} \langle\uparrow\uparrow|\hat{\rho}|\uparrow\uparrow\rangle + \langle\uparrow\downarrow|\hat{\rho}|\uparrow\downarrow\rangle & \langle\uparrow\uparrow|\hat{\rho}|\downarrow\uparrow\rangle + \langle\uparrow\downarrow|\hat{\rho}|\downarrow\downarrow\rangle \\ \langle\downarrow\uparrow|\hat{\rho}|\uparrow\uparrow\rangle + \langle\downarrow\downarrow|\hat{\rho}|\uparrow\downarrow\rangle & \langle\downarrow\uparrow|\hat{\rho}|\downarrow\uparrow\rangle \quad \langle\downarrow\downarrow|\hat{\rho}|\downarrow\downarrow\rangle \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

pure simple state

$$\begin{tikzcd} & |\alpha\rangle \otimes |\beta\rangle \arrow[dl] \arrow[dr] & \\ \hat{\rho}_A^{red} & & \hat{\rho}_B^{red} \end{tikzcd}$$

$|\alpha\rangle\langle\alpha|$ $|\beta\rangle\langle\beta|$

$$\begin{tikzcd} & \text{entangled state} \arrow[dl, bend right] \arrow[dr, bend left] & \\ \hat{\rho}_A \text{ mixed} & & \hat{\rho}_B \text{ mixed} \end{tikzcd}$$

End of Midterm 1 material

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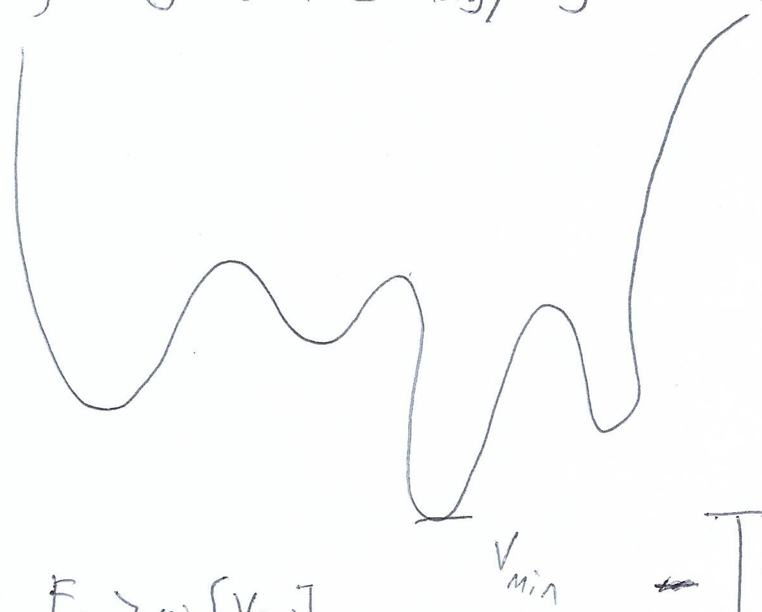
Part II : Approximation Methods

Estimating the ground state energy E_g



← no states exist with $E < V_{min}$

Lower Bound : $E_g > \min[V(x)]$

Upper Bound?

For any state, $\langle E \rangle \geq E_g$

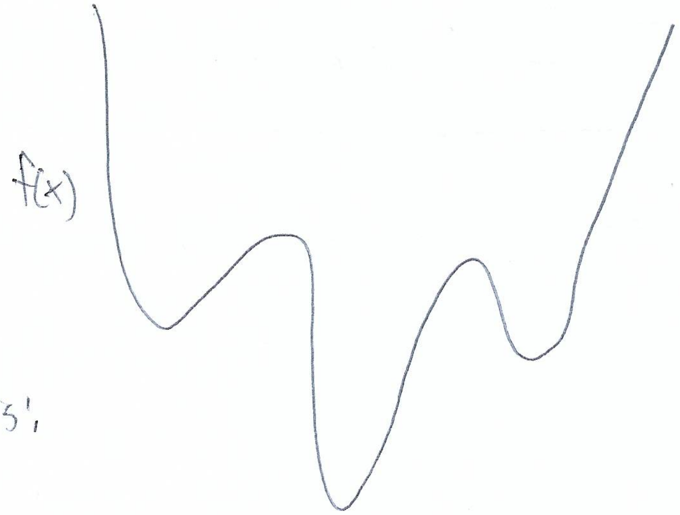
$$|\alpha\rangle = \sum_{n,\mu} c_{n,\mu} |n,\mu\rangle \quad \text{with} \quad \hat{H}|n,\mu\rangle = E_n |n,\mu\rangle$$

$$\langle E \rangle = \sum_{n,\mu} E_n |c_{n,\mu}|^2 = \sum_{n\mu} E_n P(E_n) \geq E_g$$

Define the energy functional $\mathcal{E}[|\alpha\rangle]$ or $\mathcal{E}[\psi_\alpha(x)]$

$\mathcal{E} : \mathcal{H} \to \mathbb{R}$

$$\mathcal{E}[|\alpha\rangle] \equiv \frac{\langle \alpha|\hat{H}|\alpha\rangle}{\langle \alpha|\alpha\rangle}$$



minima / extrema / stationary points:

$$\frac{\partial f}{\partial x} = 0 \qquad \delta f = 0$$

$$x \mapsto x + \delta x$$

$$f \mapsto f + \delta f$$

The Variational Method / Principle tells us that we find our ground state by globally minimizing $\mathcal{E}[|\alpha\rangle]$ with respect to $|\alpha\rangle$

If $|\alpha\rangle \mapsto |\alpha\rangle + \delta|\alpha\rangle$ (for arbitrary, small $\delta|\alpha\rangle$)

$$\Rightarrow \delta\mathcal{E} = 0 + \mathcal{O}(\varepsilon^2)$$

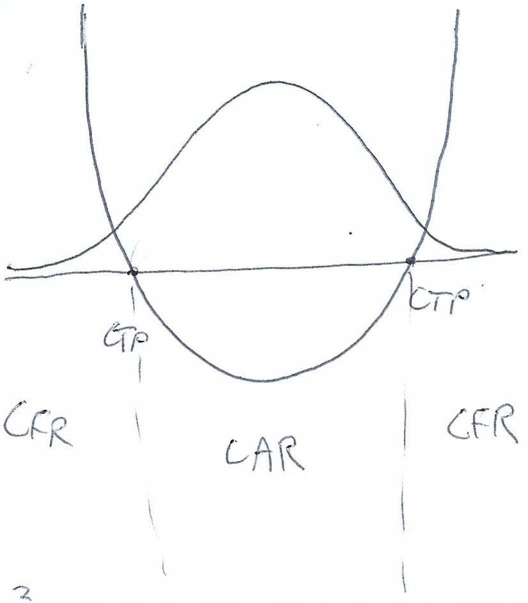
then $|\alpha\rangle$ is an energy eigenstate

* Work with wavefunction $\psi(\vec{x})$

1) Sketch the ground state wave function

2) Propose a simple to integrate ansatz with a small number of adjustable parameters

$\psi(x) \overset{?}{=} Ne^{-ax^2}$



3) $$E[|\alpha\rangle] = \frac{\langle\alpha|\hat{H}|\alpha\rangle}{\langle\alpha|\alpha\rangle}$$

$$\psi_\alpha(x) = Ne^{-ax^2} \quad \langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |N|^2 e^{-2ax^2} dx$$

$$= |N|^2 \sqrt{\frac{\pi}{2a}} \Rightarrow N = \left(\frac{2a}{\pi}\right)^{1/4}$$

$$E(a) = \int_{-\infty}^{\infty} \psi_a^* \hat{H} \psi_a dx = \sqrt{\frac{2a}{\pi}} \int_{-\infty}^{\infty} e^{-ax^2}\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}e^{-ax^2} + \frac{1}{2}\mu\omega^2 x^2 e^{-ax^2}\right)dx$$

$$= \sqrt{\frac{2a}{\pi}}\left[-\frac{\hbar}{\mu}(-a)\underbrace{\int e^{-2ax^2} dx}_{\sqrt{\frac{\pi}{2a}}} - \frac{\hbar}{2\mu}4a^2\underbrace{\int x^2 e^{-2ax^2} dx}_{\sqrt{\frac{\pi}{2a}}\frac{1}{4a}} + \frac{1}{2}\mu\omega^2\underbrace{\int x^2 e^{-2ax^2} dx}\right)$$

$$= \frac{\hbar^2 a}{2\mu} + \frac{\mu\omega^2}{8a}$$

4) Minimize! $$\frac{\partial E}{\partial a} = \frac{\hbar^2}{2\mu} - \frac{\mu\omega^2}{8a^2} = 0 \qquad a = \frac{\mu\omega}{2\hbar}$$

$$\Rightarrow E_{min} = \frac{1}{2}\hbar\omega$$

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Variational Method continued

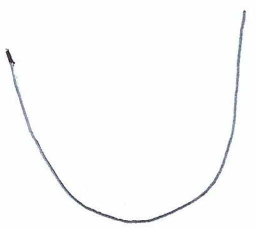
$$\tilde{E}[|\alpha\rangle] \equiv \langle E \rangle = \frac{\langle \alpha | \hat{H} | \alpha \rangle}{\langle \alpha | \alpha \rangle}$$

$$E_{\text{ground}} \leq \tilde{E}[|\alpha\rangle] \text{ for any } |\alpha\rangle$$

Last time: SHO $V(x) = \frac{1}{2}\mu w^2 x^2$

Trial: $\psi = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}$

$E(a) = \frac{\hbar^2 a}{2\mu} + \frac{\mu w^3}{8\alpha}$ $\quad a_{min} = \frac{\mu w}{2\hbar} \Rightarrow \min E(a) = \frac{1}{2}\hbar w$



$\hat{\pi}|gs\rangle = +|gs\rangle$

$\hat{\pi}|fs\rangle = -|fs\rangle$

sym ψ

antisym ψ under parity

$\Rightarrow \langle gs | fs \rangle = 0$

$|\text{antisym}\rangle = c_1 |fs\rangle + \dots$

eg try $N x e^{-ax^3}$ for SHO $\quad \langle E \rangle \geq E_1$

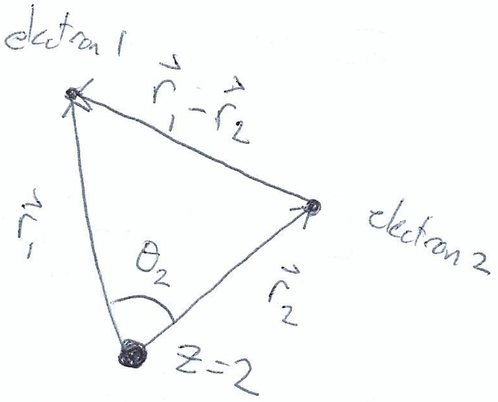
eg try Nxe^{-ax^2} for the SHO

eg for Hydrogen

$$\psi(\vec{r}) = (\text{guess})(r)\, Y_{\ell}^{m}(\theta,\phi)$$

$\langle E \rangle \geq$ lowest energy eigenvalue consistant with ℓ and m

$$|\vec{r}_1 - \vec{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}$$



Helium

Experimental gs $\simeq -79\,eV$

$$\hat{H}_{He} = \frac{\hat{p}_1^2}{2m_e} + \frac{\hat{p}_2^2}{2m_e} - \frac{2e^2}{4\pi\epsilon_0}\frac{1}{\vec{r}_1} - \frac{2e^2}{4\pi\epsilon_0}\frac{1}{\vec{r}_2} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

$$\left.\hat{H}_Z = \frac{\hat{p}^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{\hat{r}}\right\} \psi_{100}^{Z}(\vec{r}) = \sqrt{\frac{Z^3}{\pi a^3}}\, e^{-Zr/a} \quad , a = \frac{\hbar}{m_e c \alpha}$$

$$\hat{V}_{ee} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|} \qquad E_{100}^{Z} = Z^2 E_1 \qquad , E_1 = -\frac{1}{2}mc^2\alpha^2$$

$$\frac{e^2}{4\pi\epsilon_0} = -2aE_1$$

$$\hat{H}_{He} = \hat{H}_{Z1} + \hat{H}_{Z2} + \hat{V}_{ee}$$

1) Ignore V_{ee}

$$\psi_{gs}(\vec{r}_1, \vec{r}_2) = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a} \quad , E_{gs} = 8E_1 \simeq -109\,eV$$

2) use ψ_{gs} as our trial

$$\langle H \rangle = 8E_1 + \langle V_{ee} \rangle = 8E_1 - 2aE_1\left(\left\langle \frac{1}{\vec{r}_1 - \vec{r}_2} \right\rangle\right)$$

$$\left(\frac{8}{\pi a^3}\right)^2 \iint \frac{e^{-4(r_1+r_2)/a}}{|\vec{r}_1 - \vec{r}_2|}\, d^3r_1\, d^3r_2 = \frac{5}{4a} \qquad \langle E \rangle = \cancel{8}\, \frac{11}{2}E_1 \simeq -75\,eV$$

$$\Psi_{trial}(\vec{r}_1, \vec{r}_2) = \frac{Z^3}{\pi a^3} e^{-Z(r_1+r_2)/a} \qquad \frac{a}{2} \mapsto \frac{a}{Z}$$

$$\hat{H}_2 = \frac{\hat{p}^2}{2m_e} - \frac{2e^2}{4\pi\epsilon_0 \hat{r}} = \frac{\hat{p}^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0 \hat{r}} + \frac{(Z-2)e^2}{4\pi\epsilon_0 \hat{r}}$$

$$= \hat{H}_Z + \frac{(Z-2)e^2}{4\pi\epsilon_0} \frac{1}{\hat{r}}$$

$$\hat{H}_{He} = \hat{H}_{Z,1} + \hat{H}_{Z,2} - 2aE_1(Z-2)\left[\frac{1}{\hat{r}_1} + \frac{1}{\hat{r}_2}\right] + \hat{V}_{ee}$$

$$\langle E \rangle = 2Z^2 E_1 - 4aE_1(Z-2)\underbrace{\left\langle \frac{1}{r_1} \right\rangle}_{\frac{Z}{a}} - 2aE_1 \frac{5}{8} \frac{Z}{a}$$

$$\boxed{\langle E \rangle = 2E_1\left(-Z^2 + \frac{27}{8} Z\right)}$$ works for all Z

$$\frac{\partial E}{\partial Z} = 0 \Rightarrow Z = \frac{27}{16} \simeq 1.688 \qquad E_{gs} \leq 5.695 E_1 \simeq -77.5 \text{ eV}$$

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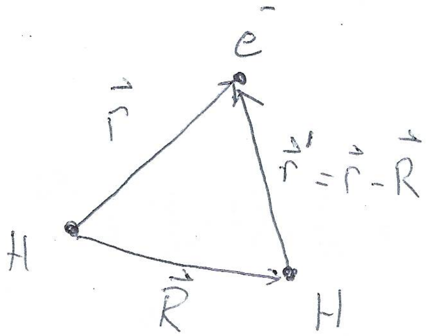
The H_2^+ ion



$$r' = \sqrt{r^2 + R^2 - 2rR\cos\theta}$$

$$\psi_0(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

$|\alpha\rangle$ such that $\langle \vec{r}|\alpha\rangle = \psi_0(\vec{r})$

$|\beta\rangle$ such that $\langle \vec{r}|\beta\rangle = \psi_0(\vec{r}') = \psi_0(\vec{r} - \vec{R})$

guess

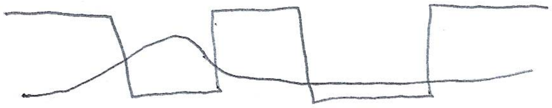
$$|\gamma_\pm\rangle = N(|\alpha\rangle \pm |\beta\rangle)$$

$$N = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1 \pm \langle \alpha|\beta\rangle}}$$

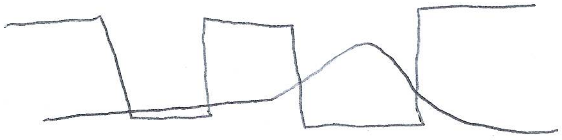
$$\langle \alpha|\beta\rangle = I = \text{"overlap integral"}$$
$$= \left[1 + \left(\frac{R}{a}\right) + \frac{1}{3}\left(\frac{R}{a}\right)^2\right] e^{-R/a}$$

~~$|\alpha\rangle$~~

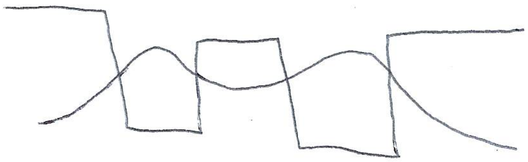
$|\alpha\rangle$



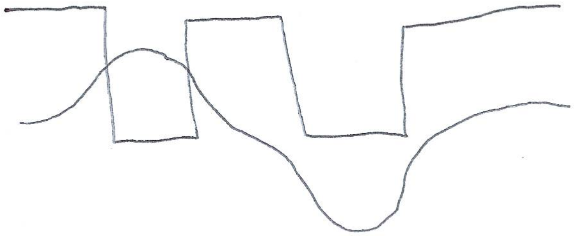
$|\beta\rangle$



$|\gamma_+\rangle$



$|\gamma_-\rangle$



$\langle E \rangle$

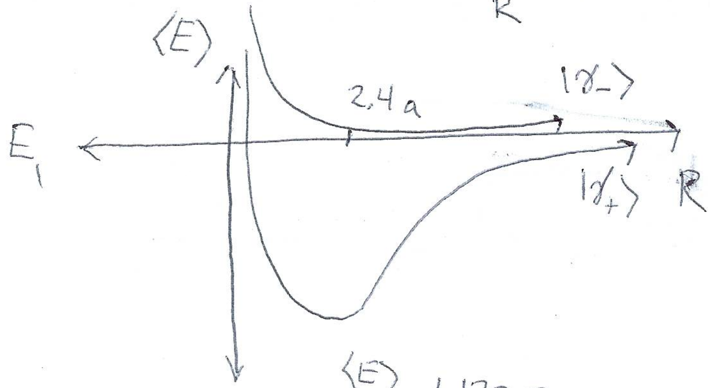
$$\hat{H} = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}'} + \frac{e^2}{4\pi\epsilon_0 R}\hat{\mathbb{1}}$$

$$\langle E \rangle = E_1\left(1+4N^2\left(D \pm X\right)\right)$$

$D = a\langle \alpha | \frac{1}{\hat{r}'} | \alpha \rangle$ "Direct integral" $= \frac{a}{R} - \left(1+\frac{a}{R}\right)e^{-2R/a}$

$X = a\langle \alpha | \frac{1}{\hat{r}} | \beta \rangle$ "exchange integral" $= \left(1+\frac{R}{a}\right)e^{-R/a}$

$$\langle E \rangle = \left(1+2\,\frac{D \pm X}{1 \pm I}\right)E_1 - \frac{2a}{R}E_1$$

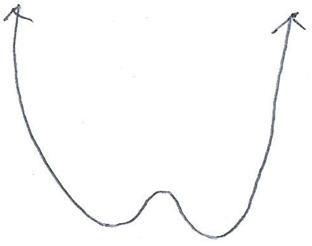


$\langle E \rangle = 1.132\,E_1$

Covalent bonded hydrogen

Perturbation Theory

- Time-Independent
- Non-degenerate



$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

full Hamiltonian

Our 0th order Hamiltonian with known solutions

perturbing Hamiltonian

eg)

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

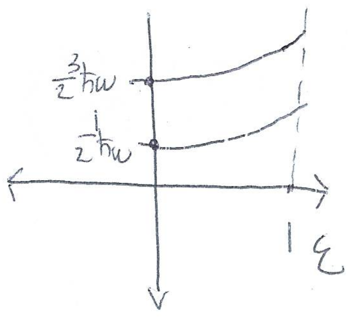
$$H_1 =$$

$$\hat{H}(\varepsilon) = \hat{H}_0 + \varepsilon\hat{H}_1$$

$\varepsilon = 0 \Rightarrow$ unperturbed

$\varepsilon = 1 \Rightarrow$ fully perturbed

The energy eigenvalues and eigenstates continuously vary/evolve as ε goes from 0 to 1



Energies $E_n(\varepsilon)$ ~~E_n~~

Eigenstates $|\phi_n, \varepsilon\rangle$

$$E_n(\varepsilon) = \sum_m \varepsilon^m E_n^{(m)}$$

$$|\phi_n, \varepsilon\rangle = \sum_m \varepsilon^m |\phi_n^{(m)}\rangle$$

$$\hat{H}(\varepsilon)|\phi_n, \varepsilon\rangle = E_n(\varepsilon)|\phi_n, \varepsilon\rangle$$

$$(\hat{H}_0 + \varepsilon \hat{H}_1)\left(\sum_j \varepsilon^j |\phi_n^{(j)}\rangle\right) = \left(\sum_q \varepsilon^q E_n^{(q)}\right)\left(\sum_f \varepsilon^f |\phi_n^{(f)}\rangle\right)$$

$$\sum_{m=0}^{\infty} \varepsilon^m (\text{stuff})^{(m)} = \sum_{m=0}^{\infty} \varepsilon^m (\text{other stuff})^{(m)}$$

$m=0]$ $\hat{H}_0|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(0)}\rangle$ ← our unperturbed solutions

$m=1]$ $\hat{H}_0|\phi_n^{(1)}\rangle + \hat{H}_1|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}|\phi_n^{(0)}\rangle$

$m=2]$ $\hat{H}_0|\phi_n^{(2)}\rangle + \hat{H}_1|\phi_n^{(1)}\rangle = E_n^{(0)}|\phi_n^{(2)}\rangle + E_n^{(1)}|\phi_n^{(1)}\rangle + E_n^{(2)}|\phi_n^{(0)}\rangle$

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Perturbation Theory

Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$

Expansions

$$\hat{H}(\varepsilon) \equiv \hat{H}_0 + \varepsilon \hat{H}_1$$

$$E_n(\varepsilon) = \sum_{i=0}^{\infty} \varepsilon^{i} E_n^{(i)}$$

$$|n, \varepsilon\rangle = \sum_{i=0}^{\infty} \varepsilon^{i} |n^{(i)}\rangle$$

$$\hat{H}(\varepsilon)|n, \varepsilon\rangle = E_n(\varepsilon)|n, \varepsilon\rangle$$

$$\Downarrow$$

$$\sum_{i=0}^{\infty} \varepsilon^{2} \left(\hat{H}_0 |n^{(i)}\rangle + \hat{H}_1 |n^{(i-1)}\rangle\right)$$

$$= \sum_{i=0}^{\infty} \varepsilon^{i} \left(\sum_{j=0}^{i} E_n^{(j)} |n^{(i-j)}\rangle\right)$$

Example: SHO

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega_0^2 \hat{x}^2 \qquad \text{Ladder } \hat{a}_\pm$$

$$E_n^{(0)} = \hbar\omega_0 (n + \tfrac{1}{2}) \qquad \text{states } |n^{(0)}\rangle$$

$$\omega_0 \mapsto \omega + \delta\omega$$

$$\hat{H}_1 = \left(m\omega_0 \delta\omega + \tfrac{1}{2} m (\delta\omega)^2\right)\hat{x}^2$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m (\omega_0 + \delta\omega)^2 \hat{x}^2$$

$$E_n = \hbar(\omega + \delta\omega)(n + \tfrac{1}{2})$$

ε^0

$$\hat{H}_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle \qquad \text{unperturbed eigenvalue equation}$$

ε^1

$$\hat{H}_0 |n^{(1)}\rangle + \hat{H}_1 |n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle$$

$$(\hat{H}_0 - E_n^{(0)} \mathbb{1})|n^{(1)}\rangle + (\hat{H}_1 - E_n^{(1)} \mathbb{1})|n^{(0)}\rangle = 0$$

Use $\{|n^{(0)}\rangle\}$ as a basis

$$|n^{(1)}\rangle = \sum_m{}' C_n^m |m^{(0)}\rangle$$

$$C_n^m = \langle m^{(0)}|n^{(1)}\rangle$$

$$\langle m^{(0)}|(\hat{H}_0 - E_n^{(0)}\mathbb{1})|n^{(1)}\rangle + \langle m^{(0)}|(\hat{H}_1 - E_n^{(1)}\mathbb{1})|n^{(0)}\rangle = 0$$

$$\langle m^{(0)}|(\hat{E}_m^{(0)} - E_n^{(0)}\mathbb{1})|n^{(1)}\rangle + \langle m^{(0)}|\hat{H}_1|n^{(0)}\rangle - E_n^{(1)}\langle m^{(0)}|n^{(0)}\rangle$$

$$(E_m^{(0)} - E_n^{(0)})\langle m^{(0)}|n^{(1)}\rangle + \underbrace{\langle m^{(0)}|\hat{H}_1|n^{(0)}\rangle}_{\text{Computable}} - E_n^{(1)}\delta_{mn} = 0$$

$\underline{m = n}$

$$\langle n^{(0)}|\hat{H}_1|n^{(0)}\rangle - E_n^{(1)} = 0$$

$$E_n^{(1)} = \langle n^{(0)}|\hat{H}_1|n^{(0)}\rangle$$

Example

$$E_n^{(0)} = \hbar\omega_0(n + \tfrac{1}{2})$$

$$E_n^{(1)} = \langle n^{(0)}|(m\omega_0\delta\omega + \tfrac{1}{2}(\delta\omega)^2)\hat{x}^2|n^{(0)}\rangle$$

$$= (m\omega_0\delta\omega + \tfrac{1}{2}m(\delta\omega)^2)\langle n^{(0)}|\hat{x}^2|n^{(0)}\rangle$$ Ladder Operators!

$$\hat{x} = \sqrt{\frac{\hbar}{2\omega_0 m}}(\hat{a}_+ + \hat{a}_-)$$

$$(m\omega_0\delta\omega + \tfrac{1}{2}m(\delta\omega)^2)\frac{\hbar}{2\omega_0 m}\Big(\langle n^{(0)}|\hat{a}_+^2|n^{(0)}\rangle + \langle n^{(0)}|\hat{a}_-^2|n^{(0)}\rangle + \langle n^{(0)}|\hat{a}_+\hat{a}_-|n^{(0)}\rangle$$
$$+ \langle n^{(0)}|\hat{a}_-\hat{a}_+|n^{(0)}\rangle$$

$$=A(n\langle n^{(0)}|n^{(0)}\rangle + (n+1)\langle n^{(0)}|n^{(0)}\rangle) = (2n+1)(m\omega_0\delta\omega + \tfrac{1}{2}m(\delta\omega)^2)\frac{\hbar}{2\omega_0 m}$$

~~$= \hbar\omega_0\delta\omega$~~

$$= \hbar\delta\omega(n + \tfrac{1}{2}) + \frac{\hbar(\delta\omega)^2}{2\cancel{\delta}\omega_0}(n + \tfrac{1}{2})$$

$$\hbar\omega_0(n + \tfrac{1}{2}) + \varepsilon\hbar\delta\omega(n + \tfrac{1}{2}) + \varepsilon\frac{\hbar(\delta\omega)^2}{2\cancel{\delta}\omega_0}(n + \tfrac{1}{2}) + \mathcal{O}(\varepsilon)$$

$m \neq n$

$$\left(E_m^{(0)} - E_n^{(0)}\right)\langle m^{(0)} | n^{(1)}\rangle + \langle m^{(0)} | \hat{H}_1 | n^{(0)}\rangle$$

$$C_n^m = \langle m^{(0)} | n^{(1)}\rangle = \frac{\langle m^{(0)} | \hat{H}_1 | n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}$$

$$|n,\varepsilon\rangle = (1 + ia\varepsilon)|n^{(0)}\rangle + \varepsilon \sum_{m\neq n}\left(\frac{\sim}{\sim}\right) + \mathcal{O}(\varepsilon^2)$$

ia phase in hiding

$$|n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle m^{(0)} | \hat{H}_1 | n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} |m^{(0)}\rangle + (?)|n^{(0)}\rangle$$

$$1 + ia\varepsilon + \frac{(ia\varepsilon)^2}{2} + \dots$$

$$= e^{ia\varepsilon}$$

$$\langle n,\varepsilon | n,\varepsilon\rangle = 1$$

$$1 = \langle n^{(0)} | n^{(0)}\rangle + \varepsilon\left[\langle n^{(0)} | n^{(1)}\rangle + \langle n^{(1)} | n^{(0)}\rangle\right] + \mathcal{O}(\varepsilon^2)$$

$$\Rightarrow \langle n^{(0)} | n^{(0)}\rangle = 1$$

$$\mathrm{Re}\,\langle n^{(0)} | n^{(1)}\rangle = 0$$

$$\langle n^{(0)} | n^{(1)}\rangle = 0$$

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Degenerate Perturbation Theory

We need to find "good states" that anticipate how degeneracy will break so that the states evolve continuously as perturbation parameter is turned on.

$$\hat{H}(\varepsilon) \doteq \begin{bmatrix} 2 & \varepsilon & \varepsilon \\ \varepsilon & 2 & \varepsilon \\ \varepsilon & \varepsilon & 4 \end{bmatrix} \qquad E_1 = 2-\varepsilon \quad \chi_1 \doteq \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

$$E_2 = 2+\varepsilon-\varepsilon^2+\mathcal{O}(\varepsilon^3) \quad \chi_2 \doteq \begin{bmatrix} 1-\varepsilon \\ 1-\varepsilon \\ -\varepsilon \end{bmatrix} + \mathcal{O}(\varepsilon^2)$$

$$E_3 = 4+\varepsilon^2+\mathcal{O}(\varepsilon^3) \quad \chi_3 \doteq \begin{bmatrix} \varepsilon/2 \\ \varepsilon/2 \\ 1 \end{bmatrix} + \mathcal{O}(\varepsilon^2)$$

$\hat{H}_0$

Eigenbasis 1: $|n,\xi\rangle$ "bad basis"

Eigenbasis 2: $|n,\mu\rangle^{(0)}$ "good basis"

ξ, μ each run from 1 to N_n, the degeneracy of energy E_n

$$\hat{H}_0|n,\xi\rangle = E_n^{(0)}|n,\xi\rangle$$

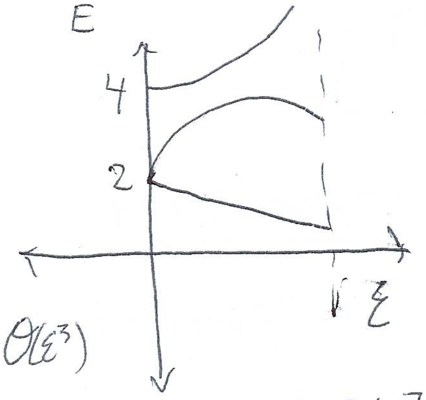
$$\hat{H}_0|n,\mu\rangle^{(0)} = E_n^{(0)}|n,\mu\rangle^{(0)}$$

$$|n,\mu\rangle^{(0)} = \sum_{\xi=1}^{N_n} c^{\xi}_{\mu}|n,\xi\rangle$$

$$|n,\mu\rangle(\varepsilon) = |n,\mu\rangle^{(0)} + \varepsilon|n,\mu\rangle^{(1)} + \cdots$$

with $|n,\mu\rangle^{(0)} = \lim_{\varepsilon\to 0}|n,\mu\rangle(\varepsilon)$

$$\hat{H}(\varepsilon) \doteq \begin{bmatrix} 2 & \varepsilon & \varepsilon \\ \varepsilon & 2 & \varepsilon \\ \varepsilon & \varepsilon & 4 \end{bmatrix}$$



$$E_1 = 2-\varepsilon \quad \chi_1 \doteq \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

$$E_2 = 2+\varepsilon-\varepsilon^2+\mathcal{O}(\varepsilon^3) \quad \chi_2 \doteq \begin{bmatrix} 1-\varepsilon \\ 1-\varepsilon \\ -\varepsilon \end{bmatrix} + \mathcal{O}(\varepsilon^3)$$

$$E_3 = 4+\varepsilon^2+\mathcal{O}(\varepsilon^3) \quad \chi_3 \doteq \begin{bmatrix} \varepsilon/2 \\ \varepsilon/2 \\ 1 \end{bmatrix} + \mathcal{O}(\varepsilon^3)$$

$$\chi_1^{(0)} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

$$\chi_2^{(0)} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

$$\chi_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\hat{H}_0 \doteq \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix} \quad \hat{H}_1 \doteq \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

$$\hat{H}(\varepsilon) = \hat{H}_0 + \varepsilon\hat{H}_1$$

$$|n,\mu\rangle(\varepsilon) = |n,\mu\rangle^{(0)} + \varepsilon|n,\mu\rangle^{(1)} + \dots$$

$$|n,\mu\rangle^{(0)} = \sum_{\xi}^{N_n} c_\mu^\xi |n,\xi\rangle \qquad E_{n\mu}(\varepsilon) = E_n^{(0)} + \varepsilon E_{n,\mu}^{(1)} + \dots$$

$$\hat{H}(\varepsilon)|n,\mu\rangle(\varepsilon) = E_{n\mu}(\varepsilon)|n,\mu\rangle(\varepsilon)$$

$$\hat{H}_1|n,\mu\rangle^{(0)} - E_{n\mu}^{(1)}|n,\mu\rangle^{(0)} = -\hat{H}_0|n,\mu\rangle^{(1)} + E_n^{(0)}|n,\mu\rangle^{(1)}$$

Projections!

$$\hat{P}_n^{(0)} = \sum_\xi |n,\xi\rangle\langle n,\xi| \qquad \hat{P}_n^{(0)}\hat{P}_n^{(0)} = \hat{P}_n^{(0)} \qquad \hat{P}_n^{(0)}\hat{P}_m^{(0)} = 0 \text{ if } n\neq m$$

$$\hat{P}_n^{(0)}\hat{H}_1|n,\mu\rangle^{(0)} - E_{n,\mu}^{(1)}\hat{P}_n^{(0)}|n,\mu\rangle^{(0)} = -\hat{P}_n^{(0)}\hat{H}_0|n,\mu\rangle^{(1)} + E_n^{(0)}\hat{P}_n^{(0)}|n,\mu\rangle^{(1)}$$

$$\hat{P}_n^{(0)}|n,\mu\rangle^{(0)} = |n,\mu\rangle^{(0)} \qquad \hat{H}_0 = \sum_m E_m^{(0)}\hat{P}_m^{(0)}$$

$$\hat{P}_n^{(0)}\hat{H}_1\hat{P}_n^{(0)}|n,\mu\rangle^{(0)} - E_{n,\mu}^{(1)}|n,\mu\rangle^{(0)} = -\sum_m \hat{P}_n^{(0)}\hat{P}_m^{(0)}E_m^{(0)}|n,\mu\rangle^{(1)} + \sim\sim$$

$$= 0$$

$$\Big(\underbrace{\hat{P}^{(0)}_n \hat{H}_1 \hat{P}^{(0)}_n}_{\hat{W}_n} - E^{(1)}_{n,\mu} \mathbb{1}\Big)|n,\mu\rangle^{(0)} = 0$$

$$\left[\begin{array}{cc|c} 0 & 1 & 1 \\ 1 & 0 & 1 \\ \hline 1 & 1 & 0 \end{array}\right]$$

only care about stuff inside our eigenspace

$$W_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad W_4 = [0]$$

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

$$\hat{W}_n|n,\mu\rangle^{(0)} = E^{(1)}_{n\mu}|n,\mu\rangle^{(0)}$$

$$\hat{H}(\varepsilon) = \begin{bmatrix} 2 & \varepsilon & \varepsilon \\ \varepsilon & 2 & \varepsilon \\ \varepsilon & \varepsilon & 4 \end{bmatrix}$$

$$\begin{tikzcd}
\hat{W}_2 \arrow[r] \arrow[dr] & \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} +1 = \lambda & |E=2,1\rangle^{(0)} \quad E = 2+\varepsilon+O(\varepsilon^2) \arrow[l] \\
& \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} -1 = \lambda & |E=2,2\rangle^{(0)} \quad E = 2-\varepsilon+O(\varepsilon^2) \arrow[l]
\end{tikzcd}$$

Let A be some observable that commutes with $\hat{H}_0$, $\hat{H}_1$ and let the simultaneous eigenstates of $\hat{H}_0$ and $\hat{A}$ be such that $\hat{A}$ fully breaks the degeneracy

Then the simultaneous A and H_0 eigenstates are good eigenstates to all orders in degenerate perturbation theory

Hydrogen (better)

Relativistic terms in hiding

$$E_{\text{hydrogen}} = \underset{\mathcal{O}(\alpha^0)}{\overset{m_e c^2}{(\text{rest mass energy})}} + \underset{\mathcal{O}(\alpha^2)}{\overset{E_n = \frac{E_1}{n^2} = \frac{-\frac{1}{2} m_e c^2 \alpha^2}{n^2}}{(\text{Bohr energies})}} + \underset{\mathcal{O}(\alpha^4)}{(\text{fine structure})}$$

"Gross structure*
of Hydrogen"

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Degenerate Perturbation Theory

The "Good States" Theorem

Let $\hat{H}_0$ be unperturbed Hamiltonian

$\hat{H}_1$ be perturbation

Let $\{\hat{A}_i\}$ be a set of mutually commuting Hermitian operators

such that: ① $[\hat{A}_i, \hat{H}_0] = [\hat{A}_i, \hat{H}_1]$

② A choice of simultaneous $\{\hat{H}_0, \hat{A}_i\}$ eigenvalues uniquely picks out a state

The simultaneous $\{\hat{H}_0, \hat{A}_i\}$ eigenstate are "good states" for the perturbation $\hat{H}_1$. At this point we can go back to using non-degenerate perturbation theory

2D SHO

$$\hat{H}_0 = \frac{\hat{p}_x^2}{2\mu} + \frac{\hat{p}_y^2}{2\mu} + \frac{1}{2}m\omega^2(\hat{x}^2+\hat{y}^2)$$

Energies: $\hbar\omega(n_x+n_y+1)$

States $|n_x, n_y\rangle$

gs $|0,0\rangle$ $E_{00} = \hbar\omega$ non degenerate

1st $E = 2\hbar\omega$ $\{|1,0\rangle, |0,1\rangle\}$

$$\hat{H}_0 = \frac{\hat{p}_x^2}{2\mu} + \frac{\hat{p}_y^2}{2\mu} + \frac{1}{2}\mu\omega^2(\hat{x}^2+\hat{y}^2) \qquad \hat{H}_1 = \varepsilon\mu\omega^2\hat{x}\hat{y}$$

$$\hat{M}\,|n_x,n_y\rangle \equiv |n_y,n_x\rangle$$

$$\hat{M}^2 = \hat{\mathbb{1}} \qquad \hat{M}^\dagger = \hat{M}^{-1} \qquad \hat{M} = \hat{M}^\dagger$$

$$[\hat{M},\hat{A}] = \hat{M}\hat{A} - \hat{A}\hat{M} = (\hat{M}\hat{A}\hat{M}^\dagger - \hat{A})\hat{M}$$

$$\hat{M}\hat{x}\hat{M}^\dagger = \hat{y}$$

$$\hat{M}\hat{y}\hat{M}^\dagger = \hat{x} \qquad [\hat{M},\hat{H}_1] = (\hat{H}_1 - \hat{H}_1)\hat{M} = 0$$

$$|+\rangle = |n_x+n_y=1, m=+1\rangle = \frac{1}{\sqrt{2}}(|1,0\rangle + |0,1\rangle)$$

$$|-\rangle = |n_x+n_y=1, m=-1\rangle = \frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle)$$

$$E_\pm^{(1)} = \langle\pm|\hat{H}_1|\pm\rangle$$

$$= \frac{1}{2}\varepsilon\mu\omega^2((\langle 10| \pm \langle 01|)(\hat{x}\hat{y})(|10\rangle \pm |01\rangle))$$

$$\langle 10|\hat{x}\hat{y}|10\rangle \leftarrow \cancel{\langle 1|x|1\rangle}\langle 0|y|0\rangle$$

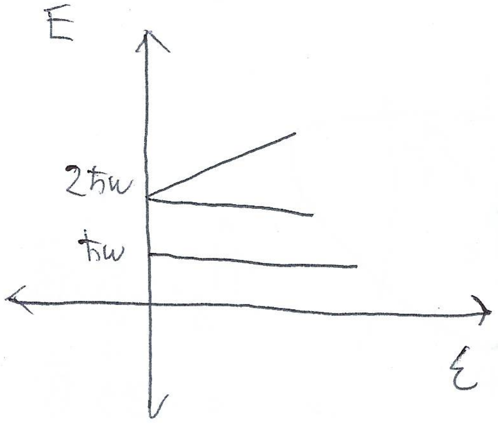
$$\pm\langle 10|\hat{x}\hat{y}|01\rangle \rightarrow \pm\langle 1|x|0\rangle\langle 0|y|1\rangle$$

$$\pm\langle 01|\hat{x}\hat{y}|10\rangle \rightarrow \pm\langle 0|x|1\rangle\langle 1|y|0\rangle$$

$$\pm\langle 01|\hat{x}\hat{y}|01\rangle \rightarrow \pm\cancel{\langle 0|x|0\rangle}\langle 1|y|1\rangle$$

$$= \frac{1}{2}\varepsilon\mu\omega^2\langle 1|\hat{x}|0\rangle\langle 0|\hat{y}|1\rangle$$

$$E_\pm^{(1)} = \pm\varepsilon\frac{\hbar\omega}{2}$$



$$E = m_e c^2 + \left(-\frac{1}{2} m_e c^2 \alpha^2\right)\frac{1}{n^2} + \text{fine structure}$$

$$\boxed{\hat{H}_0 = \frac{\hat{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}}}$$

Relativistic KE Correction

$$E^2 = p^2c^2 + m^2c^4$$

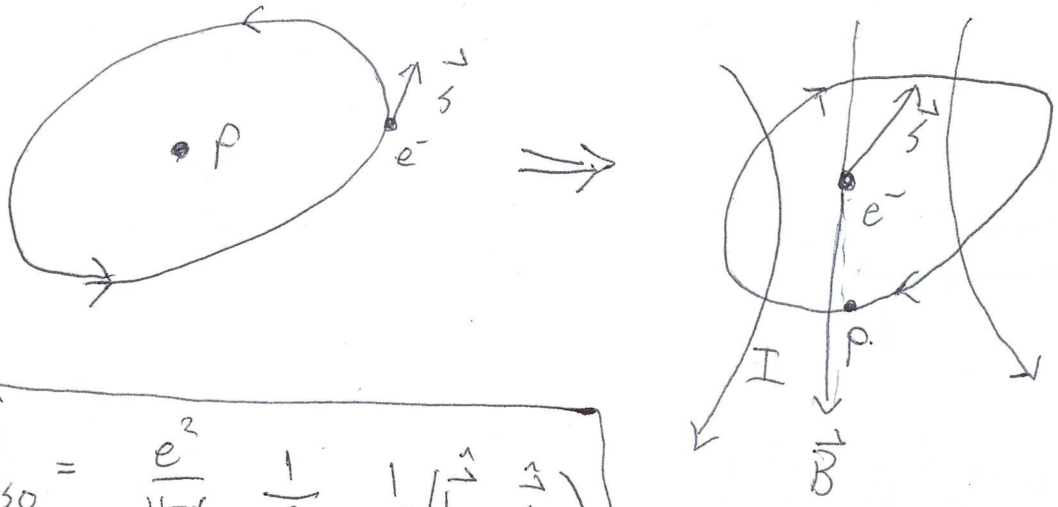
$$E = \sqrt{p^2c^2 + m^2c^4}$$

$$KE = E - m_e c^2 = m_e c^2\left(\sqrt{1 + \left(\frac{p}{m_e c}\right)^2} - 1\right)$$

$$\approx m_e c^2\left(\frac{1}{2}\left(\frac{p}{m_c}\right)^2 - \frac{1}{8}\left(\frac{p}{m_c}\right)^4 + \dots\right)$$

$$\approx \frac{p^2}{2m_e} - \frac{1}{8}\frac{p^4}{m^3c^2} + \dots$$

$$\boxed{\hat{H}_{rel} = -\frac{\hat{p}^4}{8 m_e^3 c^2}}$$



$$\hat{H}_B = -\vec{\mu}\cdot\vec{B}$$
$$= -\gamma\vec{S}\cdot\vec{B}$$
$$= \frac{e}{m}\vec{S}\cdot\vec{B}$$

$$\vec{B} = \frac{e}{4\pi\epsilon_0}\frac{1}{m_e c^2 r^3}\vec{L}$$

$$\boxed{\hat{H}_{so} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{2m_e^2c^2}\frac{1}{\hat{r}^3}(\hat{\vec{L}}\cdot\hat{\vec{S}})}$$

zitterbewegung

$$\hat{H}_D = \left(\frac{e^3}{4\pi\epsilon_0}\right)\frac{4\pi\hbar^2}{8m_e^2c^2}\delta(\hat{\vec{r}})$$

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Hydrogen Fine Structure

$$\hat{H}_{rel} = -\frac{\hat{p}^4}{8m_e^2c^2} \qquad \hat{H}_{SO} = \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{2m_e^2c^2}\frac{1}{|\hat{r}|^3}\hat{\vec{L}}\cdot\hat{\vec{S}}$$

$$\hat{H}_D = \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{4\pi\hbar^2}{8\,2m^2c^2}\,\delta^3(\vec{r})$$

Gross Structure

$$\hat{H}_0 = \frac{\hat{p}^2}{2m_e} - \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{\hat{r}}$$

States $|n\,l\,m_e\,m_s\rangle$ Energies $E_n^{(0)} = \frac{E_1}{n^2}$

Degeneracies $2n^2$

$$E_1 = -\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{m}{2\hbar^2} = -\frac{\hbar^2}{2m_e a_0^2} = -\frac{1}{2}\alpha^2 m_e c^2$$

$$\alpha = \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{\hbar c} \approx \frac{1}{137{,}036} \ll 1$$

$$\frac{e^2}{4\pi\epsilon_0} = -2a_0E_1$$

Uncoupled Basis

$|n\,l\,m_e\,m_s\rangle$ $\quad \hat{A}_i = \{\hat{L}^2, \hat{L}_z, \hat{S}_z\}$

$\hat{S}^2$

Coupled Basis

$|n\,l\,j\,m_j\rangle$ $\quad \hat{A}_c = \{\hat{L}^2, \hat{J}^2, J_z\}$

$$\vec{J} = \vec{L} + \vec{S} \qquad J^2 = (\hat{\vec{L}} + \hat{\vec{S}}) \cdot (\hat{\vec{L}} + \hat{\vec{S}})$$

$$\Rightarrow \hat{\vec{L}} \cdot \hat{\vec{S}} = \frac{\hat{J}^2 - \hat{L}^2 - \hat{S}^2}{2}$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2 a_0}$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{l + \frac{1}{2}} \frac{1}{n^3 a_0^2}$$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{l(l+\frac{1}{2})(l+1)} \frac{1}{n^3 a_0^3}$$

$$\langle n l j m_j | (\hat{H}_{rel} + \hat{H}_{so} + \hat{H}_D) | n l j m_j \rangle = E^{(1)}_{nljm_j}$$

$$\langle nljm_j | \hat{H}_{rel} | nljm_j \rangle \qquad \hat{H}_{rel} = -\frac{1}{2m_e c^2}\left(\frac{\hat{p}^2}{2m_e}\right)^2$$

$$\frac{\hat{p}^2}{2m_e} |nljm_j\rangle \qquad \frac{\hat{p}^2}{2m_e} = \hat{H}_0 + \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{\hat{r}}$$

$$= \left(\hat{H}_0 + \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{\hat{r}}\right)|nljm_j\rangle$$

$$= \left(\frac{E_1}{n^2} + \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{\hat{r}}\right)|nljm_j\rangle$$

$$\langle nljm_j | \frac{-1}{2m_e c^2}\left(\frac{\hat{p}^2}{2m_e}\right)^2 |nljm_j\rangle = -\frac{1}{2m_e c^2}\left\| \frac{\hat{p}^2}{2m_e}|nljm_j\rangle \right\|^2$$

$$= \frac{-1}{2m_e c^2}\left(\langle nljm_j | \left(\frac{E_1}{n^2} + \left(\frac{e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}}\right)\right)\left(\frac{E_1}{n^2} + \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{\hat{r}}\right)|nljm_j\rangle\right)$$

$$= -\frac{1}{2m_e c^2}\left(\frac{E_1^2}{n^4} + \frac{2E_1}{n^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)\left\langle\frac{1}{r}\right\rangle + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left\langle\frac{1}{r^2}\right\rangle\right)$$

$$-\frac{1}{2m_ec^2}\left(\frac{E_1}{n^2}\right)^2\left(1-4a_0n^2\left\langle\frac{1}{r}\right\rangle+4a_0^2n^4\left\langle\frac{1}{r^2}\right\rangle\right)$$

$$=-\frac{E_n^{(0)2}}{2m_ec^2}\left(1-4+\frac{4n}{l+\frac{1}{2}}\right)$$

$$E^1_{n\,rel}=-\frac{E_n^{(0)2}}{2m_ec^2}\left(\frac{4n}{l+\frac{1}{2}}-3\right)$$

$$\langle n l j m_j|\hat{H}_{SO}|n l j m_j\rangle$$

$$\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{1}{m_e^2c^2}\right)\langle n l j m_j|\frac{1}{\hat{r}^3}\hat{\vec{L}}\cdot\hat{\vec{S}}|n l j m_j\rangle$$

$$\hat{\vec{L}}\cdot\hat{\vec{S}}|n l j m_j\rangle=\frac{\hbar^2}{2}\left(j(j+1)-l(l+1)-\underset{\underset{\frac{3}{4}}{\downarrow}}{s(s+1)}\right)|n l j m_j\rangle$$

$$\left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{\hbar^2}{4m_e^2c^2}\right)\left(j(j+1)-l(l+1)-\frac{3}{4}\right)\left\langle\frac{1}{\hat{r}^3}\right\rangle$$

if $l=0$, this is zero

if $l\neq 0$

$$(-2a_0E_1)\left(\frac{\hbar^2}{4m_e^2c^2}\right)\frac{1}{n^3a_0^3}\left(\frac{j(j+1)-l(l+1)-\frac{3}{4}}{l(l+\frac{1}{2})(l+1)}\right)$$

$$=\frac{E_n^{(0)2}}{m_ec^2}\left(\frac{j(j+1)-l(l+1)-\frac{3}{4}}{l(l+1)(l+\frac{1}{2})}\right)$$

$$\langle n l j m_j | \hat{H}_D | n l j m_j \rangle$$

$$(-2a_0 E_1)\frac{\pi\hbar^3}{2m_e^2c^2}\underbrace{|\psi(0)|^2}_{0 \text{ if } l \neq 0}$$

$$\frac{1}{\pi a_0^3 n^3} \text{ if } l=0$$

$$E^{(1)}_{n,D} = \frac{-E_n^{(0)2}}{2m_ec^2}\left(-4n\right) \quad l=0$$

$$\frac{j(j+1)-l(l+1)-\frac{3}{4}}{l(l+\frac{1}{2})(l+1)} \quad \text{when } j=\frac{1}{2}$$

$$= \frac{l}{l(l+\frac{1}{2}(l+1)} = \frac{1}{(l+\frac{1}{2})(l+1)} = 2 \text{ if } l=0$$

$$E^{(1)}_{nj} = -\frac{E_n^{(0)2}}{2m_ec^2}\left(\frac{4n}{j+\frac{1}{2}}-3\right) = -\frac{1}{8}\alpha^4(m_ec^2)\left(\frac{4n}{j+\frac{1}{2}}-3\right)$$

residual degeneracy of $\underset{\substack{\uparrow \\ l=j\pm\frac{1}{2}}}{2}\underbrace{(2j+1)}_{m_j \text{ values}}$

$$j=\frac{1}{2},\ldots,n-\frac{1}{2}$$

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$$E^1_{nj} = \langle n l j m_j | (\hat{H}_{rel} + \hat{H}_{so} + \hat{H}_D) | n l j m_j \rangle$$

$$= \frac{-(E_n^0)^2}{2m_e c^2}\left(\left(\frac{2n}{l+\frac{1}{2}} - \frac{3}{2}\right) - \frac{n}{l+\frac{1}{2}}\left(\frac{j(j+1) - l(l+1) - \frac{3}{4}}{l(l+1)} \right) \right)$$

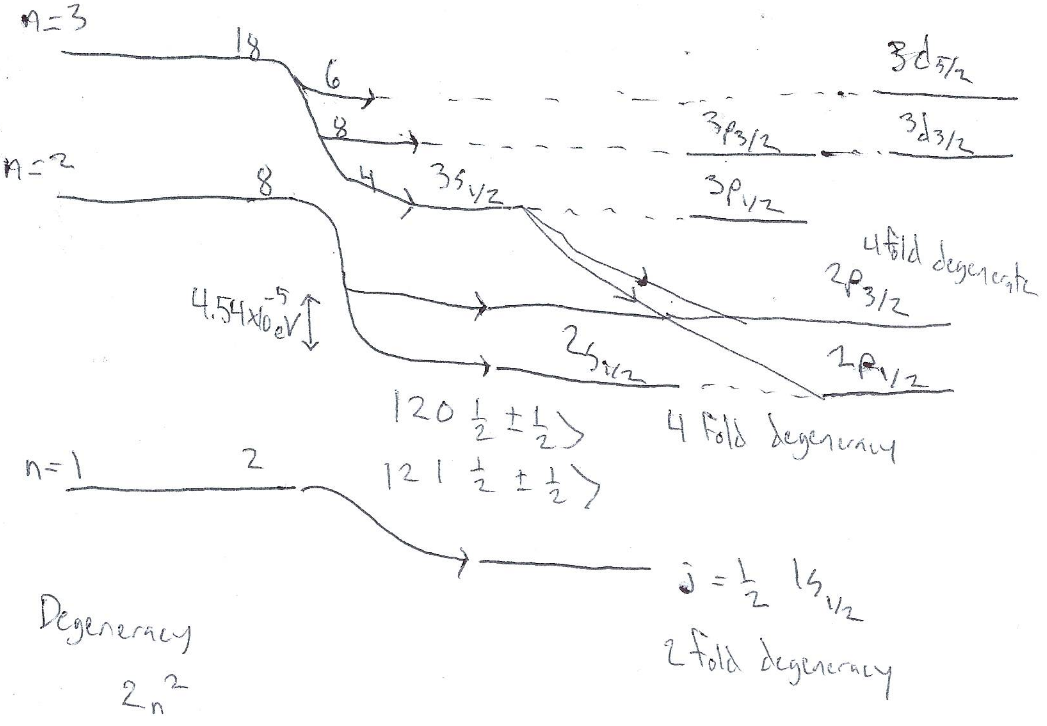
$$= \frac{-(E_n^0)^2}{2m_e c^2}\left(\frac{4n}{j+\frac{1}{2}} - 3\right) = -\frac{1}{8}\underbrace{\alpha^4 m_e c^2}_{1.8\times10^{-4}\,eV}\frac{1}{n^4}\left(\frac{4n}{j+\frac{1}{2}} - 3\right)$$

$$E_n^0 = -\left(\frac{1}{2}\alpha^2 m_e c^2\right)\frac{1}{n^2}$$

$$E_{nj} = E_n^0\left(1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right) + \mathcal{O}(\alpha^4)\right)$$

$$\underset{\#}{n}\,\overset{\text{a letter}}{l}_{j \leftarrow \#}$$

Gross



$l, s = \frac{1}{2}$

$j = l \pm \frac{1}{2}$

$l = 0, 1, \ldots, n-1$

$j = \frac{1}{2}, \frac{3}{2}, \ldots, n - \frac{1}{2}$

n possibilities

$j \leq n - \frac{1}{2}$

$$\frac{4n}{j+\frac{1}{2}} - 3 \geq 1$$

$E^1_{nj} < 0$

Bohr $n=3 \rightarrow n=2$: $\Delta E = 1.8897\ \text{eV}$

$\Delta l = \pm 1$

$3s_{1/2} \rightarrow 2p_{1/2}$

1.8886888eV

$3s_{1/2} \rightarrow 2p_{3/2}$

1.88864343 eV

$n, j < n - \frac{1}{2}$ degeneracy: $2(2j+1)$

$n, j = n - \frac{1}{2}$

Dirac Equation Solution

$$E_{nj} = m_e c^2 \left(\frac{1}{\sqrt{1 + \frac{\alpha}{n - (j + \frac{1}{2}) + \sqrt{(j+\frac{1}{2})^2 - \alpha^2}}}} - 1 \right)$$

Lamb Shift

$$E^{1}_{lamb,2s} = 4.372\times10^{-6}\,eV \qquad \mathcal{O}(\alpha^5 \ln\alpha)$$

Hydrogen in B-Field: Zeeman Effect
E-field: Stark Effect

Zeeman Effect

Apply an external magnetic field to hydrogen, $\vec{B}$.

$$\hat{H}_Z = -(\hat{\vec{\mu}}_l + \hat{\vec{\mu}}_s)\cdot\vec{B}$$

$$\vec{\mu} = g\frac{q}{2m} \qquad \hat{\vec{\mu}}_l = -\frac{e}{2m}\hat{\vec{L}} \qquad \hat{\vec{\mu}}_s = -\frac{e}{m}\hat{\vec{S}}$$

$$\hat{H}_Z = \frac{e}{2m_e}(\hat{\vec{L}} + 2\hat{\vec{S}})\cdot\vec{B}$$

$$\vec{B} = B_0\check{z}$$

$$\hat{H}_Z = \frac{eB_0}{2m_e}(\hat{L}_z + 2\hat{S}_z)$$

$$\hat{H} = \hat{H}_0 + \hat{H}_{fs} + \hat{H}_Z$$

① $B_{ext} \ll B_{int} \overset{\text{Start}}{\Rightarrow} (\hat{H}_0 + \hat{H}_{fs}) + \hat{H}_Z$

② $B_{ext} \gg B_{int} \Rightarrow (\hat{H}_0 + \hat{H}_Z) + \hat{H}_{fs}$

③ $B_{ext} \approx B_{int} \Rightarrow \hat{H}_0 + (\hat{H}_{fs} + \hat{H}_Z)$

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Zeeman Effect

Hydrogen in a magnetic field

Let $\vec{B} = B_0 \check{z}$

$$H_z = \frac{e}{2m_e}\vec{B}\cdot\left(\hat{\vec{L}}+2\hat{\vec{S}}\right) = \frac{e}{2m_e}\vec{B}\cdot\left(\hat{\vec{J}}+\hat{\vec{S}}\right) = \frac{eB}{2m_e}\left(\hat{J}_z+\hat{S}_z\right)$$

Weak-field $\hat{H} = \overbrace{\boxed{\hat{H}_0 + \hat{H}_{fs}}}^{\text{unperturbed}} + \hat{H}_z \rightarrow$ perturbation

Intermediate field $\hat{H} = \overset{\text{uperturbed}}{\hat{H}_0} + \boxed{\hat{H}_{fs} + \hat{H}_z}$ perturbation

Strong Field $\hat{H} = \underbrace{\hat{H}_0 + \overset{\text{perturbation}}{\hat{H}_{fs}} + \hat{H}_z}_{\text{uperturbed}}$

Weak-Field

States $|n\,l\,j\,m_j\rangle$ energies E_{nj}

$|n\;l\;j\;m_j\rangle$

$\hat{H}_0, \hat{L}^2, \hat{J}^2, \hat{J}_z$ $\hat{L}^2, \hat{J}_z$ label our degeneracy

1st order shifts

$$\langle n l j m_j | \hat{H}_Z | n l j m_j \rangle$$

$$\frac{eB_0}{2m_e}\left(\langle J_z \rangle + \langle S_z \rangle \right) = \frac{eB_0}{2m_e}\left(m_j \hbar + \langle S_z \rangle \right)$$

$$\langle n l j m_j | S_z | n l j m_j \rangle$$

Clebsch Gordon time!

$$| l\, s=\tfrac{1}{2}\, j m_j \rangle = \sum_{m_s=-\frac{1}{2}}^{\frac{1}{2}} \langle l\, s=\tfrac{1}{2}\, \overset{m_j - m_s}{m_l}\, m_s | j m_j \rangle \, | l\, s=\tfrac{1}{2}\, m_l m_s \rangle$$

$$\hat{S}_z | l\, s=\tfrac{1}{2}\, j m_j \rangle = \sum_{m_s=-\frac{1}{2}}^{\frac{1}{2}} \langle l\, s=\tfrac{1}{2}\, m_l m_s | j m_j \rangle \, \hbar m_s \, | l\, s=\tfrac{1}{2}\, m_l m_s \rangle$$

$$\langle l\, s=\tfrac{1}{2}\, j m_j | \hat{S}_z | l s j m_j \rangle = \sum_{m_s=-\frac{1}{2}}^{\frac{1}{2}} \hbar m_s \left| \langle l\, s=\tfrac{1}{2}\, m_l m_s | j m_j \rangle \right|^2$$

~~$\langle l\, s=\frac{1}{2}\quad j=l\pm\frac{1}{2}\quad m_j$~~

$$\langle l, s=\tfrac{1}{2}, \underbrace{(m_j - \tfrac{1}{2})}_{m_l}\, m_s=\tfrac{1}{2} | j = l \pm \tfrac{1}{2}, m_j \rangle$$

$$= \sqrt{\frac{l+\frac{1}{2} \pm m_j}{2l+1}}$$

$$\langle l\, s=\tfrac{1}{2}\, (m_j + \tfrac{1}{2})\, m_s = -\tfrac{1}{2} | j = l \pm \tfrac{1}{2}, m_j \rangle = \pm \sqrt{\frac{l+\frac{1}{2} \mp m_j}{2l+1}}$$

$$\sum_{m_s=-\frac{1}{2}}^{\frac{1}{2}} \hbar m_s \left|\langle l \; s=\tfrac{1}{2} \; m_l m_s | j m_j \rangle\right|^2$$

$$= \hbar\left(\tfrac{1}{2}\right)\frac{l+\frac{1}{2}\pm m_j}{2l+1} + \hbar\left(-\tfrac{1}{2}\right)\frac{l+\frac{1}{2}\mp m_j}{2l+1} = \pm\frac{\hbar m_j}{2l+1}$$

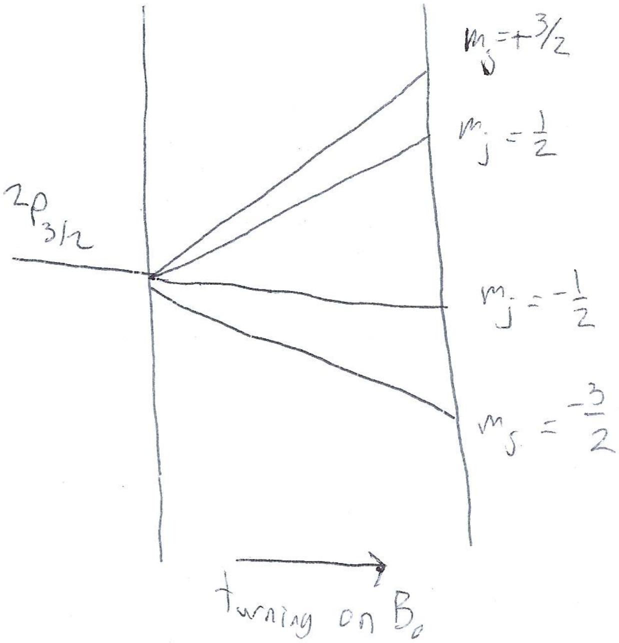
$$E'_z - \frac{e\hbar}{2m_e} B_0 \left(1 \pm \frac{1}{2l+1}\right) m_j$$

$j = l \pm \frac{1}{2}$

$$g_J = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)} \qquad \mu_B = \frac{e\hbar}{2m_c}$$

$$E'_z = \mu_B B_0 g_J m_j$$

weak field



Strong Field

$$\hat{H}_Z = \frac{eB_0}{2m_e}\left(\hat{L}_z + 2\hat{S}_z\right)$$

$$|n\, l\, m_l\, m_s\rangle$$

$$E_n^0 = \frac{E_1}{n^2} \xRightarrow{\text{Zeeman first}} E_Z^1 = \langle n\, l\, m_l\, m_s | \hat{H}_Z | n\, l\, m_l\, m_s\rangle$$

$$\hat{H}_0, \underbrace{\hat{L}^2, \hat{L}_z, \hat{S}_z}_{\text{degenerate states}}$$

$$= \frac{eB_0}{2m_e}\hbar\left(m_l + 2m_s\right)$$

$$= \frac{eB_0}{2m_e}\hbar\left(m_j + m_s\right)$$

energy determined by $n\ m_j\ m_s$

two fold degeneracy of l

$$\frac{E_1}{n^2} + \mu_B B_0\left(m_j + m_s\right) + \frac{E_1}{n^2}\left(\frac{\alpha^2}{n^2}\left\{\frac{l(l+1) - m_l m_s}{l(l+\frac{1}{2})(l+1)} n\right\} - \frac{3}{4}\right)$$

Hyperfine interaction

$$\hat{H}_B = \frac{e}{2m_e}\vec{B}\cdot\left(\vec{L} + 2\vec{S}\right) \Rightarrow \hat{H}_{hfs} = \frac{e}{2m_e}\vec{B}_{nuc}\cdot\left(\vec{L} + 2\vec{S}\right)$$

$$\vec{\mu}_N = \frac{g_N Ze}{2m_N}\vec{I}$$

Hydrogen $I = \frac{1}{2}$ $m_N = 1836 m_e$ $g_N = 5.59$

Deuterium $I = 1$ $m_N = 3671 m_e$ $g_N = 1.71$

$$\vec{B} = \frac{\mu_0}{4\pi r^3}\left(3(\vec{\mu}\cdot\hat{r})\hat{r} - \vec{\mu}\right) + \frac{2\mu_0}{3}\delta^3(\vec{r})\vec{\mu}$$

just look at $l = 0$

$$\langle \hat{H}_{hfs} \rangle = (\text{stuff that is } 0) + \frac{2\mu_0}{3}\frac{g_N Ze}{2m_N}\frac{e}{2m_e}2\left\langle \delta^3(\vec{r})\vec{I}\cdot\vec{S} \right\rangle$$

$$\langle H_{hfs} \rangle = \frac{1}{n^3}\frac{\mu_0 g_N e^2}{3\pi m_e m_N a_0^3}\langle \vec{I}\cdot\vec{S} \rangle$$

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Hydrogen Hyperfine Structure

- Electron's Angular Momentum interacts with protons spin

For s states in Hydrogen:

$$\hat{H}_{hfs} = (\text{stuff that will not contribute}) + \frac{2\mu_0}{3}\frac{e^2}{m_e}\frac{g_N}{2m_p}\delta(\hat{\vec{r}})\underbrace{(\hat{\vec{I}}\cdot\hat{\vec{S}})}$$

$$\frac{\mu_0}{3}\frac{e^2 g_N}{m_e m_p}\delta(\vec{r})\frac{\hat{F}^2 - \hat{I}^2 - \hat{S}^2}{2} \qquad \vec{F} = \vec{I} + \vec{S}$$

States: $|n, l=0, f, m_f\rangle = |n, l=0, I, s=\frac{1}{2}, f, m_f\rangle$

$$E^1_{hfs} = \frac{\mu_0}{3}\frac{e^2 g_N}{m_e m_p}|\psi(0)|^2 \frac{\hbar^2(f(f+1) - I(I+1) - \frac{3}{4})}{2}$$

$$= \frac{2}{3} g_N \left(\frac{m_e}{m_p}\right)\alpha^4 m_e c^2 \left(\frac{f(f+1) - I(I+1) - \frac{3}{4}}{n^3}\right)$$

Hydrogen ^1H

$I = \frac{1}{2}$

$m_p = 1836 m_e$

$g_p = 5.59$

$\underline{n=1}$

$$E^1_{hfs} = (2.94\times10^{-6}\,eV) \times \left(F(F+1) - \frac{3}{2}\right)$$

$\Delta E = 5.88\times10^{-6}\,eV$

$\lambda = 21\,cm$

Deuterium ^2H

nucleus is $1p + 1n$

$I = 1$

$g_D = 0.855$

$\Delta E = 1.36 \times 10^{-6}\, eV$

$\lambda = 91\, cm$

A transformation is carried out by a unitary Operator $\hat{U}^\dagger = \hat{U}^{-1}$

Active

Leave Basis fixed, act on the states

$$|\alpha\rangle \mapsto \underbrace{\hat{U}|\alpha\rangle}_{\text{different state}} \qquad \hat{A} \mapsto \hat{U}\hat{A}\hat{U}^\dagger$$

Space translations

$$\hat{T}(a) = e^{-i\hat{p}a/\hbar}$$

$\hat{T}|\alpha\rangle$ ← shifts state

$$\psi_\alpha(x) \mapsto \psi_\alpha(x-a)$$

$$\hat{T}\hat{x}\hat{T}^\dagger = \hat{x} - a\hat{\mathbb{1}}$$

$$\langle\alpha|\hat{x}|\alpha\rangle \mapsto \langle\alpha|\hat{T}^\dagger\hat{T}\hat{x}\hat{T}^\dagger\hat{T}|\alpha\rangle = \langle\alpha|\hat{x}|\alpha\rangle$$

Passive

Change of Basis

$|f\rangle^{i} = U^{i}{}_{j}|e^{j}\rangle$

$\alpha^{i} = \langle e^{i}|\alpha\rangle \qquad \vec{\alpha} \mapsto U^{\dagger}\vec{\alpha}$

$A^{i}{}_{j} = \langle e^{i}|\hat{A}|e_{j}\rangle \qquad \overleftrightarrow{A} \mapsto U^{\dagger}\overleftrightarrow{A}U$

Discrete

exchange $\hat{P}_{1\leftrightarrow 2}$

Parity $\hat{\Pi}$

Continuous

Space translation

Time translation

Rotation

Discrete Example: Parity

$\hat{\Pi}^{\dagger} = \hat{\Pi}^{-1}$ Unitary

$\hat{\Pi}^{2} = \hat{1}$ "$\mathbb{Z}_2$ symmetry"

$\hat{\Pi}^{\dagger} = \hat{\Pi}$ Hermitian

eigenvalues are ±1

"even parity states" $\hat{\Pi}|\text{even}\rangle = |\text{even}\rangle$

"odd parity states" $\hat{\Pi}|\text{odd}\rangle = -|\text{odd}\rangle$

"parity eigenoperators"

"even parity operator"

$$\hat{\Pi}\hat{A}_{even}\hat{\Pi} = \hat{A}_{even}$$

eg $\hat{X}^2$, $\hat{\vec{L}}$

"odd parity operators"

$$\hat{\Pi}\hat{A}_{odd}\hat{\Pi} = -\hat{A}_{odd}$$

eg $\hat{\vec{X}}$, $\hat{\vec{P}}$

$\hat{A}_{even}|even\rangle$ is even parity

$A_{even}|odd\rangle$ is odd parity

$\hat{A}_{odd}|even\rangle$ is odd parity

$\hat{A}_{odd}|odd\rangle$ is even parity

Let $|\alpha\rangle$, $|\beta\rangle$, $\hat{A}$ all be definite parity objects

$\hat{\Pi}|\alpha\rangle = \Pi_\alpha|\alpha\rangle$ $\quad \Pi|\beta\rangle = \Pi_\beta|\beta\rangle$ $\quad \hat{\Pi}\hat{A}\hat{\Pi} = \Pi_A \hat{A}$

$$\langle\alpha|\hat{A}|\beta\rangle = \Pi_\alpha\langle\alpha|\hat{\Pi}\hat{A}\hat{\Pi}|\beta\rangle\Pi_\beta = \langle\alpha|\hat{1}\hat{A}\hat{1}|\beta\rangle$$

$$= \langle\alpha|\hat{\Pi}\hat{\Pi}\hat{A}\hat{\Pi}\hat{\Pi}|\beta\rangle = \Pi_\alpha\Pi_A\Pi_\beta\langle\alpha|\hat{A}|\beta\rangle$$

if $\Pi_\alpha\Pi_\beta\Pi_A = -1$ then $\langle\alpha|\hat{A}|\beta\rangle = -\langle\alpha|\hat{A}|\beta\rangle = 0$

$|n\,l\ldots\rangle$ states of hydrogen have parity $(-1)^l$

Continuous

Given a Hermitian operator $\hat{G}$ ← the "generator"

a parameter b such that $Gb/\hbar$ is dimensionless

$\hat{P}$

x

We define a family of unitary operators

$$\hat{U}(b) = e^{-i\hat{G}b/\hbar} \simeq \hat{\mathbb{1}} - \frac{i\hat{G}b}{\hbar} + \frac{1}{2}\left(\frac{i\hat{G}b}{\hbar}\right)^2 + \cdots$$

Momentum generates space translations $\hat{T}(\vec{a}) = e^{-i\vec{a}\cdot\hat{\vec{P}}/\hbar}$

Energy generates time translations $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$

Orbital Angular momentum generates spatial rotations $\hat{R}_{space}(\phi,\check{n}) = e^{-i\phi\hat{n}\cdot\hat{\vec{L}}/\hbar}$

Spin Angular momentum generates spin Rotations $\hat{R}_{spin}(\phi,\check{n}) = e^{-i\phi\check{n}\cdot\hat{\vec{S}}/\hbar}$

Total Angular momentum generates Full Rotations $\hat{R}(\phi,\hat{n}) = e^{-i\phi\check{n}\cdot\hat{\vec{J}}/\hbar}$

Let $\hat{A}$ be invariant under a transformation

$$\boxed{\hat{U}\hat{A}\hat{U}^{\dagger} = \hat{A}}$$

Let's look at a wee transformation

$$\hat{U}(\delta b) = \hat{1} - \frac{i\hat{G}\delta b}{\hbar} + \mathcal{O}(\delta b^2)$$

$$\left(\hat{1} - \frac{i\hat{G}\delta b}{\hbar} + \mathcal{O}(\delta b^2)\right)\hat{A}\left(\hat{1} + \frac{i\hat{G}\delta b}{\hbar} + \mathcal{O}(\delta b^2)\right)$$

$$= \hat{1}\hat{A}\hat{1} + \hat{1}\hat{A}\left(\frac{i\hat{G}\delta b}{\hbar}\right) - \left(\frac{i\hat{G}\delta b}{\hbar}\right)\hat{A}\hat{1} + \mathcal{O}(\delta b^2)$$

$$= \hat{A} + \frac{i}{\hbar}\delta b\left[\hat{A},\hat{G}\right] + \mathcal{O}(\delta b^2) = \hat{A}$$

$$\left[\hat{A},\hat{G}\right] = 0$$

Symmetry tends to imply degeneracy

Hamiltonian $\hat{H}$ energy eigenstate $|\alpha\rangle$ with energy eigenvalue E_α

H invariant under transformations generated by $\hat{G} \Rightarrow [\hat{H},\hat{G}] = 0$

Define $|\beta\rangle \equiv \hat{G}|\alpha\rangle$

$$\hat{H}|\beta\rangle = E_\alpha|\beta\rangle$$

Possibility 1: $\hat{G}|\alpha\rangle = 0$

Possibility 2: $\hat{G}|\alpha\rangle = g|\alpha\rangle$

Possibility 3: $\hat{G}|\alpha\rangle \neq g|\alpha\rangle$

$|\beta\rangle$ is a linearly independent state from $|\alpha\rangle$ with the same energy E_α

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Continuous Symmetries

Hermitian Op / Generator $\hat{G}$

Unitary Op / Transformation $\hat{U}(b) = e^{-i\hat{G}b/\hbar}$

$\hat{A}$ invariant under $\hat{U} \longleftrightarrow \hat{U}(b)\hat{A}U^{\dagger}(b) = \hat{A}$

$\longleftrightarrow [\hat{G}, \hat{A}] = 0$

Hamiltonian $\hat{H}$

Eigenstate $|\alpha\rangle$ with eigenvalues E_α

Let $[\hat{G}, \hat{H}] = 0$ and $|\beta\rangle \equiv \hat{G}|\alpha\rangle$

$$\left.\right\} \hat{H}|\beta\rangle = E_{\alpha}|\beta\rangle$$

Gross Structure Hydrogen

Symmetries: Spin Rotation
Space Rotation

Predicted: $2(2l+1)$ actual: $2n^2$

Fine Structure Hydrogen

Symmetries: Overall Rotations

$(2j+1)$

3D Rotations: Group SO(3)

Hydrogen/Coulomb/Inverse Square

Exta Symmetry generated by Laplace-Runge-Lenz vector

$$\hat{M}_+|n\,l\,m_x^{+l}\rangle = C|n, l+1, m_{x+1}^{+l}\rangle$$

$$\hat{M}_+ = \hat{M}_x + i\hat{M}_y$$

$$[\hat{\vec{M}}, \hat{H}_0] = 0$$

$$\hat{\vec{M}} = \frac{\hat{\vec{p}} \times \hat{\vec{L}} - \hat{\vec{L}} \times \hat{\vec{p}}}{2m_e} - \frac{e^2}{4\pi\epsilon_0}\frac{\hat{\vec{r}}}{|\hat{\vec{r}}|}$$

Rotations

Consider total angular momentum $\vec{J}$

Scalar Operators

Invariant under rotations

Definition: A scalar operator $\hat{A}$ is one that is invariant under rotations.

$$\longleftrightarrow \cancel{[\hat{\vec{J}}, \hat{A}} \quad [\hat{\vec{J}}, \hat{A}] = 0$$

$$\frac{p^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hat{r}} \qquad\qquad \frac{eB_0}{2m_e}\left(\hat{L}_z + 2\hat{S}_z\right)$$

scalar   not scalar

Vector Operators

A set of three operators $\hat{V}_a$, $a = 1,2,3$ or x,y,z that get "mixed up" under rotations the same way regular vectors do.

$$\check{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \xrightarrow[\text{about } z \text{ axis}]{\text{rotate } 90°} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \check{y} \qquad \hat{R}(\phi, \check{n})\hat{V}_a \hat{R}^\dagger(\phi, \check{n}) = \sum_b \mathcal{R}_a^b(\phi, \check{n})\hat{V}_b$$

$$\hat{V}_x \longrightarrow \hat{V}_y \qquad \mathcal{R} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\hat{R}\hat{\vec{V}}_x\hat{R}^\dagger = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{V}_x \\ \hat{V}_y \\ \hat{V}_z \end{bmatrix} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$\hat{\vec{V}}$ is a vector operator if $\left[\hat{J}_a, \hat{V}_b\right] = \sum_c i\hbar \varepsilon_{abc} \hat{V}_c$

$\left[\hat{J}_a, \hat{J}_b\right] = \sum_c i\hbar \varepsilon_{abc} \hat{J}_c \qquad \left[\hat{J}_a, \hat{S}_b\right] = \sum_c i\hbar \varepsilon_{abc} \hat{S}_c$

$\left[\hat{J}_a, \hat{L}_b\right] = \sum_c i\hbar \varepsilon_{abc} \hat{L}_c$

$\hat{V}_{+1} \equiv -\frac{1}{\sqrt{2}}\left(\hat{V}_x + i\hat{V}_y\right)$

$\hat{V}_0 \equiv \hat{V}_z$

$\hat{V}_{-1} \equiv \frac{1}{\sqrt{2}}\left(\hat{V}_x - i\hat{V}_y\right)$

$Y_1^1 = -\frac{1}{\sqrt{2}} \frac{x+iy}{r} \qquad Y_0^1 = \frac{z}{r} \qquad Y_{-1}^1 = \frac{1}{\sqrt{2}} \frac{x-iy}{r}$

$\left[\hat{J}_z, \hat{V}_{+1}\right] = \hbar \hat{V}_{+1}$

$\left[\hat{J}_z, \hat{V}_0\right] = 0$

$\left[\hat{J}_z, \hat{V}_{-1}\right] = -\hbar \hat{V}_{-1}$

$\hat{J}_z |1,1\rangle = \hbar |1,1\rangle$

$\hat{J}_z |1,0\rangle = 0$

$\hat{J}_z |1,-1\rangle = -\hbar |1,-1\rangle$

$[\hat{J}_+, \hat{V}_{+1}] = 0$ $\quad$ $[\hat{J}_-, \hat{V}_{+1}] = \hbar\sqrt{2}\,\hat{V}_0$

$[\hat{J}_+, \hat{V}_0] = \sqrt{2}\,\hbar\,\hat{V}_{+1}$ $\quad$ $[\hat{J}_-, \hat{V}_0] = \hbar\sqrt{2}\,\hat{V}_{-1}$

$[\hat{J}_+, \hat{V}_{-1}] = \sqrt{2}\,\hbar\,\hat{V}_0$ $\quad$ $[\hat{J}_-, \hat{V}_{-1}] = 0$

$$[\hat{J}_\pm, \hat{V}_m] = \hbar\sqrt{1(1+1) - m(m\pm1)}\;\hat{V}_{m\pm1}$$

$m = -1, 0, 1$

$$\sum_a [\hat{J}_a, [\hat{J}_a, \hat{V}_b]] = \underset{\uparrow\; 1(1+1)}{2}\hbar^2\hat{V}_b$$

Vector operators $\hat{V}_m$ act like they carry angular momenta!

Scalar Operator Selection Rules

States $|\underset{\substack{\uparrow \\ \text{any other quantum number}}}{n}, j, m_j\rangle$

Scalar operator $\hat{A}$

$\langle n', j', m_j' | \hat{A} | n, j, m_j\rangle$

$[\hat{J}^2, \hat{A}] = 0$

$\langle n' j' m_j' | [\hat{J}^2, \hat{A}] | n j m_j\rangle = 0 = \langle n' j' m_j' | \hat{J}^2\hat{A} - \hat{A}\hat{J}^2 | n j m_j\rangle$

$= \hbar^2 j'(j'+1)\langle n' j' m_j' | \hat{A} | n j m_j\rangle - \hbar^2 j(j+1)\langle n' j' m_j' | \hat{A} | n j m_j\rangle$

if $j \neq j'$ $\langle n' j' m_j' | \hat{A} | n j m_j\rangle$ must be zero

or if $m_j \neq m_j'$

$$0 = \langle n' j' m_j \pm 1 | [\hat{J}_\pm , \hat{A}] | n j m_j \rangle$$

$$= \langle n' j\, m_j \pm 1 | \hat{J}_\pm \hat{A} - \hat{A} \hat{J}_\pm | n j m_j \rangle$$

$$= -\hbar \sqrt{j(j+1) - m_j(m_j \pm 1)} \langle n' j m_j \pm 1 | \hat{A} | n j m_j \pm 1 \rangle$$
$$+ \hbar \sqrt{j(j+1) - m_j(m_j \pm 1 \mp 1)} \langle n' j m_j | \hat{A} | n j m_j \rangle$$

$$= \hbar \sqrt{j(j+1) - m_j(m_j \pm 1)} \left(\langle n' j m_j | A | n j m_j \rangle - \langle n' j m_j \pm 1 | A | n j m_j \pm 1 \rangle \right)$$

$\langle n' j m_j | \hat{A} | n j m_j \rangle$

is independent of m_j

$$\langle n' j' m_j' | \hat{A} | n j m_j \rangle = \delta_{jj'} \delta_{m_j m_j'} \times \langle n' j \| A \| n j \rangle$$

"reduced matrix" element

4 n=2 states of hydrogen

$$\begin{array}{c|cccc} \langle 200| \boxed{\hat{r}^2} & |200\rangle & |211\rangle & |210\rangle & |21-1\rangle \\ \hline & a & 0 & 0 & 0 \\ \langle 211| & 0 & b & 0 & 0 \\ \langle 210| & 0 & 0 & b & 0 \\ \langle 21-1| & 0 & 0 & 0 & b \end{array}$$

$a = \langle 200 | \hat{r}^2 | 200 \rangle$

$b = \langle 210 | \hat{r}^2 | 210 \rangle$

$[\hat{J}_z, \hat{V}_0] = 0 \Rightarrow \langle n'j'm_j'|\hat{V}_z|n j m_j\rangle = 0$ if $m_j' \neq m_j$

$\cancel{[\hat{J}_z, \hat{V}_{\pm 1}] = 0}$

$[\hat{J}_z, \hat{V}_{\pm 1}] = \pm\hbar \hat{V}_{\pm} \Rightarrow \langle n'j'm_j'|\hat{V}_{\pm 1}|n j m_j\rangle = 0$ if $m_j' \neq m_j \pm 1$

$$\langle n'j'm_j'|\hat{V}_{m_v}|n j m_j\rangle = \begin{pmatrix}\text{coefficient depending}\\ \text{only on } j, j', m_j, m_j' \\ \text{and } m_v\end{pmatrix} \times \begin{pmatrix}\text{common factor}\\ \text{that doesn't depend}\\ \text{on any of the } m\text{'s}\\ (\text{only on } n, n', j, j')\end{pmatrix}$$

$\uparrow$

Clebsch Gordon
Coefficients

$$C^{j1j'}_{m_j m_v m_j'} \langle n'j'||V||nj\rangle$$

To be nonzero, . . .

$|j-1| \leq j' \leq j+1 \Rightarrow \Delta j = 0, \pm 1$

$m_j + m_v = m_j' \Rightarrow \Delta m_j = 0, \pm 1$

$\langle 210|\hat{z}|320\rangle$

knowing this tells you all 45 $\langle 21 m_j|\hat{r}_{m_v}|32 m_j\rangle$

<u>Wigner - Eckart Theorem</u>

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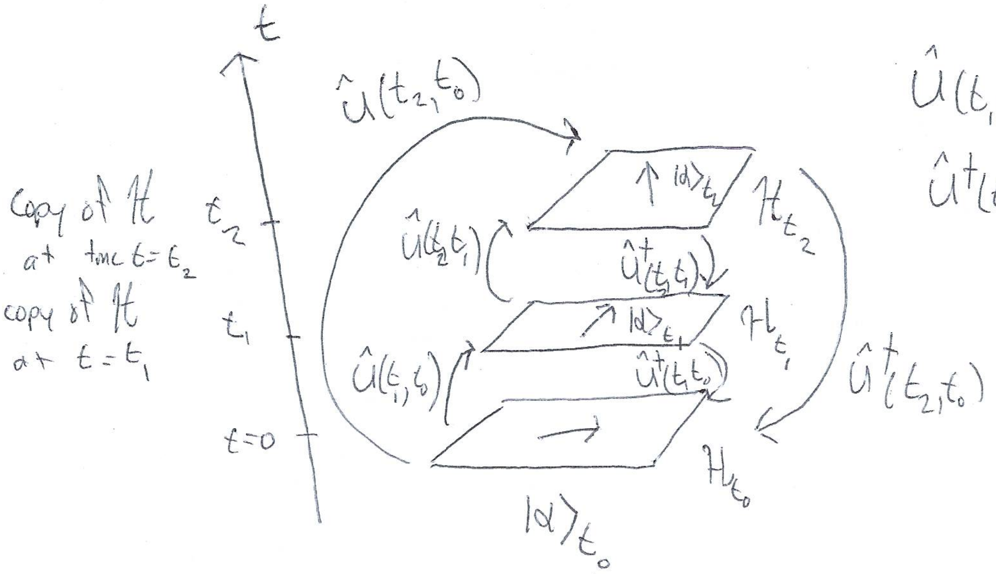
Dynamics

Time Evolution and the time translation operator



$\hat{U}(t_1,t_0): \mathcal{H}_{t_0} \to \mathcal{H}_{t_1}$

$\hat{U}^\dagger(t_1,t_0): \mathcal{H}_{t_1} \to \mathcal{H}_{t_0}$

Unitary $\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0)$

$\hat{U}(t,t) = \hat{\mathbb{1}}$ (initial condition)

Composition: $\hat{U}(t_2,t_1)\hat{U}(t_1,t_0) = \hat{U}(t_2,t_0)$

$$\underset{\mathcal{H}_t}{\underset{\cap}{|\alpha\rangle_t}} = \hat{U}(t,t_0)\underset{\mathcal{H}_{t_0}}{\underset{\cap}{|\alpha\rangle_{t_0}}}$$

$$i\hbar \frac{\partial |\alpha\rangle_t}{\partial t} = \hat{H}(t)|\alpha\rangle_t$$

$$i\hbar \frac{\partial}{\partial t}\left(\hat{U}(t,t_0)|\alpha\rangle_{t_0}\right) = \hat{H}(t)\hat{U}(t,t_0)|\alpha\rangle_{t_0} = i\hbar\frac{\partial \hat{U}(t,t_0)}{\partial t}|\alpha\rangle_{t_0} = \left(\hat{H}(t)\hat{U}(t,t_0)\right)|\alpha\rangle_{t_0}$$

Time Dependent Schrodinger Equation

$$i\hbar \frac{\partial U(t,t_0)}{\partial t} = \hat{H}(t)\hat{U}(t,t_0)$$

$$\hat{u}(t_0+\delta t, t_0) = u(t_0, t_0) + \delta t \left.\frac{\partial \hat{u}}{\partial t}\right|_{t_0} + \mathcal{O}(\delta t^2)$$

$$= \mathbb{1} + \delta t \left.\frac{H(t)\,u(t,t_0)}{i\hbar}\right|_{t_0} + \mathcal{O}(\delta t^2)$$

$$= \mathbb{1} - \frac{i}{\hbar}\hat{H}(t_0)\,\delta t + \cdots$$

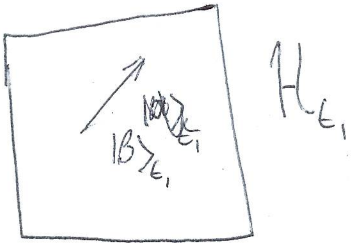
If $\frac{\partial \hat{H}}{\partial t} = 0$, $\hat{u}(t_0+\Delta t, t_0) = e^{-i\hat{H}\Delta t/\hbar}$

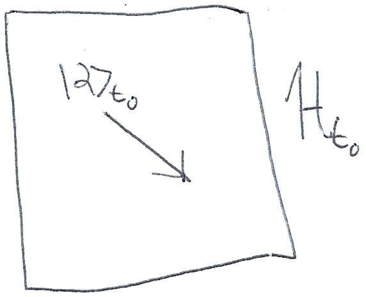
If $[\hat{H}(t_0), \hat{H}(t)] = 0 \ \forall t_0, t$

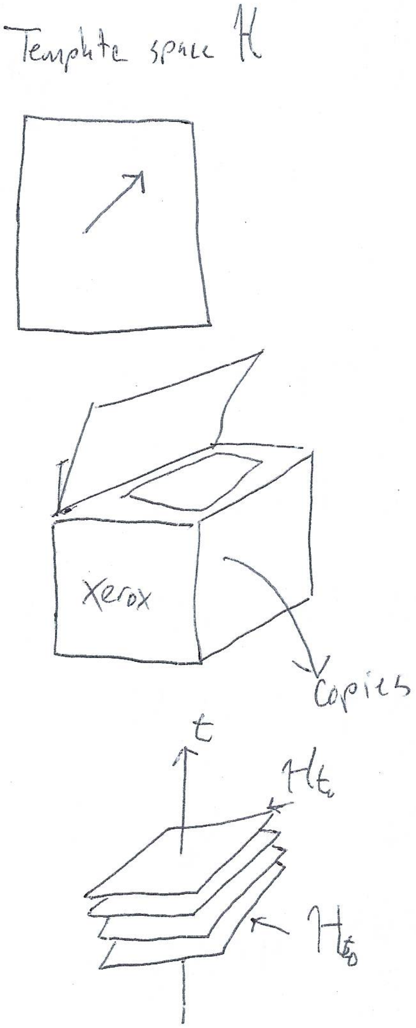
$$\hat{u}(t_1, t_0) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t_1}\hat{H}(t')\,dt'\right)$$

If $[A, B] \neq 0$

$\Rightarrow e^{\hat{A}}e^{\hat{B}} \neq e^{[\hat{A},\hat{B}]}e^{\hat{A}+\hat{B}}$







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A summary of the "pictures"

	State Evolution	Operator Evolution	TDSE
Schrödinger	$\hat{U}(t,t_0)$	$\hat{\mathbb{1}}$	$i\hbar\frac{\partial}{\partial t}\lvert\alpha(t)\rangle = \hat{H}_S\lvert\alpha(t)\rangle_S$
Heisenberg	$\hat{\mathbb{1}}$	$\hat{U}(t,t_0)$	$i\hbar\frac{\partial}{\partial t}\lvert\alpha(t)\rangle_H = 0$
Dirac	$e^{iH_0(t-t_0)/\hbar}$	$e^{-iH_0(t-t_0)/\hbar}$	$i\hbar\frac{\partial}{\partial t}\lvert\alpha(t)\rangle_D = H_{1D}(t)\lvert\alpha(t)\rangle_D$ $\hat{H}_{1D}(t) = e^{iH_0(t-t_0)/\hbar}H_1(t)e^{-iH_0(t-t_0)/\hbar}$

$$\hat{H}_S(t) = \hat{H}_0 + \hat{H}_1(t)$$

$|n\rangle$ with energy E_n^0

at $t=0$

$$\lvert\alpha(0)\rangle = \sum_n c_n(0)\lvert n\rangle$$

$$\lvert\alpha(t)\rangle_P = \sum_n c_{nP}(t)\lvert n\rangle$$

$$c_{nS}(t) = \sum_m c_m(0)\langle n\rvert\hat{U}(t,0)\lvert m\rangle$$

$$c_{nH}(t) = c_n(0)$$

$$c_{nD}(t) = e^{iE_n^0 t/\hbar}c_{nS}(t)$$

$$|\alpha(t)\rangle = \sum_n c_n(t)\, e^{-iE_n^0 t/\hbar}\,|n\rangle$$

$$\frac{dc_m}{dt} = \frac{-i}{\hbar}\sum c_n(0)\, e^{i\omega_{mn}t}\langle m|\hat{H}_1|n\rangle \quad , \quad \omega_{mn} = \frac{E_m^0 - E_n^0}{\hbar}$$

$$\hat{H}(t;\varepsilon) = \hat{H}_0 + \varepsilon \hat{H}_1(t)$$

We will ultimately set $\varepsilon = 1$

$$c_m(t) = \sum_p \varepsilon^p c_m^{(p)}(t)$$

$\underline{p=0}$

$$c_m^0(t) = c_m(0) = c_m^0$$

$\underline{p \geq 1}$

$$\frac{dc_m^{(p)}}{dt} = -\frac{i}{\hbar}\sum_n c_n^{(p-1)}(t)\, e^{i\omega_{mn}t}\langle m|\hat{H}_1|n\rangle$$

$$c_m^1(t) = \frac{-i}{\hbar}\sum_n c_n^0 \int_0^t e^{i\omega_{mn}t'}\langle m|\hat{H}_1(t')|n\rangle\, dt'$$

Start in an H_0 eigenstate at t_0

$$c_m^0 = \delta_{nm} \qquad\qquad |n\rangle \swarrow \text{starting state}$$

$$\Downarrow \Longrightarrow \quad c_m(t) = \delta_{mn} - \frac{i}{\hbar}\int_{t_0}^{t} e^{i\omega_{mn}t'}\langle m|H_1(t')|n\rangle\, dt' + \mathcal{O}(H_1^2)$$

$$P_{n\to m} \equiv |c_m(t)|^2 \quad \text{transition probability}$$

$$= |c_m^0 + c_m^1 + \ldots|^2 \cong |c_m^0|^2 + c_m^0 c_m^1 + (c_m^0 c_m^2 + c_m^{(1)2}) + \ldots$$

$$m \neq n \Rightarrow c_{m\neq n} = 0 \qquad P_{m\to m} = |c_m^1(t)|^2 + \mathcal{O}(H_1^3)$$

$n \neq m$

$$P_{n\to m} = \frac{1}{\hbar^2}\left|\int_{t_0}^{t} e^{i\omega_{mn}t'}\langle m|H_1|n\rangle dt'\right|^2$$

Example 1:

Turn a constant perturbation on at $t=0$ and off at $t=t_f$

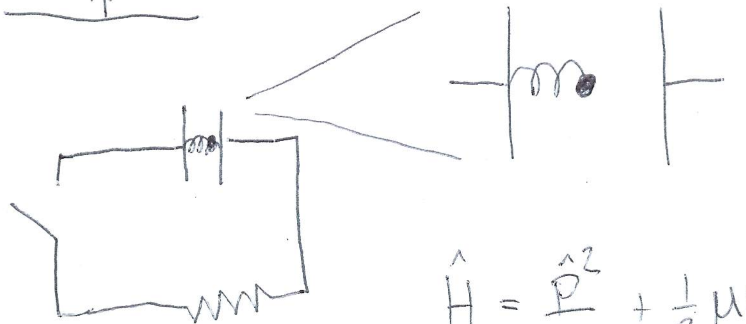
$$\hat{H}_1(t) = \begin{cases} \hat{H}_1 & 0 \leq t \leq t_f \\ 0 & \text{else} \end{cases} \qquad |n\rangle \text{ at } t<0$$

$$P_{n\to m}(t>t_f) \cong \frac{1}{\hbar^2}\left|\int_{t<0}^{t>t_f} e^{i\omega_{mn}t'}\langle m|\hat{H}_1(t')|n\rangle dt'\right|^2$$

$$= \frac{|\langle m|\hat{H}_1|n\rangle|^2}{\hbar^2}\left|\underbrace{\int_0^{t_f} e^{i\omega_{mn}t'}dt'}_{2e^{i\omega_{mn}t/2}\frac{\sin\left(\frac{\omega_{mn}t}{2}\right)}{\omega_{mn}}}\right|^2$$

$$= \frac{4|\langle m|\hat{H}_1|n\rangle|^2}{\hbar^2\omega_{mn}^2}\sin^2\left(\frac{\omega_{mn}t}{2}\right)$$

Example 2



$$\hat{H}_0 = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\tilde{\omega}\hat{x}^2$$

$$\hat{H}_1(t) = \begin{cases} -q\mathcal{E}_0\hat{x}e^{-t/\tau} & t \geq 0 \\ 0 & t < 0 \end{cases}$$

Start in ground state at $t=0$

Probability of transition to state m

$$C_m^1 = \frac{-i}{\hbar}\int_0^t dt'\, e^{im\tilde{\omega}t'}(-q\mathcal{E}_0)e^{-t/\tau}\langle m|\hat{x}|0\rangle$$

$$\omega_{m0} = \frac{E_m - E_0}{\hbar} = \frac{\hbar\tilde{\omega}(m+\frac{1}{2}) - \hbar\tilde{\omega}(\frac{1}{2})}{\hbar}$$

$\langle m|\hat{x}|0\rangle$

$= \sqrt{\frac{\hbar}{2\mu\tilde{\omega}}}$ $m=1$

$= 0$ else

~~$P_{0\to1}$~~ $C_m^1(\infty) = \frac{iq\mathcal{E}_0}{\hbar}\sqrt{\frac{\hbar}{2\mu\tilde{\omega}}}\frac{\tau}{1-i\tilde{\omega}\tau}$

$$P_{0\to1} = \frac{q^2\mathcal{E}_0^3}{2\mu\tilde{\omega}\hbar}\frac{\tau^2}{1+\tilde{\omega}^2\tau^2}$$

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$$\hat{H}_1(t) = \hat{K}^{\dagger} e^{i\omega_0 t} + \hat{K} e^{-i\omega_0 t} \qquad \Delta\omega = \omega_0 - |\omega_{fi}|$$

$$\boxed{P_{i\to f}(t) \approx \frac{4|K_{fi}|^2}{\hbar^2} \frac{\sin^2\left(\frac{\Delta\omega t}{2}\right)}{(\Delta\omega)^2}} \qquad \omega_{fi} = \frac{E_f - E_i}{\hbar}$$

$$K_{fi} = \langle f|\hat{K}|i\rangle$$

$$\lim_{t\to\infty} \frac{\sin^2\left(\frac{\Delta\omega t}{2}\right)}{(\Delta\omega)^2} = \frac{\pi}{2} t\, \delta(\Delta\omega)$$

$$P_{i\to f}(t>>1) = \frac{2\pi|K_{fi}|^2}{\hbar^2} t\, \delta(\omega_0 - \omega_{fi})$$

$$\boxed{R_{i\to f} \equiv \frac{dP_{i\to f}}{dt} = \frac{2\pi|K_{fi}|^2}{\hbar^2} \delta(\omega_0 - \omega_{fi})}$$

Continuous Spectrum of final states

$\rho(E_f)$ density of states at energy E

$\rho(E_f)\, dE_f$ is the number of states with energy between E_f and $E_f + dE_f$

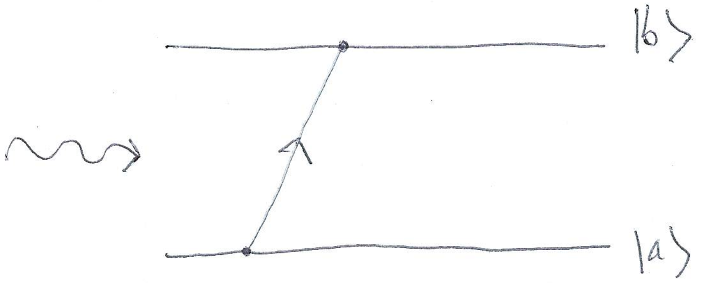
$$R_{i\to E_f} = \int_{E_f-\epsilon}^{E_f+\epsilon} R^{(E)}_{i\to f}\,\rho(E)\,dE \Rightarrow \boxed{R_{i\to E_f} = \frac{2\pi}{\hbar}\left|\langle f|\hat{K}|i\rangle\right|^2\rho(E_f)}$$

Fermi's Golden Rule

Consider a system that can interact with the EM field

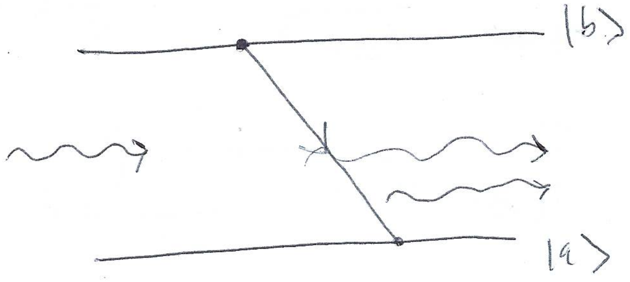
2 states $|a\rangle$ and $|b\rangle$ of $\hat{H}_0$

EM waves will act as a time dependent perturbation



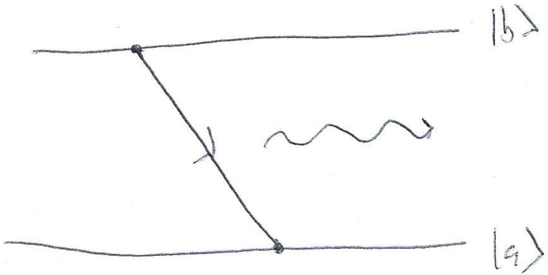
Absorption

$R_{a\to b} = B_{ab}\,\rho(\omega_{\substack{ab\\ba}})$



Stimulated emission

$R_{b\to a} = B_{ba}\,\rho(\omega_{\substack{ab\\ba}})$



Spontaneous emission

$R_{b\to a} = A_{ba}$

Look at a monochromatic (fixed ω) polarized plane wave moving in a particular direction.

$$\hat{H}_1 \propto \underset{\nwarrow\text{electric field Amplitude}}{\mathcal{E}_0} \Rightarrow R_{i\to f} \propto \mathcal{E}_0^2 \propto u_{avg}$$

energy-per unit volume in EM field $u = \frac{1}{2}\epsilon_0|\vec{E}|^2 + \frac{|\vec{B}|^2}{2\mu_0}$

$$u_{avg} = \frac{1}{2}\epsilon_0\mathcal{E}_0^2 \qquad = \epsilon_0|\vec{E}|^2$$

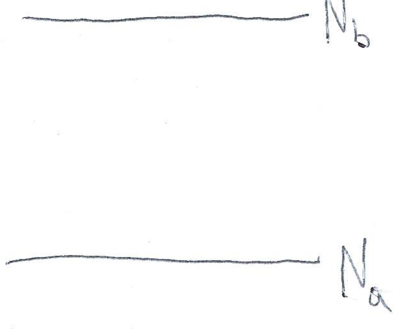
$$\vec{E} = \vec{\mathcal{E}}_0\cos(\vec{k}\cdot\vec{r} - \omega t)$$

$u_\omega \equiv \rho(\omega)d\omega$

energy density at frequency ω $\quad \omega = \frac{2\pi c}{\lambda}$

$$\rho(\omega)d\omega = \frac{1}{2}\epsilon_0\mathcal{E}_0^2(\omega) \;,\quad dR_{a\to b}(\omega) \propto \mathcal{E}_0^2(\omega) \propto \rho(\omega)d\omega$$

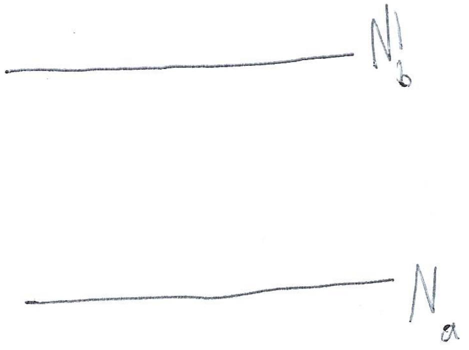
$$dR_{a\to b} = \frac{2\pi}{\hbar^2}\left|K_{fi}\right|^2\delta(\omega - \omega_{ba}) \Rightarrow R_{a\to b,tot} \propto \rho(\omega_{ba})$$



Planck $\rho(\omega) = \frac{\hbar}{\pi^2c^3}\frac{\omega^3}{e^{\hbar\omega/kT} - 1}$

Assume we are in thermal equilibrium → Boltzman

$$\frac{N_a}{N_b} = \frac{e^{-E_a/k_BT}}{e^{-E_b/k_BT}} = e^{\hbar\omega_{ba}/k_BT}$$



$$\frac{dN_a}{dt} = N_b B_{ba} \rho(\omega_{ba}) - N_a B_{ab} \rho(\omega_{ba}) + N_b A_{ba} = 0$$

$$\rho(\omega_{ba}) = \frac{A_{ba}}{\left(\frac{N_a}{N_b}\right) B_{ab} - B_{ba}} \qquad \frac{\hbar}{\pi^2 c^3} \frac{\omega_{ba}^3}{e^{\hbar\omega_{ba}/kT} - 1} = \frac{A_{ba}}{e^{\hbar\omega/kT} B_{ab} - B_{ba}}$$

$$\boxed{B_{ab} = B_{ba}} \qquad \boxed{A_{ba} = \frac{\hbar \omega_{ba}^3}{\pi^2 c^3} B_{ab}}$$

Lifetime of $|b\rangle = \frac{1}{A}$

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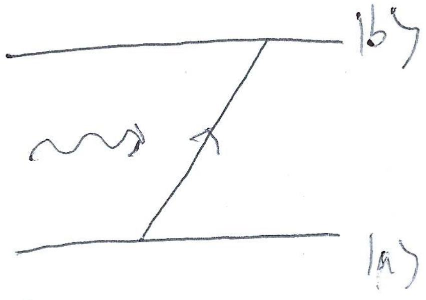
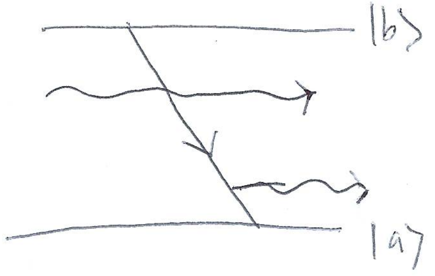


Absorption rate

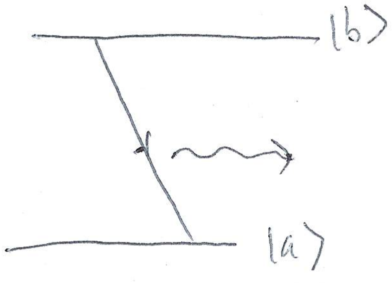
$R_{ab} = B_{ab}\rho(\omega_{ba})$

radiation density



Stimulated Emission rate

$R_{ba} = B_{ba}\rho(\omega_{ba})$



Spontaneous Emission Rate

$R_{ba} - A_{ba}$

$$B_{ba} = B_{ab} \qquad A_{ba} = \frac{\hbar\omega_{ba}^3}{\pi^2 c^3} B_{ab}$$

Monochromatic Polarized Plane wave

$\vec{k}$, $|\vec{k}| = \frac{2\pi}{\lambda}$ $\check{k}$ = propagation direction

$\omega = |\vec{k}|c$

amplitude

$\vec{E}(\vec{r},t) = \vec{\mathcal{E}}_0 \cos(\vec{k}\cdot\vec{r} - \omega t)$, $\vec{\mathcal{E}}_0 = \mathcal{E}_0 \check{\mathcal{E}}$ ← Polarization direction

$\check{\mathcal{E}} \perp \vec{k}$

$r \sim 10^{-10} m$

~~$k \gtrsim 10^{+8} m$~~ $K < 10^{8} m^{-1}$

$kr < 10^{-2}$

$\vec{E}(\vec{r},t) \cong \mathcal{E}_0 \cos\omega t\, \check{\mathcal{E}}$

Electric Dipole Approximation

Electric Dipole (E1) ← if this electric field is used in $\hat{H}_1$

rate $\propto |\langle b|\hat{\vec{r}}_q|a\rangle|^2$

"allowed transitions"

$\Delta j = 0, \pm 1 \quad \Delta m_j = 0, \pm 1$ } coupled basis

$\Delta l = \pm 1$

~~Δ~~

$\Delta l = \pm 1$ } uncoupled basis

$\Delta m_s = 0$

$\Delta m_l = 0, \pm 1$

driving frequency

$$\hat{H}_{E1} = -q(\vec{\mathcal{E}}_0 \cdot \hat{\vec{r}})\cos\omega t$$

$$= \hat{K} e^{-i\omega_0 t} + \hat{K}^\dagger e^{i\omega_0 t}$$

$\omega = \omega_0$

$$\hat{K} = -\frac{1}{2} q \mathcal{E}_0 \check{\mathcal{E}} \cdot \hat{\vec{r}}$$

a component of a vector operator

$$|K_{ba}|^2 = |\langle b| -\frac{1}{2} q \mathcal{E}_0 \check{\mathcal{E}} \cdot \hat{\vec{r}} |a\rangle|^2 = \frac{q^2 \mathcal{E}_0^2}{4} |\langle b|\hat{\vec{r}}|a\rangle|^2$$

$$R_{a\to b} = \frac{2\pi}{\hbar^2} |K_{ba}|^2 \delta(\omega - \omega_{ba}) = \frac{2\pi}{\hbar^2} \frac{q^2 \mathcal{E}_0^2}{4} |\check{\mathcal{E}} \cdot \langle b|\hat{\vec{r}}|a\rangle|^2 \delta(\omega - \omega_{ba})$$

→ monochromatic transition rate

expand to broadband with a range of ω

Last time: $\mathcal{E}_0^2 = \frac{2\rho(\omega)d\omega}{\epsilon_0}$

$$\frac{2\pi}{\hbar^2}\frac{q^2\,2\rho(\omega)d\omega}{4\,\epsilon_0}\left|\check{\mathcal{E}}\cdot\langle b|\hat{r}|a\rangle\right|^2\delta(\omega-\omega_{ba}) = dR_{a\to b}$$

$$R_{a\to b} = \frac{\pi q^2}{\hbar^2\epsilon_0}\left|\check{\mathcal{E}}\cdot\langle b|\hat{\check{r}}|a\rangle\right|^2\rho(\omega_{ba})$$ ↗ contains states of all polarization directions and propagation directions

↖ transition rate for EM radiation of fixed polarization and propagation direction

⇓ average over $\check{k}$ and $\check{\mathcal{E}}$

Our $\rho = \sum_s \int d\Omega\, \rho_{townsend}$

averaging over $\check{k}$ does nothing since our rate is $\check{k}$ independent

Consider a fixed vector $\check{V}$ and another vector $\check{\mathcal{E}}$

↑ chose $\check{z}$

$$\check{\mathcal{E}} = \begin{bmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{bmatrix} \qquad \check{V} = \begin{bmatrix}0\\0\\1\end{bmatrix}$$

$$\check{\mathcal{E}}\cdot\check{V} = \cos\theta$$

Average: $\frac{1}{4\pi}\int|\check{\mathcal{E}}\cdot\check{V}|^2\,d\cos\theta\,d\phi = \frac{1}{4\pi}\int_{-1}^{1}\cos^2\theta\,d\cos\theta\int_0^{2\pi}d\phi$

$= \frac{1}{4\pi}\frac{2}{3}2\pi = \frac{1}{3}$

average over $\check{\mathcal{E}} \Rightarrow R_{a\to b} = \frac{\pi q^2}{3\epsilon_0\hbar^2}|\langle b|\hat{r}|a\rangle|^2\rho(\omega_{ba})$

with $|\langle b|\hat{r}|a\rangle|^2 = |\langle b|\hat{x}|a\rangle|^2 + |\langle b|\hat{y}|a\rangle|^2 + |\langle b|\hat{z}|a\rangle|^2$

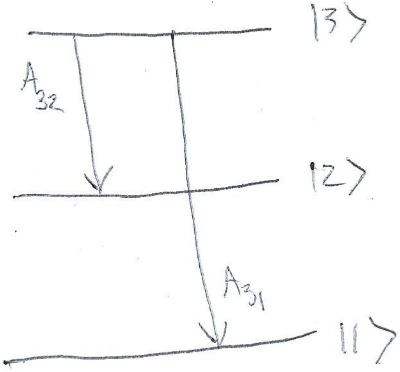
$$B_{ab} = B_{ba} = \frac{\pi q^2}{3\epsilon_0 \hbar^2} |\langle b|\hat{r}|a\rangle|^2$$

$$A_{ba} - \frac{\hbar \omega_{ba}^3}{\pi^2 c^3} \frac{\pi q^2}{3\epsilon_0 \hbar^2} |\langle b|\hat{r}|a\rangle|^2$$

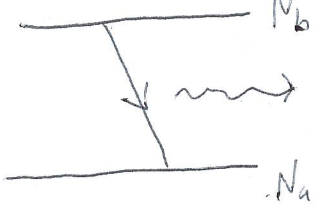
$q = e$

$$A_{ba} = \frac{4}{3} \frac{\alpha \omega_{ba}^3}{c^2} |\langle b|\vec{r}|a\rangle|^2$$

dipole
Spontaneous
emission rate



$$\tau = \frac{1}{A_{32} + A_{31}}$$



$$\frac{dN_b}{dt} = -N_b A_{ba}$$

$$N_b = N_{b0} e^{-A_{ba} t} = N_{b0} e^{-t/\tau}$$

$$\tau = \frac{1}{A_{ba}}$$

Lifetime of the 2p state

$$|\langle b|\hat{\vec{r}}|a\rangle|^2 = |\langle b|\hat{r}_{+1}|a\rangle|^2 + |\langle b|\hat{r}_0|a\rangle|^2 + |\langle b|\hat{r}_{-1}|a\rangle|^2$$

$$= \sum_{m_v} |\langle b|\hat{r}_{m_v}|a\rangle|^2$$

$2p \to 1s$

$$|a\rangle = |\overset{n\ l\ m_l}{100}\rangle$$

$$|b\rangle = |21m_l\rangle$$

$$\sum_{m_v} |\langle b|\hat{r}_{m_v}|a\rangle|^2 = \sum_{m_v} |\langle 21m_l|\hat{r}_{m_v}|100\rangle|^2$$

$0 + m_v = m_l$ for this to be nonzero

$$|\langle 21m_l|\hat{r}_{m_l}|100\rangle|^2$$

$m_l = 0$ $$\langle 210|\hat{z}|100\rangle = \overset{\swarrow 1}{C^{011}_{000}} \langle 21\|r\|10\rangle \qquad C^{0jj'}_{0mm'} = \delta_{jj'}\delta_{mm'}$$

$$\langle 21\pm|\hat{r}_{\pm}|100\rangle = \underset{\uparrow 1}{C^{011}_{0\pm1\pm1}} \langle 21\|r\|10\rangle$$

$$|\langle 2p|\hat{r}|1s\rangle|^2 = |\langle 210|\hat{z}|100\rangle|^2$$

$$E_n = \frac{1}{2n^2}\alpha^2 mc^2$$

$$\Delta E = \left(1-\frac{1}{4}\right)\frac{1}{2}\alpha^2 mc^2 = \frac{3}{8}\alpha^2 mc^2$$

$$\omega_{2p\to 1s} = \frac{3}{8}\frac{\alpha^2 mc^2}{\hbar}$$

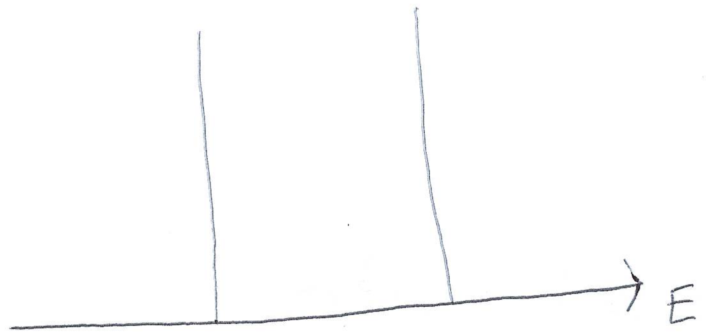
$$\left|\frac{1}{\sqrt{2}}\frac{2^8}{3^5}a\right|^2 \qquad a = \frac{\hbar}{\alpha mc}$$

$$A_{2p\to 1s} = \frac{4}{3}\alpha\frac{\omega^3}{c^2}|\langle 210|\hat{z}|100\rangle|^2$$

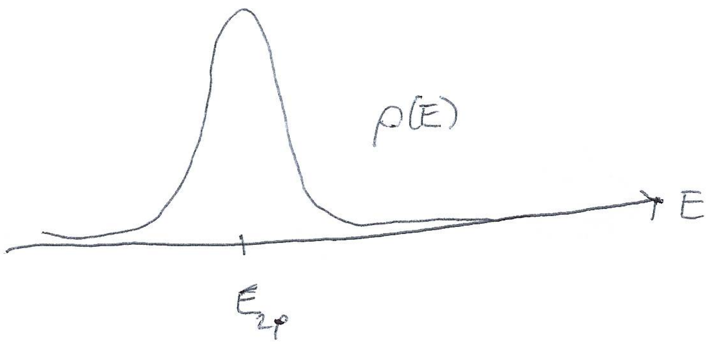
$$= \frac{2^2}{3}\alpha\frac{1}{c^2}\frac{3^3}{2^9}\frac{\alpha^6 m^3c^6}{\hbar^3}\frac{2^{16}}{2\cdot 3^{10}}\cancel{\alpha^2}\frac{\hbar^2}{\alpha^2 m^2 c^2} = \frac{2^8}{3^8}\frac{\alpha^5 mc^2}{\hbar}, \quad \tau_{2p} = \left(\frac{3}{2}\right)^8 \frac{\hbar}{\alpha^5 mc^2}$$

$$= 1.6\times 10^{-9}\,s$$

$\Delta E = \frac{\hbar}{\tau}$ $\quad \frac{\Delta E}{E_{2p}} = 1.2\times10^{-7}$



$\rho(E)$ for a discrete spectrum



Lorentzian $\rho(E) = \frac{\hbar A/2\pi}{(E-E_{2p})^2 + (\frac{\hbar A}{2})^2}$ $\quad \frac{1}{\pi}\frac{\alpha}{(E-E_{2p})^2+\alpha^2}$

$$\hat{H}(t) = \begin{cases} \hat{H}_i & t<t_0 \\ \hat{H}_T & t_0<t<t_f \\ \hat{H}_f & t_f<t \end{cases}$$

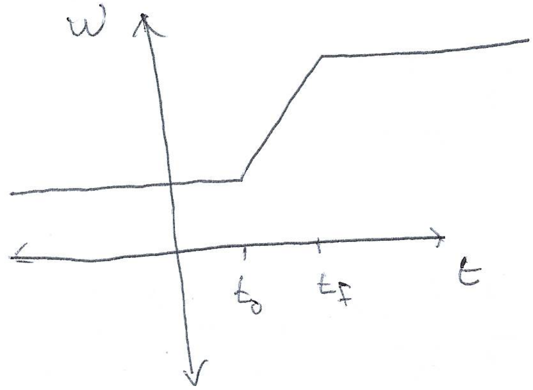
time scale: $\Delta t = t_f - t_0$

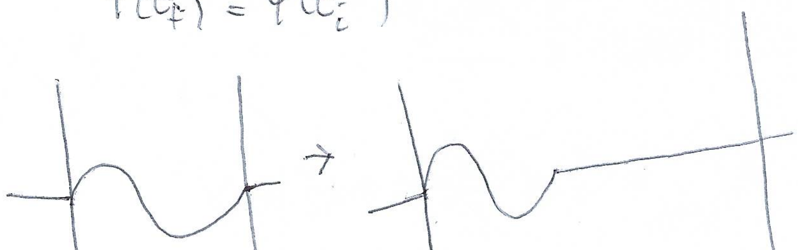
If $\Delta t \ll \frac{\hbar}{\Delta E}$ energy splitting

"Sudden Approximation"

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega(t)^2x^2$

$\Psi(t_f) = \Psi(t_i)$





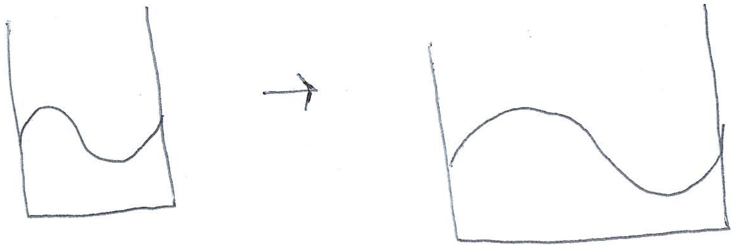
$P(i\to f) = |\langle m_f|n_i\rangle|^2$

$$\Delta t >> \frac{\hbar}{\Delta E}$$

Adiabatic Approximation

Adiabatic Theorem

If we start in the n^{th} energy eigenstate of $\hat{H}_i$ ~~and end~~ we end in the n^{th} energy eigenstate of $\hat{H}_f$



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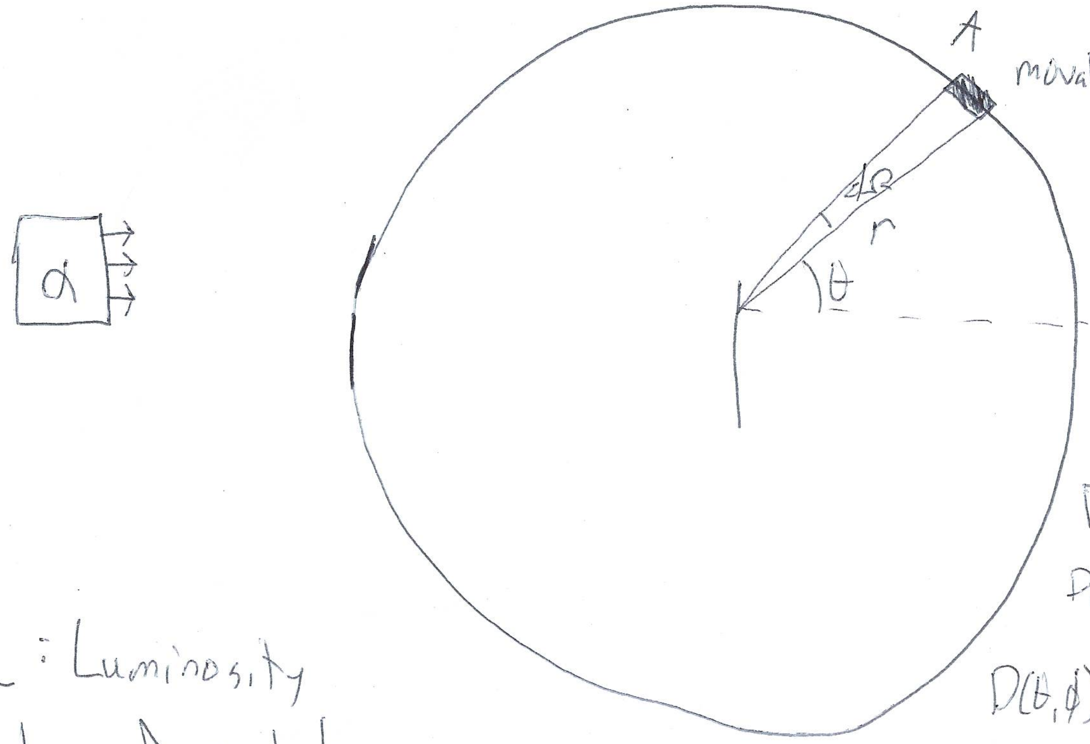
Scattering



$A = \cancel{R} d\Omega\, r$

detection rate

$dR \, \frac{\text{particles}}{\text{second}}$

$D(\theta,\phi) = \frac{d\sigma}{d\Omega}$

Differential cross section

$D(\theta,\phi) = \frac{1}{\mathcal{L}} \frac{dR}{d\Omega}$

$\frac{\text{area}}{\text{solid angle}}$

$\mathcal{L}$: Luminosity

number of particles per unit area and per unit time

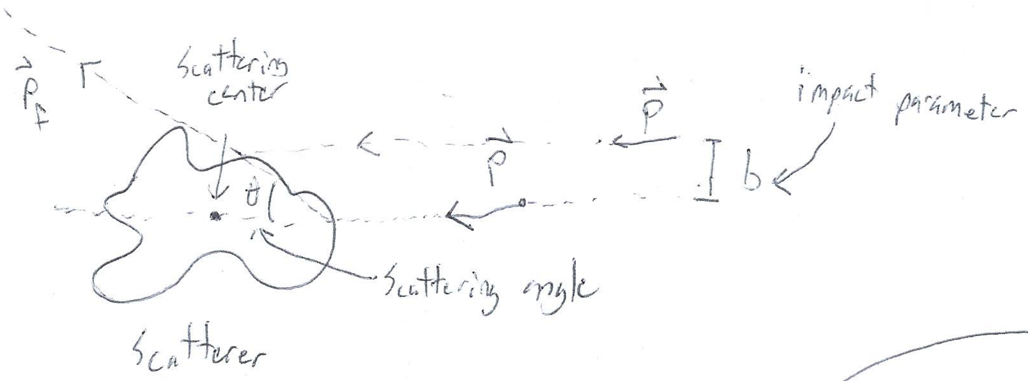
$\frac{[n]}{[A][t]}$

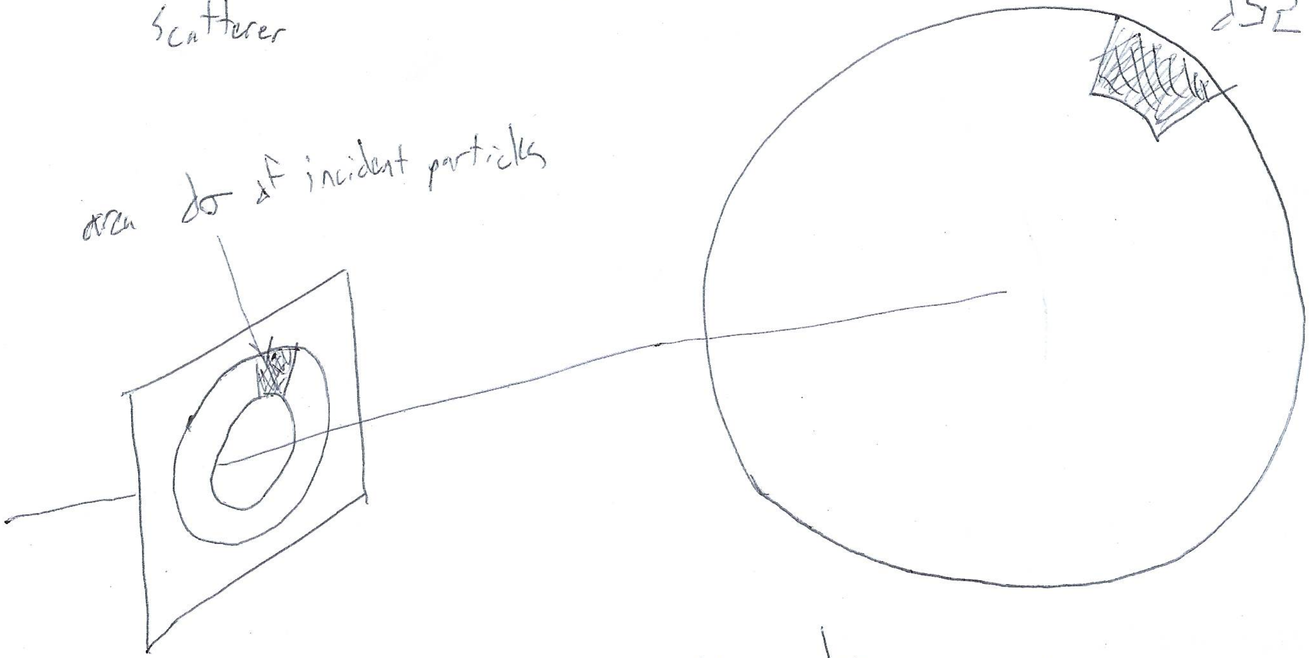
↳ barn ≈ size of a uranium nucleus

$10^{-28}\,m^2 \approx 100\,fm^2$

$\sigma = \int D(\theta,\phi)\, d\Omega$

↑ total cross section area

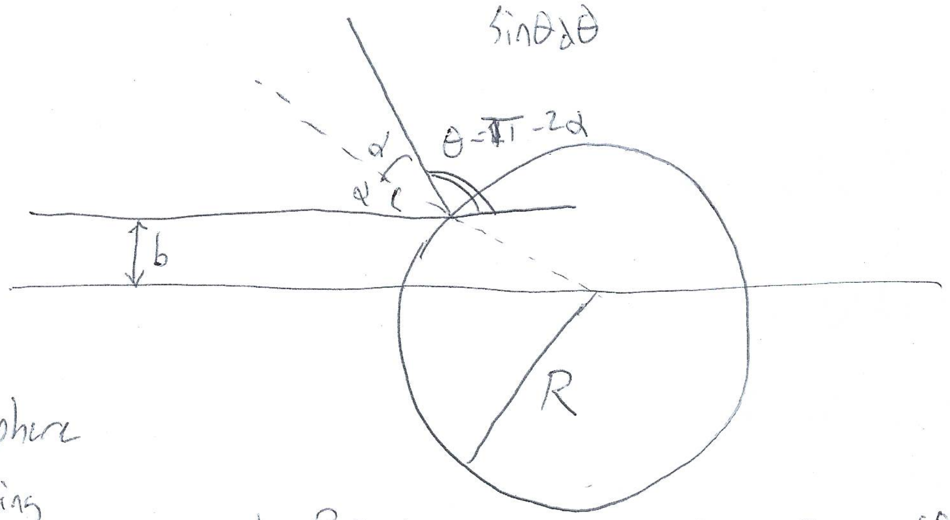




$$d\sigma = b\,db\,d\phi$$

$$D(\theta,\phi) = \frac{d\sigma}{d\Omega} = \frac{b\,db\,d\phi}{d\Omega} = \frac{b\,db\,d\phi}{\sin\theta\,d\theta\,d\phi}$$

$$= \frac{b\,db}{\sin\theta\,d\theta}$$



Hard sphere Scattering

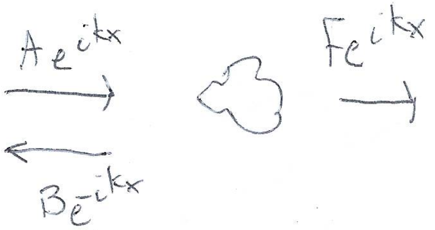
$$b = R\sin\alpha = R\cos\left(\frac{\pi}{2}-\alpha\right) = R\cos\left(\frac{\theta}{2}\right)$$

$$\frac{db}{d\theta} = -\frac{R}{2}\sin\left(\frac{\theta}{2}\right) \qquad \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\frac{R}{2}\sin\frac{\theta}{2} = \frac{R^2}{4}$$

$$\sigma = \pi R^2$$

Quantum Scattering

$V(\vec{r})$



$R=\left|\frac{B}{A}\right|^2$ reflection

$T=\left|\frac{F}{A}\right|^2$ transmission

$\lim_{r\to\infty} V(\vec{r})=0$

energy scale V_0

length scale a

$r>>a \Rightarrow V\simeq 0$

We will only concern ourselves with the far-field $r>>a$

Look for solutions of the TISE in region $r>>a$

① Plane waves States of definite momentum

$|\vec{k}\rangle$ $\hat{\vec{p}}|\vec{k}\rangle=\hbar\vec{k}|\vec{k}\rangle$ $E=\frac{\hbar^2k^2}{2\mu}$

$\psi_{\vec{k}}(\vec{r})=Ae^{i\vec{k}\cdot\vec{r}}$ $\psi_{\vec{k}}(\vec{r},t)=Ae^{i(\vec{k}\cdot\vec{r}-\omega t)}$

② Spherical waves

$\mathcal{H}_{3D}=\mathcal{H}_{ang}\otimes\mathcal{H}_{rad}$ $|state\rangle=|ang\rangle\otimes|rad\rangle$

$R(r)=\langle r|rad\rangle=\frac{u(r)}{r}$, $u(r)$ a solution to $-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2}+V_{eff}(r)u=Eu$

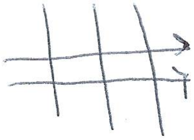
$V_{eff}=V(r)+\frac{\hbar^2 l(l+1)}{2\mu r^2}$, $r>>a$ $V_{eff}(r)=0$

$u''=-k^2u$

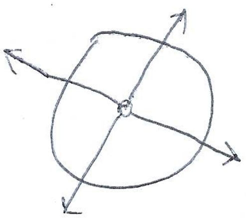
$u=e^{\pm ikr}$ $|k_\pm\rangle\doteq\frac{e^{\pm ikr}}{r}$

$f(\theta,\phi) = \langle \theta,\phi | \text{ang} \rangle$

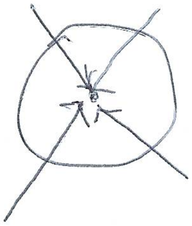
① $|\vec{k}\rangle \quad A e^{i(\vec{k}\cdot\vec{r} - wt)}$



② $|\text{ang}\rangle \otimes |k_+\rangle \quad A \frac{e^{i(kr-wt)}}{r} \quad f(\theta,\phi)$



③ $|\text{ang}\rangle \otimes |k_-\rangle \quad A \frac{e^{i(-kr-wt)}}{r} \quad f(\theta,\phi)$



Send in a plane wave
(~~definite~~ define this to be $\vec{z}$-direction)
Get out a spherical wave

$$\psi(\vec{r},t) \xrightarrow[r>>a]{} A\Big(\underset{\substack{\uparrow\\ \text{incident}}}{e^{ikz}} + f(\theta,\phi)\frac{e^{ikr}}{r}\Big)e^{-iwt}$$

$\rho = |\langle \vec{r}|\alpha\rangle|^2 = |\psi_\alpha(\vec{r})|^2$ probability density

$\vec{j} = \frac{\hbar}{2\mu i}\left(\psi^* \vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)$ probability current

$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0$

Incident Plane wave

$\rho = |A|^2$ $\quad \vec{j}_{in} = \frac{\hbar k}{\mu} |A|^2 \check{z}$

units of $\frac{\text{Probability}}{\text{area} \cdot \text{time}}$

~~will serve as our~~

will take the place of luminosity $\mathcal{L}$

$\vec{j} \cdot d\vec{A}$ = rate of detections

Outgoing Spherical

$\rho_{out} = \frac{|A|^2 |f|^2}{r^2}$ $\quad \vec{j}_{out} = \frac{\hbar k}{\mu r^2} |A|^2 |f|^2 \check{r}$

Let detector at angles θ, ϕ have ~~an~~ over vector

$$d\vec{A} = r^2 d\Omega \check{r}$$

$$\frac{1}{\mathcal{L}} \frac{\text{rate of detections}}{d\Omega} = D(\theta, \phi)$$

$$= \frac{\frac{\hbar k}{\mu r^2} |A|^2 |f|^2 r^2 d\Omega}{\frac{\hbar k}{\mu} |A|^2 d\Omega} = |f(\theta, \phi)|^2$$

$f(\theta, \phi)$ = scattering amplitude

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi = E\psi$$

$$E = \frac{\hbar^2 k^2}{2\mu}$$

$$\frac{2\mu}{\hbar^2} V(\vec{r})\psi(\vec{r})$$

$$(\nabla^2 + k^2)\psi(\vec{r}) = Q(\vec{r})$$

Let $\psi_0(\vec{r})$ be any solution of $(\nabla^2 + k^2)\psi_0 = 0$

$\psi_p(\vec{r})$ one particular solution of $(\nabla^2 + k^2)\psi_p = Q$.

$$\psi = \psi_0 + \psi_p$$

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Scattering

Incident Plane wave in z direction

(wave number $\vec{k} = k\hat{z}$, $\vec{p} = \hbar\vec{k}$, $E = \frac{\hbar^2 k^2}{2\mu}$

$r \to \infty$

$$\psi(\vec{r}) = A\left(e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\right)$$

$f(\theta,\phi)$ scattering amplitude

$D(\theta,\phi) = |f(\theta,\phi)|^2$ differential cross-section

$\sigma = \int D(\theta,\phi)\, d\Omega$ cross-section

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi = E\psi$$

$$\Downarrow$$

$$(\nabla^2 + k^2)\psi = Q \quad , \quad Q = \frac{2\mu}{\hbar^2}V\psi$$

Given one particular solution ψ_1 of $(\nabla^2+k^2)\psi = Q$

Then any solution has the form $\psi = \psi_1 + \psi_0$

$(\nabla^2+k^2)\psi_0 = 0$

ψ_1 solves $(\nabla^2+k^2)\psi_1 = f_1$

ψ_2 solves $(\nabla^2+k^2)\psi_2 = f_2$

$a\psi_1 + b\psi_2$ solves $(\nabla^2+k^2)\psi = af_1 + bf_2$

Let $G(\vec{r}; \vec{r}_0)$ solve $(\nabla^2 + k^2) G(\vec{r}; \vec{r}_0) = \delta(\vec{r} - \vec{r}_0)$

$$\Delta(\vec{r}) = \int \Delta(\vec{r}_0)\, \delta(\vec{r} - \vec{r}_0)\, d^3 r$$

incoming plane wave

$$\Rightarrow \psi(\vec{r}) = \psi_0(\vec{r}) + \iiint \Delta(\vec{r}_0)\, G(\vec{r}; \vec{r}_0)\, d^3 r_0$$

$$G(\vec{r}, \vec{r}_0) = -\frac{e^{ik|\vec{r} - \vec{r}_0|}}{4\pi |\vec{r} - \vec{r}_0|}$$

$$\psi(\vec{r}) = A e^{ikz} - \frac{\mu}{2\pi\hbar^2} \int \frac{e^{ik|\vec{r} - \vec{r}_0|}}{|\vec{r} - \vec{r}_0|} V(\vec{r}_0)\, \psi(\vec{r}_0)\, d^3 r_0$$

$r >> a \Rightarrow r >> r_0$

$|\vec{r} - \vec{r}_0| \cong \cancel{r(1+} \; r - \hat{r} \cdot \vec{r}_0 + \dots$

$\frac{1}{|\vec{r} - \vec{r}_0|} \approx \frac{1}{r} + \frac{\hat{r} \cdot \vec{r}_0}{r^2} + \dots$

$\cancel{e^{ikr}} \; \frac{e^{ik|\vec{r} - \vec{r}_0|}}{|\vec{r} - \vec{r}_0|} \approx \frac{e^{ikr}}{r} e^{-i\vec{k}_f \cdot \vec{r}_0} + \dots$

$$\psi(\vec{r}) \xrightarrow[r \to \infty]{} \cancel{A e^{i\vec{k} \cdot \vec{r}}} \; A e^{ikz} - \frac{\mu}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\vec{k}_f \cdot \vec{r}_0} V(\vec{r}_0)\, \psi(\vec{r}_0)\, d^3 r_0$$

to zeroth order in $\frac{V_0}{E}$, $\psi(\vec{r}) = A e^{ikz}$

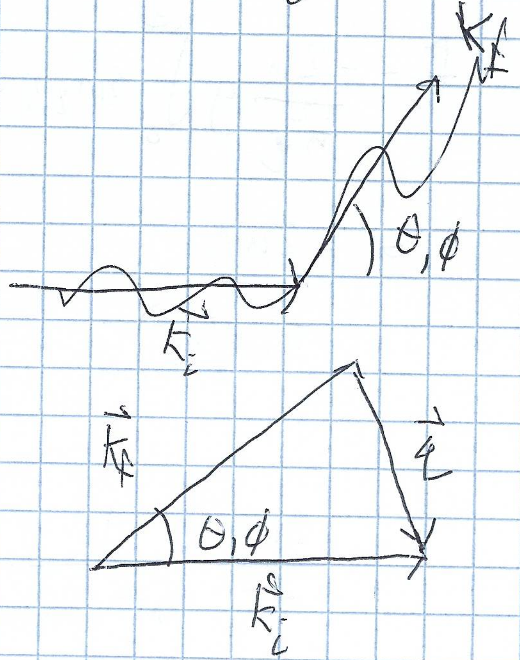
plug this into ψ_0 for first born approximation

1st Born Approximation

$$\psi \simeq Ae^{ikz} - \frac{\mu}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-i\vec{k}_f\cdot\vec{r}_0} V(\vec{r}_0) A e^{i\vec{k}_i\cdot\vec{r}_0}\, d^3 r_0$$

$$\vec{q} = k_i - k_f = k(\hat{z} - \hat{r})$$

$$A\int V(\vec{r}_0)\, e^{i\vec{q}\cdot\vec{r}_0}\, d^3 r_0$$



$$f(\theta,\phi) \approx \frac{-\mu}{2\pi\hbar^2}\int V(\vec{r}_0)\, e^{i\vec{q}\cdot\vec{r}_0}\, d^3\vec{r}_0$$

Spherically Symmetric Potentials

$$V(\vec{r}) = V(r)$$

$$\vec{q}\cdot\vec{r}_0 = q r_0 \cos\theta_0$$

$$\int V(r_0)\, e^{iqr_0\cos\theta_0}\, r_0^2\, dr_0\, d\cos\theta_0\, d\phi_0$$

$$^{*}\, f(\theta,\phi) \cong \frac{-2\mu}{\hbar^2 q}\int_0^\infty r_0 \sin(q r_0)\, V(r_0)\, dr_0$$

Yukawa Potential $V(r) = \frac{g e^{-m_0 r}}{r}$

$$f = \frac{-2\mu}{\hbar^2 q} g \int_0^\infty \sin q r_a e^{-m_0 r} dr$$

$$= \frac{-2\mu g}{\hbar^2 (m_0^2 + q^2)}$$

$$q^2 = (k_i - k_f)^2 = k_i^2 - 2k_i k_f + k_f^2$$

$$= k^2(1 - 2\cos\theta + 1)$$

$$= 2k^2(1 - \cos\theta) = 4k^2 \sin^2\frac{\theta}{2}$$

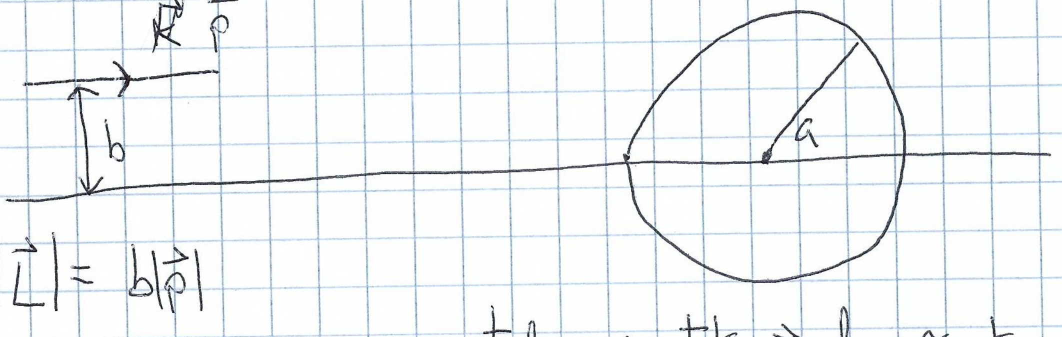
$$f = -\frac{2\mu g}{\hbar^2} \frac{1}{m_0^2 + 4k^2 \sin^2\frac{\theta}{2}}$$

$$D(\theta, \phi) = \frac{4\mu^2 g^2}{\hbar^4} \frac{1}{(m_0^2 + 4k^2 \sin^2\frac{\theta}{2})^2}$$

~~$\sigma = \frac{4\mu^2 g^2}{\hbar^4}$~~ $\sigma = \frac{8\pi\mu^2 g^2}{\hbar^4} \frac{2}{m_0^4 + 4m_0^2 k^2}$

Partial Wave Analysis

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_{lm} Y_l^m(\theta, \phi)$$



$|\vec{L}| = b|\vec{p}|$

$L_{max} \sim ap$

$\hbar l_{max} \sim a\hbar k \Rightarrow l_{max} \sim ak$

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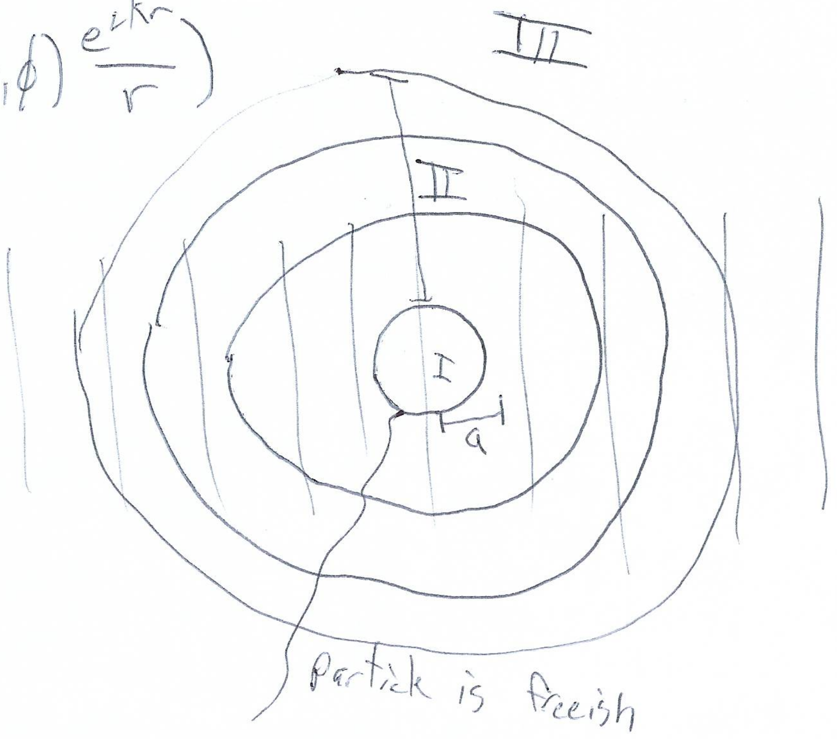
Far-field: $\psi = A\left(e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\right)$

$$D(\theta,\phi) = |f(\theta,\phi)|^2$$

$$\sigma = \int D(\theta,\phi)\Delta\Omega$$

Region I: Scattering region

$V(\vec{r})$ is not negligable



Region II: Intermediate region

$V(\vec{r})$ is negligable but centrifugal term isn't

$$V_{eff} = V + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

Region III: far-field

both V and centripetal terms are negligable

$$\psi = \sum_l \sum_m C_{lm} \frac{u_l(r)}{r} Y_l^m(\theta,\phi)$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2 u}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2}u = \frac{\hbar^2 k^2}{2\mu}u$$

$$u'' - \frac{l(l+1)}{r^2}u + k^2 u = 0$$

$$u = A_l r j_l(kr) + B_l r n_l(kr)$$

$$= C_{+l} r h_l^{(1)}(kr) + C_{-l} r h_l^{(2)}(kr)$$

$h_l^{(1)} = j_l + i n_l$ $\quad h_l^{(2)} = j_l - i n_l$

$j_0 = \frac{\sin x}{x}$ $\quad j_1 = \frac{\sin x}{x^2} - \frac{\cos x}{x}$

$n_0 = \frac{-\cos x}{x}$ $\quad n_1 = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$

$h_0^{(1)} = -i\frac{e^{ix}}{x}$ $\quad h_1^{(1)} = \left(\frac{-i}{x^2} - \frac{1}{x}\right)e^{ix}$

$$j_\ell(x) \xrightarrow[x\gg1]{} \frac{\sin(x-\frac{\ell\pi}{2})}{x}$$

$$n_\ell(x) \xrightarrow[x\gg1]{} -\frac{\cos(x-\frac{\ell\pi}{2})}{x}$$

$$h_\ell^{(1)}(x) \rightarrow (-i)^{\ell+1}\frac{e^{ix}}{x}$$

$$\psi_{II}(\vec{r}) = \sum_{\ell,m}\Big(c_{\ell m}\underset{\Downarrow\ \frac{e^{ikr}}{r}}{h_\ell^{(1)}(kr)} + d_{\ell m}\underset{\downarrow\ \frac{+e^{-ikr}}{r}}{h_\ell^{(2)}(kr)}\Big)Y_\ell^m(\theta,\phi)$$

Given an azimuthally-symmetric potential

we expect no ϕ dependence inside ψ

$\Downarrow$

Only $m=0$ contribute

$$Y_\ell^0(\theta,\phi) = \sqrt{\frac{2\ell+1}{2\pi}}\,P_\ell(\cos\theta)$$

$$\Downarrow$$

$$\psi_{II}(\vec{r}) = \sum_{\ell=0}^{\infty}\left(A_\ell h_\ell^{(1)}(kr) + B_\ell h_\ell^{(2)}(kr)\right)P_\ell(\cos\theta)$$

$\uparrow$ in practice, we can take upper limit as ka

If $V=0$ everywhere (no scattering)

$$f(\theta,\phi)=0$$

$$\psi = Ae^{ikz}$$

$$= A\sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

$$= A\sum i^l (2l+1)\left(\frac{h_l^{(1)}(kr)+h_l^{(2)}(kr)}{2}\right)P_l(\cos\theta)$$

$r \to \infty$

$$\psi = A\sum_{l=0}^{\infty} i^l(2l+1)\frac{(-i)^{l+1}e^{ikr}+i^{l+1}e^{-ikr}}{2kr}P_l(\cos\theta)$$

$$= A\sum_{l=0}^{\infty}\frac{i^l(2l+1)}{2ikr}\left(e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}\right)P_l(\cos\theta)$$

$$\psi \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty}\left(\tilde{A}_l\frac{e^{ikr}}{kr}+\tilde{B}_l\frac{e^{-ikr}}{kr}\right)P_l(\cos\theta)$$

$$|\tilde{A}_l| = |\tilde{B}_l|$$

Define c_l and δ_l so $\tilde{A}_l = \frac{c_l}{2i}e^{-i\frac{l\pi}{2}}e^{i\delta_l}$

$$\tilde{B}_l = -\frac{c_l}{2i}e^{il\pi/2}e^{-i\delta_l}$$

Free: $\delta_l=0$ $c_l=i^l(2l+1)A$

$$\psi = \sum\frac{c_l}{2ikr}\left(e^{i(kr-\frac{l\pi}{2}+\delta_l)}-e^{-i(kr-\frac{l\pi}{2}+\delta_l)}\right)P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} c_l\frac{\sin(kr-\frac{l\pi}{2}+\delta_l)}{kr}P_l(\cos\theta)$$

$$\psi - Ae^{ikr} \xrightarrow[r\to\infty]{} Af(\theta,\phi)\frac{e^{ikr}}{r}$$

$$\sum\left(\frac{C_l}{2ikr}\left(e^{i(kr-\frac{l\pi}{2}+\delta_l)} - e^{-i(kr-\frac{l\pi}{2}+\delta_l)}\right) - \frac{Ai^l(2l+1)}{2ikr}\left(e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}\right)\right.$$
$$\times P_l(\cos\theta) = Af\frac{e^{ikr}}{r}$$

$$C_l = A(2l+1)i^l e^{i\delta_l}$$

$$f(\theta,\phi) = \sum_l^{\infty}(2l+1)\left(\frac{e^{i\delta_l}\sin\delta_l}{k}\right)P_l(\cos\theta)$$

$$\sigma = \sum_{l=0}^{\infty}\frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$$

At low energies $\sigma \approx \frac{4\pi}{k^2}\sin^2\delta_0$

Hard-sphere Scattering

$$V(r) = \begin{cases} 0 & r > r_0 \\ \infty & r < r_0 \end{cases}$$

Low energy $kr_0 \ll 1$ $\quad l_{max} = 0$

$$\sigma = \frac{4\pi}{k^2}\sin^2\delta_0$$

$$\psi \approx C_0\frac{\sin(kr+\delta_0)}{kr}P_0(\cos\theta)$$

$$\psi(r=r_0) = 0 \Rightarrow \delta_0 = -kr_0$$

$$\sigma = \frac{4\pi}{k^2}\sin^2 kr_0 \approx \frac{4\pi}{k^2}k^2r_0^2 = 4\pi r_0^2$$

$kr_0 \gg 1$

$$\sum_{l=0}^{kr_0} \frac{4\pi}{k^2} \sin^2 \delta_l \cancel{P_l(\cos\theta)} (2l+1)$$

$\nwarrow$ is probably $\frac{1}{2}$ ish

$$\frac{4\pi}{2k^2} \sum_{l=0}^{kr_0} (2l+1) = \frac{2\pi}{k^2} k^2 r_0^2 = 2\pi r_0^2$$

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Discussion

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Problem 2: Coherent States

Def $|z_0\rangle = \sum_{n=0}^{\infty} \frac{z_0^n}{\sqrt{n!}} e^{-|z_0|^2/2} |n\rangle$ where n is the nth QHO eigenstate (n=0,1,2,...)

~~$\hat{H} = \frac{\hat{p}^2}{2m}$~~ $\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2\hat{x}^2 = \hbar\omega(\hat{a}_+\hat{a}_- + \frac{1}{2})$

$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar\omega\mu}}(\mp i\hat{p} + \mu\omega\hat{x})$

$E_n = (n+\frac{1}{2})\hbar\omega$ $[\hat{a}_-, \hat{a}_+] = 1$

You will show that $\hat{a}_-|z_0\rangle = z_0|z_0\rangle$

~~$\hat{a}_-|0\rangle$~~ $\hat{a}_-|z_0=0\rangle = 0|z_0=0\rangle = 0$

$\hat{a}_-|n=0\rangle = 0|n=0\rangle = 0$

$|z_0=0\rangle = |n=0\rangle = |0\rangle$

Ex Solve for $|0\rangle$

$$\frac{1}{\sqrt{2\hbar\omega\mu}}(i\hat{p} + \mu\omega\hat{x})|0\rangle = 0 = \frac{1}{\sqrt{2\hbar\omega\mu}}\left(\frac{\hbar i}{i}\frac{\partial}{\partial x} + \mu\omega x\right)|0\rangle = 0$$

$$\frac{\hbar\partial\psi}{\partial x} = -\mu\omega x \qquad \hbar\psi = -\frac{1}{2}\mu\omega x^2$$

$$\psi = |0\rangle = \frac{1}{2\hbar}\mu\omega x^2 \qquad (?)$$

$$\frac{d|0\rangle}{|0\rangle} = -\frac{\mu\omega}{\hbar} x\, dx$$

$$\ln(|0\rangle) = \frac{-\mu\omega}{2\hbar} x^2 + C$$

$$|0\rangle = A e^{-\frac{\mu\omega}{2\hbar} x^2} \qquad A = \left(\frac{\mu\omega}{\pi\hbar}\right)^{1/4}$$

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

Displacement Operator $\hat{D}(z)$

$$\hat{D}(z)|z_0\rangle = |z_0 + z\rangle$$

$$|z_0\rangle = \hat{D}(z_0)|0\rangle \quad , \quad \hat{D}^{+}(z)\hat{D}(z) = \hat{D}(z)\hat{D}^{+}(z) = \hat{\mathbb{1}}$$

$$\hat{D}(z) = e^{z\hat{a}_+ - z^*\hat{a}_-}$$

<u>Baker - Campbell - Hausdorff</u> (Zazzenhaus)

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A},\hat{B}]} \quad \ldots$$

this if $[A,[A,B]] = [B,[A,B]] = 0$

$$\hat{D}(z) = e^{-\frac{1}{2}|z|^2} e^{z\hat{a}_+} e^{-z^*\hat{a}_-}$$

use taylor series to expand

$$= \left(1 - \frac{|z|^2}{2} + \frac{|z|^4}{4(2)} + \ldots\right)\left(1 + z\hat{a}_+ + \frac{(z\hat{a}_+)^2}{2} + \ldots\right)\left(1 - \frac{z^*\hat{a}_-}{1} + \frac{(z^*\hat{a}_-)^2}{2} + \ldots\right)$$

$$= \left(1 - \frac{|z|^3}{2} + \frac{|z|^4}{8} + \ldots\right)\left(1 - \frac{z^*\hat{a}_-}{1} + \ldots\right)$$

$$|z_0\rangle = \hat{D}(z_0)|0\rangle = e^{-\frac{1}{2}|z_0|^2} e^{z_0\hat{a}_+} \underbrace{e^{-z_0^*\hat{a}_-}|0\rangle}_{①}$$

$$① = \sum_{n=0}^{\infty} \frac{(-z_0^*)^n}{n!} a_-^n |0\rangle = |0\rangle$$

$$\hat{a}_+|0\rangle = |1\rangle$$
$$\hat{a}_+|1\rangle = \sqrt{2}|2\rangle$$
$$\hat{a}_+\sqrt{2}|2\rangle = \sqrt{6}|3\rangle = \sqrt{3!}|3\rangle$$
$$\hat{a}_+^n|0\rangle = \sqrt{n!}|n\rangle$$

$$|z_0\rangle = e^{-\frac{1}{2}|z_0|^2} \sum_{n=0}^{\infty} \frac{(z_0)^n}{n!}\hat{a}_+^n|0\rangle$$
$$= e^{-\frac{1}{2}|z_0|^2} \sum_{n=0}^{\infty} \frac{(z_0)^n}{\sqrt{n!}}|n\rangle$$

$$\int d^3z\, |z\rangle\langle z| = \pi\, \mathbb{1}$$

Problem 4

$$V(\vec{x}) = \frac{1}{2}\mu\omega^2(r_1^2 + r_2^2)$$

Each oscillator has its own independent raising and lowering operators

$\hat{a}_{\pm 1}, \hat{a}_{\pm 2}$ or $\hat{a}_{\pm}, \hat{b}_{\pm}$

$$[\hat{a}_-, \hat{a}_+] = [\hat{b}_-, \hat{b}_+] = 1 \qquad [\hat{a}_\pm, \hat{b}_\pm] = 0$$

Eigenstates are $|n_1 n_2\rangle$ $\quad \hat{a}_+\hat{a}_-|n_1 n_2\rangle = n_1|n_1, n_2\rangle$

$$\hat{b}_+\hat{b}_-|n_1 n_2\rangle = n_2|n_1, n_2\rangle$$

$$J_x = \frac{\hbar}{2}(\hat{a}_+\hat{b}_- + \hat{a}_-\hat{b}_+)$$

$n_1 + n_2$ remains the same

$$J_y = \frac{\hbar}{2}(-i\hat{a}_+\hat{b}_- + i\hat{a}_-\hat{b}_+)$$

$N = n_1 + n_2 =$ "total spin"

$$J_z = \frac{\hbar}{2}(\hat{a}_+\hat{a}_- - \hat{b}_+\hat{b}_-)$$

$n_1 n_2 =$ "z component" of N (not quite)

$$m = \frac{n_1 - n_2}{2}$$

$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ $\hat{J}_+ = \hbar\hat{a}_+\hat{b}_-$, $\hat{J}_- = \hbar\hat{a}_-\hat{b}_+$

$$\hat{J}_+|n_1 n_2\rangle = \hbar\hat{a}_+\hat{b}_-|n_1 n_2\rangle = \hbar\sqrt{n_1+1}\,\hat{b}_-|n_1+1, n_2\rangle$$

$$= \hbar\sqrt{(n_1+1)n_2}\,|n_1+1, n_2-1\rangle$$ ~~$N = n_1+n_2$~~ $j = n_1+n_2$

$$= \hbar\sqrt{j(j+1)-m(m+1)}\,|n_1+1, n_2-1\rangle$$ $m = \dfrac{n_1-n_2}{2}$

$$[\hat{J}_x, \hat{J}_y] = \frac{\hbar^2}{4}\Big(\overset{\nearrow 0}{[a_+b_-, -ia_+b_-]} + [a_-b_+, -ia_+b_-]$$
$$+ [a_+b_-, ia_-b_+] + \underset{\searrow 0}{[a_-b_+, ia_-b_+]}\Big)$$

$$= \frac{\hbar^2}{4}\left(a_+b_-a_-b_+ - a_-b_+a_+b_- - a_-b_+a_+b_- + a_+b_-a_-b_+\right)$$

$$= \frac{\hbar^2}{i2}\left(a_+b_-a_-b_+ - a_-b_+a_+b_-\right)$$ play with orders of a, b

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Discussion

Suppose we have two spin $\frac{1}{2}$ particles

One way is in the uncoupled basis

$|m_1\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$

$|m_2\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$

$|m_1 m_2\rangle = |m_1\rangle \otimes |m_2\rangle \in \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$

if $H = A\vec{S}_1 \cdot \vec{S}_2$ this basis might not work well

we define total angular momentum operator

$$\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2$$

$$\hat{S}_z|m_1,m_2\rangle = (\hat{S}_{1z}+\hat{S}_{2z})|m_1,m_2\rangle = \hbar(m_1+m_2)|m_1,m_2\rangle = \hbar m|m_1,m_2\rangle$$

$m = m_1 + m_2$

$|\uparrow\uparrow\rangle$: $m=1$

$|\uparrow\downarrow\rangle$ $m=0$

$|\downarrow\uparrow\rangle$ $m=0$

$|\downarrow\downarrow\rangle$ $m=-1$

$$S^2 = (\vec{S}_1+\vec{S}_2)^2 = S_1^2 + S_2^2 + 2\vec{S}_1\cdot\vec{S}_2 \neq S_1^2 + S_2^2$$

~~unless $S_1 = S_2$~~

unless S_1 is orthogonal to S_2

$S^2|\uparrow\uparrow\rangle = 2\hbar^2|\uparrow\uparrow\rangle$

$S^2|\uparrow\downarrow\rangle = \hbar^2(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

~~$|S=1, m=1\rangle = |\uparrow\uparrow\rangle$~~

$S^2|\downarrow\uparrow\rangle = \hbar^2(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$S^2|\downarrow\downarrow\rangle = 2\hbar^2|\downarrow\downarrow\rangle$

$$S^2\left(\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}}\right) = 2\hbar^2\left(\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}}\right)$$ Spin 1 state

$$S^2\left(\frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}\right) = 0$$

Spin 0 state

Triplet states

$$|s=1, m=1\rangle = |\uparrow\uparrow\rangle \qquad |s=1, m=0\rangle = \frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}} \qquad |s=1, m=-1\rangle = |\downarrow\downarrow\rangle$$

Singlet state

$$|s=0, m=0\rangle = \frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}$$

General Problem combining 2 angular momentum

Combine $\vec{L}$ and $\vec{S}$ to get a total angular momentum $\vec{J}$

In the uncoupled basis we index states as $\{|l, s, m_l, m_s\rangle\}$

ie. by the eigenvalues of $\{\hat{L}^2, \hat{S}^2, \hat{L}_z, \hat{S}_z\}$

Alternatively we can write states in the coupled basis $\{|l, s; j, m_j\rangle\}$

ie by the eigenvalues of $\{\hat{L}^2, \hat{S}^2, \hat{J}^2, \hat{J}_z\}$

$$|l, s, m_l, m_s\rangle = \sum_{j=|l-s|}^{l+s} C^{lsj}_{m_l m_s m_j} |l, s; j, m_j\rangle \quad , \quad C^{lsj}_{m_l m_s m_j}$$ Clebsch Gordan Coefficients

$$C^{lsj}_{m_l m_s m_j} = \langle l, s, m_l, m_s | l, s; j, m_j\rangle \equiv \langle l, s, m_l, m_s | j, m_j\rangle$$

1. $\langle l, s, m_l, m_s | l', s'; j, m_j\rangle = 0$ unless $l = l'$, $s = s'$

2. $\langle l, s, m_l, m_s | j, m_j\rangle = 0$ unless $|l-s| \leq j \leq l+s$

3. $\langle l, s, m_l, m_s | j, m_j\rangle = 0$ unless $m_j = m_l + m_s$

Uncoupled   fixed l and s

$$(2l+1)(2s+1) \text{ basis vectors}$$

Coupled   (assume $l \geq s$)

$$\sum_{l-s}^{l+s}(2j+1) = \sum_{0}^{l+s}(2j+1) - \sum_{0}^{l-s}(2j+1) = \cancel{\left(\frac{(2j+1)(2j+2)}{2}\right)}$$

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2}$$

$$= \left((l+s)(l+s+1) + (l+s+1)\right) - \left((l-s-1)(l-s) + (l-s)\right)$$

$$= (l+s+1)^2 - (l-s)^2 = (2l+1)(2s+1)$$

∴ same number of basis vectors

1. $|l,s,l,s\rangle = |l,s;\, l+s, l+s\rangle$

Act with $\hat{L}_- + \hat{S}_- = \hat{J}_-$

$$\langle l,s,l+s-1,l+s-1 \,|\, l,s,l+s,l+s-1\rangle = 0$$

$|l,s,l-1,s\rangle$, $|l,s,l,s-1\rangle$ are orthogonal

Clebsch-Gordan Table

Individual Tables are labeled by $\ell \times s$

rows correspond to m_ℓ, m_s

Columns correspond to j, m_j

$\langle 1,1,1,-1 | 2,0 \rangle$

1x1 table

1 -1 row $\rightarrow \frac{1}{\sqrt{6}}$

2 0 column

$\langle 2,\frac{1}{2},1,\frac{1}{2} | \frac{3}{2},\frac{3}{2} \rangle$

$2\times\frac{1}{2}$ table

$1\ \frac{1}{2}$ row $\rightarrow \frac{-1}{\sqrt{5}}$

$\frac{3}{2}\ \frac{3}{2}$ column

To write an uncoupled state in terms of coupled states look at row of the table

$$|1,1,0\,0\rangle = \sqrt{\frac{2}{3}}\,|1,1;2,0\rangle - \frac{1}{\sqrt{3}}\,|1,1;0,0\rangle$$

1x1 table

0 0 row

other way around for opposite direction

$$|2,1;3,-1\rangle = \sqrt{\frac{2}{5}}\,|2,1,0,-1\rangle + \sqrt{\frac{8}{15}}\,|2,1,-1,0\rangle + \frac{1}{\sqrt{15}}\,|2,1,-2,1\rangle$$

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Discussion

Systems of multiple Particles

$$|\Psi(r_1, r_2, t)|^2 dr_1^3 dr_2^3$$

Probability of simultaneously finding particle 1 in a volume dr_1^3 and particle 2 in dr_2^3

$$\int_V dr_2^3 \left(|\Psi(r_1, r_2, t)| d^3 r_1 \right)$$

If V is time independent we can use separation of variables and get

$$\Psi(r_1, r_2, t) = \psi(r_1, r_2) e^{-iEt/\hbar}$$

with ψ satisfying the two particle TISE

$$\left(\frac{-\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(r_1, r_2) \right) \psi = E\psi$$

Often $V(\vec{r}_1, \vec{r}_2) = V(|\vec{r}_1 - \vec{r}_2|)$. In this case it is useful to define new coordinates $\vec{r} = \vec{r}_1 - \vec{r}_2$ (separation of particles)

$$\vec{R} = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2} \text{ (CoM position)}$$

CoM acts like a free particle with no potential and the other particle acts as if in potential $V(|\vec{r}_1 - \vec{r}_2|)$

$$H = H_{CoM} + H_{rel} \qquad H_{CoM} = \frac{-\hbar^2}{2M} \nabla_2^2$$

$H = H_{CoM} + H_{rel}$ $M = m_1 + m_2$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$H_{CoM} = \frac{-\hbar^2}{2M} \nabla_R^2$$

$$H_{rel} = \frac{-\hbar^2}{2\mu} \nabla_r^2 + V(\vec{r})$$

If $q(x_1, x_2, \dots, x_n)$

$$\frac{\partial}{\partial q} = \sum_i \frac{\partial x_i}{\partial q} \frac{\partial}{\partial x_i}$$

Suppose we have 2 particles in states ψ_a and ψ_b so then the overall state of the system is ~~$\psi(r_1, r$~~

$$\psi(r_1, r_2) = \psi_a(r_1)\psi_b(r_2)$$

$$\psi(r_1, r_2) = \sum_i \psi_{a_i}(r_1)\,\psi_{b_i}(r_2)$$

$$\psi_s = N_s(\psi_a(r_1)\psi_b(r_2) + \psi_b(r_1)\psi_a(r_2)) \quad \text{bosons}$$

$$\psi_{as} = N_{as}(\psi_a(r_1)\psi_b(r_2) - \psi_b(r_1)\psi_a(r_2)) \quad \text{fermions}$$

Bosons (symmetric) integer spin

Fermions (antisymmetric) half integer spin

Suppose $\psi_a = \psi_b$ Pauli Exclusion Priciple

$\psi_{ab} \to 0$

Two fermions can't be in the same state

Exchange Operator P

$\hat{P}\psi(r_1, r_2) = \psi(r_2, r_1)$ $\hat{P}^2\psi(r_1, r_2) = \psi(r_1, r_2)$

$\hat{P}^2 = \hat{\mathbb{1}}$ $\hat{P}^2\psi(r_1, r_2) = \lambda^2\psi(r_1, r_2)$

$\lambda = \pm 1$

If I have 2 identical particles $m_1 = m_2$ and $V(r_1, r_2) = V(r_2, r_1)$

$[\hat{H}, \hat{P}] = 0$

Two particles in ψ_a, ψ_b $r^2 = (x_1 - x_2)^2$

~~$\langle r^2\rangle_S \neq < \langle r^2$~~

$\langle r^2\rangle_S < \langle r^2\rangle_D < \langle r^2\rangle_{AS}$

$$\langle r^2\rangle_D = \int dx_1 \int dx_2 \psi_a^*(x_1)\psi_b^*(x_2)(x_1 - x_2)^2 \psi_a(x_1)\psi_b(x_2)$$

$$= \langle \psi_a(x_1)\psi_b(x_2)|(x_1 - x_2)^2|\psi_a(x_1)\psi_b(x_2)\rangle$$

$$= \left(\int dx_1 x_1^2 |\psi(x_1)|^2\right)\left(\int dx_2 |\psi_b(x_2)|^2 = -2\left(\int dx_1 x_1 |\psi_a(x_1)|^2\right.\right.$$

$$\langle x^2\rangle_a - 2\langle x\rangle_a\langle x\rangle_b + \langle x^2\rangle_b$$

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Discussion

Identical Particles

Two Bosons $\frac{1}{\sqrt{2}}\left(\psi_a(x_1)\psi_b(x_2) + \psi_b(x_1)\psi_a(x_2)\right)$

Two Fermions $\frac{1}{\sqrt{2}}\left(\psi_a(x_1)\psi_b(x_2) - \psi_b(x_1)\psi_a(x_2)\right)$

Suppose we want the wavefunction of N identical particles.

The wave function needs to be totally symmetric or antisymmetric

$$\hat{P}_{i\leftrightarrow j}\psi(x_1,\dots,x_N) = \pm\psi(x_1,\dots,x_N)$$

for all (i,j) pairs

The wave function of N identical fermions (if the single particle wavefunctions are orthonormal) is given by the Slater determinant

$$\psi(x_1,\dots,x_N) = \frac{1}{\sqrt{N!}}\det\left(\begin{bmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_N(x_1) \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \\ \psi_1(x_N) & \cdots & \cdots & \psi_N(x_N)\end{bmatrix}\right)$$

Automatically totally antisymmetric and obeys Pauli Exclusion

For Bosons :

$$\psi(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \text{perm}\left(\begin{bmatrix} \psi_1(x_1) & \cdots & \psi_N(x_1) \\ \vdots & \ddots & \vdots \\ \psi_1(x_N) & \cdots & \psi_N(x_N) \end{bmatrix}\right)$$

is like determinant except not negatives

Second Quantization

Describe states in fock - space

Say individual particles have a local hilbert space of size M.

eg $M = 3$, $\{|\psi_a\rangle, |\psi_b\rangle, |\psi_c\rangle\}$

states can be written as

$$|n_a = 3, n_b = 1, n_c = 0\rangle$$

Density Matrices

we can consider instead of a single wave function $|\psi\rangle$ a statistical ensemble of particles in different states

eg) N spin $\frac{1}{2}$ particles where spin up / spin down correspond to ~~wave~~ have energy $\sigma \pm \varepsilon$

$\beta = \frac{1}{k_b T}$ $\quad \frac{N e^{\beta}}{e^{\beta \varepsilon}}$

More generally, say we have an orthonormal basis

$$\{|1\rangle, \ldots, |M\rangle\}$$

we describe the system by a set of probabilities

$(P_1, \ldots, P_M)$ for a randomly chosen particle to be in state $|i\rangle$

We can equivalently express this set of P's as a density matrix

$$\rho = \sum_i P_i |i\rangle\langle i| \qquad \sum_i P_i = 1$$

If $\rho = |\psi\rangle\langle\psi|$ for some $|\psi\rangle$, ρ is a pure state

If $\rho^2 = \rho$ iff ρ is a pure state

if ρ is not pure, we call it a mixed state

To take an expectation value with respect to a density matrix,

$$\langle \hat{A} \rangle = \sum_i P_i \langle i|\hat{A}|i\rangle = tr(\rho \hat{A})$$

Properties of the trace

$Tr(\hat{A}) = \sum$ diagonal entries $= \sum \langle i|\hat{A}|i\rangle \qquad Tr(ABC) \neq Tr(BAC)$

$Tr(A^T) = Tr(A) \qquad Tr(A+B) = TrA + TrB$

$Tr(cA) = cTr(A) \qquad Tr(AB) = Tr(BA)$

Properties of ρ

$\rho = \rho^\dagger$ $\quad \rho^2 = \rho$ iff ρ is pure

$\mathrm{Tr}\rho = 1$ $\quad \rho = \frac{1}{M}\hat{\mathbb{1}}$ for maximally mixed state

$\mathrm{tr}\rho^2 \leq 1$ equality for a pure state

We can define the Von-Neumann entropy S of a density matrix by

$$S = -\sum_i P_i \log_e(P_i) = -\mathrm{Tr}(\rho \ln(\rho))$$

$S = 0$ for a pure state

$S = \ln M = -\sum \frac{1}{M}\log_e(\frac{1}{M})$ for maximally mixed state

$$\frac{\partial|\psi\rangle}{\partial t} = \frac{-i}{\hbar}\hat{H}|\psi\rangle \qquad \frac{\partial\langle\psi|}{\partial t} = \frac{i}{\hbar}\langle\psi|\hat{H} \qquad \rho = |\psi\rangle\langle\psi|$$

$$\frac{\partial\rho}{\partial t} = \frac{\partial|\psi\rangle\langle\psi|}{\partial t} = \left(\frac{\partial|\psi\rangle}{\partial t}\right)\langle\psi| + |\psi\rangle\left(\frac{\partial\langle\psi|}{\partial t}\right)$$

$$= \frac{-i}{\hbar}\hat{H}|\psi\rangle\langle\psi| + \frac{i}{\hbar}|\psi\rangle\langle\psi|\hat{H}$$

$$= \frac{-i}{\hbar}\hat{H}\rho + \frac{i}{\hbar}\cancel{\hat{H}}\rho\hat{H} = \frac{-i}{\hbar}[\hat{H},\rho]$$

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Discussion

Bloch Sphere / Ball

ρ for a two state system

$\rho = \rho^\dagger$, $\mathrm{tr}\,\rho = 1$

$a, b, c \in \mathbb{R}$

$$\begin{bmatrix} a & b-ic \\ b+ic & 1-a \end{bmatrix} = \begin{bmatrix} \frac{1}{2}+(a-\frac{1}{2}) & b-ic \\ b+ic & \frac{1}{2}-(a-\frac{1}{2}) \end{bmatrix}$$

$$= \frac{1}{2}(\mathbb{1} + \vec{h}\cdot\vec{\sigma}) \qquad \vec{h} = (2b, 2c, 2a-1)$$

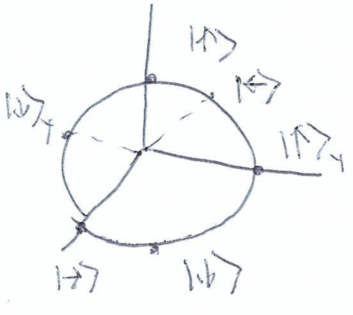
$$|\vec{h}| \leq 1$$

$h = n$

One to one correspondence between density matrices for two state systems and points in a ball of radius 1

if $\vec{n} = \hat{z}$, $\rho = \frac{1}{2}(\mathbb{1}+\sigma_z) = \frac{1}{2}\left(\begin{bmatrix}1&0\\0&1\end{bmatrix} + \begin{bmatrix}1&0\\0&-1\end{bmatrix}\right) \doteq \begin{bmatrix}1&0\\0&0\end{bmatrix} = |\uparrow\rangle\langle\uparrow|$

$\vec{n} = -\hat{z}$, $\rho = \frac{1}{2}(\mathbb{1}-\sigma_z) \doteq \begin{bmatrix}0&0\\0&1\end{bmatrix} = |\downarrow\rangle\langle\downarrow|$

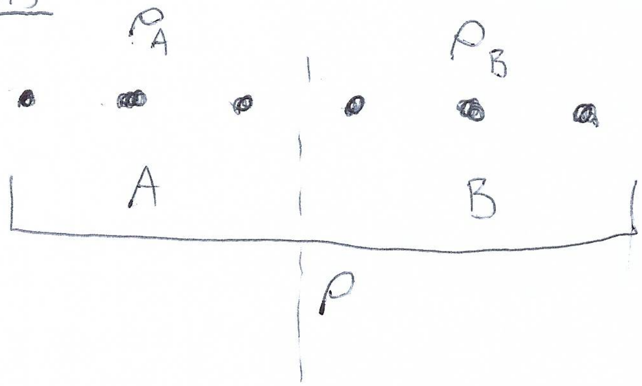


$\vec{n} = \hat{x}$ $\rho = \frac{1}{2}(\mathbb{1}+\sigma_x) = \frac{1}{2}\begin{bmatrix}1&1\\1&1\end{bmatrix} \doteq |\rightarrow\rangle\langle\rightarrow|$

$|\rightarrow\rangle \doteq \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$

It turns out All points on the surface of the Bloch Ball are pure states. Points in the interior are mixed states. The origin is the maximally mixed state.

Subsystems



We find eg ρ_A by computing the partial trace of ρ over B

$$\rho_A = tr_B(\rho) \qquad \rho_B = tr_A(\rho)$$

$$\rho_A = tr_B(\rho) = \sum_b \langle b|\rho|b\rangle$$

$$\langle a_1|\rho|a_2\rangle = \sum_b \langle a_1, b|\rho|a_2, b\rangle$$

$$\rho = |\uparrow\uparrow\rangle\langle\uparrow\uparrow|$$

$$\rho_A = \sum_i {}_2\langle i|\rho|i\rangle_2 = {}_2\langle\uparrow|\uparrow\uparrow\rangle\langle\uparrow\uparrow|\uparrow\rangle_2 + {}_2\langle\downarrow|\uparrow\uparrow\rangle\langle\uparrow\uparrow|\downarrow\rangle_2$$

$$\langle\uparrow|\uparrow\uparrow\rangle = \langle\uparrow|(|\uparrow\rangle_1 \otimes |\uparrow\rangle_2) = |\uparrow\rangle_1$$

$$\rho_A = {}_1|\uparrow\rangle\langle\uparrow|_1$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}\left(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|\right)$$

$$\rho_A = \begin{bmatrix} \sum_i \langle\uparrow_i|\rho|\uparrow_i\rangle & \sum_i \langle\uparrow_i|\rho|\downarrow_i\rangle \\ \sum_i \langle\downarrow_i|\rho|\uparrow_i\rangle & \sum_i \langle\downarrow_i|\rho|\downarrow_i\rangle \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

The entanglement entropy of A and B is defined by

$$S(\rho_A) = -\mathrm{Tr}_A\left(\rho_A \log_e(\rho_A)\right) = -\mathrm{Tr}_B\left(\rho_B \log_e(\rho_B)\right) = S(\rho_B)$$

$$S = -\mathrm{tr}\left(\begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}\begin{bmatrix} \ln\frac{1}{2} & 0 \\ 0 & \ln\frac{1}{2} \end{bmatrix}\right) = \mathrm{tr}\left(\begin{bmatrix} \frac{1}{2}\ln 2 & 0 \\ 0 & \frac{1}{2}\ln 2 \end{bmatrix}\right) = \cancel{\log}\ \ln 2$$

Ramsey Pulse Sequence

$$\hat{H} = \Delta|\uparrow\rangle\langle\uparrow| + \Omega\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)$$

$$= \begin{bmatrix} \Delta & \Omega \\ \Omega & 0 \end{bmatrix} \qquad \Omega \propto |\vec{E}|$$

Two cases:

$$\Omega = 0 \qquad H = \begin{bmatrix} \Delta & 0 \\ 0 & 0 \end{bmatrix} \qquad U(t) = e^{-iHt/\hbar} = \begin{bmatrix} e^{-i\Delta t} & 0 \\ 0 & 1 \end{bmatrix}$$

$$\Omega >> \Delta \qquad H \cong \begin{bmatrix} 0 & \Omega \\ \Omega & 0 \end{bmatrix} = \Omega\sigma_x \qquad U = e^{-i\Omega\sigma_x t/\hbar} \quad \text{choose } t = \frac{\pi}{4\Omega}$$

$$e^{i\theta(\vec{n}\cdot\vec{\sigma})} = \cos\theta\,\mathbb{1} + i\sin\theta\cdot(\vec{n}\cdot\vec{\sigma}) \qquad \downarrow \quad U^x_{\pi/2} = \frac{1}{\sqrt{2}}\left(\mathbb{1} - i\sigma_x\right) = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}$$

Procedure:

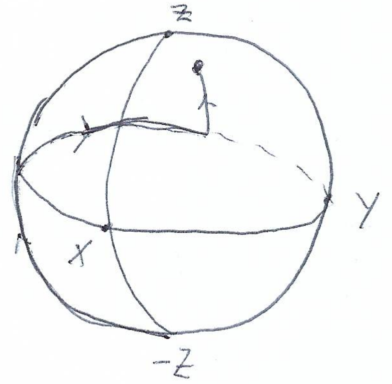
1) Prepare a state in $|\downarrow\rangle$

2) Apply a $\frac{\pi}{2}$ pulse about $\check{X}$

3) Turn off pulse and allow the system to evolve for a time τ

4) Apply $\frac{\pi}{2}$ pulse about $\check{X}$

5) Measure $|\downarrow\rangle$



$$|\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$U^{x}_{\frac{\pi}{2}} \rightarrow \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} -i \\ 1 \end{bmatrix}$$

$$U(t) \rightarrow \begin{bmatrix} e^{-i\Delta t} & 0 \\ 0 & 1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} -i \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} -ie^{-i\Delta\tau} \\ 1 \end{bmatrix}$$

$$U^{x}_{\frac{\pi}{2}} \rightarrow \cancel{\frac{1}{\sqrt{2}}\begin{bmatrix} -ie^{-i\Delta\tau} \\ 1 \end{bmatrix}} \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ -i & 1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} -ie^{-i\Delta\tau} \\ 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} -i(1+e^{-i\Delta\tau}) \\ 1-e^{-i\Delta\tau} \end{bmatrix}$$

$$|\langle\downarrow|\psi_f\rangle|^2 = \sin^2\left(\frac{\Delta\tau}{2}\right)$$

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Discussion

Degenerate Perturbation Theory

$|a^0\rangle, |b^0\rangle$ such that $H^0|a^0\rangle = E^0|a^0\rangle$

$$H^0|b^0\rangle = E^0|b^0\rangle$$

$$\langle a^0|b^0\rangle = 0$$

$|\psi^0\rangle = \alpha|a^0\rangle + \beta|b^0\rangle$, $|\alpha|^2 + |\beta|^2 = 1$

is still an eigenstate of $\hat{H}^0$ with energy E^0 ~~$\langle H$~~ $H^0|\psi^0\rangle = E^0|\psi^0\rangle$

$H(\varepsilon) = H^0 + \varepsilon H'$

$H(\varepsilon)|\psi\rangle = E|\psi\rangle$

$E = E^0 + \varepsilon E^1 + \varepsilon^2 E^2 + \dots$

$|\psi\rangle = |\psi^0\rangle + \varepsilon|\psi^1\rangle + \varepsilon^2|\psi^2\rangle + \dots$

$(H^0 + \varepsilon H')(|\psi\rangle + \varepsilon|\psi'\rangle + \varepsilon^2|\psi^2\rangle + \dots) = (E^0 + \varepsilon E^1 + \varepsilon^2 E^2 + \dots)(|\psi^0\rangle + \varepsilon|\psi'\rangle + \dots)$

$H^0|\psi^0\rangle + \varepsilon(H'|\psi^0\rangle + H^0|\psi'\rangle) + \dots = E^0|\psi^0\rangle + \varepsilon(E'|\psi^0\rangle + E^0|\psi'\rangle) + \dots$

ε^1: $H'|\psi^0\rangle + H^0|\psi'\rangle = E'|\psi^0\rangle + E^0|\psi'\rangle$ ☆

Apply $\langle a^0|$ to ☆

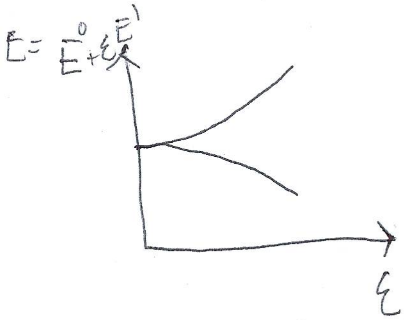
$\langle a^0|H'|\psi^0\rangle + \langle a^0|H^0|\psi^1\rangle = E^1\langle a^0|\psi^0\rangle + E^0\langle a^0|\psi^1\rangle$

$\alpha\langle a^0|H'|a^0\rangle + \beta\langle a^0|H'|b^0\rangle + E^0\langle a^0|\psi'\rangle = E'\alpha + E^0\langle a^0|\psi'\rangle$

$\alpha\langle b^0|H'|a^0\rangle + \beta\langle b^0|H'|b^0\rangle = \beta E'$

$$\underbrace{\begin{bmatrix} \langle a^0|H'|a^0\rangle & \langle a^0|H'|b^0\rangle \\ \langle b^0|H'|a^0\rangle & \langle b^0|H'|b^0\rangle \end{bmatrix}}_{W}\begin{bmatrix}\alpha \\ \beta\end{bmatrix} = E^1\begin{bmatrix}\alpha \\ \beta\end{bmatrix}$$

E^1 is an eigenvalue of this matrix W



Say A is an Hermitian operator that commutes with the perturbation $[A, H'] = 0$ furthermore suppose that $|a^0\rangle$ and $|b^0\rangle$ are simultaneous eigenstates of H^0 and A such that

$A|a^0\rangle = \mu|a^0\rangle$, $A|b^0\rangle = \nu|b^0\rangle$, $\mu \neq \nu$

Pf: $\langle a^0|[A, H']|b^0\rangle = 0 = \langle a^0|AH'|b^0\rangle - \langle a^0|H'A|b^0\rangle$

$= \mu\langle a^0|H'|b^0\rangle - \nu\langle a^0|H'|b^0\rangle = (\mu-\nu)\langle a^0|H'|b^0\rangle \Rightarrow \langle a^0|H'|b^0\rangle = 0$

Ex1 In Special Relativity $T \neq \frac{p^2}{2m}$

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2 = mc^2\left(\sqrt{1+\left(\frac{p}{mc}\right)^2} - 1\right)$$

$$= mc^2\left(1 + \frac{1}{2}\left(\frac{p}{mc}\right)^2 - \frac{1}{8}\left(\frac{p}{mc}\right)^4 - 1\right) = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}$$

$$H' = \frac{-p^4}{8m^3c^2} \qquad |n\ell m\rangle, \ E_n^0 = \frac{-13.6\,eV}{n^2}$$

$$[H', L^2], [H', L_z]$$

Ex 2: particle on a ring of circumference L

$$H^0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad -\frac{L}{2} < x < \frac{L}{2}$$

$$|n\rangle = \frac{1}{\sqrt{L}} e^{2\pi i n x/L} \qquad n \in \mathbb{Z}$$

$$E_n = \frac{2}{m}\left(\frac{n\pi\hbar}{L}\right)^2 \qquad E_n = E_{-n}$$

$$H' = -V_0 e^{-x^2/a^2}, \quad a \ll L$$

$$\langle n|H'|n\rangle = \langle -n|H'|-n\rangle = -\frac{V_0}{L}\int_{-L/2}^{L/2} e^{-x^2/a^2}\,dx \approx \frac{-V_0}{L}\int_{-\infty}^{\infty} e^{-x^2/a^2}\,dx$$

$$= \frac{-V_0 a}{L}\sqrt{\pi}$$

$$\gamma$$

$$\langle -n|H'|n\rangle = \langle n|H'|-n\rangle^*$$

$$\approx \frac{-V_0}{L}\int_{-\infty}^{\infty} e^{-x^2/a^2} e^{4\pi n i x/L}\,dx$$

$$\approx -\frac{V_0}{L}\int_{-\infty}^{\infty} e^{-(x-2\pi i n a^2/L)^2/a^2} e^{-4\pi^2 n^2 a^2/L^2}\,dx$$

$$= -\frac{V_0 a}{L}\sqrt{\pi}\, e^{-4\pi^2 n^2 a^2/L^2} \equiv \delta$$

$$W = \begin{bmatrix} \gamma & \delta \\ \delta & \gamma \end{bmatrix} \qquad \begin{vmatrix} \gamma - E' & \delta \\ \delta & \gamma - E' \end{vmatrix} = (\gamma - E')^2 - \delta^2$$

$$E'_{\pm} = \gamma \pm \delta = -\frac{V_0 a}{L}\sqrt{\pi}\left(1 \pm e^{-4\pi^2 n^2 a^2/L^2}\right)$$

$$\left[\begin{array}{cc|c} \gamma-(\gamma\pm\delta) & \delta & 0 \\ \delta & \gamma-(\gamma\pm\delta) & 0 \end{array}\right] = \left[\begin{array}{cc|c} \mp\delta & \delta & 0 \\ \delta & \mp\delta & 0 \end{array}\right]$$

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |-\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|n\rangle \pm |-n\rangle\right) = \sqrt{\frac{2}{L}}\,\frac{1}{2}\left(e^{2\pi n i x/L} \pm e^{-2\pi n i x/L}\right)$$

$$|+\rangle = \sqrt{\frac{2}{L}}\cos\left(\frac{2\pi n x}{L}\right) \qquad |-\rangle = i\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi n x}{L}\right)$$

$$H'(-x) = H'(x)$$

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Discussion

Perturbative Corrections to Hydrogen

The relativistic correction to the Hamiltonian is given by

$$H'_r = \frac{-p^4}{8m^3c^2} \qquad [\hat{L}^2, \hat{H}'_r] = [\hat{L}_z, \hat{H}'_r] = 0 \checkmark$$

$|nlm\rangle$ are "good states"

$$\langle\psi^0|p^4|\psi^0\rangle = \langle p^2\psi^0|p^2\psi^0\rangle$$

$$p^2|\psi^0\rangle = 2m(E^0 - V)|\psi^0\rangle$$

$$\langle p^4\rangle = 4m^2\langle(E^0-V)^2\rangle \qquad V = \frac{-e^2}{4\pi\epsilon_0 r}$$

$$E'_r = \langle H'_r\rangle = -\frac{1}{2mc^2}\left((E_n^0)^2 + 2E_n^0 \frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r}\right\rangle + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left\langle\frac{1}{r^2}\right\rangle\right.$$

$$E'_{nlm,r} = -\frac{(E_n^0)^3}{2mc^2}\left(\frac{4n}{l+\frac{1}{2}} - 3\right) = -\frac{1}{8}\alpha^4\frac{mc^2}{n^4}\left(\frac{4n}{l+\frac{1}{2}} - 3\right)$$

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$$ fine structure constant.

$$\frac{E_n^0}{mc^2} \approx 2\times10^{-5}$$

$H'_{so} \sim -\vec{\mu} \cdot \vec{B}$ $\quad \mu \propto S \quad \vec{B} \propto \vec{L}$

$$H'_{so} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{m^2c^2r^3} \vec{S} \cdot \vec{L} \frac{1}{2}(3)$$

$$E'_{fs} = E'_r + E'_{so} = \frac{(E_n^0)^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right) = \frac{\alpha^4 mc^2}{8n^4}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)$$

degeneracy in j is lifted by H'_{fs}

<u>Zeeman Effect</u> (external magnetic field)

$H'_z = -(\vec{\mu}_\ell + \vec{\mu}_s) \cdot \vec{B}$ $\quad \vec{\mu}_s = \frac{-e}{m}\vec{S}, \vec{\mu}_\ell = \frac{-e}{2m}\vec{L}$

$$= \frac{+e}{2m}(\vec{L} + 2\vec{S}) \cdot \vec{B}$$

$$B_{int} = \left\langle \frac{1}{4\pi\epsilon_0} \frac{e^2}{mc^2r^3} L \right\rangle$$

Weak Field Zeeman Effect $B << B_{int}$ $\quad \langle \vec{S} \rangle = \frac{\langle (\vec{S} \cdot \vec{J}) J \rangle}{\langle J^2 \rangle}$

Fine structure H starting point and H_z perturbs that

Need coupled states $E'_z = \langle n \ell j m_j | H'_z | n \ell j m_j \rangle = \frac{e^2}{2m} B \cdot \langle \vec{J} + \vec{S} \rangle$

~~Strong Field Zeeman Effect $B >> B_{int}$~~

$$S \cdot J = \frac{1}{2}(J^2 + S^2 - L^2)$$

$\mu_B = \frac{e\hbar}{2m}$ (Bohr magneton)

$$E_z^1 = \frac{e^2}{2m} \vec{B} \cdot \langle J + S \rangle = \frac{e^2}{2m} \vec{B} \cdot \left\langle \left(1 + \frac{S \cdot J}{J^2}\right) J \right\rangle$$

$$= \frac{e^2}{2m} \underbrace{\left(1 + \frac{j(j+1) - \ell(\ell+1) + \frac{3}{4}}{2j(j+1)}\right)}_{g_J} \vec{B} \cdot \langle \vec{J} \rangle = \mu_B g_J B m_j$$ lifts degeneracy in m_j

Strong Field Zeeman Effect

$B >> B_{in}$

Zeeman perturbation first and then the fine structure perturbation

Use uncoupled basis

$$E_z^1 = \frac{e}{2m} B \langle n l m_l m_s | L_z + 2S_z | n l m_l m_s \rangle$$

$$= \frac{e\hbar}{2m} B (m_l + 2m_s) = \mu_B B (m_l + 2m_s)$$

$\langle \vec{L} \cdot \vec{S} \rangle = \hbar^2 m_l m_s$ for fine structure

Intermediate Field Zeeman Effect $B \approx B_{in}$

Treat them together as a single perturbation

Stark Effect (external electric field)

$$H_s^1 = -eE\hat{z} = -Er\cos\theta$$

eg n=2 states

$|200\rangle$ $|211\rangle$ $|210\rangle$ $|21-1\rangle$

$$W = -eE \begin{bmatrix} \langle 200|z|200\rangle & \cdots \\ \langle 211|z|200\rangle & \\ \langle 210|z|200\rangle & \\ \langle 21-1|z|200\rangle & \end{bmatrix}$$

Phys 137B 06 Nov 19

Discussion

Schrödinger Picture

$$i\hbar \frac{\partial}{\partial t}|\psi_s(t)\rangle = H(t)|\psi_s(t)\rangle$$

$$|\psi_s(t)\rangle = U(t)|\psi_s(0)\rangle$$

$$i\hbar \frac{\partial U}{\partial t}|\psi_s(0)\rangle = H(t)U|\psi_s(0)\rangle$$

$$i\hbar \frac{\partial U}{\partial t} = HU$$

If H is time independent, we can solve this to find $U(t) = e^{-iHt/\hbar}$

Alternatively, we can consider that operators evolve and states are static

Heisenberg Picture

$$|\psi_H(t)\rangle = U^\dagger(t)\underbrace{|\psi_s(t)\rangle}_{U(t)|\psi_s(0)\rangle} = |\psi_s(0)\rangle = |\psi_H(0)\rangle$$

$\langle\psi_a|\hat{A}|\psi_b\rangle$ needs to be picture independent

$$\hat{A}_H = U^\dagger(t)\hat{A}_s U(t)$$

$$\langle\psi_H|\hat{A}_H|\psi_H\rangle = (\langle\psi_s|U)(U^\dagger A_s U)(U^\dagger|\psi_s\rangle) = \langle\psi_s|A_s|\psi_s\rangle$$

$$\frac{\partial A_H}{\partial t} = \frac{\partial}{\partial t}\left(U^\dagger A_s U\right) = \left(\frac{\partial U^\dagger}{\partial t}\right) A_s H + U^\dagger A_s \left(\frac{\partial U}{\partial t}\right) + U^\dagger \frac{\partial A_s}{\partial t} U$$

$$i\hbar \frac{\partial U}{\partial t} = HU \qquad -i\hbar \frac{\partial U^\dagger}{\partial t} = U^\dagger H$$

$$i\hbar \frac{\partial A_H}{\partial t} = -U^\dagger H \underset{\underset{UU^\dagger}{\uparrow}}{} A_s U + U^\dagger A_s \underset{\nwarrow}{} H U + i\hbar U^\dagger \frac{\partial A_s}{\partial t} U$$

$$= -(U^\dagger H U)(U^\dagger A_s U) + (U^\dagger A_s U)(U^\dagger H U) + i\hbar U^\dagger \frac{\partial A_s}{\partial t} U$$

$$= \left[A_H, H_H\right] + i\hbar \left(\frac{\partial A}{\partial t}\right)_H$$

$$\frac{\partial A_H}{\partial t} = \frac{-i}{\hbar}\left[A_H, H_H\right] + \left(\frac{\partial A}{\partial t}\right)_H$$

Interaction Picture

We can also make an intermediate choice and put some time dependence on both states and operators

$$H(t) = H_0 + H_1(t)$$

We want to move time dependence due to H_0 onto the operators and leave the remaining time dependence on the states.

Define unitaries U, U_0

Evolution under H_0: $|\psi_0(t)\rangle_s = U_0(t)|\psi_0(t)\rangle_s$

$|\psi(t)\rangle_s = U(t)|\psi(t)\rangle_s$

We then know that $i\hbar \frac{\partial U}{\partial t} = H(t)U$ and $i\hbar \frac{\partial U_0}{\partial t} = H_0 U_0$

Under the assumption that H_0 is time independent,
$U_0(t) = e^{-iH_0 t/\hbar}$

we define states in the interaction picture as

$|\psi_I(t)\rangle = U_0^\dagger(t)|\psi_s(t)\rangle$ Note $|\psi_I(0)\rangle = |\psi_s(0)\rangle$

$A_I(t) = U_0^\dagger A_s U_0$ so $\langle\psi_I|A_I|\psi_I\rangle = \langle\psi_s|A_s|\psi_s\rangle$

We define a unitary W such that W is a time evolution operator in the interaction picture.

$|\psi_I(t)\rangle = W(t)|\psi_I(0)\rangle$

$|\psi_I(t)\rangle = U_0^\dagger|\psi_s(t)\rangle = U_0^\dagger U|\psi_s(0)\rangle = U_0^\dagger U|\psi_I(0)\rangle$

$U_0^\dagger U = W(t)$

$$i\hbar\frac{\partial W}{\partial t} = i\hbar\frac{\partial}{\partial t}(U_0^\dagger U) = i\hbar\frac{\partial U_0^\dagger}{\partial t}U + i\hbar U_0^\dagger\frac{\partial U}{\partial t}$$

$$= -(U_0^\dagger H_0)U + U_0^\dagger(HU) = U_0^\dagger(H-H_0)U = U_0^\dagger H_1(t)\overset{U_0U_0^\dagger}{\downarrow}U$$

$$= (U_0^\dagger H_1 U_0)U_0^\dagger U \quad = (U_0^\dagger H_1 U_0)W$$

Time Evolution in the interaction picture looks like time evolution under the "effective hamiltonian" H_{eff}

$$H_{eff} = U_0^\dagger H_1 U_0 = U_0^\dagger(H-H_0)U_0 = U_0^\dagger H U_0 - H_0 = H_{1,I}$$

We can consider other transformations

$$|\psi\rangle \to U|\psi\rangle, \quad \hat{A} \to U\hat{A}U^{\dagger} \text{ for any unitary } U$$

$U(\eta) = e^{-i\eta\hat{G}/\hbar}$, $\hat{G}$ is the generator of the transformation

η determines strength of transformation

Ex

Transformation	Unitary	Generator
time evolution	$U(t) = e^{-i\hat{H}t/\hbar}$	$\hat{H}$
Spatial translation	~~$U(t) =$~~ $T(x) = e^{-i\hat{p}_x x/\hbar}$	$\hat{p}$
Rotation	$R_{space}(\theta) = e^{-i\theta\check{n}\cdot\vec{L}/\hbar}$	$\check{n}\cdot\vec{L}$. (Rotation about $\check{n}$)
Spin Rotation	$R_{spin}(\theta) = e^{-i\theta\check{n}\cdot\vec{S}/\hbar}$	$\check{n}\cdot\vec{S}$ (Rotation about $\check{n}$)
Total Rotation	$R(\theta) = e^{-i\theta\check{n}\cdot\vec{J}/\hbar}$	$\check{n}\cdot\vec{J}$ (Rotation about $\check{n}$)

If $\hat{A}$ is invariant under U, then

$UAU = A$, so for an infinitessimal transformation,

$$\left(1 - \frac{i\varepsilon G}{\hbar}\right)A\left(1 + \frac{i\varepsilon G}{\hbar}\right) = A + \frac{i\varepsilon}{\hbar}[A, G] = A$$

the $[A, G] = 0$

A is invariant under U

Vector operators:

$$[J_i, V_j] = i\hbar\,\varepsilon_{ijk}V_k \qquad \vec{r}:\ V_{\pm 1} = \mp(V_x \pm iV_y),\ V_0 = V_z$$

Phys 137B 16Nov19
Midterm 2 Review

1. particle in 1D SHO potential

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \quad , \quad \hat{H}_1 = \alpha \hat{p}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

a) $$\tilde{E}_0 \leq \langle 0 | H_0 + H_1 | 0 \rangle = \overbrace{\langle 0 | H_0 | 0 \rangle}^{E_0} + \langle 0 | H_1 | 0 \rangle$$

$$\langle 0 | H_1 | 0 \rangle = \alpha \langle 0 | \hat{p} | 0 \rangle \qquad \langle 0 | \hat{p} | 0 \rangle = \langle 0 | \hat{\pi} \hat{\pi} \hat{p} \hat{\pi} \hat{\pi} | 0 \rangle$$

$$= 0 \qquad\qquad = - \langle 0 | \hat{p} | 0 \rangle$$

$$\tilde{E}_0 \leq E_0$$

since $\hat{p}$ is odd under parity and $|0\rangle$ is even

b) $E_n^0 = (n + \frac{1}{2})\hbar\omega$, $|n\rangle$, $\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)$

$$E_n^1 = \langle n | H_1 | n \rangle = i\alpha \sqrt{\frac{\hbar m \omega}{2}} \left(\langle n | a^\dagger - a | n \rangle \right) = 0$$

$$|n^1\rangle = \sum_{m \neq n} \frac{\langle m | H_1 | n \rangle}{E_n^0 - E_m^0} |m\rangle \qquad E_n^0 - E_m^0 = (n-m)\hbar\omega$$

$$\langle m | H_1 | n \rangle = i\alpha \sqrt{\frac{\hbar m \omega}{2}} \langle m | a^\dagger - a | n \rangle = i\alpha \sqrt{\frac{\hbar m\omega}{2}} \langle m | \left(\sqrt{n+1} |n+1\rangle - \sqrt{n} |n-1\rangle \right)$$

$$= i\alpha \sqrt{\frac{\hbar m\omega}{2}} \left(\sqrt{n+1}\, \delta_{m,n+1} - \sqrt{n}\, \delta_{m,n-1} \right)$$

$$|n^1\rangle = i\alpha \sqrt{\frac{\hbar m\omega}{2}} \sum_{m \neq n} \frac{\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}}{\hbar\omega(n-m)} |m\rangle$$

$$= -i\alpha \sqrt{\frac{m}{2\hbar\omega}} \left(\sqrt{n+1} |n+1\rangle + \sqrt{n} |n-1\rangle \right)$$

$$E_n^2 = \langle n | H_1 | n' \rangle = \sum_{m \neq n} \frac{|\langle m | H_1 | n \rangle|^2}{E_n^0 - E_m^0} = \alpha^2 \frac{\hbar m \omega}{2} \frac{1}{\hbar \omega} \left(-(n+1) + n \right)$$

$$= -\frac{m\alpha^2}{2}$$

2. 2D Harmonic Oscillator

$$\hat{H}_0 = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m} + \frac{1}{2} m \omega^2 (\hat{x}^2 + \hat{y}^2)$$

$$|n,m\rangle = |n\rangle_x \otimes |m\rangle_y$$

$a, a^\dagger$ lowering, raising operators for x

$b, b^\dagger$ lowering, raising operators for y

$$E^0_{n,m} = (n+m+1)\hbar\omega$$

$$\hat{H}_1 = A \hat{x} \hat{y}$$

a) $E^0_{n,m} = N\hbar\omega = (n+m+1)\hbar\omega$ $\quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$

degeneracy of $N\hbar\omega$ is N and the states are ~~$|N,0\rangle, |N-1,1\rangle$~~

$|N-1,0\rangle, |N-1,1\rangle, \ldots, |0,N-1\rangle$

b) $E_0 = 3\hbar\omega$ states

$|2,0\rangle, |1,1\rangle, |0,2\rangle$

$$\langle a,b | H_1 | c,d \rangle = \frac{\hbar A}{2m\omega} \langle a | a + a^\dagger | c \rangle \langle b | b + b^\dagger | d \rangle$$

$$= \frac{\hbar A}{2m\omega} \left(\sqrt{c}\, \delta_{a,c-1} + \sqrt{c+1}\, \delta_{a,c+1} \right) \left(\sqrt{d}\, \delta_{b,d-1} + \sqrt{d+1}\, \delta_{b,d+1} \right)$$

$$W_3 = \frac{\hbar A}{2m\omega}\begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix} \rightarrow \lambda = 0, \pm\frac{\hbar A}{m\omega} = E^1$$

$$V_0 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left(|2,0\rangle - |0,2\rangle\right)$$

$$V_\pm = \frac{1}{2}\begin{bmatrix} 1 \\ \pm\sqrt{2} \\ 1 \end{bmatrix} = \frac{1}{2}\left(|2,0\rangle \pm \sqrt{2}|1,1\rangle + |0,2\rangle\right)$$

$2\hbar\omega$ subspace: $|1,0\rangle, |0,1\rangle$

$$W_2 = \frac{\hbar A}{2m\omega}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \rightarrow E^1 = \pm\frac{\hbar A}{2m\omega},\ V_\pm = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left(|1,0\rangle \pm |0,1\rangle\right)$$

$$V_\pm^1 = \sum_{\substack{i \neq \pm \\ i = |2,1\rangle \\ |1,2\rangle}} \frac{\langle i|H_1|V_\pm^0\rangle}{2\hbar\omega - \underset{\downarrow\ 4\hbar\omega}{E_i^0}}|i\rangle = \frac{-1}{2\hbar\omega}\frac{\hbar A}{2m\omega}\left(\langle 1,2|(a+a^\dagger)(b+b^\dagger)\overset{|V_\pm\rangle|1,2\rangle}{\cancel{|1,2\rangle}} + \langle 2,1|(a+a^\dagger)(b+b^\dagger)|V_\pm\rangle|2,1\rangle\right)$$

$$\boxed{?} = -\frac{A}{4m\omega^2}\sqrt{2}\,\frac{1}{\sqrt{2}}\left(\pm|1,2\rangle + |2,1\rangle\right) = \frac{A}{4m\omega^2}\left(\mp|1,2\rangle - |2,1\rangle\right)$$

$$E_\pm^2 = \langle V_\pm^0|H_1|V_\pm^1\rangle$$

$$= \frac{\hbar A}{2m\omega}\frac{1}{\sqrt{2}}\left(\langle 1,0| \pm \langle 0,1|\right)(a^\dagger + a)(b + b^\dagger)\frac{A}{4m\omega^2}\left(\mp|1,2\rangle - |2,1\rangle\right)$$

$$= \frac{-\hbar A}{2m\omega}\frac{1}{\sqrt{2}}\frac{A}{4m\omega^2}\left(\sqrt{2} + \sqrt{2}\right) = \frac{-\hbar A^2}{4m^2\omega^3}$$

3. Variational principle with the ansatz $|\psi(a)\rangle = Ne^{-ar^2}$ for hydrogen

$$\int_0^\infty e^{-ar^2}\,dr = \frac{1}{2}\sqrt{\frac{\pi}{a}} \rightarrow \int_0^\infty r^{2n} e^{-ar^2}\,dr = (-1)^n \frac{1}{2}\frac{d^n}{da^n}\left(\sqrt{\frac{\pi}{a}}\right)$$

$$\int_0^\infty r^2 e^{-ar^2}\,dr = \frac{1}{4}\sqrt{\frac{\pi}{a^3}} \qquad \int_0^\infty r^4 e^{-ar^2}\,dr = \frac{3}{8}\sqrt{\frac{\pi}{a^5}}$$

$$\int_0^\infty r e^{-ar^2}\,dr \xrightarrow[dt=2r\,dr]{t=r^2} \frac{1}{2}\int_0^\infty e^{-at}\,dt = \frac{1}{2a}$$

$$\langle\psi(a)|\psi(a)\rangle = 4\pi N^2 \int_0^\infty e^{-2ar^2} r^2\,dr = \frac{4\pi N^2}{4}\sqrt{\frac{\pi}{8a^3}}, \quad N = \left(\frac{8a^3}{\pi^3}\right)^{1/4} = \left(\frac{2a}{\pi}\right)^{3/4}$$

4π

$$\langle\hat{T}\rangle = \frac{-\hbar^2}{2m}\langle\nabla^2\rangle = \frac{-\hbar^2}{2m}\left(\frac{2a}{\pi}\right)^{3/2} 4\pi \int_0^\infty e^{-ar^2}\frac{1}{r}\frac{d^2}{dr^2}\left(re^{-ar^2}\right) r^2\,dr$$

$$= \frac{+\hbar^2}{2m}\left(\frac{2a}{\pi}\right)^{3/2} 4\pi \int_0^\infty 2a\left(3r^2 - 2ar^4\right)e^{-2ar^2}\,dr$$

$$= \frac{\hbar^2}{2m}\left(\frac{2a}{\pi}\right)^{3/2} 8\pi a\left(\frac{3}{4}\sqrt{\frac{\pi}{8a^3}} - \frac{3}{4}a\sqrt{\frac{\pi}{32a^5}}\right) = \frac{3\hbar^2 a}{2m}$$

$$\langle\hat{V}\rangle = -\left(\frac{2a}{\pi}\right)^{3/2} 4\pi \int_0^\infty \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}e^{-2ar^2} r^2\,dr$$

$$= -\left(\frac{2a}{\pi}\right)^{3/2}\frac{e^2}{\epsilon_0}\frac{1}{4a} = \frac{-e^2}{\epsilon_0}\sqrt{\frac{a}{2\pi^3}}$$

$$E(a) = \frac{3\hbar^2 a}{2m} - \frac{e^2}{\epsilon_0}\sqrt{\frac{a}{2\pi^3}}$$

$$\frac{\partial E}{\partial a} = \frac{3\hbar^2}{2m} - \frac{e^2}{\epsilon_0}\sqrt{\frac{1}{8\pi^3 a}} = 0$$

$$a = \frac{m^2 e^4}{18\pi^3\hbar^4\epsilon_0^2} = \frac{8}{9\pi a_0^2} \qquad E(a)_{min} = \frac{-me^4}{12\pi^3\hbar^2\epsilon_0^2} = \frac{8}{3\pi}E_1 \simeq -11{,}5\,\text{eV}$$

4. Stark Effect for n=3 hydrogen

$$\hat{H}_1 = -eE\check{z}\hat{z}$$

a) use selection rules to find out which elements of W are nonzero

$$\langle n'l'm'|\hat{z}|nlm\rangle = \langle n'l'm'|\hat{\Pi}^\dagger\hat{\Pi}\hat{z}\hat{\Pi}^\dagger\hat{\Pi}|nlm\rangle$$

$$= (-1)^{l+l'+1}\langle n'l'm'|\hat{z}|nlm\rangle$$

$\langle n'l'm'|\hat{z}|nlm\rangle = 0$ unless $l+l' = 1 \pmod 2$

$$|300\rangle, |31\begin{smallmatrix}1\\0\\-1\end{smallmatrix}\rangle, |32\begin{smallmatrix}2\\1\\0\\-1\\-2\end{smallmatrix}\rangle$$

$$[\hat{L}_z, \hat{z}] = 0$$

$$\langle n'l'm'|[\hat{L}_z, \hat{z}]|nlm\rangle = 0$$

$$= \hbar(m'-m)\underbrace{\langle n'l'm'|z|nlm\rangle}_{0 \text{ unlesss } m'=m} = 0$$

→ 8 nonzero matrix elements

$\langle 300|H_1|310\rangle = 3\sqrt{6}\,ea_0E$

$\langle 310|H_1|320\rangle = 3\sqrt{3}\,ea_0E$

$\langle 31\pm1|H_1|32\pm1\rangle = \frac{9}{2}ea_0E$

$$ea_0E\left[\begin{array}{c|c|c} 0 & 0\ \ 3\sqrt{6}\ \ 0 & \\ \hline \begin{matrix}0\\3\sqrt{6}\\0\end{matrix} & O & \begin{matrix}0&9/2&0&0\\0&0&0&0\\0&0&9/2&0\end{matrix} \\ \hline O & \begin{matrix}0&0&0\\9/2&0&0\\0&3\sqrt{3}&0\\0&0&9/2\\0&0&0\end{matrix} & O\end{array}\right]$$

$E^1 = \pm 9ea_0E$: $\sqrt{\frac{1}{3}}|300\rangle \pm \sqrt{\frac{1}{2}}|310\rangle + \frac{1}{\sqrt{6}}|320\rangle$

$E^1 = \pm\frac{9}{2}a$ (2x degenerate): $\frac{1}{\sqrt{2}}(|311\rangle \pm |321\rangle)$, $\frac{1}{\sqrt{2}}(|31-1\rangle \pm |32-1\rangle)$

$E^1 = 0$ (3x degenerate) $|322\rangle$, $|32-2\rangle$, $\frac{1}{\sqrt{3}}|300\rangle - \sqrt{\frac{2}{3}}|320\rangle$

c) $\left[\hat{L}^2, [\hat{L}^2, \hat{r}]\right] = 2\hbar^2(\hat{r}\hat{L}^2 + \hat{L}^2\hat{r})$

$|\alpha'\rangle = |n'l'm'\rangle \quad |\alpha\rangle = |nlm\rangle$

$\langle\alpha'|[\hat{L}^2,[\hat{L}^2,\hat{r}]]|\alpha\rangle$

$= \langle\alpha'|\hat{L}^2[\hat{L}^2,\hat{r}] - [\hat{L}^2,\hat{r}]\hat{L}^2|\alpha\rangle$

$= \hbar^2(l'(l'+1) - l(l+1))\langle\alpha'|[\hat{L}^2,\hat{r}]|\alpha\rangle$

$= \hbar^2(l'(l'+1) - l(l+1))^2\langle\alpha'|r|\alpha\rangle$

$= \langle\alpha'|2\hbar^2(rL^2+L^2r)|\alpha\rangle = 2\hbar^4(l'(l'+1)+l(l+1))\langle\alpha'|r|\alpha\rangle$

$\langle\alpha'|r|\alpha\rangle = 0$ unless

$(l'(l'+1) - l(l+1))^2 = 2(l'(l'+1)+l(l+1))$

$l'(l'+1) - l(l+1) = (l'+l+1)(l'-l)$

$2(l'(l'+1)+l(l+1)) = (l'+l+1)^2 + (l'-l)^2 - 1$

$(l'+l+1)^2(l'-l)^2 - (l'+l+1)^2 - (l'-l)^2 + 1 = 0$

$((l'+l+1)^2-1)((l'-l)^2-1) = 0$

$(l'-l)^2 - 1 = 0 \to l' - l = \pm 1$

$l' = l \pm 1$

Phys 137B 13 Dec 19
Final Review

1. Atom with nondegenerate states $|1\rangle, |2\rangle, |3\rangle, \ldots$ is driven with a perturbation $H' = \Omega(r)\sin(\omega t)$

Denote $\Omega_{mn} = \langle m|\Omega(r)|n\rangle$ and assume $\Omega_{nn} = 0 \ \forall n$.

We'll further assume that $\hbar\omega << E_m - E_n = \hbar\omega_{mn} \ \forall m \neq n$

a) calculate the energy shift ΔE_m for state $|m\rangle$ using 2nd order TDPT $\quad d_m(0) = 1$

$$d_m(t) = e^{-i\Delta E_n t/\hbar} \simeq 1 - \frac{i\Delta E_n t}{\hbar}$$

$$\Delta E_n \simeq i\hbar \frac{\partial}{\partial t} d_m(t)$$

$$e^{-i\omega_{mn}t'} \downarrow \qquad e^{i\omega_{mn}t''} \downarrow$$

$$d_m^{(2)}(t) = 1 - \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_0^t dt' \int_0^{t'} dt'' \langle n|\Omega|m\rangle\langle m|\Omega|n\rangle \sin\omega t' \sin\omega t'' e^{i\omega_{mn}(t''-t')}$$

$$= 1 + \sum_m \frac{\Omega_{nm}\Omega_{mn}}{4\hbar^2} \int_0^t dt' \int_0^{t'} dt'' \left(e^{i\omega t'} - e^{-i\omega t'}\right) \underbrace{\left(e^{i\omega t''} - e^{-i\omega t''}\right) e^{i\omega_{mn}(t''-t')}}_{e^{i(\omega+\omega_{mn})t''} - e^{-i(\omega+\omega_{mn})t''}}$$

$$= 1 + \sum_m \frac{\Omega_{mn}\Omega_{nm}}{4\hbar^2} \int_0^{t'} dt' \left(e^{i(\omega-\omega_{mn})t'} - e^{-i(\omega+\omega_{mn})t'}\right)\left(\frac{e^{i(\omega+\omega_{mn})t'} - 1}{i(\omega+\omega_{mn})} - \frac{e^{-i(\omega-\omega_{mn})t'} - 1}{i(\omega_{mn}-\omega)}\right)$$

$$d_n^2 = 1 + \sum_m \frac{\Omega_{mn}\Omega_{nm}}{4\hbar^2}\left(t\left(\frac{i}{\omega+\omega_{mn}} + \frac{i}{\omega_{mn}-\omega}\right) + \cdots\right)$$

$$\Delta E_n = -\sum \frac{\Omega_{mn}\Omega_{nm}\omega_{mn}}{2\hbar(\omega_{mn}^2 - \omega^2)} \approx -\sum_m \frac{\Omega_{mn}\Omega_{nm}}{2\hbar\,\omega_{mn}}$$

if instead $\omega = \omega_{mn} + \delta$
$\delta << \omega_{mn}$

$$-\sum_m \frac{\Omega_{mn}\Omega_{nm}\omega_{mn}}{4\hbar\omega_{mn}\delta}$$

2. 2 level system with $H = \hbar(\Delta\sigma_z + \Omega(t)\sigma_x) = \hbar\begin{bmatrix}\Delta & \Omega(t)\\ \Omega(t) & -\Delta\end{bmatrix}$

a) $H_0 = \hbar\begin{bmatrix}\Delta & 0\\ 0 & -\Delta\end{bmatrix}$ $E_\pm = \pm\hbar\Delta$ $|+\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ $|-\rangle = \begin{bmatrix}0\\1\end{bmatrix}$

b) $\Omega(t) = \frac{\Omega_0}{1+(\nu t)^2}$, ~~$d_+^{(1)}(t)$~~

$\omega_\pm = \frac{1}{\hbar}[E_+ - E_-] = 2\Delta$

$d_+^{(1)}(\infty) = \frac{-i}{\hbar}\int\langle+|\hbar\Omega(t)\sigma_x|-\rangle e^{2i\Delta t}dt$

$|\psi(-\infty)\rangle = |-\rangle$

$[1\ 0]\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = 1$

$$d_+^{(1)}(\infty) = -i\int_{-\infty}^{\infty} e^{2i\Delta t}\frac{\Omega_0}{1+(\nu t)^2}dt = \frac{-i\Omega_0\pi}{\nu}e^{-2\Delta/\nu}$$

$$P_+(\infty) \simeq |d_+^{(1)}(\infty)|^2 = \left(\frac{\Omega_0\pi}{\nu}\right)^2 e^{-4\Delta/\nu}$$

If $\Delta = 0$ $H = H' = \hbar\Omega(t)\sigma_x \to [H(t), H(t')] = \Omega(t)\Omega(t')[\sigma_x, \sigma_x] = 0$

$$U(t_0, t_f) = \mathcal{T}e^{\frac{-i}{\hbar}\int_{t_0}^{t_f}H(t)dt} = e^{-i\int_{t_0}^{t_f}\Omega(t)dt\,\sigma_x}$$

$$= e^{-i\theta(t_0,t_f)\sigma_x} = \cos(\theta(t_0,t_f))\mathbb{1}_{2\times2} - i\sin(\theta(t_0,t_f))\sigma_x$$

$$\theta(-\infty,\infty) = \int_{-\infty}^{\infty}\frac{\Omega_0}{1+(\nu t)^2}dt = \frac{\Omega_0\pi}{\nu}$$

$$U(-\infty,\infty) = \cos\left(\frac{\Omega_0\pi}{\nu}\right)\mathbb{1} - i\sin\left(\frac{\Omega_0\pi}{\nu}\right)\sigma_x$$

$$|\psi(\infty)\rangle = U(-\infty,\infty)|\psi(-\infty)\rangle = \cos\left(\frac{\Omega_0\pi}{\nu}\right)|-\rangle - i\sin\left(\frac{\Omega_0\pi}{\nu}\right)|+\rangle$$

$P_+(\infty) = \sin^2\left(\frac{\Omega_0\pi}{\nu}\right)$ PT is good for $\frac{\Omega_0\pi}{\nu} \ll 1$

3. Gaussian potential: $V(r) = V_0 e^{-r^2/2a^2}$

$$f(\theta,\phi) \approx \frac{-m}{2\pi\hbar^2}\int e^{i(\vec{k}'-\vec{k})\cdot\vec{r}\,'} V(r')\,d^3\vec{r}\,' \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

$\vec{k}' = k\check{z}$, $\vec{k} = k\check{r}$

$\vec{q} = \vec{k}' - \vec{k} \rightarrow \vec{q}\cdot\vec{r}\,' = qr'\cos\theta'$

put $\check{z}'$ along $\vec{q}$

$f(\theta,\phi)$ only a function of θ due to spherical symmetry

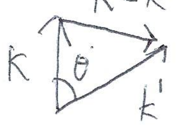
$$f(\theta) = \frac{-m}{2\pi\hbar^2}\int e^{iqr'\cos\theta'} V(r')\sin\theta'\,d\theta'\,d\phi'\,(r')^2\,dr'$$

$$= -\frac{2m}{\hbar^2 q}\int_0^\infty r V(r)\sin(qr)\,dr$$

$$= \frac{-2mV_0}{\hbar^2 q}\int_0^\infty r e^{-r^2/2a^2}\sin qr\,dr = \frac{-2m}{\hbar^2 q}\Big(\overset{0}{\nearrow}\;\; -a^2 e^{-r^2/2a^2}\sin qr\Big)\Big|_0^\infty + a^2 q\int_0^\infty e^{-r^2/2a^2}\cos qr\,dr\Big)$$

$$= \frac{-2mV_0 a^2}{\hbar^2}\operatorname{Re}\left(\int_0^\infty e^{-r^2/2a^2} e^{-iqr}\,dr\right) = \frac{-2mV_0 a^2}{\hbar^2}\operatorname{Re}\left(\frac{\sqrt{2\pi a^2}}{2} e^{-q^2a^2/2}\right)$$

$$= \frac{-\sqrt{2\pi}\,mV_0 a^3}{\hbar^2} e^{-q^2a^2/2} = f(\theta)$$



$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{2\pi m^2 V_0^2 a^6}{\hbar^4} e^{-q^2a^2}$$

law of cosines

$$q^2 = k^2 + k^2 - 2k^2\cos\theta$$

$$= 2k^2(1-\cos\theta)$$

$$= 4k^2\sin^2\frac{\theta}{2}$$

$$e^{-q^2/a^2} = e^{\frac{2k^2a^2}{\cancel{2}}(1-\cos\theta)}$$

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi \frac{2\pi m^2 V_0^2 a^6}{\hbar^4} \int_0^{\pi} e^{-2k^2a^2(1-\cos\theta)} \sin\theta \, d\theta$$

$t = 1-\cos\theta$

$dt = \sin\theta \, d\theta$

$$= \frac{4\pi^2 m^2 V_0^2 a^6}{\hbar^4} \int_0^2 e^{-2k^2a^2 t} dt$$

$$= \frac{2\pi^2 m^2 V_0^2 a^6}{\hbar^4 k^2} \left(1 - e^{-4k^2a^2}\right)$$

low energy limit $(ka \ll 1)$ $e^{-4k^2a^2} \approx 1 - 4k^2a^2$

$$\sigma \approx \frac{8\pi^2 m^2 V_0^2 a^6}{\hbar^4} = 4\pi \left(\frac{\sqrt{2\pi}\, m V_0 a^3}{\hbar^2} \right)^2$$

$|a_l|^2 \sim (ka)^{4l+2}$ (?)   (?) $h_l^{(1)}(x) = j_l(x) + i n_l(x)$

$V(r) = \alpha \delta(r-a)$ Ignore $l>0$ terms

Want to find phase shift

$$\psi(r,\theta) = \tilde{A} \sum_{l=0}^{\infty} i^l (2l+1)\left(j_l(kr) + ika_l h_l^{(1)}(kr)\right) P_l(\cos\theta) \quad r>a$$

$$a_l = \frac{1}{k} e^{i\delta_l} \sin\delta_l$$

δ_l is the l^{th} phase shift

ignore $l>0$

$$\psi(r,\theta) = \tilde{A}\left(j_0(kr) + ika_0 h_0^1(kr)\right) P_0(\cos\theta)$$

$$= \tilde{A}\left(\cancel{j_0(kr)} \frac{\sin kr}{kr} + a_0 \frac{e^{ikr}}{r}\right) = \tilde{A}\left(\frac{\sin kr}{kr} + \frac{e^{i\delta_0}\sin\delta_0 e^{ikr}}{kr}\right)$$

$$= \frac{Ae^{i\delta_0}}{kr}\left(e^{-i\delta_0}\sin kr + \sin\delta_0 e^{ikr}\right) = \frac{A}{r}(\sin kr + \delta_0)$$

$$A = \frac{\tilde{A} e^{i\delta_0}}{k}$$

In general $\psi(r,\theta)$ is a LC of $n_l(kr)$ and $j_l(kr)$

$$\psi(r,\theta) = b j_0(kr) = b\frac{\sin kr}{kr} = B\frac{\sin kr}{r} \quad B = \frac{b}{k}$$

Boundary Conditions

1. ψ is continuous at $r = a$

$$u(r) = r R(r)$$

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(\alpha\delta(r-a) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u = Eu$$

$$\int_{a-\varepsilon}^{a+\varepsilon} \frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(\alpha\delta(r-a) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - E\right)u = 0$$

$$= -\frac{\hbar^2}{2m}\Delta u'(r) + \alpha u(a) = 0$$

$$\rightsquigarrow \cancel{\Delta} \quad \Delta u'(r) = \cancel{\frac{\hbar^2}{2m}} \frac{2m\alpha}{\hbar^2}u(a) = \frac{\beta}{a}u(a)$$

$$\beta = \frac{2ma\alpha}{\hbar^2}$$

1. u continuous

$$A\sin(ka + \delta_0) = B\sin ka \rightarrow B = A\frac{\sin(ka+\delta)}{\sin ka}$$

2. $$Ak\cos(ka+\delta) - Bk\cos ka = \frac{\beta}{a}A\sin(ka+\delta)$$

$$Ak\cos(ka+\delta) - Ak\frac{\sin(ka+\delta)}{\sin ka}\cos ka$$

$$\cos(ka+\delta)\sin ka - \sin(ka+\delta)\cos ka$$

$$\sin(ka - ka - \delta) = \sin(-\delta) = -\sin\delta$$

$$= \frac{\beta}{ka}\sin ka \sin(ka+\delta) = \frac{\beta}{ka}\sin ka(\sin ka\cos\delta + \cos ka\sin\delta)$$

$$1 = \frac{-\beta}{ka}(\sin ka\cot\delta + \cos ka)\sin ka$$

$$\cot\delta = -\cot ka - \frac{ka}{\beta}\csc^2 ka$$

b) $ka << 1 \rightarrow \cot ka \approx \csc ka \approx \frac{1}{ka}$

$$\cot \delta \approx \frac{-1}{ka} - \frac{1}{\beta ka}$$

$$\tan \delta \approx -\frac{ka\beta}{1+\beta} \qquad \delta \approx \arctan\left(-\frac{ka\beta}{1+\beta}\right) \approx -\frac{ka\beta}{1+\beta}$$

$$a_0 = \frac{1}{k} e^{i\delta} \sin\delta \approx -\frac{a\beta}{1+\beta}$$

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) a_l P_l(\cos\theta) \cong a_0 = \frac{-a\beta}{1+\beta}$$

$$D(\theta) = \frac{a^2\beta^2}{(1+\beta)^2}$$

$$\sigma = \int D(\theta) d\Omega \approx 4\pi \left(\frac{a\beta}{1+\beta}\right)^2$$

$$= 4\pi \sum_{l=0}^{\infty} (2l+1)|a_l|^2$$