I. Spinors

II. The matrices and eigenspinors of S_x and S_y

II. Spinors

This is an example of using the matrix formulation of Quantum Mechanics

"Matrix Mechanics"

with 2-component $|i\rangle$ and $|f\rangle$ states

• Recall that a particle can have 2 kinds of angular momentum
-spin angular momentum and orbital angular momentum

• Recall that spin (a kind of angular momentum) can have components,
in particular a z-component

• Recall that z-component of spin can have only 2 values:

$$|S_z = \text{up}\rangle \text{ and } |S_z = \text{down}\rangle$$

also called $\quad |+\rangle \quad$ and $|-\rangle \quad\quad$ (no $|0\rangle$)

- Recall that a particle's m quantum number concerns the z-component of its angular momentum

orbital angular momentum
and spin angular momentum

If the particle has no orbital angular momentum ($m_\ell = 0$)

Then $m = m_s$ only.

- Recall that the general operator that represents the measurement of m is J_z

like L_z but generalized to measure m_{spin} AND m_ℓ

So in general $J_z |\Psi\rangle = m\hbar |\Psi\rangle$

if $\ell = 0$, this is m_{spin}

Recall on (?) we showed that quantum # j (like ℓ but including spin) can take values given by $\dfrac{integer}{2}$

I. Spinors (continued)

II. The matrices and eigenspinors of S_x and S_y

Also $m_{J \, max} = +j$ and $m_{J \, min} = -j$

And $(m_{J \, max} - m_{J \, min}) = $ integer

The way to satisfy all of this for a 2-state system is for $j = \dfrac{1}{2}$

$m_{J \, max} = +\frac{1}{2}$

$m_{J \, min} = -\frac{1}{2}$

No othe m_J values allowed.

So if $\ell = 0$, so j = spin only then we have $\begin{cases} m_{spin \, max} = +\frac{1}{2} \\ m_{spin \, min} = -\frac{1}{2} \end{cases}$

Make a matrix to reflect $\underbrace{J_z}$ when j = spin only:

Call it "S_z"

$$\left\langle \Psi_f \left| S_z \right| \Psi_i \right\rangle = \left\langle \Psi_f \left| m_{spin} \hbar \right| \Psi_i \right\rangle = m_{spin} \hbar \left\langle \Psi_f \middle| \Psi_i \right\rangle = m_{spin} \hbar \delta_{if}$$

$$S_z = \begin{array}{c} \\ \langle + | \\ \langle - | \end{array} \begin{array}{cc} m_{spin \, final} & \\ |+\rangle & |-\rangle \end{array} \left(\begin{array}{cc} +\frac{1}{2}\hbar & 0 \\ 0 & -\frac{1}{2}\hbar \end{array} \right)$$

$m_{spin \, initial}$

δ_{if}

Recap what we know:

Dirac notation stuff

$|+\rangle$ and $|-\rangle$ exist

They are eigenfunctions of the spin measurement, S_z

Their eigenvalues are $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$

We can summarize this information as:

$S_z|+\rangle = \frac{\hbar}{2}|+\rangle$ and $S_z|-\rangle = -\frac{\hbar}{2}|-\rangle$

Matrix notation stuff

The matrix representation for S_z is $\begin{pmatrix} +\frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}$

What are the matrix representations for $|+\rangle$ and $|-\rangle$?

To answer this we need to solve

$$\begin{pmatrix} +\frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}\begin{pmatrix} u_+^z \\ v_+^z \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} u_+^z \\ v_+^z \end{pmatrix}$$

$\underset{S_z}{\uparrow}$ $\underset{|+\rangle}{\searrow\quad\nearrow}$

and

$$\begin{pmatrix} +\frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}\begin{pmatrix} u_-^z \\ v_-^z \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} u_-^z \\ v_-^z \end{pmatrix}$$

$\underset{S_z}{\uparrow}$ $\underset{|-\rangle}{\searrow\quad\nearrow}$

The solutions are

alternative symbol

$$|S, S_z\rangle = |+\tfrac{1}{2}, +\tfrac{1}{2}\rangle$$

$$|+\rangle = \begin{pmatrix} u_+^z \\ v_+^z \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \chi_+^{(z)}$$

eigenfunctions of $S_z = |+\tfrac{1}{2}, -\tfrac{1}{2}\rangle$

$$|-\rangle = \begin{pmatrix} u_-^z \\ v_-^z \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \chi_-^{(z)}$$

*Any 2 component vector is called a spinor

*These two-component column vectors which are the eigenfunctions of S_z in the $|m_s\rangle$ basis   — also called the S_z basis
are called the eigenfunctions of S_z

We could also write for example a matrix S_x to describe the measurement of the x-component of spin

That matrix would have different eigenfunctions χ_+^z and χ_+^z , the "eigenspinors of S_x "

Any pair of spinors:

(1) are orthogonal: $\langle \chi_+ | \chi_+ \rangle = 0$

(2) are normalized: $\langle \chi_+ | \chi_+ \rangle = \langle \chi_- | \chi_- \rangle = 1$

(3) form a basis in "spin space": any state of arbitrary spin χ can be represented by a linear combination of them

$$\chi = a\chi_+ + b\chi_-$$

coefficients

II. The matrices and eigenspinors of S_x and S_y

Recall in P 491 we *showed* that

$$[L_x, L_y] = i\hbar L_z \qquad \text{(and cyclic x} \to \text{y} \to \text{z)}$$

and we postulated that

$$[J_x, J_y] = i\hbar J_z \qquad \text{(and cyclic x} \to \text{y} \to \text{z)}$$

Now postulate that S_x, S_y, S_z are related in the same way:

$$\boxed{[S_x, S_y] = i\hbar S_z} \qquad \text{(and cyclic x} \to \text{y} \to \text{z)}$$

Also recall from P 491 the definition of the general angular momentum raising and lowering operators:

$$J_+ \equiv J_x + iJ_y$$

$$J_- \equiv J_x - iJ_y$$

Since these are general, they raise or lower both

orbital angular momentum and *spin* angular momentum

$$\underbrace{\qquad\qquad\qquad\qquad}_{L} \qquad \underbrace{\qquad\qquad\qquad\qquad}_{S}$$

When L=0, they act only on S, so we could call them in that case:

$$S_+ \equiv S_x + iS_y$$

$$S_- \equiv S_x - iS_y$$

To make the matrix for S_x (in the m_s or the S_z basis) we need the matrices for S_+ and S_- in the m_s basis:

Recall:

$$J_+ \left| j, m_j \right\rangle = \hbar \sqrt{j(j+1) - m_j(m_j+1)} \left| j, m_j + 1 \right\rangle \qquad\qquad J_- \left| j, m_j \right\rangle = \hbar \sqrt{j(j+1) - m_j(m_j-1)} \left| j, m_j - 1 \right\rangle$$

In general $j=\ell+s$ and $m_j = m_\ell + m_s$

Suppose $\ell = m_\ell = 0$

Then $j=s$ and $m_j = m_s$

Then

$$S_+ \left| s, m_s \right\rangle = \hbar \sqrt{s(s+1) - m_s(m_s+1)} \left| s, m_s + 1 \right\rangle \qquad\qquad S_- \left| s, m_s \right\rangle = \hbar \sqrt{s(s+1) - m_s(m_s-1)} \left| s, m_s - 1 \right\rangle$$

<div align="center">But $s = \frac{1}{2}$ only</div>

$$= \hbar \sqrt{\tfrac{1}{2}(\tfrac{3}{2}) - m_s(m_s+1)} \left| s, m_s + 1 \right\rangle \qquad\qquad = \hbar \sqrt{\tfrac{1}{2}(\tfrac{3}{2}) - m_s(m_s-1)} \left| s, m_s - 1 \right\rangle$$

So

$$\left\langle s, m_s' \right| S_+ \left| s, m_s \right\rangle = \hbar \sqrt{\tfrac{3}{4} - m_s(m_s+1)} \, \delta_{m_s', m_s+1} \qquad\qquad \left\langle s, m_s' \right| S_- \left| s, m_s \right\rangle = \hbar \sqrt{\tfrac{3}{4} - m_s(m_s-1)} \, \delta_{m_s', m_s-1}$$

Make the matrices:

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$$S_+ = \quad m_s': \quad \begin{array}{c} +\frac{1}{2} \\ -\frac{1}{2} \end{array} \begin{array}{cc} & \overset{m_s:}{} \quad +\frac{1}{2} \qquad\qquad -\frac{1}{2} \\ \begin{pmatrix} 0 & \hbar\sqrt{\frac{3}{4} - (-\frac{1}{2})(-\frac{1}{2}+1)} \\ 0 & 0 \end{pmatrix} \end{array}$$

$$S_- = \quad m_s': \quad \begin{array}{c} +\frac{1}{2} \\ -\frac{1}{2} \end{array} \begin{array}{cc} & \overset{m_s:}{} \quad +\frac{1}{2} \qquad\qquad -\frac{1}{2} \\ \begin{pmatrix} 0 & 0 \\ \hbar\sqrt{\frac{3}{4} - (\frac{1}{2})(\frac{1}{2}-1)} & 0 \end{pmatrix} \end{array}$$

$$= \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}$$

Combine these to get

$$S_x = \frac{S_+ + S_-}{2} = \frac{1}{2}\left[\begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}\right] = \frac{1}{2}\begin{pmatrix} 0 & \hbar \\ \hbar & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_y = \frac{S_+ - S_-}{2i} = \frac{1}{2i}\left[\begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}\right] = \frac{-i}{2}\begin{pmatrix} 0 & \hbar \\ -\hbar & 0 \end{pmatrix} = \frac{\hbar}{2i}\begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$$

Now find their eigenspinors

eigenvectors in the m_s basis

To find $\chi^x_\pm$ and their eigenvalues λ, solve

$$S_+\chi^x_\pm = \lambda_\pm\chi^x_\pm$$

$$\begin{pmatrix} 0 & \frac{\hbar}{2} \\ \frac{\hbar}{2} & 0 \end{pmatrix}\begin{pmatrix} u^x \\ v^x \end{pmatrix} = \lambda\begin{pmatrix} u^x \\ v^x \end{pmatrix}$$

$$\begin{pmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{pmatrix}\begin{pmatrix} u^x \\ v^x \end{pmatrix} = 0$$

$$\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = 0$$

$$\lambda^2 - \frac{\hbar^2}{4} = 0$$

$$\lambda = \pm\frac{\hbar}{2}$$

To get the eigenvectors (spinors) plug these λ back in:

$$\begin{pmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{pmatrix}\begin{pmatrix} u^x \\ v^x \end{pmatrix} = 0$$

Plug in $\lambda = +\frac{\hbar}{2}$ for (u^x_+, v^x_+)

$$-\frac{\hbar}{2}u^x_+ + \frac{\hbar}{2}v^x_+ = 0$$

$$u^x_+ = v^x_+$$

Normalized

$$\boxed{\begin{pmatrix} u^x_+ \\ v^x_+ \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \chi^x_+ \quad \text{this is the spinor that goes with eigenvalues } +\frac{\hbar}{2}}$$

Similarly,

$$\chi_-^x = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ +\frac{1}{\sqrt{2}} \end{pmatrix}$$
  this is the spinor that goes with $-\frac{\hbar}{2}$

We can similarly find eigenfunctions (spinors) of S_y :

$$\chi_+^y = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$
  for $\lambda = \frac{\hbar}{2}$

$$\chi_-^y = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix}$$
  for $\lambda = -\frac{\hbar}{2}$

Example:

Suppose an SG filter produces an e^- in state S_z = down.

Then the e^- enters another SG filter designed to select S_y = up or down.

What is the probability that the e^- will be found to have S_y = up?

Answer:

$$\langle \alpha | i \rangle = \chi_-^z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle \alpha | f \rangle = \chi_+^y = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

$$P = \left| \langle f | \alpha \rangle \langle \alpha | i \rangle \right|^2 = \left| \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{2}$$

complex conjugate

Read Chapter 16

I. The Pauli Matrices

II. The Transformation Matrix

III. The Pauli Matrices

Recall:

$$S_x = \begin{pmatrix} 0 & \frac{\hbar}{2} \\ \frac{\hbar}{2} & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \longleftarrow \quad "\sigma_x"$$

$$S_y = \begin{pmatrix} 0 & -\frac{i\hbar}{2} \\ +\frac{i\hbar}{2} & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} \longleftarrow "\sigma_y"$$

$$S_z = \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \longleftarrow \quad "\sigma_z"$$

These matrices (without $\frac{\hbar}{2}$'s) are called the Pauli matrices σ_i

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Facts about the Pauli matrices

1) The set of σ_x, σ_y, σ_z and $I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ form a *basis* for the space of 2x2 matrices

i.e. any 2x2 matrix can be expressed as a linear combination of σ_x, σ_y, σ_z and I

2) $\sigma_i^2 = 1$ i=1, 2, 3

3) $\sigma_x \sigma_y = i\sigma_z$ and cyclic x → y → z → x

4) $\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij}$ since there is a + instead of a -, we say they "anti-commute"

$$\{\sigma_i, \sigma_j\}$$

5) $\left[\sigma_x, \sigma_y \right] = 2i\sigma_z$ and cyclic x → y → z → x

6) They are Hermitian. This makes sense because

$$\sigma_i^\dagger = \sigma_i$$

$\sigma_i = $ (a real number)*S_i

S_i measures spin, a physical observable

Operators reflecting physical observables are always Hermitian.

So we have 3 separate matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Forget for a moment that those σ_i are matrices.

Focus on the symbols. They look like the components of a 3-D vector:

$$"\vec{\sigma}" = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}$$

We will use this vector. So for example if we have some other vector $\bar{v}$, then $\bar{v} \cdot \vec{\sigma} =$

$$v_x \sigma_x + v_y \sigma_y + v_z \sigma_z$$

$$= v_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + v_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + v_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & v_x \\ v_x & 0 \end{pmatrix} + \begin{pmatrix} 0 & -iv_y \\ iv_y & 0 \end{pmatrix} + v_z \begin{pmatrix} v_z & 0 \\ 0 & -v_z \end{pmatrix}$$

$$= \begin{pmatrix} v_z & v_x - iv_y \\ v_x + iv_y & -v_z \end{pmatrix}$$

I. The Transformation Matrix

Plan:

(i) Present plan of what calculation we need to learn how to do

(ii) Show why one might want to do it

(iii) Show how to do it

(iv) Examples

Carry out plan:

(i) Suppose a particle is prepared in a particular basis state, example it is prepared to have S_z = up.

But we actually want to know its S_y state

<div align="center">i.e. its probability of S_y = up and S_y = down</div>

So we need a translation dictionary that says

"If the state is S_z = _____ , it has Amplitude = _____ to be found in

state S_y = _____ (i.e. want the projection of one set of basis vectors onto another set.)

Table: all possible S_z states → ☐   ☐   ☐   ☐···

           all possible S_y states ☐

           ↓   ☐ $\begin{pmatrix} & \text{each element of this} \\ & \text{matrix is the amplitude} \\ & \text{that relates (projects) an} \\ & S_z \text{ state to an } S_y \text{ state} \end{pmatrix}$

               ☐

               ☐

This matrix is called the Transformation Matrix from the S_z basis to the S_y basis.

Call it $U_{S_z \to S_y}$

It's matrix elements look like

$$\langle S_y = f | S_z = i \rangle \qquad \text{where for example i = +, 0, - and f = +, 0, -}$$

So if you know all of the elements of the matrix between 2 bases, then if you know a particle's state in one basis, you can translate it into the other basis.

(ii) Why would you want to do that?

It is hard to see why if you consider just $|S_z\rangle$ and $|S_y\rangle$

Example of other possible bases: $|x\rangle$ (position)

or $|E\rangle$ (energy)

unlike the S_z basis,
which has 3 states for
a spin -1 particle, these
have ∞ # of states.
But they are *still* bases.

So you might want to know for example, $\langle x | E \rangle$

Recall how Dirac notation works:

$|E\rangle =$ a state with energy, E

$\langle x | E \rangle$ means project it from Hilbert

space into position space

so $\langle x | E \rangle = \Psi_E(x)$

So when we say we find the elements of a Transformation Matrix we are really finding the possible wavefunctions of a particle which is entirely specified by 2 of its properties

say (E and x) or (S_z and S_y)

(iii) How to construct $U_{S_z \to S_y}$

Recall what the S_z basis is:

It is the set of m $_s$ states which can be arranged to make the matrix representation of S_z diagonal

i.e. quantum # m +s $\leq$ m $\leq$ -s

like $+\ell < m_\ell < -\ell$

Recall that in the S_z basis,

the eigenspinors of S_z are $\chi_+^z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_-^z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

eigenfunctions   in S_z basis   in S_z basis

while the eigenspinors of operator S_y represented in the S_z basis are

$\chi_+^y = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$ and $\chi_-^y = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix}$

Recall that in the S_z basis, the S_y operator looks like

$S_y = \begin{pmatrix} 0 & -\frac{i\hbar}{\sqrt{2}} \\ \frac{i\hbar}{\sqrt{2}} & 0 \end{pmatrix}$ $\Rightarrow$ it is not diagonal

There must be some basis in which S_y is diagonal (i.e., we coudl diagonalize S_y)

Before we do that let's call that basis in which S_y would be diagonalized, "the S_y basis"

In the S$_y$ basis, S$_y$ would look like

$$\left|S_y = +\right\rangle \quad \left|S_y = -\right\rangle$$

$$S_y = \begin{matrix} \left|S_y = +\right\rangle \\ \left|S_y = +\right\rangle \end{matrix} \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & \frac{\hbar}{2} \end{pmatrix}$$

And *in the S$_y$ basis*, the eigenspinors of S$_y$ would look like

$$\chi_+^y = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi_-^y = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$\uparrow$ $\uparrow$

in S$_y$ basis   in S$_y$ basis

We need a translation U which simultaneously guarantees

Name of eigen spinor   Representation in S$_y$ basis   =   U ·   Representation in S$_z$ basis

$$\chi_+^y \quad\quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad = \quad U \cdot \quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix}$$

AND

$$\chi_-^y \quad\quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad = \quad U \cdot \quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix}$$

The U that satisfies both is

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}$$

The recipe to make a U that translates from some arbitrary basis to an operator's "home" basis is this:

here S$_z$ here S$_y$

1) Because the operator is diagonal in its home basis (that is the definition of a home basis), its eigenvectors in that basis will always look like

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \ldots \ldots \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \text{ etc.}$$

2) Find its eigenvectors in the basis that you want to translate *out* of

Suppose they are

$$\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$$

↑ where this has the lowest eigenvalue

↑ this has the next lowest

↑ this has the highest eigenvalue

3) Take the Hermitian conjugate of each

HC=transpose complex conjugate

$(a_1^* \ a_2^* \ \ldots \ a_n^*) \quad (b_1^* \ b_2^* \ \ldots \ b_n^*) \quad (c_1^* \ c_2^* \ \ldots \ c_n^*)$

4) arrange the HC eigenvectors in rows in order of decreasing eigenvalues

$$U = \begin{pmatrix} c_1^* & c_2^* & \ldots & c_n^* \\ b_1^* & b_2^* & \ldots & b_n^* \\ a_1^* & a_2^* & \ldots & a_n^* \end{pmatrix}$$

So to summarize:

$$U_{S_z \to S_y} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}$$

we could have done a similar calculation for

$$U_{S_z \to S_x} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

save these for later

I. The Transformation Matrix is unitary

II. Why we diagonalize matrices in QM

III. Writing the Hamiltonian operator as a matrix

II. The Transformation Matrix U is unitary

U has the important feature that $U^{-1} = U^{\dagger}$

To see this:

Recall that the inverse M^{-1} of any matrix M must have the property that $M^{-1}M=1$.

For any matrix M,

$$M^{-1} = \frac{1}{\det M}\tilde{C}$$

transpose of the matrix of cofactors of M

Example: Suppose

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

Then $\det M = ad-bc$

$C_{ij} = (-1)^{i+j} \cdot \det(\text{submatrix obtained by deleting row i and column j from M})$

$$C = \begin{pmatrix} d & (-1)c \\ (-1)b & a \end{pmatrix}$$

$$\tilde{C} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

So $M^{-1} = \dfrac{1}{(ad-bc)}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

Also recall $M^{\dagger} = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}$

Plug in the specific transformation matrix $U_{S_z \to S_y}$ for M:

$$U_{S_z \to S_y} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}$$

$$U^{-1} = \frac{1}{\left(\frac{1}{\sqrt{2}}\frac{i}{\sqrt{2}} - \left(\frac{-i}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\right)\right)} \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$= -i \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix}$$

Also

$$U^{\dagger} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}^{*} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix}$$

So $U^{-1} = U^{\dagger}$

What is the *physical* importance of being unitary?

1) Recall that applying U to each element of a basis $|\alpha\rangle$ projects it onto another basis $|\beta\rangle$

For any element of basis $|\beta\rangle$:

$$|\beta\rangle = 1 \cdot |\beta\rangle$$

$$\text{Insert } 1 = \sum_{\alpha} |\alpha\rangle\langle\alpha|$$

$$= \sum_{\alpha} |\alpha\rangle\langle\alpha|\beta\rangle$$

$$\langle\beta|\alpha\rangle^{*} = U_{\beta\alpha}^{*}$$

$$|\beta\rangle = \sum_{\alpha} |\alpha\rangle U_{\beta\alpha}^{*}$$

Take the complex conjugate of this equation:

$$\langle\beta| = \sum_{\alpha} U_{\beta\alpha}^{*} \langle\alpha|$$

Now consider some arbitrary state $|\Psi\rangle$

Project it onto the new basis $\langle\beta|$

It will have components in that basis given by

$$\Psi'_{\beta} = \langle\beta|\Psi\rangle$$
$$= \sum_{\alpha} \langle\beta|\alpha\rangle\underbrace{\langle\alpha|\Psi\rangle}$$
$$= \sum_{\alpha} U_{\beta\alpha} \Psi_{\alpha}$$

these are the components of Ψ in the "old" basis $\alpha \rightarrow \Psi_{\alpha}$
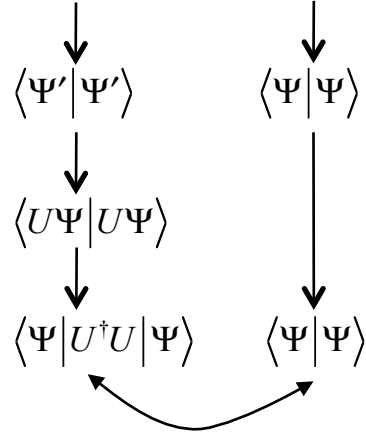
These subscripts concern individual components of the state. Generalize to the full state

$$\Psi' = U\Psi$$

Recall that changing basis is like changing coordinate systems. The length of a vector Ψ should not depend on which coordinate system is is measured in.

So we expect

length of $\Psi' =$ length of Ψ

$$\langle \Psi' | \Psi' \rangle \qquad \langle \Psi | \Psi \rangle$$

But $|\Psi'\rangle = U|\Psi\rangle$

$$\langle U\Psi | U\Psi \rangle$$

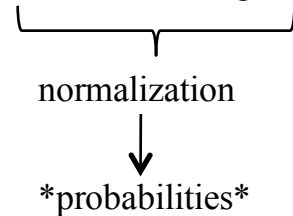$$\langle \Psi | U^\dagger U | \Psi \rangle \qquad \langle \Psi | \Psi \rangle$$

These can only be equal if $U^\dagger U = 1$

But $U^{-1} U = 1$ by definition of U^{-1}

So these can only be equal if $U^\dagger = U^{-1}$

Fortunately $U^\dagger$ does $= U^{-1}$

So unitarity transformation preserves state vector lengths

normalization

probabilities

under change of basis.

This is important because probabilities are what is actually measured, and they cannot depend on choice of basis.
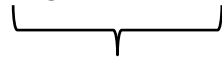
III. Why do we diagonalize matrices in QM

Suppose we are working in some basis (Ex: the S_z basis)

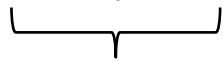We have an operator that is not diagonalized in this basis

(Ex: the S_y basis)

We find $U_{S_z \to S_y}$ that relates the form of the eigeinvectors of the operator

Example: χ_+^y and χ_-^y

in the arbitrary basis to these in the home basis

S_z basis S_y basis

Thus far we have considered only the effect of U on the χ's.

Now consider the effect of U on the operator itself:

$$US_y U^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{-i\hbar}{2} \\ \frac{-i\hbar}{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & \frac{-\hbar}{2} \end{pmatrix}$$

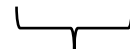*Applying U, U^{-1} to the non-diagonal operator diagonalizes it.

Who cares?

The goal of many QM calculations is to answer "What are the possible results (=eigenvalues) I could get if Imake a particular measurement?"

(i) When an operator is in non-diagonalized form, every vector that it operates on gets changed into a different vector. So you learn from this what changes this operator (Ex L_+) can cause in nature.

(ii) If you want to find what are the stationary states of an operator, the states of definite energy, the states that can appear as possible results of measurements, then you need the eigenvectors and eigenvalues of the operator.

(iii) A diagonal form of the operator is the only form that leads to an eigenvalue equation. The U matrix converts an aperator into a diagonal form.

(iv) As a bonus, the U gives the amplitude for observation of every possible physical state which can be found by that measurement (Ex: S_y) given the initial prepared state.

in S_z

I. Writing the Hamiltonian operator as a matrix

Recall the time-dependent Schrodinger Equation:

$$i\hbar \frac{\partial}{\partial t}\Psi = H\Psi$$

Consider situation where

(i) Ψ is not just a scalar but is an object that can be axpanded in a basis. So

$$\Psi \to |\Psi\rangle$$

(ii) We are interested only in the time-development of Ψ. So

$$\frac{\partial}{\partial t} \to \frac{d}{dt}$$

$$i\hbar \frac{d}{dt}\Psi = H\Psi$$

Recall it is difficult to work on $|\Psi\rangle$ as a Hilbert space object, so project

into some (unspecified) basis $\langle j|$

$$\left\langle j \left| i\hbar \frac{d}{dt} \right| \Psi \right\rangle = \left\langle j | H | \Psi \right\rangle$$

Insert $1 = \sum_i |i\rangle\langle i|$

$$i\hbar \frac{d}{dt}\langle j|\Psi\rangle = \sum_i \langle j|H|i\rangle\langle i|\Psi\rangle$$

similarly this is c_i

call this c_j, the amplitude that Ψ is in state j

H_{ji}, element of the H matrix

Reunite:

$$i\hbar \frac{d}{dt} c_j = \sum_i H_{ji} c_i$$

This equation is true for a $|\Psi\rangle$ with any number of components

i.e any number of possible states what a measurement could find it to be in.

Consider a $|\Psi\rangle$ which can only ever be in 2 states

then i:(1,2)

j:(1,2)

So this represents 2 equations

When j=   the equation reads:

1

$$i\hbar \frac{d}{dt} c_1 = H_{11} c_1 + H_{12} c_2$$

2

$$i\hbar \frac{d}{dt} c_2 = H_{21} c_1 + H_{22} c_2$$

an alternative form of this is:

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$
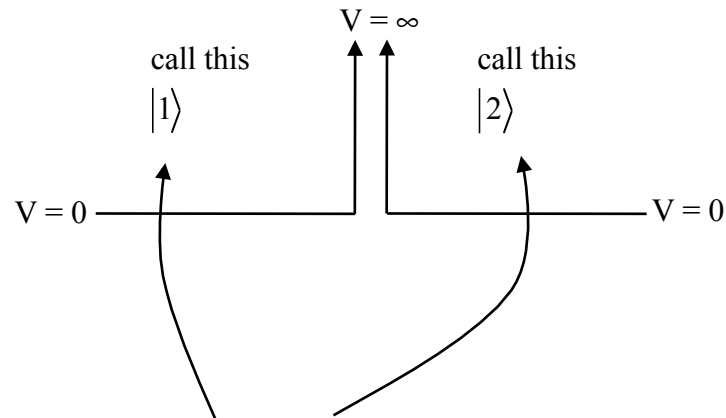
I. The meaning of diagonal and non-diagonal matrices

II. The ammonia molecule

Read handout on NMR

II. The meaning of diagonal and non-diagonal matrices

Consider a potential in which 2 states are theoretically possible

$$V = \infty$$

call this $|1\rangle$ call this $|2\rangle$

$V = 0$ ——————————— $V = 0$

Ψ could be here or here but because the barrier is ∞, Ψ can never tunnel from one state to the other.

Recall we showed in Section 6.4 that when the Hamiltonian acts on a state, it evolves the state forward in time.

If the particle can never tunnel from $|1\rangle \rightarrow |2\rangle$ or $|2\rangle \rightarrow |1\rangle$

Then $H|1\rangle = $ [possibly some constant]$|1\rangle$

and $H|2\rangle = [\quad]|2\rangle$

but $H|1\rangle = 0 \cdot |2\rangle$

and $H|2\rangle = 0 \cdot |1\rangle$

Another way to express this is

initial states $\rightarrow$ $|1\rangle$ $|2\rangle$

final states $\downarrow$

$$H= \begin{array}{c} |1\rangle \\ |2\rangle \end{array} \begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} \end{pmatrix}$$

Now recall from Chapter 3 that $H\Psi=E\Psi$, so the [possible some constant] $= E_0$

Since the $|1\rangle$ and $|2\rangle$ are both in regions where V=0, expect both to have same energy, so

$$H = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}$$

Now suppose that the barrier is not infinitely high, so there is some probability that as time passes that a state in $|1\rangle \rightarrow |2\rangle$ or a state in $|2\rangle \rightarrow |1\rangle$

as the H acts

Suppose that after a certain length of time, the probability that $|1\rangle \rightarrow |2\rangle$ is A^2

Let the amplitude $= \sqrt{A^2} = -A$

Similarly for $|2\rangle \rightarrow |1\rangle$

Now

$$H = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

II. The Ammonia molecule

An example of a physical case where 2 states are related by $\begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$ is the 2 physical states

of the NH_3 molecule.

The 3 H's make a triangle which has repulsive potential

Coulomb repulsion up

and down
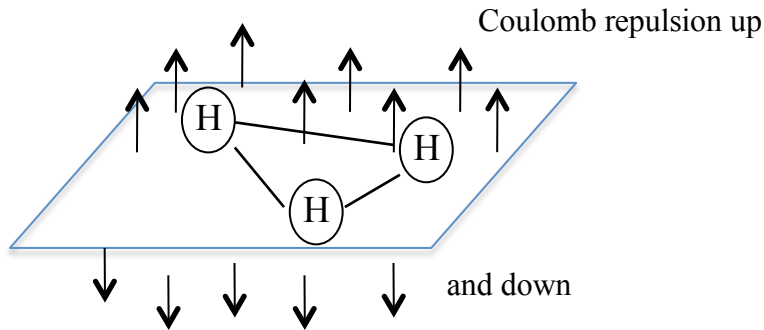
If the N is above, it sees a coulombic barrier that prevents it from moving below.

If it is below, it is barricaded from moving up.

So there are 2 states

call this $|1\rangle$

and

call this $|2\rangle$
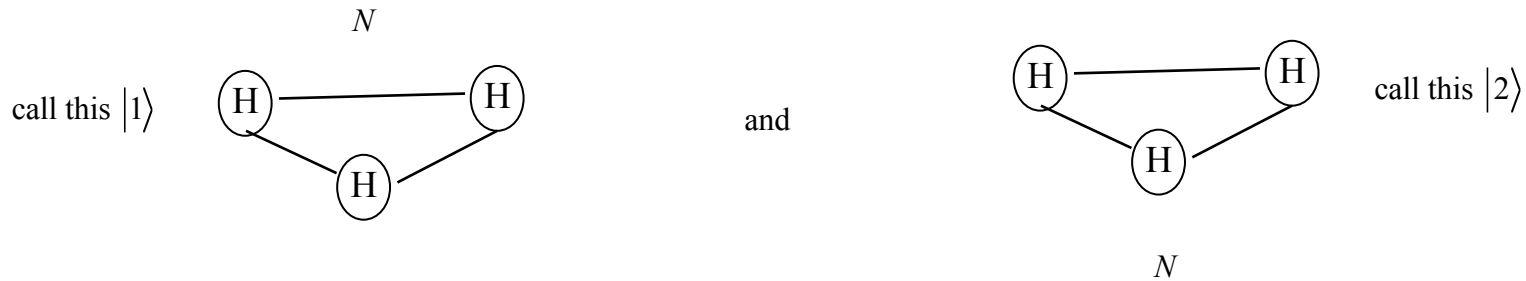
But the Coulomb potential is not ∞ so there is some amplitude for the N to tunnel from above to below.

call it -A

Compare:

effect of a diagonal H

$$H = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

Time-dependent Schrodinger Equation:

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$i\hbar \frac{d}{dt} c_1 = E_1 c_1 \quad \text{and} \quad i\hbar \frac{d}{dt} c_2 = E_1 c_2$$

$$c_1 = A e^{-iE_1 t / \hbar} \qquad c_2 = B e^{-iE_2 t / \hbar}$$

Notice about this:

We can write $|\Psi\rangle$ as an expansion (or linear combination)

in the basis:

$$|\Psi\rangle = |1\rangle\langle 1|\Psi\rangle + |2\rangle\langle 2|\Psi\rangle$$
$$= |1\rangle c_1 + |2\rangle c_2$$
$$= A e^{-iE_1 t / \hbar} |1\rangle + B e^{-iE_2 t / \hbar} |2\rangle$$

So $|1\rangle$ is a stationary state with energy E_1 and

$|2\rangle$ energy E_2

and c_1 and c_2 are the amplitude for finding $|\Psi\rangle$ in

"stationary state" means a measurement of the energy
and state of this system will always find one or the
other, but no combination or other option.

effect of a non-diagonal H:

$$H = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

To find the stationary states we have
to diagonalize this

$$\begin{vmatrix} E_0 - \lambda & -A \\ -A & E_0 - \lambda \end{vmatrix} = 0$$

$$\downarrow$$

$$\lambda_I = E_0 + A \equiv "E_I"$$
$$\lambda_{II} = E_0 - A \equiv "E_{II}"$$

We need to find the eigenvectors (basis vectors)

$|I\rangle$ that goes with λ_I

$|II\rangle$ that goes with λ_{II}

To visualize them, let us write $|I\rangle\ |II\rangle$ as linear combinations of $|1\rangle$ and $|2\rangle$

N above H's   N below H's
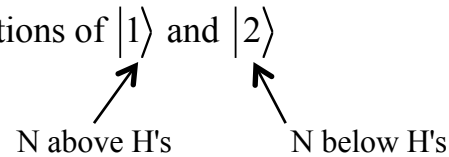
i.e. we want

$$|I\rangle = \sum_i |i\rangle\langle i|I\rangle$$

$$= |1\rangle\langle 1|I\rangle + |2\rangle\langle 2|I\rangle$$

$$= |1\rangle\langle I|1\rangle^* + |2\rangle\langle I|2\rangle^*$$
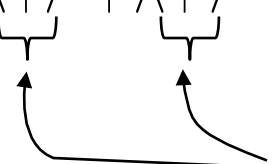
but $\langle I|1\rangle$ and $\langle I|2\rangle$ are matrix elements of the transformation matrix

that transforms H from non-diagonalized form to diagonal form

which has eigenvectors   which has eigenvectors

$|1\rangle,\ |2\rangle$ $|I\rangle,\ |II\rangle$

So we need to find U

To find U,

Recall $H = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$

*Every 2x2 matrix can be written as a linear combination of the Pauli matrices and the identity matrix:

$= E_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - A \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = E_0 \mathbf{1} - A\sigma_x$

So to diagonalize H we just need to diagonalize σ_x

But $\sigma_x = \frac{2}{\hbar} S_x$

So to diagonalize H we just need to diagonalize S_x

The U that diagonalizes S_x is $U_{S_z \to S_x}$ (see notes from last lecture)

$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$ ← eigenvector corresponds to S_x eigenvalue $= +\frac{\hbar}{2}$ (or σ_x eigenvalue +1)

← eigenvector corresponds to S_x eigenvalue $= -\frac{\hbar}{2}$ (or σ_x eigenvalue -1)

(Remember to arrange eigenvectors in order of decreasing eigenvalue)

Now the eigenvalues of H are $\begin{cases} E_0 + A \\ E_0 - A \end{cases}$

Now the eigenvalues of 1 are $\begin{cases} 1 \\ 1 \end{cases}$

Now the eigenvalues of σ_x are $\begin{cases} +1 \\ -1 \end{cases}$

So to create the U that diagonalizes H, order the eigenvectors from

Row 1 high eigenvalue $E_0 + A$ $E_0(1) + A(-1)$ eigenvector of σ_x corresponds to -1

↓

Row 2 low eigenvalue $E_0 - A$ $E_0(1) - A(-1)$ eigenvector of σ_x corresponds to +1

I. The ammonia molecule (continued)

II. Ammonia oscillation frequency

Reach Chapter 18

Feynman pages 8-10 to 9-5

So

$$U = \begin{array}{c} \\ |\text{I}\rangle \\ |\text{II}\rangle \end{array} \begin{array}{cc} |1\rangle & |2\rangle \\ \left(\begin{array}{cc} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{array} \right) \end{array}$$

Now we have

$$\langle \text{I} | 1 \rangle = \frac{-1}{\sqrt{2}} = \langle \text{I} | 1 \rangle^*$$

$$\langle \text{I} | 2 \rangle = \frac{+1}{\sqrt{2}} = \langle \text{I} | 2 \rangle^*$$

So $|\text{I}\rangle = |1\rangle\langle 1|\text{I}\rangle + |2\rangle\langle 2|\text{I}\rangle$

$$= |1\rangle\langle 1|\text{I}\rangle^* + |2\rangle\langle 2|\text{I}\rangle^*$$

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

$$\boxed{|\text{I}\rangle = \frac{1}{\sqrt{2}}\left(-|1\rangle + |2\rangle\right)}$$

We could do a similar calculation to find that

$$\boxed{|\text{II}\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right)}$$

Interim conclusion #1: If H is expanded in the basis $|1\rangle$, $|2\rangle$ it *is not* diagonal. But if it is expanded in the basis $|\text{I}\rangle$, $|\text{II}\rangle$ it *is* diagonal.

So we can write:

$$\begin{array}{cc} & |\mathrm{I}\rangle \qquad |\mathrm{II}\rangle \end{array}$$

$$H = \begin{array}{c} |\mathrm{I}\rangle \\ |\mathrm{II}\rangle \end{array} \begin{pmatrix} E_0 + A & 0 \\ 0 & E_0 - A \end{pmatrix}$$

Now we have the basis in which H is diagonal.

Now solve the Schrodinger Equation in this basis.

Recall in general the Schrodinger Equation can be written as
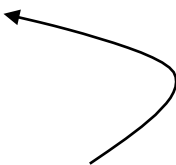
$$i\hbar \frac{d}{dt}|\Psi\rangle = H\Psi$$

$$\downarrow \qquad \text{apply } \langle j|$$

$$i\hbar \frac{d}{dt}\underbrace{\langle j|\Psi\rangle}_{c_j} = \langle j|H|\Psi\rangle = \sum_i \underbrace{\langle j|H|i\rangle}_{H_{ji}}\underbrace{\langle i|\Psi\rangle}_{c_i}$$

$$i\hbar \frac{d}{dt}c_j = \sum_i H_{ji}c_i$$

For 2-D, this is:

$$\left\{ \begin{array}{l} i\hbar \dfrac{d}{dt}c_1 = H_{11}c_1 + H_{12}\cancel{c_2}^{\,0} \\[2mm] i\hbar \dfrac{d}{dt}c_2 = H_{21}\cancel{c_1}^{\,0} + H_{22}c_2 \end{array} \right.$$

In the $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$ basis, $H_{12} = H_{21} = 0$ and

$$H_{11} = E_0 + A$$

$$H_{22} = E_0 - A$$

Since we are in the $|I\rangle$, $|II\rangle$ basis, call

$$c_1 \to c_I \equiv \langle I|\Psi\rangle$$

$$c_2 \to c_{II} \equiv \langle II|\Psi\rangle$$

Then we have

$$\left\{ \begin{array}{ll} i\hbar\dfrac{d}{dt}c_I = (E_0 + A)c_I & \to c_I = C\exp\left[-i(E_0+A)t/\hbar\right]|I\rangle \\[3mm] i\hbar\dfrac{d}{dt}c_{II} = (E_0 - A)c_{II} & \to c_{II} = D\exp\left[-i(E_0-A)t/\hbar\right]|II\rangle \end{array} \right.$$

$|\Psi\rangle$ can be expanded in any basis that spars its space:

$$|\Psi\rangle = \sum_i |i\rangle\langle i|\Psi\rangle$$

In particular

$$= |I\rangle\langle I|\Psi\rangle + |II\rangle\langle II|\Psi\rangle$$

$$= \underbrace{C\exp\left[-i(E_0+A)t/\hbar\right]|I\rangle}_{|\Psi_I\rangle} + \underbrace{D\exp\left[-i(E_0-A)t/\hbar\right]|II\rangle}_{|\Psi_{II}\rangle}$$

So the stationary states of this system are

$|\Psi_I\rangle$ which has $E = E_0 + A$ $\Big\}$ *these are the only 2 possible results of a measurement on this system.

$|\Psi_{II}\rangle$ which has $E = E_0 - A$ You would never measure just E_0, or some linear combination of $|\Psi_I\rangle + |\Psi_{II}\rangle$

I. Ammonia oscillation frequency

II. MRI

Read Chapter 17

I. Ammonia Oscillation Frequency

Recall that physically the ammonia molecule can be in either of 2 states, and can tunnel through a barrier to get from one to the other. Because it can switch between them, those are NOT the stationary states. However, they are real physical states.

Calculate the Frequency with which the molecule changes state from $|1\rangle$ to $|2\rangle$:

$\downarrow$

frequency at which the N tunnels back and forth

This will help clarify the meaning of different basis we have used

Recall the two basis we have worked in for this problem:

Basis $|1\rangle$, $|2\rangle$

correspondes to *physical* states

N

$|1\rangle = \triangle$

$|2\rangle = \triangledown$

N
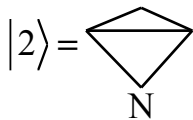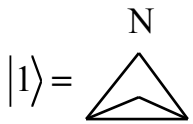
In this basis,

$H = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$

Basis $|I\rangle$, $|II\rangle$

correspondes to stationary states with unchanging energies

$|I\rangle$: state with $E = E_0 + A$

$|II\rangle$: state with $E = E_0 - A$

In this basis,

$H = \begin{pmatrix} E_0 + A & 0 \\ 0 & E_0 - A \end{pmatrix}$

Define time-dependent Schrodinger Equations:

$c_1 = \langle 1 | \Psi \rangle$ and $c_2 = \langle 2 | \Psi \rangle$

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$\downarrow$

$$\left\{ \begin{array}{l} i\hbar \dfrac{d}{dt} c_1 = E_0 c_1 - A c_2 \\[3mm] i\hbar \dfrac{d}{dt} c_2 = -A c_1 - E_0 c_2 \end{array} \right\} \text{coupled eq.} \rightarrow \text{transitions}$$

"Eq 1"
"Eq 2"

We never solved for c_1, c_2

The basis in which H is nondiagonal gives information about transitions between states

Because we want to study transitions (i.e. tunnelling frequency) we will work in this basis.
So we need to find c_1, c_2
To find c_1, c_2 first
(i) Add Eq 1 and Eq 2

$$i\hbar \frac{d}{dt}(c_1 + c_2) = (E_0 - A)(c_1 + c_2)$$

$$(c_1 + c_2) = a e^{\frac{-i}{\hbar}(E_0 - A)t} \qquad \text{"Eq 3"}$$

$\qquad \qquad \hookleftarrow$ unspecified normalization

$c_I = \langle I | \Psi \rangle$ and $c_{II} = \langle II | \Psi \rangle$

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_I \\ c_{II} \end{pmatrix} = \begin{pmatrix} E_0 + A & 0 \\ 0 & E_0 - A \end{pmatrix}\begin{pmatrix} c_I \\ c_{II} \end{pmatrix}$$

$\downarrow$

$$\left\{ \begin{array}{l} i\hbar \dfrac{d}{dt} c_I = (E_0 + A) c_I \\[3mm] i\hbar \dfrac{d}{dt} c_{II} = (E_0 - A) c_{II} \end{array} \right\} \text{uncoupled eq.} \rightarrow \text{no transitions}$$

We solved for c_I, c_{II} : we get

$$c_I = C \exp\left[{-i(E_0 + A)t}/{\hbar} \right]$$

$$c_{II} = D \exp\left[{-i(E_0 - A)t}/{\hbar} \right]$$

Notice the basis which makes H diagonal yields the energies (eigenvalues) which are possible results of measurements.

(ii) subtract Eq 1 - Eq 2

$$i\hbar \frac{d}{dt}(c_1 - c_2) = (E_0 + A)(c_1 - c_2)$$

$$c_1 - c_2 = be^{\frac{-i}{\hbar}(E_0 + A)t} \qquad \text{"Eq 4"}$$

—unspecified normalization

(iii) Solve Eq 3 and Eq 4 simultaneously to get

$$c_1(t) = \frac{a}{2}e^{\frac{-i}{\hbar}(E_0 - A)t} + \frac{b}{2}e^{\frac{-i}{\hbar}(E_0 + A)t}$$

$$c_2(t) = \frac{a}{2}e^{\frac{-i}{\hbar}(E_0 - A)t} - \frac{b}{2}e^{\frac{-i}{\hbar}(E_0 + A)t}$$

Question: Suppose at t=0 the molecule is in state $|1\rangle$. What is the probability that it will be found in $|2\rangle$ at t=t′ ?

Answer:

starting condition:

$$c_1(0) = \langle 1 | \Psi(t=0)\rangle = 1 \quad \text{AND} \quad c_2(0) = \langle 2 | \Psi(t=0)\rangle = 0$$

$$\frac{a}{2} + \frac{b}{2} = 1 \qquad\qquad\qquad \frac{a}{2} - \frac{b}{2} = 0$$

a=b=1

Plug in a, b into c_1, c_2 :

$$c_1(t) = \frac{1}{2} e^{\frac{-i}{\hbar}(E_0 - A)t} + \frac{1}{2} e^{\frac{-i}{\hbar}(E_0 + A)t} = e^{\frac{-i}{\hbar}(E_0)t} \cos\left(\frac{At}{\hbar}\right)$$

$$c_1(t) = \frac{1}{2} e^{\frac{-i}{\hbar}(E_0 - A)t} - \frac{1}{2} e^{\frac{-i}{\hbar}(E_0 + A)t} = i e^{\frac{-i}{\hbar}(E_0)t} \sin\left(\frac{At}{\hbar}\right)$$

So the probability that the system is in $|2\rangle$ at t=t′ is

$$\left|\langle 2|\Psi(t')\rangle\right|^2$$

$$\left|c_2(t')\right|^2 = \left|i e^{\frac{-i}{\hbar}(E_0)t} \sin\left(\frac{At'}{\hbar}\right)\right|^2 = \boxed{\sin^2\left(\frac{At'}{\hbar}\right)}$$

II. NMR = MRI

This is another example of a 2-state system

Consider a particle with charge q, mass m, and magnetic moment $\vec{M}$ in a magnetic field $\vec{B}$.

Recall from classical E&M that it develops potential energy $E = -\vec{M} \cdot \vec{B}$

Guess that the QM Hamiltonian for this process looks similar so

$H = -\vec{M} \cdot \vec{B}$

Recall from Chapter 13 that $\vec{M}$ is related to angular momentum

$$\vec{M} = \frac{qg\vec{L}}{2mc}$$

generalize this from $\vec{L}$ to $\vec{S}$

$$\vec{M}_{\substack{\text{due to spin} \\ \text{when L=0}}} = \frac{qg\vec{S}}{2mc}$$

the gyromagnetic ratio g, depends on the particle involved and whether
the angular momentum is due to $\vec{L}$ or $\vec{S}$.

For NMR, the particle is the proton and the angular momentum is $\vec{S}$.

In that case, $g = g_p = 5.6$ also $q = +e$ and $m = m_p$

So $H = -\vec{M} \cdot \vec{B} = \dfrac{-eg_p \vec{S} \cdot \vec{B}}{2m_p c}$

Recall the spin operator $\vec{S}$ is related to the composite vector $\vec{\sigma}$ made

I. MRI (continued)

II. The medical application of MRI

III. Time Independent Perturbation Theory

Read Chapter 22, Sections 1,2,6 only

from the Pauli matrices, so

$$\bar{S} = \frac{\hbar}{2} \bar{\sigma}$$

Then $\bar{H} = \dfrac{-eg}{2mc} \dfrac{\hbar}{2} \bar{\sigma} \cdot \bar{B}$ $\qquad \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$

call this μ_p

If $\bar{B}$ is purely $B_z \hat{z}$, then $\bar{\sigma} \cdot \bar{B} = \sigma_z B_z$ only

$$= \sigma_z |B|$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} B$$

Then H would $= -\mu_p B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$= \begin{array}{c} \\ \\ \end{array} \begin{array}{cc} |s_z = +\rangle & |s_z = -\rangle \end{array}$$

$$= \begin{array}{c} |s_z = +\rangle \\ |s_z = -\rangle \end{array} \begin{pmatrix} -\mu_p B & 0 \\ 0 & +\mu_p B \end{pmatrix}$$

The diagonal form would mean that the presence of the $\bar{B}$ would not change the state of the p's spin.

the effect of H on the initial state of p

There are no matrix elements that convert $|-\rangle \rightarrow |+\rangle$ or $|+\rangle \rightarrow |-\rangle$

Now suppose we add another component to $\bar{B}$

Let $\bar{B} = B_x \hat{x} + B_z \hat{z}$

$B_x = B_1 \cos \omega t$ $\qquad$ still constant, call it B_0. It has no time dependence.

$B_1 = (e^{i\omega t} + e^{-i\omega t})/2$

Then $\vec{\sigma} \cdot \vec{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$

$$\frac{B_1\left(e^{i\omega t} + e^{-i\omega t}\right)}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad B_0\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$H = -\mu_p \vec{\sigma} \cdot \vec{B} = \begin{pmatrix} -\mu_p B_0 & \dfrac{-\mu_p B_1\left(e^{i\omega t} + e^{-i\omega t}\right)}{2} \\ \dfrac{-\mu_p B_1\left(e^{i\omega t} + e^{-i\omega t}\right)}{2} & +\mu_p B_0 \end{pmatrix}$$

Now there is a possibility for the proton to flip its spin between $|+\rangle$ and $|-\rangle$ in response to $\vec{B}$.

If we define $E_0 \equiv -\mu_p B_0$

and $\qquad A \equiv \dfrac{\mu_p B_1\left(e^{i\omega t} + e^{-i\omega t}\right)}{2}$

Then $H = \begin{pmatrix} E_0 & -A \\ -A & -E_0 \end{pmatrix}$

So we could do calculations identical to the ones we did for the ammonia 2-state system, assume that the protons begin with spin up, then find the probability of finding spin down at t=t′.

For real MRI, the B field is usually a little more complicated.

Still have $\qquad B_z = B_0$

and $\qquad \boxed{B_x = B_1 \cos \omega t}$ $\qquad \leftarrow$ so the B field rotates in the x-y plane

but we also have $\boxed{B_y = -B_1 \sin \omega t}$

So $H_{MRI} = -\mu_p \sigma \cdot \vec{B}$

$= -\mu_p (\sigma_x B_x + \sigma_y B_y + \sigma_z B_z)$

$= -\mu_p \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} B_x + \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} B_y + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} B_z \right]$

$= -\mu_p \begin{bmatrix} B_0 & (B_1 \cos \omega t + i B_1 \sin \omega t) \\ (B_1 \cos \omega t - i B_1 \sin \omega t) & -B_0 \end{bmatrix}$

want to solve

$-i\hbar \dfrac{d}{dt} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = H \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

Solve 2 equations silmutaneously $c_1 =$ ....

$$c_2 = \text{..........}$$

Now assume that at t=0 $c_1 = \langle 1 | \Psi \rangle = 1$ and $c_2 = \langle 2 | \Psi \rangle = 0$

This gives normalization so you get

$c_1(t) =$ ....

$$c_2(t) = \frac{\dfrac{i \mu_p B_1}{\hbar}}{\left[\left(\dfrac{\mu_p B_0}{\hbar} - \dfrac{\omega}{2} \right)^2 + \dfrac{\mu_p^2 B_1^2}{\hbar^2} \right]^{\frac{1}{2}}} \cdot \sin \left\{ \left[\left(\dfrac{\mu_p B_0}{\hbar} - \dfrac{\omega}{2} \right)^2 + \dfrac{\mu_p^2 B_1^2}{\hbar^2} \right]^{\frac{1}{2}} t \right\} e^{-i\frac{\omega}{2} t}$$

At any time t=t′, the probability that a spin has flipped from + to - is

$\left| c_2(t') \right|^2 =$

I. The medical application of MRI

II. Time-Independent Perturbation Theory

$$|c_2(t)|^2 = \frac{\dfrac{\mu_p^2 B_1^2}{\hbar^2}}{\left[\left(\dfrac{\mu_p B_0}{\hbar} - \dfrac{\omega}{2}\right)^2 + \dfrac{\mu_p^2 B_1^2}{\hbar^2}\right]} \cdot \sin^2\left\{\left[\left(\dfrac{\mu_p B_0}{\hbar} - \dfrac{\omega}{2}\right)^2 + \dfrac{\mu_p^2 B_1^2}{\hbar^2}\right]^{\frac{1}{2}} t\right\}$$

when $\omega = \dfrac{2\mu_p B_0}{\hbar}$, the denominator is minimized so the probability of spin flip is maximal.

This is a *magentic resonance.*

How to use this for medical imaging

I. The medical purpose of MRI is to distinguish normal from non-normal tissue. How this works:

(i) When $B_0(\hat{z})$ is turned on but $B_1(xy)$ is off, then

$|S_z = +\rangle$ is a *lower* energy state $\qquad (H_{11} = -\mu_p B_0)$

$|S_z = -\rangle \qquad\qquad\qquad\qquad\qquad (H_{22} = +\mu_p B_0)$

So most protons are in the $|S_z = +\rangle$ state. If $N_0 =$ total # protons

$$\frac{\text{# protons in } |S_z = +\rangle}{\text{# protons in } |S_z = -\rangle} = \frac{N_0 \exp\left(-E_+/kT\right)}{N_0 \exp\left(-E_-/kT\right)} = \frac{\exp\left(-\left(-\mu_p B_0\right)/kT\right)}{\exp\left(-\left(+\mu_p B_0\right)/kT\right)} = \exp\left(2\mu_p B_0/kT\right)$$

(ii) Turn on B_1 $\rightarrow$ most spins flip from $|+\rangle$ to $|-\rangle$

(iii) Turn off B_1

the spins in normal tissue relax to $|+\rangle$ at a different rate than do the spins in abnormal tissue.

Measure relaxation rate by placing a coil near the tissue (but outside the body) and measure $\sum_i \vec{M}_i$ by the current induced in the coil.

I. Intro to addition of angular momentum

II. Example method for Clebsch-Gordan coefficient construction

Read Chapter 8 Section 2 (WKB approximation)

I. Intro to Addition of Angular Momentum

A) Why total angular momentum is important in QM:

• Most physical systems actually have > angular momentum contributor

Example: e^- in Hydrogen has $\bar{L}$ and $\bar{S}$

       multi-atom system has multiple $J_i\text{'}s$

• only the total J for the system is conserved (ie $\langle \Psi | J | \Psi \rangle \neq$ f) is called a "constant of motion"

(responds only to external forces)

commutes with the Hamiltonian H

has stationary states with definite eigenvalues

• Those eigenvalues occur as measurements (eg reflected in spectroscopy of allowed energy levels of a system)

Example: In particular relativistic corrections introduced into the hydrogen atom Hamiltonian a

term $\sim L \cdot S$ so need to describe the probabilites for different composite J values correctly

B) What we typically have:

math expressions for eigenfunctions, eigenvalues in terms of:

J_1^2 m_1 J_2^2 m_2

↑   ↑   ↑   ↑

total angular momentum (of particle) 1	eigenvalue of J_z (of particle) 1	total angular momentum (of particle) 2	eigenvalue of J_z (of particle) 2

Call these eigenfunctions $\left| J_1, m_1 \right\rangle$ and $\left| J_2, m_2 \right\rangle$

Then characteristic that

$$J_1^2 \left| j_1, m_1 \right\rangle = j_1(j_1 + 1)\hbar^2 \left| j_1, m_1 \right\rangle$$

$$J_2^2 \left| j_2, m_2 \right\rangle = j_2(j_2 + 1)\hbar^2 \left| j_2, m_2 \right\rangle$$

$$J_{1z} \left| j_1, m_1 \right\rangle = m_1 \hbar \left| j_1, m_1 \right\rangle$$

$$J_{2z} \left| j_2, m_2 \right\rangle = m_2 \hbar \left| j_2, m_2 \right\rangle$$

C) What we typically want is eigenvalues , eigenfunctions for J_{tot}^2, m_{tot}.

Call them $\left| j, m \right\rangle$ such that $J_{tot}^2 \left| j, m \right\rangle = j(j+1)\hbar^2 \left| j, m \right\rangle$ and $J_{z\,tot} \left| j, m \right\rangle = m\hbar \left| j, m \right\rangle$

So we need a transformation matrix
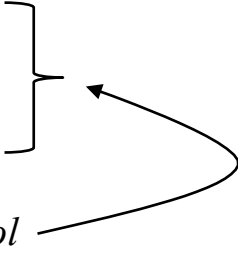
from $\left| j_1, m_1 \right\rangle \left| j_2, m_2 \right\rangle \rightarrow \left| j, m \right\rangle$

i.e. Need this

$$\left| j, m \right\rangle = \sum_{m_1 + m_2 = m} \left| j_1, m_1, j_2, m_2 \right\rangle \left\langle j_1, m_1, j_2, m_2 \middle| j, m \right\rangle$$

They are called the Clebsch-Gordan coefficients. They tell how much of each old $\left| j_1, m_1, j_2, m_2 \right\rangle$ eigenket contribute to each new $\left| j, m \right\rangle$ eigenket.

Note: the $\left| j_1, m_1, j_2, m_2 \right\rangle$ form a basis

    the $\left| j, m \right\rangle$ form a different basis

members in each basis are *orthoganol*

Show that the eigenfunctions of a mermitian operator (for example J) are orthogoanl; as this is important in constructing the C-G coefficients

Let hermitian operator be $A = A^{\dagger}$

Let eigenfunctions be Ψ_1 and Ψ_2, so

$A\Psi_1 = a_1 \Psi_1$ Eq 1

and

$A\Psi_2 = a_2 \Psi_2$ Complex conjugate this:

$[A\Psi_2]^* = a_2^* \Psi_2^*$ but Herimitian operators have real eigenvalues so $a_2^* = a_2$. Then

$[A\Psi_2]^* = a_2 \Psi_2^*$ Eq 2

Take $\int dx \Psi_2^* \cdot Eq1$ $\qquad \Rightarrow \int dx \Psi_2^* A \Psi_1 = \int dx \Psi_2^* a_1 \Psi_1$ $\qquad$ Eq 3

and $\quad \int dx \cdot Eq2 \cdot \Psi_1$ $\qquad \Rightarrow \int dx [A\Psi_2]^* \Psi_1 = \int dx a_2 \Psi_2^* \Psi_1$ $\qquad$ Eq 4

Eq3 − Eq4 :

$$\int dx \Psi_2^* A \Psi_1 - \int dx [A\Psi_2]^* \Psi_1 = (a_1 - a_2) \int dx \Psi_2^* \Psi_1$$

LHS:

$$\int dx \Psi_2^* A \Psi_1 - \int dx [A\Psi_2]^* \Psi_1 = \int dx \Psi_2^* A \Psi_1 - \int dx \Psi_2^* A^\dagger \Psi_1 \qquad \text{for hermitian A}$$

$$= \int dx \Psi_2^* (A - A^\dagger) \Psi_1 = 0$$

RHS:

If $a_1 \neq a_2$, $\int dx \Psi_2^* \Psi_1 = 0$

i.e. Ψ_1 and Ψ_2 are orthogonal

II. Examples of Clebsch Gordan Coefficient construction

The C-G are available in tables--example of how some are constructed:

Let $j_1 = j_2 = 1$. There are 9 possible combined states $\left| j_1, m_1, j_2, m_2 \right\rangle$:

1 1 1 1

1 1 1 0

1 1 1 -1

1 1 0 1

1 1 0 0

1 1 0 -1

1 1 -1 1

1 1 -1 0

1 1 -1 -1

For fixed $j_1 = 1$, $j_2 = 1$, call these states $\left| m_1, m_2 \right\rangle$ to simplify notation.

There are 9 possible $\left| jm \right\rangle$ states to which they contribute.

How to see this:

m=$m_1 + m_2$ (sum of z-components)

Bothe m_1 and m_2 can separately be 1, 0, -1

So m can be $\{2,1,0,-1,-2\}$

But m is the eigenvalue of J_z

$\left| J_z \right| \leq J$

So J can be 0, 1, or 2.

The 9 possible $\left| jm \right\rangle$ states are

2 2

2 1

2 0

2 -1

2 -2

1 1

1 0

1 -1

0 0

For notation, use prime to indicate $\left| j, m \right\rangle$

i.e. $\left| 1,1 \right\rangle' \equiv \left| j = 1, m = 1 \right\rangle$

Use unprimed to indicate $\left| m_1, m_2 \right\rangle$

i.e. $\left| 1,1 \right\rangle \equiv \left| m_1 = 1, m_2 = 1 \right\rangle$

Notice $\left| 2,2 \right\rangle' = \left| 1,1 \right\rangle$

as both refer to state where $m_1 = m_2 = 1$ and m_1 and m_2 are parallel

Similarly $\left| -2,-2 \right\rangle' = \left| -1,-1 \right\rangle$

So we can find all the states for j=2 either by apply J$_-$ to $\left|2,2\right\rangle'$ or J$_+$ to $\left|2,-2\right\rangle'$

Do this:

$\left|2,2\right\rangle' = \left|1,1\right\rangle$

but J$_-$ = $(J_{1_-} + J_{2_-})$

$J_-\left|2,2\right\rangle' = (J_{1_-} + J_{2_-})\left|1,1\right\rangle$

recall for any J$_-$: $J_-\left|j,m\right\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\left|j,m\right\rangle$

(on j$_1$ = 1, m$_1$ = 1)   (on j$_2$ = 1, m$_2$ = 1)

$\hbar\sqrt{2(2+1) - 2(2-1)}\left|2,1\right\rangle' = \hbar\sqrt{1(1+1) - 1(1-1)}\left|0,1\right\rangle + \hbar\sqrt{1(1+1) - 1(1-1)}\left|1,0\right\rangle$

$\hbar\cdot 2\left|2,1\right\rangle' = \hbar\sqrt{2}\left|0,1\right\rangle + \hbar\sqrt{2}\left|1,0\right\rangle$

$$\boxed{\left|2,1\right\rangle' = \frac{1}{\sqrt{2}}\left(\left|0,1\right\rangle + \left|1,0\right\rangle\right)}$$

C-G Coefficient

Now repeat. Apply J$_-$ to both sides

I. Constructing C-G coefficients for the $j_1 = j_2 = 1$ system (continued)

II. Symmetric and antisymmetric multi-particle states

III. Example application of C-G coefficients

$$J_-|2,1\rangle' = \frac{1}{\sqrt{2}}\left(J_{1-} + J_{2-}\right)\left(|0,1\rangle + |1,0\rangle\right)$$

$$\hbar\sqrt{2(2+1)-1(1-1)}\,|2,0\rangle' =$$

$$\text{(on } j_1 = 1, m_1 = 0) \qquad \text{(on } j_2 = 1, m_2 = 1) \qquad \text{(on } j_2 = 1, m_1 = 1) \qquad \text{(on } j_2 = 1, m_2 = 0)$$

$$\frac{1}{\sqrt{2}}\hbar\left\{\sqrt{1(1+1)-0(0-1)}\,|-1,1\rangle + \sqrt{1(1+1)-1(1-0)}\,|0,0\rangle + \sqrt{1(1+1)-1(1-0)}\,|0,0\rangle + \sqrt{1(1+1)-0(0-1)}\,|1,-1\rangle\right\}$$

$$\sqrt{6}\,|2,0\rangle' = \frac{1}{\sqrt{2}}\left\{\sqrt{2}\,|-1,1\rangle + \sqrt{2}\,|0,0\rangle + \sqrt{2}\,|0,0\rangle + \sqrt{2}\,|1,-1\rangle\right\}$$

$$\boxed{\,|2,0\rangle' = \left\{\frac{1}{\sqrt{6}}|-1,1\rangle + \frac{2}{\sqrt{6}}|0,0\rangle + \frac{1}{\sqrt{6}}|1,-1\rangle\right\}\,}$$

Similarly,

$$\boxed{\begin{array}{l}|2,-1\rangle' = \frac{1}{\sqrt{2}}\left\{|0,-1\rangle + |-1,0\rangle\right\} \\[2mm] \text{and} \\[2mm] |2,21\rangle' = |-1,1\rangle\end{array}}$$

Note all 9 $|m_1, m_2\rangle$ kets needed to form the five $|j = 2, m\rangle$ kets.

"old kets" "new kets"

In general call "new kets" with a particular m values are linear combinations of old kets for which $m_1 + m_2 = m$

So we foresee that

m m_1, m_2 m_1, m_2

$$|1,1\rangle' = a|0,1\rangle + b|1,0\rangle$$

But we also know that $|1,1\rangle'$ must be orthogonal to $|2,1\rangle'$ so specifically

$$|1,1\rangle' = \frac{1}{\sqrt{2}}\left(|0,1\rangle - |1,0\rangle\right)$$

Again apply J_ to both sides to get:

$$|1,0\rangle' = \frac{1}{\sqrt{2}}\left(|1,-1\rangle - |-1,1\rangle\right)$$

$$|1,-1\rangle' = \frac{1}{\sqrt{2}}\left(|0,-1\rangle - |-1,0\rangle\right)$$

Now foresee that

$$|0,0\rangle' = a|1,-1\rangle + b|0,0\rangle + c|-1,1\rangle$$

and must be orthogonal to both $\left|2,0\right\rangle'$ and $\left|1,0\right\rangle'$

Require

$$\left\langle 2,0\right|'\left|0,0\right\rangle' = 0$$

$$\left\{\frac{1}{\sqrt{6}}\left\langle 1,-1\right| + \frac{2}{\sqrt{6}}\left\langle 0,0\right| + \frac{1}{\sqrt{6}}\left\langle 1,-1\right|\right\}\cdot\left\{a\left|1,-1\right\rangle + b\left|0,0\right\rangle + c\left|-1,1\right\rangle\right\} = 0$$

$$\underbrace{\frac{1}{\sqrt{6}}a\left\langle 1,-1\middle|1,-1\right\rangle}_{1} + \underbrace{\frac{2}{\sqrt{6}}b\left\langle 0,0\middle|0,0\right\rangle}_{1} + \underbrace{\frac{1}{\sqrt{6}}c\left\langle 1,-1\middle|1,-1\right\rangle}_{1} + \underbrace{\text{all cross terms like }\left\langle 1,-1\middle|0,0\right\rangle}_{0} = 0$$

$a + 2b + c = 0$ "Eq1"

Also require

$$\left\langle 1,0\right|'\left|0,0\right\rangle' = 0$$

$$\left\{\frac{1}{\sqrt{2}}\left\langle 1,-1\right| - \frac{1}{\sqrt{2}}\left\langle -1,1\right|\right\}\cdot\left\{a\left|1,-1\right\rangle + b\left|0,0\right\rangle + c\left|-1,1\right\rangle\right\} = 0$$

$$\underbrace{\frac{1}{\sqrt{2}}a\left\langle 1,-1\middle|1,-1\right\rangle}_{1} + \underbrace{\frac{1}{2}c\left\langle -1,1\middle|-1,1\right\rangle}_{1} + \underbrace{\text{all cross terms like }\left\langle -1,1\middle|0,0\right\rangle}_{0} = 0$$

$a - c = 0$ "Eq2"

Solve Eq1 and Eq2 simultaneously:

Eq2: c=a

Then Eq1 is:

a+2b+a=0

b=-a

So $|0,0\rangle' = a|1,-1\rangle - a|0,0\rangle + a|-1,1\rangle$

normalize $\rightarrow$ a=$\dfrac{1}{\sqrt{3}}$

$$\boxed{|0,0\rangle' = \frac{1}{\sqrt{3}}\left\{|1,-1\rangle - |0,0\rangle + |-1,1\rangle\right\}}$$

Facts about C-G coefficients

1) Handout for values of low j systems

2) $\langle j_1 m_1 j_2 m_2 | jm\rangle = (-1)^{j_1+j_2-j}\langle j_2 m_2 j_1 m_1 | jm\rangle$

3) $\langle j_1 m_1 j_2 m_2 | jm\rangle = (-1)^{j_1+j_2-j}\langle j_1,-m_1,j_2,-m_2 | jm\rangle$

4) $\langle j_1 m_1 j_2 m_2 | jm\rangle = (-1)^{j_1-m_1}\left(\dfrac{2j+1}{2j_2+1}\right)^{\frac{1}{2}}\langle j_1,m_1,j,-m | j_2,-m_2\rangle$

II. Symmetric and antisymmetric multiparticle states

Consider 2 identical spin 1/2 particles. Each can be independently spin up or spin down so there are 4 possible combined states.

$$m_{s_i} = +\tfrac{1}{2} \qquad m_{s_i} = -\tfrac{1}{2}$$

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

$+\tfrac{1}{2} \quad +\tfrac{1}{2}$

$+\tfrac{1}{2} \quad -\tfrac{1}{2}$

$-\tfrac{1}{2} \quad +\tfrac{1}{2}$

$-\tfrac{1}{2} \quad -\tfrac{1}{2}$

Find form of combined state $\left| s, m_s \right\rangle$

Analogous to converting $\left| m_1 m_2 \right\rangle \rightarrow \left| jm \right\rangle$

Note $m_s = m_{s_1} + m_{s_2}$ can be

$\quad 1 \quad \left(+\tfrac{1}{2}\right) \left(+\tfrac{1}{2}\right)$

$\quad 0 \quad \left(+\tfrac{1}{2}\right) \left(-\tfrac{1}{2}\right)$ or $\left(-\tfrac{1}{2}\right) \left(+\tfrac{1}{2}\right)$

$\quad -1 \quad \left(-\tfrac{1}{2}\right) \left(-\tfrac{1}{2}\right)$

Since $|S_z| \le |S|$

if $|m_s|_{max} = 1$, then $S_{max} = 1$, so S can be 0 or 1.

Then allowed $|S, m_s\rangle'$ are

$$
\begin{array}{cc}
1 & 1 \\
1 & 0 \\
1 & -1 \\
0 & 0
\end{array}
$$

Begin with $\boxed{|1,1\rangle' = |\frac{1}{2}, \frac{1}{2}\rangle}$ (both spin up) Apply S_- to both:

$S_- |1,1\rangle' = (S_{1-} + S_{2-}) |\frac{1}{2}, \frac{1}{2}\rangle$ (analogous to J's)

$$
\boxed{|1,0\rangle' = \frac{1}{\sqrt{2}}\left(|\frac{-1}{2}, \frac{1}{2}\rangle + |\frac{1}{2}, \frac{-1}{2}\rangle \right)}
$$

Note $|0,0\rangle'$ has $m_s = 0$ so must be built of kets with $m_1 + m_2 = 0$, i.e. also $|\frac{1}{2}, \frac{-1}{2}\rangle$ and $|\frac{-1}{2}, \frac{1}{2}\rangle$

But also $|0,0\rangle'$ must be *orthogonal* to $|1,0\rangle'$ so it is

$$
\boxed{|0,0\rangle' = \frac{1}{\sqrt{2}}\left(|\frac{-1}{2}, \frac{1}{2}\rangle - |\frac{1}{2}, \frac{-1}{2}\rangle \right)}
$$

Lastly by inspection $\left|1,-1\right\rangle' = \left|\frac{-1}{2},\frac{-1}{2}\right\rangle$ (both particles spin down)

Rewrite the 4 coupled states

$$\left|1,1\right\rangle' = \left|\frac{1}{2},\frac{1}{2}\right\rangle$$

$$\left|1,0\right\rangle' = \frac{1}{\sqrt{2}}\left(\left|\frac{-1}{2},\frac{1}{2}\right\rangle + \left|\frac{1}{2},\frac{-1}{2}\right\rangle\right)$$

$$\left|1,-1\right\rangle' = \left|\frac{-1}{2},\frac{-1}{2}\right\rangle$$

Set of 3 "Triplet States"
all are symmetric under interchange $m_{s_1} \leftrightarrow m_{s_2}$

$$\left|0,0\right\rangle' = \frac{1}{\sqrt{2}}\left(\left|\frac{-1}{2},\frac{1}{2}\right\rangle - \left|\frac{1}{2},\frac{-1}{2}\right\rangle\right)$$

"Singlet State"
is anti-symmetric under interchange $m_{s_1} \leftrightarrow m_{s_2}$

Where Pauli Principle demands

Fermions: total wavefunction antisymmetric

(spatial) $\cdot$ (spin)

$$\Psi_{n\ell m} \cdot \chi$$

$\Psi_{n\ell m}$ are hydrogenic wavefunctions

$\boxed{\textit{These}}$ are χ

I. Example application of coupled basis

II. Intro to WKB

I. Example application of couples basis

Goswami problem 17-7

Consider a 2-particle Hamiltonian for a spin system

$H=A+BS_1 \cdot S_2$

Calculate the eigenvalues and eigenstates for 2 identical spin 1/2 particles

(i) using uncoupled representation $\left| m_{s_1}, m_{s_2} \right\rangle$

(ii) using coupled representation $\left| s, m_s \right\rangle$

Solution:

(i) $H=A+B(S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z})$

Recall $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$, so

$$S_x = \frac{S_+ + S_-}{2} \quad \text{and} \quad S_y = \frac{S_+ - S_-}{2i}$$

Then $H=A+B(S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}) =$

$$A+B\left[\left(\frac{S_{1+} + S_{1-}}{2} \right)\left(\frac{S_{2+} + S_{2-}}{2} \right) + \left(\frac{S_{1+} - S_{1-}}{2i} \right)\left(\frac{S_{2+} - S_{2-}}{2i} \right) + S_{1z}S_{2z} \right]$$

$$= A + \frac{B}{4}\left[S_{1+}S_{2+} + S_{1-}S_{2-} + S_{1+}S_{2-} + S_{1-}S_{2+} - S_{1+}S_{2+} - S_{1-}S_{2-} + S_{1-}S_{2+} + S_{1+}S_{2-} \right] + BS_{1z}S_{2z}$$

$$= A + \frac{B}{2}\left[S_{1+}S_{2-} \right] + \frac{B}{2}\left[S_{1-}S_{2+} \right] + BS_{1z}S_{2z}$$

$$A\left| m_{s_1}, m_{s_2} \right\rangle = A\left| m_{s_1}, m_{s_2} \right\rangle$$

$$BS_{1z}S_{2z}\left| m_{s_1}, m_{s_2} \right\rangle = B\hbar^2 m_{s_1} m_{s_2}\left| m_{s_1}, m_{s_2} \right\rangle$$

$$\frac{B}{2}S_{1+}S_{2-} = \frac{B}{2}\hbar^2 \sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right) - m_{s_1}\left(m_{s_1}+1\right)}\sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right) - m_{s_2}\left(m_{s_2}-1\right)}\left| m_{s_1}+1, m_{s_2}-1 \right\rangle$$

$$\frac{B}{2}S_{1-}S_{2+} = \frac{B}{2}\hbar^2 \sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right) - m_{s_1}\left(m_{s_1}-1\right)}\sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right) - m_{s_2}\left(m_{s_2}+1\right)}\left| m_{s_1}-1, m_{s_2}+1 \right\rangle$$

	$\left\vert\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\vert\frac{1}{2},\frac{-1}{2}\right\rangle$	$\left\vert\frac{-1}{2},\frac{1}{2}\right\rangle$	$\left\vert\frac{-1}{2},\frac{-1}{2}\right\rangle$
$\left\vert\frac{1}{2},\frac{1}{2}\right\rangle$	$A+\dfrac{B\hbar^2}{4}$	0	0	0
$\left\vert\frac{1}{2},\frac{-1}{2}\right\rangle$	0	$A-\dfrac{B\hbar^2}{4}$	$\dfrac{B\hbar^2}{2}$	0
$\left\vert\frac{-1}{2},\frac{1}{2}\right\rangle$	0	$\dfrac{B\hbar^2}{2}$	$A-\dfrac{B\hbar^2}{4}$	0
$\left\vert\frac{-1}{2},\frac{-1}{2}\right\rangle$	0	0	0	$A+\dfrac{B\hbar^2}{4}$

2 eigenvectors are given by diagonals:

$\left|\frac{1}{2},\frac{1}{2}\right\rangle$ has E=A+$\dfrac{B\hbar^2}{4}$

$\left|\frac{-1}{2},\frac{-1}{2}\right\rangle$ has E=A+$\dfrac{B\hbar^2}{4}$

To find others, diagonalize 2x2 submatrix to get:

$\dfrac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{-1}{2}\right\rangle+\left|\frac{-1}{2},\frac{1}{2}\right\rangle\right]$ with E=A+$\dfrac{B\hbar^2}{4}$

$\dfrac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{-1}{2}\right\rangle-\left|\frac{-1}{2},\frac{1}{2}\right\rangle\right]$ with E=A-$\dfrac{3B\hbar^2}{4}$

(ii) In the coupled basis:

Recall H=A+B$S_1 \cdot S_2$

If we let S=$S_1 + S_2$, then

$$S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 S_2$$

Then $S_1 S_2 = \dfrac{S^2}{2} - \dfrac{S_1^2}{2} - \dfrac{S_2^2}{2}$

$S^2\left|s,m_s\right\rangle = \hbar^2 s(s+1)\left|s,m_s\right\rangle$

$S_1^2\left|s,m_s\right\rangle = \hbar^2 s_1(s_1+1)\left|s,m_s\right\rangle$

$S_2^2\left|s,m_s\right\rangle = \hbar^2 s_2(s_2+1)\left|s,m_s\right\rangle$

Eigenvalues:

when S=1, $S_1 = \frac{1}{2}$, $S_2 = \frac{1}{2}$

$$\begin{cases} \left| s = 1, m_s = 1 \right\rangle \\ \left| s = 1, m_s = 0 \right\rangle \\ \left| s = 1, m_s = -1 \right\rangle \end{cases}$$

$$E = A + \frac{B}{2}\hbar^2 \left[1(1+1) - \tfrac{1}{2}(\tfrac{1}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}+1) \right] = A + \frac{B\hbar^2}{4}$$

When S=0, $S_1 = \frac{1}{2}$, $S_2 = \frac{1}{2}$ $\begin{cases} \left| s = 0, m_s = 0 \right\rangle \end{cases}$

$$E = A + \frac{B}{2}\hbar^2 \left[0(0+1) - \tfrac{1}{2}(\tfrac{1}{2}+1) - \tfrac{1}{2}(\tfrac{1}{2}+1) \right] = A - \frac{3B\hbar^2}{4}$$
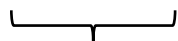
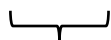I. Time-independent perturbation theory

I. Time-independent perturbation Theory

For every kind of *interaction* in the world there is a Hamiltonian H

force measurement etc.

In general one wants to predict the *results* that could be

eigenvalues, eigenvectors = possible
stationary states and their energies

obtained by studying that interaction.

So one wants to diagonalize the H to get

$H|\Psi_n\rangle = E_n|\Psi_n\rangle$ for all states n.

Recall $H = \dfrac{-\hbar^2}{2m} + V$

It turns out that most physical V's are so complicated that it is not possible to solve $H|\Psi_n\rangle = E_n|\Psi_n\rangle$ analytically for them.

For some of these H's we can still get an approximate solution IF we can write them in this form:

$H = H_{\substack{known \\ eigenfunctions}} + H'$ where H' is "small" compared to H. We will say what "small" means.

Call this H_0 Return this $H' = \lambda H_1$

*Assume for now that $H' \neq f(t)$

I. Time-independent perturbation Theory (continued)

So $H = H_0 + \lambda H_1$ and our goal is to *solve* $\left(\text{get } E_n \text{ and } |\Psi_n\rangle \right)$

$$\left(H_0 + \lambda H_1 \right) |\Psi_n\rangle = E_n |\Psi_n\rangle$$

To solve this we make the following assumption:

i) there exist known solutions "$E_n^{(0)}$" and $|\varphi_n\rangle$ to the equation

$$H_0 |\varphi_n\rangle = E_n^{(0)} |\varphi_n\rangle$$

ii) If $\lambda \to 0$, the unknown $|\Psi_n\rangle \to$ the known $|\varphi_n\rangle$ and

the unknown $E_n \to$ the known E_n^0

iii) Because the $|\varphi_n\rangle$ are eigenvectors, they form a basis, so we can expand $|\Psi_n\rangle$ in terms of them

$$|\Psi_n\rangle = \sum_k |\varphi_k\rangle\langle\varphi_k|\Psi_n\rangle$$

$$= \langle\varphi_k|\Psi_n\rangle |\varphi_n\rangle + \sum_{k \neq n} |\varphi_k\rangle\langle\varphi_k|\Psi_n\rangle$$

the amount this overlaps depends on the value of λ.

call this term $N(\lambda)$

$$= N(\lambda)\left[|\varphi_n\rangle + \sum_{k \neq n} |\varphi_k\rangle \frac{\langle\varphi_k|\Psi_n\rangle}{N(\lambda)} \right]$$

call this C_{nk}

In order that $\left|\Psi_n\right\rangle \xrightarrow[\lambda\to 0]{} \left|\varphi_n\right\rangle$, must have $N(\lambda = 0)=1$

(iv) The c_{nk} represent the amount of admixture between $\left|\Psi_n\right\rangle$ and the unperturbed states $\left|\varphi_k\right\rangle$.

So the c_{nk} are functions of λ.

Assume they can be written as

$$c_{nk}(\lambda) \equiv \cancel{c_{nk}^{(0)}} + \lambda c_{nk}^{(1)} + \lambda^2 c_{nk}^{(2)} + ...$$

we assume that when $\lambda=0$, $\left|\Psi_n\right\rangle = \left|\varphi_n\right\rangle$ (there is no admixture between

$\left|\Psi_n\right\rangle$ and $\left|\Psi_{n\neq k}\right\rangle$), so $c_{nk}(\lambda = 0) = 0$. this means $c_{nk}^{(0)} =0$.

(v) Also assume $E_n \equiv E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...$

So $E_n \xrightarrow[\lambda\to 0]{} E_n^{(0)}$ naturally

Plug in the expansions:

$$\left(H_0 + \lambda H_1\right)\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$

$$\left(H_0 + \lambda H_1\right)N(\lambda)\left\{\left|\varphi_n\right\rangle + \sum_{k\neq n}\left|\varphi_k\right\rangle c_{nk}\right\} = \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...\right)N(\lambda)\left\{\left|\varphi_n\right\rangle + \sum_{k\neq n}\left|\varphi_k\right\rangle c_{nk}\right\}$$

plug in $c_{nk} = \lambda c_{nk}^{(1)} + \lambda^2 c_{nk}^{(2)} + ...$

$$\left(H_0 + \lambda H_1\right)\left\{\left|\varphi_n\right\rangle + \sum_{k \neq n}\lambda c_{nk}^{(1)}\left|\varphi_k\right\rangle + \sum_{k \neq n}\lambda^2 c_{nk}^{(2)}\left|\varphi_k\right\rangle + ...\right\} =$$

$$\left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...\right)\left\{\left|\varphi_n\right\rangle + \sum_{k \neq n}\lambda c_{nk}^{(1)}\left|\varphi_k\right\rangle c_{nk} + \sum_{k \neq n}\lambda^2 c_{nk}^{(2)}\left|\varphi_k\right\rangle c_{nk} + ...\right\}$$

Require that this equation be true for arbitrary λ, so the coefficients of each power of λ on both sides must be equal.

$\lambda^0 :$ $\boxed{H_0\left|\varphi_n\right\rangle = E_n^{(0)}\left|\varphi_n\right\rangle}$ presumably all these terms are known

$\lambda^1 :$ $H_0 \sum_{k \neq n}c_{nk}^{(1)}\left|\varphi_k\right\rangle + H_1\left|\varphi_n\right\rangle = E_n^{(0)}\sum_{k \neq n}c_{nk}^{(1)}\left|\varphi_k\right\rangle + E_n^{(1)}\left|\varphi_n\right\rangle$

$\lambda^2 :$ $H_0 \sum_{k \neq n}c_{nk}^{(2)}\left|\varphi_k\right\rangle + H_1 \sum_{k \neq n}c_{nk}^{(1)}\left|\varphi_k\right\rangle + H_2\left|\varphi_n\right\rangle = E_n^{(0)}\sum_{k \neq n}c_{nk}^{(2)}\left|\varphi_k\right\rangle + E_n^{(1)}\sum_{k \neq n}c_{nk}^{(1)}\left|\varphi_k\right\rangle + E_n^{(2)}\left|\varphi_n\right\rangle$

$\lambda^3 :$ ....

$\boxed{\text{We will solve for } E_n^{(1)},\ c_{nk}^{(1)},\ E_n^{(2)},\ N(\lambda)}$

To find $E_n^{(1)}$: Rewrite the λ coefficients' equations emphasize $E_n^{(1)}$:

$$E_n^{(1)}\left|\varphi_n\right\rangle = H_1\left|\varphi_n\right\rangle + \sum_{k \neq n}c_{nk}^{(1)}H_0\left|\varphi_k\right\rangle - E_n^{(0)}\sum_{k \neq n}c_{nk}^{(1)}\left|\varphi_k\right\rangle$$

plug in

$$E_n^{(1)}\left|\varphi_n\right\rangle = H_1\left|\varphi_n\right\rangle + \sum_{k \neq n}c_{nk}^{(1)}E_k^{(0)}\left|\varphi_k\right\rangle - E_n^{(0)}\sum_{k \neq n}c_{nk}^{(1)}\left|\varphi_k\right\rangle$$

$$= H_1\left|\varphi_n\right\rangle + \sum_{k \neq n}\left(E_k^{(0)} - E_n^{(0)}\right)c_{nk}^{(1)}\left|\varphi_k\right\rangle \qquad\qquad \text{"Eq1"}$$

Multiply equation by $\left\langle\varphi_n\right|$:

$$E_n^{(1)} \underbrace{\langle \varphi_n | \varphi_n \rangle}_{1} = \langle \varphi_n | H_1 | \varphi_n \rangle + \sum_{k \neq n} \left(E_k^{(0)} - E_n^{(0)} \right) c_{nk}^{(1)} \underbrace{\langle \varphi_n | \varphi_k \rangle}_{\delta_{nk} \to 0}$$

So $E_n^{(1)} = \langle \varphi_n | H_1 | \varphi_n \rangle$

$$\boxed{\lambda E_n^{(1)} = \langle \varphi_n | \lambda H_1 | \varphi_n \rangle}$$

the first order   =   the diagonal element of the matrix of the
correction to the   perturbative hamiltonian
energy

the expectation value of λH_1

To find $c_{nk}^{(1)}$:

Multiply Eq1 by $\langle \varphi_m |$ (m $\neq$ n):

$$E_n^{(1)} \underbrace{\langle \varphi_m | \varphi_n \rangle}_{0} = \langle \varphi_m | H_1 | \varphi_n \rangle + \sum_{k \neq n} \left(E_k^{(0)} - E_n^{(0)} \right) c_{nk}^{(1)} \underbrace{\langle \varphi_m | \varphi_k \rangle}_{\delta_{mk} \to 1 \text{ only when k=m}}$$

$$0 = \langle \varphi_m | H_1 | \varphi_n \rangle + \left(E_m^{(0)} - E_n^{(0)} \right) c_{nm}^{(1)}$$

$$\boxed{c_{nm}^{(1)} = \frac{\langle \varphi_m | H_1 | \varphi_n \rangle}{E_n^{(0)} - E_m^{(0)}}}$$

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I. Time-independent perturbation theory (continued)

II. The Stark Effect

III. Degenerate perturbation theory

Read Chapter 22 Sections 1 and 2 only

Facts about the first-order mixing coefficient $c_{nm}^{(1)}$:

(i) H_1 will naturally have some off-diagonal elements (if it did not, we would not have had to define a "λH_1", we could have incorporated it into H_0).

Call some non-diagonal H_1 element "H_{1mn}". Then we say that "states $|\varphi_m\rangle |\varphi_m\rangle$ are connected by the pater bation" i.e., H_1 causes the system to make transitions between $|\varphi_m\rangle$ and $|\varphi_n\rangle$.

(ii) Recall c_{nk} represents the amount of admixture $|\varphi_k\rangle$ that the perturbation causes to be superposed into $|\varphi_n\rangle$. We see that the magnitude of admixture depends on 2 things:

$$\underbrace{}$$
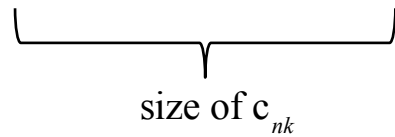
size of c_{nk}

1) the overlap $\langle \varphi_k | H_1 | \varphi_n \rangle$ i.e. "how much H_1 changes $|\varphi_n\rangle$ to be like $|\varphi_k\rangle$"

2) the unperturbed energy deifference between the states: $E_n^{(0)} - E_k^{(0)}$

    so the closer in energies the unperturbed states $|\varphi_n\rangle$ and $|\varphi_k\rangle$ are, the more of $|\varphi_k\rangle$ will be mixed into $|\varphi_n\rangle$ by the perturbation.

3) The size of $c_{nk}^{(1)}$ defines whether a perturbation is "small", i.e. whether it was ok to expand everything in terms of λ.

I. Time-independent perturbation theory (continued)

II. Example of T-I-P-T: Stark Effect Energies

III. Degenerate perturbation theory

IV. Example of DPT: Stark Effect wavefunctions

Read Goswami Chapter 22

To find $E_n^{(2)}$:

Recall the λ^2 coefficient's equation:

$$H_0 \sum_{k \neq n} c_{nk}^{(2)} |\varphi_k\rangle + H_1 \sum_{k \neq n} c_{nk}^{(1)} |\varphi_k\rangle + H_2 |\varphi_n\rangle = E_n^{(0)} \sum_{k \neq n} c_{nk}^{(2)} |\varphi_k\rangle + E_n^{(1)} \sum_{k \neq n} c_{nk}^{(1)} |\varphi_k\rangle + E_n^{(2)} |\varphi_n\rangle$$

Rewrite to emphsasize $E_n^{(2)}$:

$$E_n^{(2)} |\varphi_n\rangle = \sum_{k \neq n} c_{nk}^{(2)} H_0 |\varphi_k\rangle + \sum_{k \neq n} c_{nk}^{(1)} H_1 |\varphi_k\rangle - E_n^{(0)} \sum_{k \neq n} c_{nk}^{(2)} |\varphi_k\rangle - E_n^{(1)} \sum_{k \neq n} c_{nk}^{(1)} |\varphi_k\rangle$$

$$E_k^{(0)} |\varphi_k\rangle$$

Multiply on left with $\langle \varphi_n |$:

$$E_n^{(2)} \underbrace{\langle \varphi_n | \varphi_n \rangle}_{1} = \sum_{k \neq n} c_{nk}^{(2)} E_k^{(0)} \underbrace{\langle \varphi_n | \varphi_k \rangle}_{0} + \sum_{k \neq n} c_{nk}^{(1)} \langle \varphi_n | H_1 | \varphi_k \rangle - E_n^{(0)} \sum_{k \neq n} c_{nk}^{(2)} \underbrace{\langle \varphi_n | \varphi_k \rangle}_{0} - E_n^{(1)} \sum_{k \neq n} c_{nk}^{(1)} \underbrace{\langle \varphi_n | \varphi_k \rangle}_{0}$$

I. Time-independent perturbation theory (continued)

II. Example of T-I-P-T: Stark Effect Energies

III. Degenerate perturbation theory

IV. Example of Degenerate Perturbation Theory

$$E_n^{(2)} \langle \varphi_n | \varphi_n \rangle = \sum_{k \neq n} c_{nk}^{(1)} \langle \varphi_n | H_1 | \varphi_k \rangle$$

$$\text{plug in } c_{nk}^{(1)} = \frac{\langle \varphi_k | H_1 | \varphi_n \rangle}{E_n^{(0)} - E_k^{(0)}}$$

$$= \sum_{k \neq n} \frac{\langle \varphi_k | H_1 | \varphi_n \rangle}{E_n^{(0)} - E_k^{(0)}} \underbrace{\langle \varphi_n | H_1 | \varphi_k \rangle}$$

$$\langle \varphi_k | H_1 | \varphi_n \rangle^*$$

$$\boxed{E_n^{(2)} = \sum_{k \neq n} \frac{\left| \langle \varphi_k | H_1 | \varphi_n \rangle^2 \right|}{E_n^{(0)} - E_k^{(0)}}}$$

Notice:

1) To get $E_n^{(2)}$ for any level n, you have to sum over the connections to all other states

2) when n=0, we are considering the ground state. Then since $k \neq 0$ all E_k are by definition higher energy states, so all the $E_n^{(0)} - E_k^{(0)}$ are *negative*.

To get N(λ):

Require $\langle \Psi_n | \Psi_n \rangle = 1$

$$1 = N^2(\lambda)\left\{\underbrace{\langle\varphi_n|\varphi_n\rangle}_{1} + \lambda^2\sum_{n\neq k}\left|c_{nk}^{(1)}\right|^2\underbrace{\langle\varphi_k|\varphi_k\rangle}_{1} + \ldots\right\}$$

$$1 = N^2(\lambda)\left\{1 + \lambda^2\sum_{n\neq k}\left|c_{nk}^{(1)}\right|^2 + \ldots\right\}$$

So to first order in λ, $N(\lambda)=1$

Plug in N and $c_{nk}^{(1)}$ to $\left|\Psi_n\right\rangle$:

$$\left|\Psi_n\right\rangle = \left|\varphi_n\right\rangle + \sum_{n\neq k}\frac{\langle\varphi_k|H_1|\varphi_n\rangle}{E_n^{(0)} - E_k^{(0)}}\left|\varphi_k\right\rangle + \ldots$$

II. Example use of time-independent Perturbation Theory: Stark Effect Energies

Regular hydrogen atom normally experiences V=$\dfrac{-e^2}{r}$ only.

Suppose it is embedded in an external electric field $\bar{E}$.

How does this effect its energy levels?

So we want to find $\lambda E_n^{(1)} = \langle\varphi_n|\lambda H_1|\varphi_n\rangle$ and $\lambda E_n^{(2)} = \sum_{n\neq k}\dfrac{\left|\langle\varphi_k|\lambda H_1|\varphi_n\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}$

$\left(\text{Now absorb } \lambda \text{ in } E_n \text{ and } H_1\right)$

Recall the $|\varphi_n\rangle$ are the unperturbed eigenfunctions. For the hydrogen atom these are the

$$\Psi_{n\ell m} = R_{n\ell}Y_{\ell m} = |\varphi_n\rangle$$

To find λH_1 recall that an $\vec{E}$ only affects an object's energy if that object has a dipole moment $q\vec{r}$. Here q=e

So $H_1 = e\vec{E}\vec{r}$

$$\text{Let } \vec{E}=E\hat{z}$$

$$H_1 = eEz$$

Then $E_n^{(1)} = \langle \Psi_{n\ell m} | eEz | \Psi_{n\ell m} \rangle$ where z=rcosθ

$$= eE \int_r R_{n\ell}^* r R_{n\ell} r^2 \, dr \underbrace{\int_{\theta,\phi} Y_{\ell m}^* \cos\theta Y_{\ell m} \sin\theta d\theta d\phi}_{0}$$

So $E_n^{(1)} = 0$ for any level n

To ilustrate how to find $E_n^{(2)}$, choose a specific set of quantum numbers n=1, ℓ=0, m=0 (ground state)

$$E_{100}^{(2)} = e^2 E^2 \sum_{n\ell m \neq 100} \frac{\left|\langle \Psi_{n\ell m} | z | \Psi_{100} \rangle\right|^2}{E_{100}^{(0)} - E_{n\ell m}^{(0)}}$$

I. Degenerate Perturbation Theory

II. Using Degenerate Perturbation theory on the Stark Effect

III. Time-Dependent Perturbation Theory

$$\langle \Psi_{n\ell m} | eEz | \Psi_{100} \rangle = \int_r r^2 \, dr R_{n\ell}^* r R_{10} \int_{\theta,\phi} \sin\theta \, d\theta \, d\phi \, Y_{\ell m}^* \cos\theta \, Y_{00}$$

$$\underbrace{\qquad}_{\sqrt{\frac{1}{3}} Y_{10}} \quad \text{list of } Y_{\ell m}\text{'s Goswami eq 11.43}$$

$$\frac{1}{\sqrt{3}} \delta_{\ell 1} \delta_{m0}$$

So

$$E_{100}^{(2)} = \frac{e^2 E^2}{3} \sum_{n\ell m \neq 100} \delta_{\ell 1} \delta_{m0} \left[\int_r r^2 \, dr R_{n\ell}^* r R_{10} \right]^2 \frac{1}{E_{100}^{(0)} - E_{n\ell m}^{(0)}}$$

this is an infinite sum over n.

III. Degenerate Perturbation Theory

Recall with Perturbation Theory,

$$c_{nk}^{(1)} = \frac{\langle \varphi_k | H_1 | \varphi_n \rangle}{E_n^{(0)} - E_k^{(0)}} \quad \text{and} \quad E_n^{(2)} = \sum_{n \neq k} \frac{|\langle \varphi_k | H_1 | \varphi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

So if 2 levels (k and n) have the same UNperturbed energies $E_k^{(0)}$ and $E_n^{(0)}$, that will cause a $\div 0$ which will make these expressions meaningless.

This $\div 0$ is a sign that here is a case where the perturbation expansion is not being done right. Recall the expansion is only allowed if the $c_{nk}^{(1)}$ are small, i.e. if $\langle \varphi_k | H_1 | \varphi_n \rangle \ll \left(E_n^{(0)} - E_k^{(0)} \right)$

I. Degenerate Perturbation Theory (continued)

II. Stark Effect eigenfunctions

III. Time-Dependent Perturbation Theory

Read Goswami Chapter 23

General plan to fix this

(i) diagonalize the part at the H_1 matrix which connects $\langle \varphi_k |$ and $| \varphi_n \rangle \rightarrow$ then these $\langle \varphi_k | H_1 | \varphi_n \rangle$
will $= 0$

(ii) Recall perturbation theory depends on H_0 being diagonal (must have known eigenvalues and eigenfunctions) so we do not want to damage that.

(iii) It is not in general possible to change the basis to one which diagonalizes H_1 without "undiagonalizing" H_0. So to be careful we have to actually diagonalize $H_0 + H_1$ (absorbed λ into H_1)

So in general:

$H = H_0 + H_1 =$

$$
\begin{pmatrix}
E_1 & & & & \\
& E_2 & & & \\
& & \begin{pmatrix} E_i & A \\ A & E_i \end{pmatrix} & & \\
& & & E_6 &
\end{pmatrix}
$$

diagonalize this (call is "matrix E_i")

(iv) A trick: if matrix E_i is the whole matrix or if you don't care about the states outside of it, the you only have to diagonalize H_1, not H_0. This is because in the matrix E_i, H_0 is not just diagonal but also proportional to the unit matrix $\mathbf{1}$. Since H_1 (and all matrices) commute with $\mathbf{1}$, *in this subspace* you can diagonalize H_1 without affecting H_0. This is what we will do. But if one does this it is important afterwards not to discuss the re-diagonalized E_i subspace states and the non-E_i subspace states together, the are in different bases.

(v) Limit focus to the E_i subspace. Diagonalize H_1

$$\underbrace{}$$

call it H_1'

(vi) Get the new E_i', c_{nk}', Ψ_n' associated with H_1'

(vii) Apply non-degenerate perturbation theory within this subspace since the E_i' are all different. If some of the E_i' are still degenerate must diagonalize *their* subspace and iterate (this is called second order Degenerate Perturbation Theory; we will not do it.)

I. Example of degenerate perturbation theory: the Stark Effect

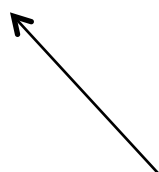II. Time-dependent Perturbation Theory

IV. Example of Degenerate Perturbation Theory: The Stark Effect

Recall $H_0 + H_1 =$

$$\left(\frac{p^2}{2m} - \frac{e^2}{r}\right) + eEz$$

Coulomb field   static electric field in $\hat{z}$

(i) Recall that the solutions to H_0 are the $\Psi_{n\ell m}$'s

Recall their energies are determined only by their "n" quantum number

$$E = \frac{-mZ^2 e^4}{2\hbar^2 n^2}$$

So for example $\begin{Bmatrix} \Psi_{200} \\ \Psi_{211} \\ \Psi_{210} \\ \Psi_{21-1} \end{Bmatrix}$ all have the same energy

Ignore Ψ_{211} and Ψ_{21-1} for now and apply degenerate perturbation theory to Ψ_{200} and Ψ_{210} :

(ii) Recall usually we would have to diagonalize $H_0 + H_1$ but if we confine our attention to the degenerate state only, then we can just diagonalize H_1 for the states that are degenerate.

Do this:

$$H_1 \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = E^{(1)} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix}$$

$$\downarrow$$

$$\left| \Psi_{200} \right\rangle \qquad \left| \Psi_{210} \right\rangle$$

$$\begin{array}{c} \left\langle \Psi_{200} \right| \\ \left\langle \Psi_{210} \right| \end{array} \begin{pmatrix} \left\langle \Psi_{200} \middle| eEz \middle| \Psi_{200} \right\rangle & \left\langle \Psi_{200} \middle| eEz \middle| \Psi_{210} \right\rangle \\ \left\langle \Psi_{210} \middle| eEz \middle| \Psi_{200} \right\rangle & \left\langle \Psi_{210} \middle| eEz \middle| \Psi_{210} \right\rangle \end{pmatrix} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = E^{(1)} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix}$$

Calculate the elements of the H_1 matrix: (use r=zcosθ)

$$\left\langle \Psi_{200} \middle| eEz \middle| \Psi_{200} \right\rangle = eE \int r^2 \, dr \, R_{20} r R_{20} \int \sin\theta \, d\theta \, d\phi \, Y_{00} \underbrace{\cos\theta Y_{00}}_{\substack{\sim Y_{10}}} = 0$$

$$\underbrace{\phantom{\cos\theta Y_{00}}}_{\delta_{1,0}}$$

Similarly, $\left\langle \Psi_{210} \middle| eEz \middle| \Psi_{210} \right\rangle = 0$

$$\left\langle \Psi_{200} \middle| eEz \middle| \Psi_{210} \right\rangle = \left\langle \Psi_{210} \middle| eEz \middle| \Psi_{200} \right\rangle =$$

$$\int_0^\infty r^2 \, dr \, \frac{1}{(2a_0)^{\frac{3}{2}}} 2 \left(1 - \frac{r}{2a_0} \right) e^{-r/2a_0} r \frac{1}{(2a_0)^{\frac{3}{2}}} \frac{1}{\sqrt{3}} \left(\frac{r}{a_0} \right) e^{-r/2a_0} \cdot \int \underbrace{Y_{00} \cos\theta Y_{10}}_{\sim Y_{10}} \sin\theta \, d\theta \, d\phi = -3a_0 eE$$

Then $H_1 \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = E^{(1)} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix}$ becomes

$$\begin{pmatrix} 0 & -3eEa_0 \\ -3eEa_0 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix} = E^{(1)} \begin{pmatrix} u_1 \\ v_1 \end{pmatrix}$$

Diagonalize:

$$\begin{vmatrix} -E^{(1)} & -3eEa_0 \\ -3eEa_0 & -E^{(1)} \end{vmatrix} = 0$$

$$E^{(1)} = \pm 3eEa_0$$

For $E_+^{(1)} = +3eEa_0$, $\begin{pmatrix} u_1 \\ v_1 \end{pmatrix}_+ = \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ remember this is in the basis $\begin{pmatrix} \Psi_{200} \\ \Psi_{210} \end{pmatrix}$

For $E_-^{(1)} = -3eEa_0$, $\begin{pmatrix} u_1 \\ v_1 \end{pmatrix}_- = \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

*Conclusion:

The perturbations converts Ψ_{200} and Ψ_{210} both with $E = \dfrac{-mZe^4}{2\hbar^2 n^2} + 3eEa_0$ into

$$\boxed{\begin{aligned} & \Psi_+ = \tfrac{1}{\sqrt{2}} \left(\Psi_{200} - \Psi_{210} \right), \quad \text{with energy } E = \frac{-mZe^4}{2\hbar^2 n^2} + 3eEa_0 \\ & \text{and} \\ & \Psi_- = \tfrac{1}{\sqrt{2}} \left(\Psi_{200} + \Psi_{210} \right), \quad \text{with energy } E = \frac{-mZe^4}{2\hbar^2 n^2} - 3eEa_0 \end{aligned}}$$