The Ammonia Molecule can be thought of as a two-state system. The TDSE in Matrix Mechanics form is

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

In this notation, the state $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ stands for N atom up, & the state $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ stands for N atom down

If we know the H_{ij}, and the initial conditions $c_1(t=0)$ & $c_2(t=0)$, then we can solve for $c_1(t)$ & $c_2(t)$ for all time

What Hamiltonian should we use?? Remember, in QM we have no general purpose rules to determine the Hamiltonian. All we can do is guess, and then compare the results that we calculate to observations.

just one useful rules of thumb:

The simplest guess that we can make for $\hat{H}$ is that it is diagonal: $H_{ij} = E_i \delta_{ij}$ or

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

By making this guess, we are essentially guessing that the |N atom up⟩ state and |N atom down⟩ state are stationary states (or eigenstates of $\hat{H}$).

The TDSE reads as

$$i\hbar \frac{dc_1(t)}{dt} = E_1 c_1(t) \quad \Rightarrow \quad \text{Solv.} \quad c_1(t) = c_1(t=0)\, e^{-i\omega_1 t}$$

$$\& \quad i\hbar \frac{dc_2(t)}{dt} = E_2 c_2(t) \qquad c_2(t) = c_2(t=0)\, e^{-i\omega_2 t}$$

When H is diagonal, the two states evolve independent of each other. If we assume an initial condition such as

$$\begin{pmatrix} c_1(t=0) \\ c_2(t=0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

(Assume that NH_3 molecule starts with N atom up)

Then the particular solution is

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} e^{-i\omega_1 t} \\ 0 \end{pmatrix}, \quad \omega_1 \equiv E_1/\hbar$$

As time goes forward, what's the probability to find N atom up? Answer $P(\text{N atom up}) = |c_1(t)|^2 = 1$.

Similarly, $P(\text{N atom down}) = |c_2(t)|^2 = 0$.

Nothing is changing in time because we assumed that the $|\text{N atom up}\rangle$ state is an eigenstate of energy, (i.e., a stationary state.) We made this assumption by guessing that the Hamiltonian is diagonal in the $\{|\text{up}\rangle, |\text{down}\rangle\}$ basis.

We can go one step further and guess that $E_1 = E_2$, because the NH_3 molecule is symmetric. So there is no reason why $|up\rangle$ should have a different energy than $|down\rangle$. In this case the NH_3 molecule has only one energy, E_0, and the $|up\rangle$ & $|down\rangle$ states are <u>stationary</u>.

<u>However</u>, our observations of NH_3 reveal that it has <u>two</u> energies. To accomodate this, we can either abandon our assumption that NH_3 is symmetric, or abandon our guess that $\hat{H}$ is diagonal in the $\{|up\rangle, |down\rangle\}$ basis. Since we have good reason for believing that NH_3 is symmetric, and no reason for believing that $\hat{H}$ is diagonal, we should try a non-diagonal $\hat{H}$.

Let's guess $\hat{H} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$, E_0, A real.

Now the TDSE reads as

$$i\hbar \frac{dc_1(t)}{dt} = E_0 c_1(t) - A c_2(t)$$
$$i\hbar \frac{dc_2(t)}{dt} = -A c_1(t) + E_0 c_2(t).$$

Roughly speaking, the off-diagonal term (A) couples the two states together. Physically it means that $|up\rangle$ & $|down\rangle$ ... not stay

A nice way to solve these equations is to add them & subtract them:

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

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

Now define $c_I(t) \equiv c_1(t) + c_2(t)$

and $c_{II}(t) \equiv c_1(t) - c_2(t)$. Then

$$i\hbar \frac{dc_I(t)}{dt} = (E_0 - A)c_I(t) \Rightarrow c_I(t) = c_I(t=0)e^{-i\omega_I t}$$

$$i\hbar \frac{dc_{II}(t)}{dt} = (E_0 + A)c_{II}(t) \Rightarrow c_{II}(t) = c_{II}(t=0)e^{-i\omega_{II} t}$$

We have found two states which are stationary. Their time evolution is simple (just multiply by $e^{-i\omega t}$), and each has one energy: $E_0 - A = E_I$, $E_0 + A = E_{II}$. We see that E_0, which is H_{11} & H_{22}, is not an eigenvalue of $\hat{H}$, so it will not be an observed energy. The eigenvalues are $E_0 - A$ & $E_0 + A$.

So our eigenstates are

$$c_I \equiv c_1 + c_2 \quad \& \quad c_{II} \equiv c_1 - c_2.$$

We can write these as $|I\rangle = |\text{Na atom up}\rangle + |\text{Na atom down}\rangle$

& $|II\rangle = |\text{Na atom up}\rangle - |\text{Na atom down}\rangle$.

But to normalize them we should write

$$|I\rangle = \frac{1}{\sqrt{2}}|\text{up}\rangle + \frac{1}{\sqrt{2}}|\text{down}\rangle, \quad \text{energy} = E_0 - A$$

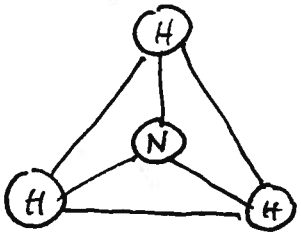
& $$|II\rangle = \frac{1}{\sqrt{2}}|\text{up}\rangle - \frac{1}{\sqrt{2}}|\text{down}\rangle, \quad \text{energy} = E_0 + A.$$

Lecture 32.5

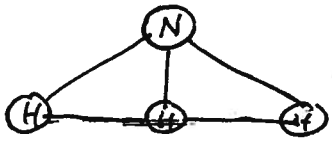
Two-State System: Ammonia Molecule (NH_3)

A triangle of H-atoms: Nitrogen above or below

"pyramid shape"

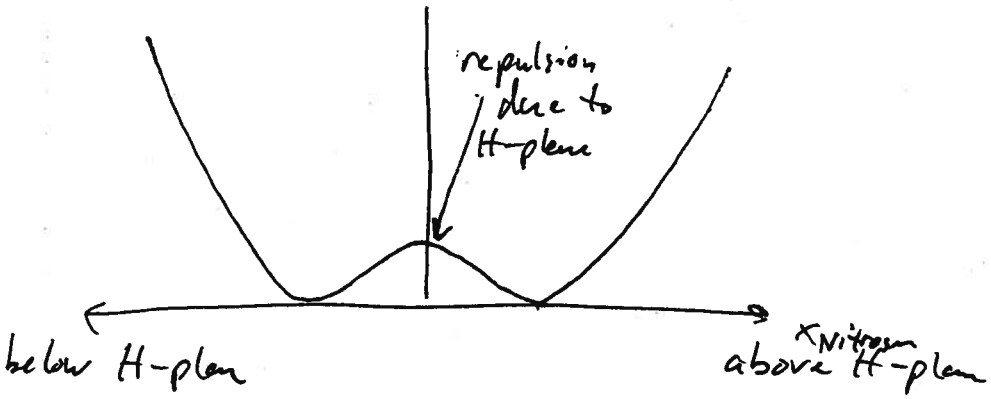


Top View



side view

Potential Seen by N atom:



Roughly speaking, N-atom takes one of two positions: up & down. This is an approximate two-state system

TDSE in Matrix Mechanics Form

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

State $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ stands for N atom up

State $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ stand for N atom down.

$C_1(t)$ = amplitude to observe N-atom up

$C_2(t)$ = " N-atom down

Hamiltonian is $\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$.

If we guess

$$H = \begin{pmatrix} H_{11} & \phi \\ \phi & H_{22} \end{pmatrix}$$

we are guessing that N-atom-up is stationary with energy H_{11}, & we are guessing that N-atom-down is stationary with energy H_{22}.

The potential $V(x)$ is symmetric, so, up & down should have same energy. Thus $H_{11} = H_{22}$. But we observe that Ammonia has 2 energies. So we must add a non-diagonal term $\Longrightarrow$ N-atom-up & N-atom-down are not stationary

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

$$i\hbar \frac{dc_1(t)}{dt} = E_0 c_1(t) - A c_2(t)$$

$$i\hbar \frac{dc_2(t)}{dt} = -A c_1(t) + E_0 c_2(t).$$

Solve by adding & subtracting both equations.

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

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

Define $c_1(t) + c_2(t) \equiv c_I(t)$

$c_1(t) - c_2(t) \equiv c_{II}(t)$

Then solution: $c_I(t) = c_I(t=0)\, e^{-i\omega_I t}$ $\quad \omega_I \equiv \frac{E_0 - A}{\hbar}$

$c_{II}(t) = c_{II}(t=0)\, e^{-i\omega_{II} t}$ $\quad \omega_{II} \equiv \frac{E_0 + A}{\hbar}$

c_I & c_{II} are stationary. They have a simple time dependence

Use Dirac Notation:

$$|I\rangle = |\text{Atom up}\rangle + |\text{Atom down}\rangle$$

$$|II\rangle = |\text{Atom up}\rangle - |\text{Atom down}\rangle$$

But Normalize them correctly:

$$|I\rangle \equiv \frac{1}{\sqrt{2}}\left(|up\rangle + |down\rangle\right) \quad \text{energy} = E_0 - A = E_I$$

$$|II\rangle \equiv \frac{1}{\sqrt{2}}\left(|up\rangle - |down\rangle\right) \quad \text{energy} = E_0 + A = E_{II}$$

Let's explicitly confirm that $|I\rangle$ & $|II\rangle$ are eigenstates of $\hat{H}$:

$$\begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \overset{??}{=} E_I \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$\hat{H}$ $\quad |I\rangle$ $\quad E_I\ |I\rangle$

Is this true?? Answer's key

Multiply the Matrix [illegible]

How do $|I\rangle$ & $|II\rangle$ evolve in time? Answer:

Answer: $|I\rangle_t = |I\rangle e^{-i\omega_I t}$ $\quad |II\rangle_t = |II\rangle e^{-i\omega_{II} t}$

How does $|up\rangle$ evolve in time?

Answer: $|I\rangle = \frac{1}{\sqrt{2}}|up\rangle + \frac{1}{\sqrt{2}}|down\rangle$

$|II\rangle = \frac{1}{\sqrt{2}}|up\rangle - \frac{1}{\sqrt{2}}|down\rangle$

i.e. $|up\rangle = \frac{1}{\sqrt{2}}|I\rangle + \frac{1}{\sqrt{2}}|II\rangle$

So at $t > t = 0$,

$|up\rangle_t = \frac{1}{\sqrt{2}}|I\rangle e^{-i\omega_I t} + \frac{1}{\sqrt{2}}|II\rangle e^{-i\omega_{II} t}$

$|up\rangle_t = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}|up\rangle + \frac{1}{\sqrt{2}}|down\rangle\right] e^{-i\omega_I t} + \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}|up\rangle - \frac{1}{\sqrt{2}}|down\rangle\right] e^{-i\omega_{II} t}$

$= \frac{1}{2}\left[e^{-i\omega_I t} + e^{-i\omega_{II} t}\right]|up\rangle + \frac{1}{2}\left[e^{-i\omega_I t} - e^{-i\omega_{II} t}\right]|down\rangle$

Also, $\omega_I = \frac{E_0 - A}{\hbar}$, $\omega_{II} = \frac{E_0 + A}{\hbar}$

$|up\rangle_t = \frac{1}{2} e^{-iE_0 t/\hbar}\left(e^{iAt/\hbar} + e^{-iAt/\hbar}\right)|up\rangle +$

$\frac{1}{2} e^{-iE_0 t/\hbar}\left(e^{iAt/\hbar} - e^{-iAt/\hbar}\right)|down\rangle$

$$\boxed{|up\rangle_t = e^{-iE_0 t/\hbar}\left[\cos(At/\hbar)|up\rangle + i\sin(At/\hbar)|down\rangle\right]}$$

If we start the system with N-atom-up, the system evolves in time like this.

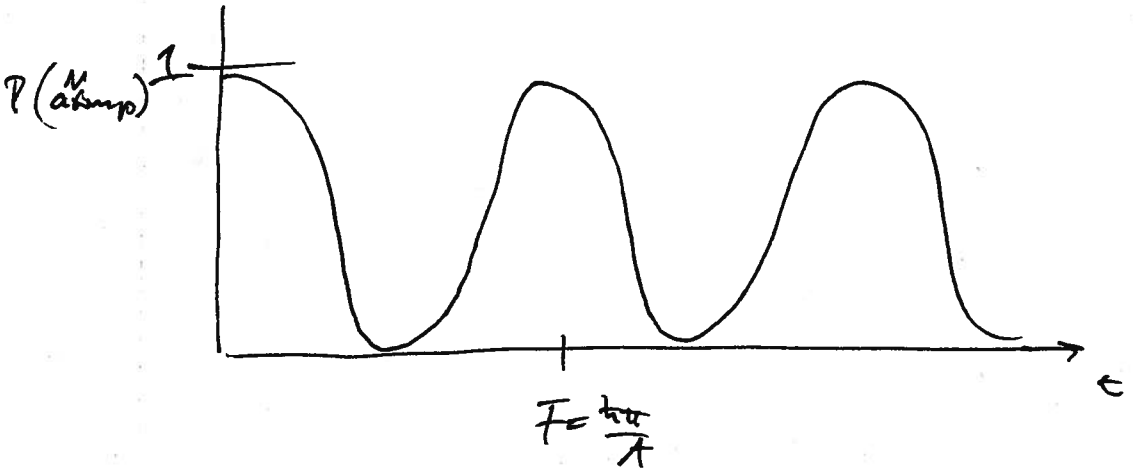
What does this mean? For example, what is the probability to observe N-atom-up as a function of time?

Amplitude to observe N-atom-up

$$= \langle up|up\rangle_t = e^{-iE_0 t/\hbar}\cos(A t/\hbar)$$

($|up\rangle$: base state; $|up\rangle_t$: state evolving in time)

$$P(up,t) = |\langle up|up\rangle_t|^2 = \cos^2(A t/\hbar)$$



Probability sloshes back and forth between $|up\rangle$ & $|down\rangle$. The only way to "stop the sloshing" is to put the system in an energy eigenstate like $|II\rangle$ or $|I\rangle$. But $|up\rangle_t$ never evolves into an energy eigenstate on its own

For the two-state Ammonia Molecule we have

$|N\text{atom up}\rangle = |up\rangle \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ in column vector form

$|N\text{atom down}\rangle = |down\rangle \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Essentially, we are imagining that the position of the N atom takes only two discrete values, up & down. This is a good approximation for this molecule

In our column vector notation, $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$, c_1 is the amplitude to find the N atom up, & c_2 is the amplitude to find N atom down. As time goes forward, these amplitudes can change.

∴ Our state vector is $\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$ for this system

& $|c_1(t)|^2 = P(N\text{atom up})$, $|c_2(t)|^2 = P(N\text{atom down})$

We can also use ket notation:

$$|\psi\rangle = c_1(t)\,|up\rangle + c_2(t)\,|down\rangle$$

Since any state can be written this way, $|up\rangle$ & $|down\rangle$ form a complete set.

Our Hamiltonian is

$$\hat{H} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$ in the $\{|up\rangle, |down\rangle\}$ basis.

We explicitly solved the TDSE for this system and we found stationary states

$|I\rangle \sim$ State I $\sim \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$, energy $= E_0 - A$

$|II\rangle \sim$ State II $\sim \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$, energy $= E_0 + A$.

We have put in the $\frac{1}{\sqrt{2}}$ factors to <u>normalize</u> these states: $\langle I|I\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} + \frac{1}{2} = 1$

and $\langle II|II\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} + \frac{1}{2} = 1$ ✓

~~The stationary states evolve in time as~~

We can explicitly confirm that $|I\rangle$ & $|II\rangle$ are stationary by showing that they are eigenstates of $\hat{H}$:

$\hat{H}|I\rangle \stackrel{?}{=} E_I|I\rangle$?? Is this true? Try it:

$$\underbrace{\begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}}_{\hat{H}} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(E_0 - A) \\ \frac{1}{\sqrt{2}}(E_0 - A) \end{pmatrix} = \underbrace{(E_0 - A)}_{\text{eigenvalue}} \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}}_{\text{eigenvector}} \checkmark$$

Similarly, $\hat{H}|II\rangle = E_{II}|II\rangle$ (Try it.)

states $|I\rangle$ & $|II\rangle$ evolve in time & in a very simple manner:

IF $|\psi\rangle_{t=0} = |I\rangle$, then $|\psi\rangle_t = |I\rangle e^{-iE_I t}$

If $|\psi\rangle_{t=0} = |II\rangle$, then $|\psi\rangle_t = |II\rangle e^{-iE_{II} t}$

How do the $|up\rangle$ and $|down\rangle$ states evolve in time?

To answer, re-write $|up\rangle$ & $|down\rangle$ in terms of $|I\rangle$ & $|II\rangle$

This is I, II in terms of up, down

$$\boxed{\begin{aligned} |I\rangle &= \tfrac{1}{\sqrt{2}}|up\rangle + \tfrac{1}{\sqrt{2}}|down\rangle \\ |II\rangle &= \tfrac{1}{\sqrt{2}}|up\rangle - \tfrac{1}{\sqrt{2}}|down\rangle \end{aligned}}$$ } Add & Subtract these equations

$\therefore$
$$|I\rangle + |II\rangle = \sqrt{2}|up\rangle$$
$$|I\rangle - |II\rangle = \sqrt{2}|down\rangle$$

$\therefore$
$$\boxed{\begin{aligned} |up\rangle &= \tfrac{1}{\sqrt{2}}|I\rangle + \tfrac{1}{\sqrt{2}}|II\rangle \\ |down\rangle &= \tfrac{1}{\sqrt{2}}|I\rangle - \tfrac{1}{\sqrt{2}}|II\rangle \end{aligned}}$$

This is up, down in terms of I, II.

Now we can write down how $|up\rangle$ & $|down\rangle$ evolve in time

IF $|\psi\rangle = |up\rangle$ at $t = 0$, then

$$|\psi\rangle_t = \tfrac{1}{\sqrt{2}}|I\rangle e^{-i\omega_I t} + \tfrac{1}{\sqrt{2}}|II\rangle e^{-i\omega_{II} t}$$

= Now substitute I, II → up, down on right hand side

If $|\psi\rangle = |up\rangle$ at $t = 0$,

$$|\psi\rangle_t = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|up\rangle + \frac{1}{\sqrt{2}}|down\rangle\right)e^{-i\omega_I t} + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|up\rangle - \frac{1}{\sqrt{2}}|down\rangle\right)e^{-i\omega_{II} t}$$

$$= \frac{1}{2}\left(e^{-i\omega_I t} + e^{-i\omega_{II} t}\right)|up\rangle + \frac{1}{2}\left(e^{-i\omega_I t} - e^{-i\omega_{II} t}\right)|down\rangle.$$

∴ If we start with the Nitrogen atom up, the amplitude to find it up at a later time is

$$\langle up|\psi\rangle_t = \frac{1}{2}\left(e^{-i\omega_I t} + e^{-i\omega_{II} t}\right)$$ (Since $\langle up|up\rangle = 1$ & $\langle up|down\rangle = 0$

We can simplify further using $\omega_I = (E_0 - A)/\hbar$

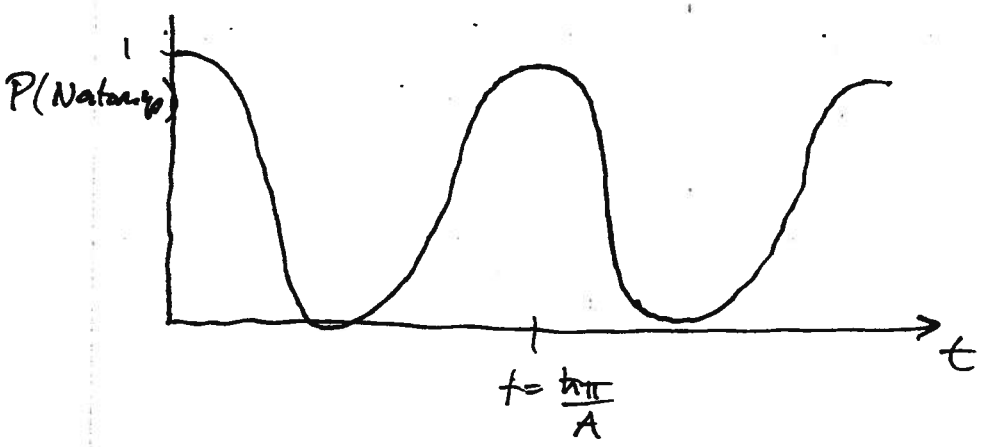
& $\omega_{II} = (E_0 + A)/\hbar$

$$\langle up|\psi\rangle_t = \frac{1}{2}e^{-iE_0 t/\hbar}\left(e^{iAt/\hbar} + e^{-iAt/\hbar}\right) = e^{-iE_0 t/\hbar}\cos(At/\hbar)$$

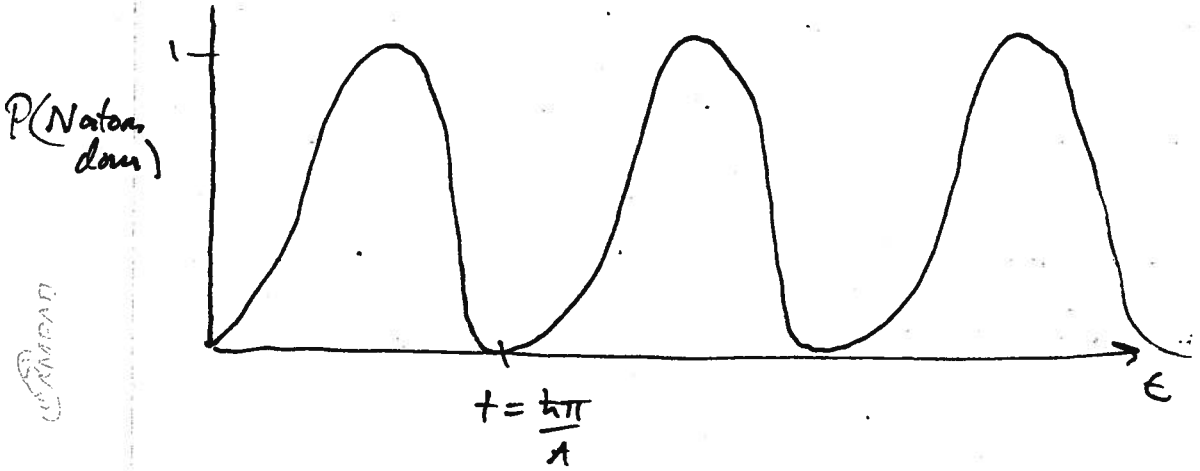
Similarly, if we start with N atom up, the amplitude to find N atom down is

$\langle down|\psi\rangle_t = e^{-iE_0 t/\hbar}\sin(At/\hbar)$

∴ If we start with N atom up, the Probability to find it up at a later time oscillates as $\cos^2(At/\hbar)$.



Where is the Probability going? Answer: into P(Natom down)



For any two state system which starts out in a non-stationary state, the probability "sloshes back and forth" between the two states. The only way to "stop the sloshing" is to start in a stationary state → an energy eigenstate.

For the Ammonia Molecule problem, we worked in the up & down basis. In this basis,

$\begin{pmatrix}1\\0\end{pmatrix}$ means N-atom-up & $\begin{pmatrix}0\\1\end{pmatrix}$ means N-atom-down

The stationary states in this basis are

$\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}$ ~ energy eigenstate I in up & down basis $E_I = E_0 - A$

$\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix}$ ~ energy eigenstate II in up & down basis $E_{II} = E_0 + A$.

The elements of these column vectors are QM amplitudes to observe N-atom-up & N-atom-down:

$\begin{pmatrix}C_1 \leftarrow \text{QM amplitude for N-atom-up}\\ C_2 \leftarrow \text{QM amplitude for N-atom-down}\end{pmatrix}$

~~We don't have to work in the up & down basis.~~

We can also work in the energy basis; where

$\begin{pmatrix}1\\0\end{pmatrix}$ means energy eigenstate I & $\begin{pmatrix}0\\1\end{pmatrix}$ means energy eigenstate II in the energy basis.

We found that up & down in terms of I & II are

$\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}$ means N-atom-up in the energy basis

$\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix}$ means N-atom-down in the energy basis

The elements of the column vectors in the energy basis are QM amplitudes

$$\begin{pmatrix} c_I \\ c_{II} \end{pmatrix}$$

c_I ← QM amplitude for energy E_I

c_{II} ← QM amplitude for energy E_{II}.

in the energy basis

We see that the meaning of the column vectors depends on the basis that we use.

Similarly, the operators an operator matrix looks different in different basis. For example

$$\hat{H} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$ in the up & down basis

$$\hat{H} = \begin{pmatrix} E_I & 0 \\ 0 & E_{II} \end{pmatrix}$$ in the energy basis

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

In general we need to be able to convert our state vectors & operators from one basis to another. How can we transform a state vector or operator matrix from one basis to another?

For a state vector, we can always expand it in another basis like this:

Let i & j label the states in basis A
Let m & n label the state in basis B

An arbitrary state in basis A is written

$$|\psi\rangle = \left(\sum_i |i\rangle\langle i|\right)|\psi\rangle = \sum_i |i\rangle \underbrace{\langle i|\psi\rangle}_{\text{call this } a_i} = \sum_i a_i |i\rangle$$

The $\{a_i\}$ are the column vector elements in basis A.
Similarly, in basis B the arbitrary state is
$|\psi\rangle = \sum_m b_m |m\rangle$, $\{b_m\}$ are the column vector elements in basis B.

Suppose we know the $\{a_i\}$, and we want to calculate the $\{b_m\}$. How can we do this?
Like this

$$b_m = \langle m|\psi\rangle = \langle m|\left(\sum_i |i\rangle\langle i|\right)|\psi\rangle$$

$$= \sum_i \langle m|i\rangle \underbrace{\langle i|\psi\rangle}_{a_i}$$

$$b_m = \sum_i a_i \langle m|i\rangle = \sum_i a_i U_{mi}, \text{ where } U_{mi} \equiv \langle m|i\rangle$$

This is a matrix equation. It says to transform from the A basis to the B basis we must know the overlap of all the basis vectors in both the bases.

In Matrix Notation

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle 1|1\rangle & \langle 1|2\rangle & \langle 1|3\rangle & \cdots \\ \langle 2|1\rangle & \langle 2|2\rangle & \langle 2|3\rangle & \cdots \\ \langle 3|1\rangle & \langle 3|2\rangle & \langle 3|3\rangle & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}$$

or $|\psi_m\rangle = \hat{U}\,|\psi_j\rangle$ in Dirac Notation

In this matrix, the bra-vectors are states in Basis B, and the ket-vectors are state in basis A. Umi

The ~~Umi~~ matrix transforms the state vector from ~~the~~ Basis A to Basis B.

Similarly, we can transform an operator matrix from A to B. Let $\hat{F}$ be some operator whose matrix elements F_{ij} are known in basis A:

$$\hat{F} = \begin{pmatrix} F_{11} & F_{12} & F_{13} & \cdots \\ F_{21} & F_{22} & F_{23} & \cdots \\ F_{31} & F_{32} & F_{33} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \qquad F_{ij} \equiv \langle i|\hat{F}|j\rangle$$

How can we calculate F_{mn}, the matrix elements in Basis B?

Answer:

$$F_{mn} = \langle m|\hat{F}|\hat{u}\rangle = \langle m|\left(\sum_i |i\rangle\langle i|\right)\hat{F}\left(\sum_j |j\rangle\langle j|\right)|n\rangle$$

$$= \sum_{ij} \langle m|i\rangle \langle i|\hat{F}|j\rangle \langle j|n\rangle$$

$$= \sum_{ij} \langle m|i\rangle F_{ij} \langle j|n\rangle$$

$$F_{mn} = \sum_{ij} U_{mi} F_{ij} U^*_{nj}$$

or $\hat{F}' = \hat{U}\hat{F}\hat{U}^{-1}$

This is a Matrix Equation it says

$$\begin{pmatrix} F_{11} & F_{12} & F_{13} \cdots \\ F_{21} & F_{22} & F_{23} \cdots \\ \vdots & \vdots & \vdots \end{pmatrix} = \begin{matrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & & \end{matrix}$$

The matrix U_{mi} is related to U_{im} because

$$U_{mi} = \langle m|i\rangle = \left(\langle i|m\rangle\right)^* = U^*_{im}$$

The $\hat{U}$ matrix is a "Unitary" matrix, which means that it preserves the normalization of state vectors which it transforms. Mathematically, for a Unitary Matrix the inverse matrix U^{-1} is the Hermitian Adjoint:

$$\hat{U}^\dagger = \hat{U}^{-1} \quad \text{for a Unitary matrix}$$

Therefore $\hat{U}\hat{U}^{-1} = 1$ ← identity matrix

$\hat{U}\hat{U}^\dagger = 1$ ✓

$$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$$

We call the transformation defined by $\hat{U}$ a "Unitary-Similarity transformation". State vectors transform as

$$|\psi'\rangle = \hat{U}|\psi\rangle$$

Operators transform as

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^{-1}$$

This is how we transform from one basis to another.

Recap of Transformation of Basis in Matrix Mechanics.

Let i & j label states in basis A

Let m & n label states in basis B

To transform a ~~state~~ column vector $\{a_i\}$ from basis A to a column vector $\{b_m\}$ in basis B do this.

$b_m = \sum_i a_i U_{mi}$ where $U_{mi} \equiv \langle m|i\rangle$ = overlap of the basis B states with the basis A states.

or same thing

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} \langle 1|1\rangle & \langle 1|2\rangle & \langle 1|3\rangle \\ \langle 2|1\rangle & \langle 2|2\rangle & \langle 2|3\rangle \\ \langle 3|1\rangle & \langle 3|2\rangle & \langle 3|3\rangle \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

or same thing

$$|\psi_m\rangle = \hat{U}|\psi_i\rangle$$

To transform a Matrix written in basis A ($F_{ij} \equiv \langle i|\hat{F}|j\rangle$) to basis B ($F_{mn} \equiv \langle m|\hat{F}|n\rangle$) do this.

~~$F_{mn} = \sum_{ij} U_{mi} F_{ij} U_{jn}$~~

$$F_{mn} = \sum_{ij} \underbrace{\langle m|i\rangle}_{U_{mi}} \underbrace{\langle i|\hat{F}|j\rangle}_{F_{ij}} \underbrace{\langle j|n\rangle}_{\text{call this } V_{jn}}$$ using Identity operator twice

Since $V_{jn} = \langle j|n\rangle = \left(\langle n|j\rangle\right)^* = U_{nj}^*$

we can write

$$F_{mn} = \sum_{ij} U_{mi} F_{ij} U^{*}_{nj}$$

The U matrix has the following property which we will prove a little later:

$$U^{*}_{nj} = (U^{-1})_{jn}$$

(U^{-1}: inverse matrix; note that these are reversed)

$$\therefore \quad F_{mn} = \sum_{ij} U_{mi} F_{ij} (U^{-1})_{jn}$$ This is a Matrix Multiplication down twice

In Matrix Notation $\boxed{F_{\text{basis B}} = U F_{\text{basis A}} U^{-1}}$

So we use the Matrix U and its inverse to convert the operator F from basis A to basis B.

Matrix Properties & the names we give them

Definition of Matrix Multiplication: AB in matrix notation

or $(AB)_{mn} = \sum_{p} A_{mp} B_{pn}$ in summation or matrix element notation

Definition of Inverse Matrix

A^{-1} is defined such that $A^{-1}A = 1$ ← identity matrix.

In Matrix Element Notation:

$$\sum_{p} (A^{-1})_{mp} A_{pn} = I_{mn} = \delta_{mn}$$

Definition of Transpose

$$(\tilde{A})_{mn} = A_{nm}$$ "reverse the rows & Columns"

(m, n reversed)

Definition of Hermitian Adjoint

From our wave mechanics definitions

$\langle \hat{A}^+ \alpha | \beta \rangle \equiv \langle \alpha | \hat{A} \beta \rangle$ definition of $\hat{A}^+$

$\downarrow$

$A_{\alpha\beta}$ in matrix element notation

Reverse this bracket by taking the complex conjugate

$\langle \beta | \hat{A}^+ \alpha \rangle^*$

$\downarrow$

$(A^+_{\beta\alpha})^*$

$\uparrow$

in matrix element notation

$$\therefore (A^+)^*_{\beta\alpha} \equiv A_{\alpha\beta}$$

(β, α reversed)

Definition of A^+ in Matrix Element notation.

Definition of a "Hermitian Matrix"

IF $A^+ = A$ we say "A is Hermitian"

Since $(A^+)^*_{\beta\alpha} \equiv A_{\alpha\beta}$ (Definition of A^+)

For a "Hermitian Matrix", $A^+ = A$, so we have

$$(A)^*_{\beta\alpha} = A_{\alpha\beta}$$ For a Hermitian Matrix

A Matrix is Hermitian if reversing rows & columns and taking the complex conjugate gives the same matrix. Example:

$\begin{pmatrix} 1 & 3+i \\ 3-i & 5 \end{pmatrix}$ is Hermitian $\qquad \begin{pmatrix} 1 & 3 \\ 3 & i \end{pmatrix}$ is not Hermitian

i violates Hermiticity

Definition of a Unitary Matrix

If $A^+ = A^{-1}$, we say "A is Unitary"

In matrix element notation,

if $(A^+)_{mn} = (A^{-1})_{mn}$ we say "A is Unitary"

$\downarrow$

if $A^*_{nm} = (A^{-1})_{mn}$ we say "A is Unitary"

if $A^*_{nm} = (A^+)_{mn}$ we say "A is unitary"

For a Unitary Matrix $AA^+ = 1$ because $A^+ = A^{-1}$

In Matrix Element notation,

$$(AA^+)_{mn} = \delta_{mn}$$

$$\text{or} \quad \sum_p A_{mp} A^+_{pn} = \delta_{mn}$$

$$\text{or} \quad \sum_p A_{mp} A^*_{np} = \delta_{mn}$$

For a unitary Matrix A

Does Uni have this property? Let's check:

$$\sum_i U_{mi} U_{ni}^* \overset{?}{=} \delta_{mn}$$ Is this true?

$$\sum_i \langle m|i\rangle \left(\langle n|i\rangle\right)^* \overset{?}{=} \delta_{mn}$$

$$\sum_i \langle m|i\rangle\langle i|n\rangle \overset{?}{=} \delta_{mn}$$

$$\langle m|\left(\sum_i |i\rangle\langle i|\right)|n\rangle \overset{?}{=} \delta_{mn}$$

$$\langle m|n\rangle \overset{?}{=} \delta_{mn} \Leftarrow \underline{\text{Yes}},$$ because the states of Basis B are orthonormal.