Lecture 34 Transformation of Bases

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:

$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

c_1 ← QM amplitude for N-atom-up

c_2 ← QM amplitude for N-atom-down

~~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

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

c_1 — QM amplitude for energy E_{I}

c_2 — QM amplitude for energy E_{II}.

in the energy basis

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

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

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

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

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

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

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

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

$$b_m = \sum_i a_i \langle m|i\rangle = \sum_i a_i U_{mi}$$

, 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 <u>overlap</u> of all the basis vectors in both bases.

U_{mi} matrix

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 $|\Psi_m\rangle = \hat{U} \cdot |\Psi_i\rangle$ in Dirac Notation

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

The U_{mi} 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:

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

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

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

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

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

~~This is a Matrix Equation it says~~

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

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:

$$\hat{U}^{+} = \hat{U}^{-1} \quad \text{for a unitary matrix}$$

Therefore $\hat{U}\hat{U}^{-1} = 1 \leftarrow$ identity matrix $\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$

$$\hat{U}\hat{U}^{+} = 1$$

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

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

Operators transform as

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

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.

⇕ same thing

or

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

or ⇕ same thing

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

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

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

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

inverse matrix

note that these are reversed

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

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

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"

reversed

Definition of Hermitian Adjoint

From our wave mechanics definition:

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

$\langle \alpha | \hat{A}\beta \rangle \downarrow A_{\alpha\beta}$ in matrix element notation

Reverse this bracket by taking the complex conjugate

$$\langle \hat{A}^{+}\alpha | \beta \rangle \downarrow \left(\langle \beta | \hat{A}^{+}\alpha \rangle \right)^{*} \downarrow \left(A^{+}_{\beta\alpha} \right)^{*}$$

in matrix element notation

$$\boxed{\therefore \; (A^{+})^{*}_{\beta\alpha} \equiv A_{\alpha\beta}}$$ Definition of A^{+} in Matrix Element notation.

reversed

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 <u>and</u> taking the complex conjugate gives the same matrix. Example:

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

violates Hermiticity

<u>Definition of a Unitary Matrix</u>

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

In ~~oth~~ matrix element notation,

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

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 U_{mi} have this property? Let's check:

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

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

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

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

$\langle m|n\rangle \stackrel{?}{=} \delta_{mn} \leftarrow$ <u>Yes</u>, because the states of Basis B are orthonormal.

Some simple QM systems in 1D position spac

Schroedinger Eq in position space: $\psi''(x) = -\frac{2m}{\hbar^2}(E-V(x$

Classically Allowed Region (CAR): $E - V(x) > 0$

$\Rightarrow \psi(x)$ oscillates with spatial ~~wavenumber~~ ~~wavelength~~ wavenumber

Classically Forbidden Region (CFR): $E - V(x) < \emptyset$

$\Rightarrow \psi(x)$ decays

Other conditions for ψ:

1. ψ is continuous
2. ψ' is continuous when $V(x)$ is not infinite
3. ψ should be normalizable. (But we ignore this sometimes when considering "beams of particles")

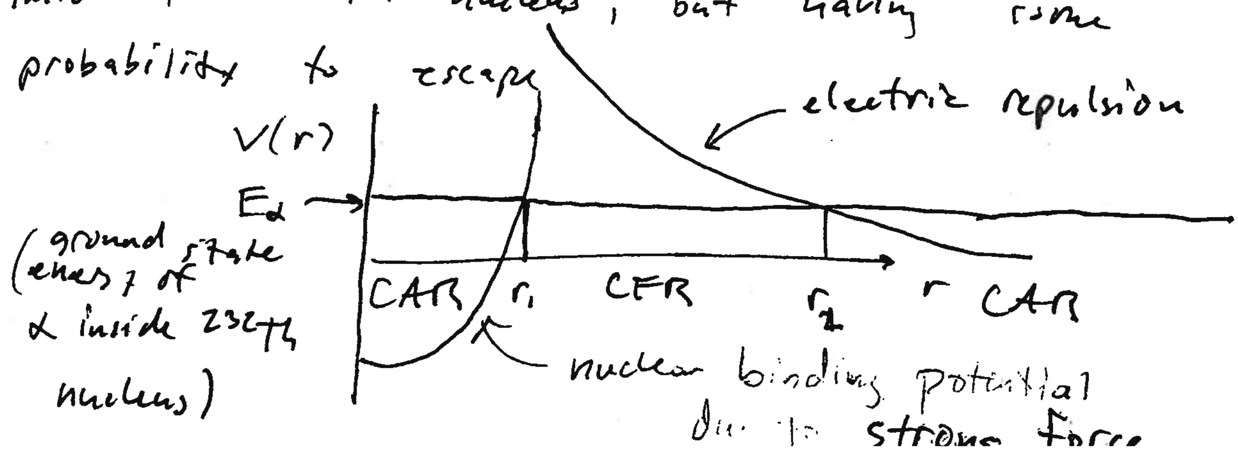
Alpha Decay

Heavy nuclei like U-238 can decay by emitting an alpha-particle (the nucleus of ^4He: ⓟⓝ ⓟⓝ)

Ex: $^{238}U \rightarrow {}^{234}Th + \alpha$ (Half-life ~ 10^9 years)

$N,Z = 238, 92$ $\quad N,Z = 234, 90 \quad N,Z = 4, 2$

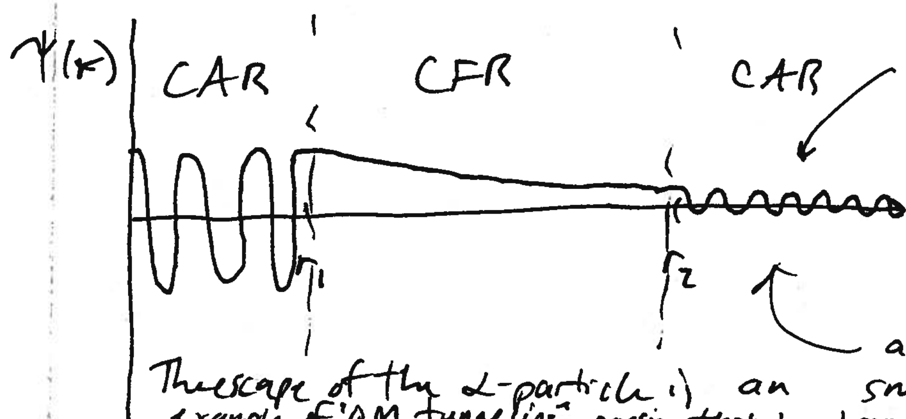
We can think of the alpha particle being bound inside the ^{234}Th nucleus, but having some probability to escape



How does the α-particle escape during α-decay?

Well, an α outside the ^{232}Th nucleus is repelled from the nucleus by the electric force (both are positively charged. So the potential must fall off like $\frac{1}{r}$.

The wavefunction must look like



The amplitude of ψ outside r_2 represents the probability of observing α-decay.

amplitude here is small because of exponential decay in the CF

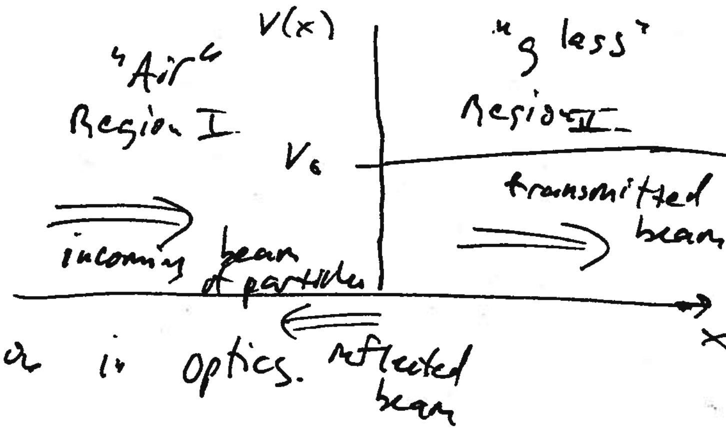
The escape of the α-particle is an example of "QM tunneling" passing through a barrier

α-decay was the first problem in nuclear physics which was explained by QM.

Potential Step

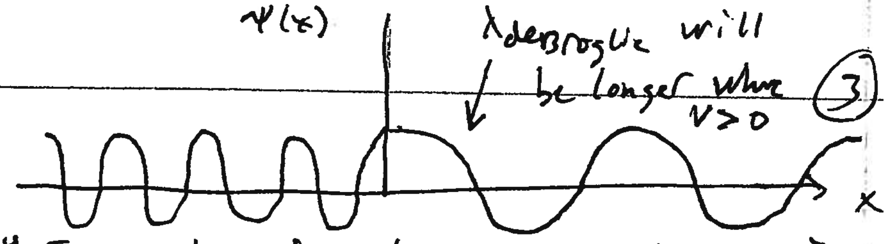
$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } x > 0 \end{cases}$$

This is the QM equivalent to a change in the index of refraction in optics.



~~[illegible]~~

We imagine a beam of particles striking the barrier from the left. How much is transmitted, and how much is reflected?



Two Cases

1 $E > V_0$ "Everywhere is classically allowed"

Assume $\psi_{incoming} = Ae^{ikx}$ ← incoming momentum eigenstate, our initial condition

Region I: $\psi_1'' = -k_1^2\psi_1$, $k_1^2 = \frac{2m}{\hbar^2}E$

Region II: $\psi_2'' = -k_2\psi_2$, $k_2^2 = \frac{2m}{\hbar^2}(E-V_0)$

$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$ ← reflected beam, travelling to the left. a

$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$ ← this represents a beam travelling to the left in Region II. We assume $D = \emptyset$.

incoming beam

transmitted beam

These wavefunctions are momentum eigenstates, which are un-normalizable. So we consider $A, B, C, \& D$ to represent the relative intensities of these beams.

Boundary Conditions

(i) $\psi_1(x=0) = \psi_2(x=0) \Rightarrow A + B = C$

(ii) $\psi_1'(x=0) = \psi_2'(x=0) \Rightarrow k_1(A-B) = k_2C$

Solution: $2k_1A = (k_1+k_2)C$ (k_1(ii) + (i))

$$\boxed{C = \left(\frac{2k_1}{k_1+k_2}\right)A} \quad \& \quad \boxed{B = \left(\frac{k_1-k_2}{k_1+k_2}\right)A}$$

relative incoming amplitude

Suppose there is no potential step: $V_0 = \emptyset$.
Then $k_1 = k_2$ & $B = \emptyset \implies$ no reflected beam
$C = 1 \implies 100\%$ transmission.

/ → Finish here

Probability Current

We can define a "probability current" $\to J$ which is analogous to electric current. Where $J > \emptyset$, particle probability is increasing to the right. Where $J < \emptyset$, particle probability is increasing to the left.

We define (in 1D) $J \equiv \frac{\hbar}{2mi}\left(\psi^* \psi' - \psi \psi^{*\prime}\right)$

(see Homework #10 for the motivation).

For the simple step,

$$J_{incoming} = \frac{\hbar}{2mi}\left(2ik_1 |A|^2\right) = \frac{\overset{\hbar k_1}{p_1}}{m}|A|^2$$

$$J_{transmitted} = \frac{\hbar k_2}{m}|C|^2$$

$$J_{reflected} = -\frac{\hbar k_1}{m}|B|^2$$

Define the Transmission Coefficient & Reflection Coefficient:

$$T \equiv \frac{|J_{transmitted}|}{|J_{incoming}|} = \frac{k_2}{k_1}\left|\frac{C}{A}\right|^2 = \frac{4k_1k_2}{(k_1+k_2)^2} = \frac{4\left(k_2/k_1\right)}{\left(1+k_2/k_1\right)^2}$$

$$R \equiv \frac{|J_{reflected}|}{|J_{incoming}|} = \left|\frac{B}{A}\right|^2 = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} = \frac{\left(1-k_2/k_1\right)^2}{\left(1+k_2/k_1\right)^2}$$

Also note that if $E = V_0$, then $k_2 = \emptyset$, & $T = \emptyset$, 100% refl.