Linear Algebra and Matrix Mechanics

Reference: Griffiths Appendix A
Griffiths Ch. 3, especially 3.6.

We've spent a great deal of time solving the Schrödinger equation,

$$\hat{H}\psi_n = E\psi_n$$

, trying to determine the energy eigenstates ψ_n. Now, let's imagine some system which has a finite number of energy levels. For concreteness, let's say there are 3 levels. We know that superposition states like

$$\psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{3}}\psi_2 + \frac{1}{\sqrt{6}}\psi_3$$

are possible.

[Remember that the probability that I'll measure a certain value of E is the square of the coefficient, so for example the probability I'll measure E_2 is $\left(\frac{1}{\sqrt{3}}\right)^2$. And, of course $\left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{3}}\right)^2 + \left(\frac{1}{\sqrt{6}}\right)^2 = 1$ so this state is normalized].

Given that this system has only 3 levels, we could represent this state as $\psi = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{3} \\ 1/\sqrt{6} \end{pmatrix}$, it looks a lot like a vector with 3 components. Any state of this system could be represented in vector form.

Here is another example of a system which we could represent this way: Last semester we learned that a system with a known value of total angular momentum $L^2 = \ell(\ell+1)\hbar^2$, can have z component of angular momentum $L_z = -\ell\hbar, -(\ell-1)\hbar, \ldots -\hbar, 0, \hbar \ldots \ell\hbar$

If we think of all possible states with $\ell = 2$, we could represent such states as a vector with 5 components, with each component representing possible values of L_z. (Possible values are $-2\hbar, -\hbar, 0, \hbar, 2\hbar$)

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As an example, consider a hydrogen atom in this state

$$\psi = \frac{1}{2}\psi_{321} + \frac{1}{2}\psi_{320} + \frac{1}{\sqrt{2}}\psi_{32-2}$$

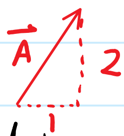
could be represented as the following vector where the possible values of L_z run from $2\hbar \ldots -2\hbar$ from top to bottom.

$$\begin{array}{cc} \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \\ 0 \\ 1/\sqrt{2} \end{pmatrix} & \begin{array}{c} (2\hbar) \\ (\hbar) \\ (0) \\ (-\hbar) \\ (-2\hbar) \end{array} \end{array}$$

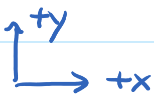
The purpose of these examples is just to illustrate how vectors (and matrices) are a natural language of QM which we want to develop now. So, we'll start by introducing some notation.

The quantum mechanical <u>state</u> of a particle is represented by the <u>state vector</u> $|\psi\rangle$. This is also called a "ket".

I think the best way to think about kets is like vectors. Go back to your intro class and suppose you have a vector $\vec{A}$



Technically, the vector is an abstract quantity represented by this arrow. Now one of you might come along and say

"I chose this coordinate system  , and then the vector has components $A_x = 1$, $A_y = 2$, $A_z = 0$

$$\vec{A} \rightarrow \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}."$$

But then someone else may come along and say

"I chose coordinates  and so the vector has components $A_x = 2$, $A_y = -1$, $A_z = 0$ so for me $\vec{A} \rightarrow \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}$"

The choice of coordinate system does not affect the vector. The vector $\vec{A}$ (the arrow drawn above) is the same for both observers. They have <u>represented</u> the vector differently by choosing different coordinate bases.

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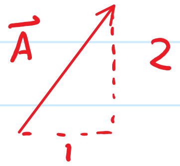
The ket $|\psi\rangle$ is like the vector. It is an abstract entity independent of any one coordinate basis. $|\psi\rangle$ can be <u>represented</u> by a column of numbers with respect to some basis

<u>Basis Vectors</u> - A basis is a set of vectors which are <u>linearly independent</u> (each one <u>cannot</u> be expressed as a combination of the others) and which span the space (meaning that <u>all</u> vectors can be expressed as combinations of the basis vectors).

Going back to the example with



, usually our basis vectors are $\hat{i}, \hat{j}, \hat{k}$ unit vectors in the x, y, z directions.

$$\hat{i} \rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \hat{j} \rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \hat{k} \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

components.

So, we can write $\vec{A} = 1 \cdot \hat{i} + 2 \cdot \hat{j} + 0\,\hat{k}$

$$\rightarrow 1\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + 2 \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + 0\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$$

rather than use $\hat{i}, \hat{j}, \hat{k}$ for a case with more dimensions (we might run out of letters), we use the notation $|e_i\rangle$ to denote the i^{th} basis vector. For the $\ell = 2$ case we could use

$$|e_1\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad |e_2\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad |e_3\rangle \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{etc...}$$

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a general vector $|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle + a_4|e_4\rangle$

$$|\alpha\rangle \rightarrow \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

where a_1, a_2, a_3, a_4 are the components of the vector.

Bras and Kets (Dirac Notation)

Suppose we have 2 kets $|\alpha\rangle$ and $|\beta\rangle$ represented as column vectors (with respect to some basis)

$$|\alpha\rangle \rightarrow \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \qquad |\beta\rangle \rightarrow \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

We now define the "bra" (you'll see why the name in a second)

$$\langle\alpha| \rightarrow (a_1^* \ a_2^* \ \ldots \ a_N^*) \qquad \langle\beta| \rightarrow (b_1^* \ b_2^* \ldots \ b_N^*)$$

In other words if you have a ket represented as a column vector, the corresponding bra is a row vector with all elements complex conjugated.

Inner Product - this is a generalization of the dot product in 3-dimensions

inner product: $\langle \text{bra}|\text{ket}\rangle$ = "bracket" (Dirac was a funny guy...)

this operation produces a number (also known as the scalar product).

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + a_3^* b_3 + \ldots$$

or, just multiply the row x column:

$$= (a_1^* \ a_2^* \ \ldots \ a_N^*) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

Poll Q: Which of the following identities is correct?

A.) $\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle$ C.) $\langle \beta | \alpha \rangle = -\langle \alpha | \beta \rangle$

B.) $\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^*$ D.) $\langle \beta | \alpha \rangle = -\langle \alpha | \beta \rangle^*$

Orthonormal Basis

Using the inner product, we can define an orthonormal basis as one where

$$\langle e_i | e_j \rangle = \delta_{ij}$$

i.e. $\langle e_1 | e_1 \rangle = \langle e_2 | e_2 \rangle = \langle e_3 | e_3 \rangle \ldots = 1$

basis vectors are normalized. This is equivalent to $\hat{i} \cdot \hat{i} = 1$

$$\langle e_1 | e_2 \rangle = \langle e_1 | e_3 \rangle = \langle e_2 | e_3 \rangle \ldots = 0$$

basis vectors are orthogonal. This is equivalent to $\hat{i} \cdot \hat{j} = 0$
$\hat{j} \cdot \hat{k} = 0$.

When working in an orthonormal basis, it is easy to pick out a particular component. For example

$$|\alpha\rangle = a_1 |e_1\rangle + a_2 |e_2\rangle + a_3 |e_3\rangle$$

sandwich each term on the left by $\langle e_2|$.

$$\langle e_2 | \alpha \rangle = a_1 \langle e_2 | e_1 \rangle + a_2 \langle e_2 | e_2 \rangle + a_3 \langle e_2 | e_3 \rangle$$
$$= 0 + a_2 + 0 = a_2$$

$a_2 = \langle e_2 | \alpha \rangle$, which generalizes to $a_i = \langle e_i | \alpha \rangle$

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Now, let's write this in a funny looking way:

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle \qquad (\{|e_i\rangle\} \text{ spans the space})$$
$$= \langle e_1|\alpha\rangle|e_1\rangle + \langle e_2|\alpha\rangle|e_2\rangle + \langle e_3|\alpha\rangle|e_3\rangle$$

using result from previous page.

$$|\alpha\rangle = |e_1\rangle\langle e_1|\alpha\rangle + |e_2\rangle\langle e_2|\alpha\rangle + |e_3\rangle\langle e_3|\alpha\rangle$$

remember $\langle e_1|\alpha\rangle$, $\langle e_2|\alpha\rangle$, $\langle e_3|\alpha\rangle$ are just numbers so it doesn't matter if you write them on the left or right of the vector (ket) $|e_i\rangle$

$$|\alpha\rangle = \sum_{i=1}^{3} |e_i\rangle\langle e_i|\alpha\rangle$$

Think about this piece as an operator, let's call it $\hat{O}$

$|\alpha\rangle = \hat{O}|\alpha\rangle$, but the only way that's possible is if $\hat{O} = \mathbb{1}$ the identity matrix.

∴ We have the strange looking relation

$$\boxed{\sum_n |e_n\rangle\langle e_n| = 1}$$

Summing this combination for an orthonormal basis gives the identity operator.

This is sometimes called the completeness relation. It is one of the most useful formulas in QM, believe it or not.

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Operators - An operator is a linear transformation, which acts on kets. In other words, after an operator acts on a ket, you end up with another ket (usually different from the first).

operator.

$$|\beta\rangle = \hat{Q}|\alpha\rangle$$

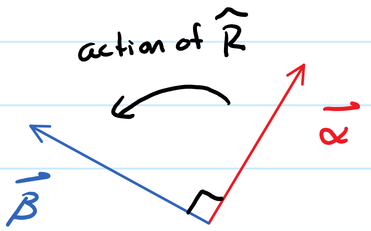
Kets

Numbers.

$$\hat{Q}\left(a_1|\alpha_1\rangle + a_2|\alpha_2\rangle\right) = a_1\hat{Q}|\alpha_1\rangle + a_2\hat{Q}|\alpha_2\rangle$$

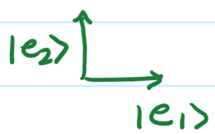
This is what we mean by a linear operator.

Going back to the graphical representation, suppose we have an operator which is an instruction to rotate a vector counterclockwise by 90°.



or, in our new notation : $|\beta\rangle = \hat{R}|\alpha\rangle$

This relationship is completely abstract. It is true in any coordinate system. Let's now specify one coordinate system.



$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle \qquad \text{(2D for simplicity)}$$
$$|\beta\rangle = b_1|e_1\rangle + b_2|e_2\rangle$$

Question: What are the components of b_i in this basis? How are they related to the components a_i?

$$|\beta\rangle = \hat{R}\underbrace{\left(\sum_j |e_j\rangle\langle e_j|\right)}_{\text{Remember, this is just } 1}|\alpha\rangle = \sum_j \hat{R}|e_j\rangle\underbrace{\langle e_j|\alpha\rangle}_{=a_j}$$

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$$|\beta\rangle = \hat{R}\underbrace{\left(\sum_j |e_j\rangle\langle e_j|\right)}_{\text{Remember, this is just } 1}|\alpha\rangle = \sum_j \hat{R}|e_j\rangle\underbrace{\langle e_j|\alpha\rangle}_{=a_j}$$

Now, multiply on the right by $\langle e_i|$ (take the inner product)

$$\langle e_i|\beta\rangle = \sum_j \underbrace{\langle e_i|\hat{R}|e_j\rangle}\, a_j$$

What's this? Its a set of numbers. In 3D, its a set of 9 numbers R_{ij}. For example:

$R_{11} = \langle e_1|\hat{R}|e_1\rangle$ which means:

1.) Take $|e_1\rangle$
2.) Use $\hat{R}$ to rotate it $90°$
3.) Take the <u>new</u> (rotated vector) and calculate the inner product with $\langle e_1|$.

Ok, So: $b_i = \sum_j R_{ij} a_j$

Now the fun part: the results are the same if we write the numbers R_{ij} in a matrix.

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \underbrace{\begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix}}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

List of components of $|\beta\rangle$ in this basis

List of components of $|\alpha\rangle$ in this basis.

Matrix representation of operator $\hat{R}$ in this basis.

Mathematical Sidenote: Converting between "component" notation and matrices is a useful skill. Suppose you're multiplying two matrices A and B, $C = A \cdot B$

$$C = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

Remember, order matters. $AB \neq BA$ in general.

For example

$$C_{11} = A_{11}B_{11} + A_{12}B_{21}$$
$$C_{12} = A_{11}B_{12} + A_{12}B_{22}$$

Look carefully at the indices

A's first index always matches
C's " "
B's 2nd index matches
C's 2nd index

The inner indices are summed.

$$C_{ij} = \sum_k A_{ik} B_{kj} \quad \longleftrightarrow \quad C = AB$$

"Component Notation" "Matrix Notation"

Make sure the summed indices are next to eachother before switching to matrix notation. This will keep the order right.

Poll Q: Consider 4 2×2 matrices W, X, Y, Z. They are related as:

$$Z_{ij} = \sum_k \sum_\ell W_{\ell j} X_{ik} Y_{k\ell}$$

in what order are the matrices multiplied?

A.) $Z = WXY$

B.) $Z = WYX$

C.) $Z = XWY$

D.) $Z = XYW$

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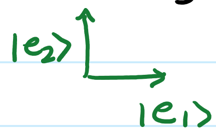
Back to the example at hand, and the calculation of R_{ij}

Poll Q

For $\hat{R}$ = a rotation by 90° (counter clockwise),
which of the following is correct?



A.) $\hat{R}|e_1\rangle = |e_1\rangle$
$\hat{R}|e_2\rangle = |e_2\rangle$

B.) $\hat{R}|e_1\rangle = |e_2\rangle$
$\hat{R}|e_2\rangle = |e_1\rangle$

C.) $\hat{R}|e_1\rangle = |e_2\rangle$
$\hat{R}|e_2\rangle = -|e_1\rangle$

D.) $\hat{R}|e_1\rangle = -|e_2\rangle$
$\hat{R}|e_2\rangle = |e_1\rangle$

So let's calculate the matrix elements:

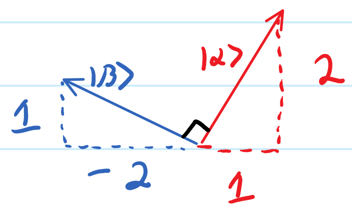
$$R_{11} = \langle e_1|\hat{R}|e_1\rangle = \langle e_1|e_2\rangle = 0$$
$$R_{12} = \langle e_1|\hat{R}|e_2\rangle = -\langle e_1|e_1\rangle = -1$$
$$R_{21} = \langle e_2|\hat{R}|e_1\rangle = \langle e_2|e_2\rangle = 1$$
$$R_{22} = \langle e_2|\hat{R}|e_2\rangle = -\langle e_2|e_1\rangle = 0$$

$i=1$ $$b_1 = R_{11}a_1 + R_{12}a_2 = 0\cdot a_1 + (-1)a_2 = -a_2$$
$i=2$ $$b_2 = R_{21}a_1 + R_{22}a_2 = 1\cdot a_1 + 0\cdot a_2 = a_1$$

This is how the components of $|\beta\rangle$ are related to those of $|\alpha\rangle$

Check for the example at hand, suppose $|\alpha\rangle \longrightarrow \begin{pmatrix}1\\2\end{pmatrix}$

$$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}\begin{pmatrix}1\\2\end{pmatrix} = \begin{pmatrix}-2\\1\end{pmatrix}$$



In fact, it works! $|\beta\rangle$ is rotated 90° compared to $|\alpha\rangle$

Conclusion: An operator $\hat{Q}$ can be represented by a matrix in a particular basis. The matrix elements Q_{ij} are given by

$$Q_{ij} = \langle e_i|\hat{Q}|e_j\rangle \quad \text{and}$$

can be found by acting with the operator on the basis states.

* Caution: If you change your basis, the matrix elements will change. This is the same with vectors: the components will change if you alter your coordinate system

Hermitian Operators

Suppose we have an operator and two kets $|\beta\rangle = \hat{Q}|\alpha\rangle$

Example: $|\alpha\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\hat{Q} \rightarrow \begin{pmatrix} 1 & i \\ 1 & 0 \end{pmatrix}$

Poll Q: if $|\beta\rangle = \hat{Q}|\alpha\rangle$, what is the representation of $\langle\beta|$ in this basis?

A.) $\begin{pmatrix} -i & 0 \end{pmatrix}$

B.) $\begin{pmatrix} -i \\ 0 \end{pmatrix}$

C.) $\begin{pmatrix} i \\ 0 \end{pmatrix}$

D.) $\begin{pmatrix} i & 0 \end{pmatrix}$

Since $|\beta\rangle = \hat{Q}|\alpha\rangle$

You might be wondering, is $\langle\beta| = \langle\alpha|\hat{Q}$?

Can be represented as a row vector

Can be represented as a matrix.

What $\langle\alpha|\hat{Q}$ in this basis?

$$\langle\alpha|\hat{Q} = \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & i \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & i \end{pmatrix}$$

Clearly you can see that $\langle\alpha|\hat{Q} \neq \langle\beta|$ in this case

$\langle\alpha|\hat{Q}$ does not match any of the choices in the poll question

So, in general if $|\beta\rangle = \hat{Q}|\alpha\rangle$, $\langle\beta| \neq \langle\alpha|\hat{Q}$

pronounced "Q-dagger"

There is a different operator called $\hat{Q}^\dagger$ for which

$$\langle\beta| = \langle\alpha|\hat{Q}^\dagger$$

this operator is called "Q-adjoint"
or, the "Hermetian Conjugate" of Q.

How are $\hat{Q}^\dagger$ and $\hat{Q}$ related?

$$\langle\beta| = \langle\alpha|\hat{Q}^\dagger$$

multiply on right by $|e_i\rangle$

$$\langle\beta|e_i\rangle = \langle\alpha|\hat{Q}^\dagger|e_i\rangle$$

insert a complete set of states.

$$\langle e_i|\beta\rangle^* = \langle\alpha|\underbrace{\left(\sum_j |e_j\rangle\langle e_j|\right)}_{1}\hat{Q}^\dagger|e_i\rangle$$

switches order of bra/ket

$$b_i^* = \sum_j \langle\alpha|e_j\rangle\langle e_j|\hat{Q}^\dagger|e_i\rangle = \sum_j \langle e_j|\alpha\rangle^* \underbrace{\langle e_j|\hat{Q}^\dagger|e_i\rangle}_{\text{matrix element}}$$

$$= \sum_j a_j^* Q^\dagger_{ji}$$

So, $b_i^* = \sum_j a_j^* (Q^\dagger)_{ji}$

But, we already know that $|\beta\rangle = \hat{Q}|\alpha\rangle \rightarrow b_i = \sum_j Q_{ij} a_j$

take the complex conjugate:

$$b_i^* = \sum_j Q_{ij}^* a_j^* = \sum_j a_j^* Q_{ij}^*$$

[order doesn't matter... the components are just numbers]

Compare with above.

$$(Q^\dagger)_{ji} = Q_{ij}^* \quad \text{or} \quad (Q^\dagger)_{ij} = Q^*_{ji}$$

to get $Q^\dagger$, transpose Q, and take its complex conjugate.

e.g. $(Q^\dagger)_{12} = Q_{21}^*$

transpose and conjugated.

So, back to our example: $\hat{Q} \rightarrow \begin{pmatrix} 1 & i \\ 1 & 0 \end{pmatrix}$ $\hat{Q}^{+} \rightarrow \begin{pmatrix} 1 & 1 \\ -i & 0 \end{pmatrix}$

Check: is $\langle \beta | = \langle \alpha | \hat{Q}^{+}$?

$|\alpha\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $\langle \alpha | \rightarrow \begin{pmatrix} 0 & 1 \end{pmatrix}$

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

✓ matches answer to poll Question.

An operator which is equal to its adjoint is called Hermitian.

$\hat{A} = \hat{A}^{+}$ [$\hat{A}$ is a Hermitian Operator]

Hermitian Operators are very important in QM, for the following reason:

$$\boxed{\text{Physical Observables in QM are represented by Hermitian Operators}}$$

Poll Q: Which of the following matrices is Hermitian (and therefore could be related to a physical observable?)

A.) $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ B.) $\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$

C.) $\begin{pmatrix} i & 1 \\ 1 & 0 \end{pmatrix}$ D.) $\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$