Quantum Mechanics Crash Course (Part 2): Mathematical Formalism

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Mathematical Methods for Quantum Mechanics

- There are two methods to perform calculations on a mathematical system:
  1. Wave Mechanics: wavefunctions are functions, operators are differential equations, most calculations involve integration
     - *Modern Physics* and most of *Quantum Mechanics*
  2. Matrix Mechanics: wavefunctions are vectors, operators are matrices, most calculations involve linear algebra
     - Some of *Quantum Mechanics* and this course
- The two methods are equivalent **BUT** one is general easier or better suited for a given application

Wavefunctions (Quantum Mechanical States) are Vectors

- In matrix mechanics wavefunctions, or quantum mechanical states, are represented by vectors using bra-ket notation: $|\psi\rangle$
  - The vectors must be normalized (meaning that they have a magnitude of 1): $\sqrt{\langle\psi|\psi\rangle} = 1$ (inner/dot product)
- Example: For each of the below states: (a) find the corresponding bra vector, (b) normalize the state if it is not already normalized.

$$|\alpha\rangle = \begin{bmatrix} i \\ 0 \end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

Computational Basis States

- For vectors of length n, the computational basis states are a set of n vectors of length n that can be used to construct all other possible vectors $\rightarrow$ these vectors are called computational basis states in quantum mechanics because they can be used to create all quantum mechanical states
- Example: For vectors of length 2 one possible computational basis is $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ (proof in HW1)
- Computational basis states must be orthonormal:
  - Orthogonal: $\langle i|j\rangle = 0$
  - Normalized: $\langle i|i\rangle = 1$
  - Proof for the length 2 basis in HW1

Create Any State with a Basis and Superposition

- With a given computational basis, you can create any quantum mechanical state through superposition
- Example:

$$|\psi\rangle = \begin{bmatrix} 3/5 \\ 4/5 \end{bmatrix} = \begin{bmatrix} 3/5 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 4/5 \end{bmatrix}$$

$$= \frac{3}{5}\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{4}{5}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle$$

- Note that the coefficients must follow the rules of probability (automatically enforced if the original matrix is normalized)
- Based on Friday: if this wavefunction is measured, you will get a result corresponding to **either** $|0\rangle$ or $|1\rangle$. These are the only two possible options.

Operators are **Hermitian** Matrices

- Operators, which are used to mathematically represent measuring a system, are represented by Hermitian matrices

$$A^{\dagger} = (A^T)^* = A$$

- Example: S_z measures the spin in the z direction of a particle (generally left in terms of $\hbar$):

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Operators are **Hermitian** Matrices (Cont.)

- Observables of a measurement are determined through an expectation value (vector-matrix multiplication)
  - The expectation value for S_z is typically represented as $\langle S_z \rangle$.
- Example: Given $|\psi\rangle$ from the previous slide, find $\langle \psi | S_z | \psi \rangle = \langle S_z \rangle$.

Observables are Eigenvalues of the Operator

- Given a matrix which describes a certain measurement of a system, there are only a finite number of observables that can be returned $\longrightarrow$ the eigenvalues of the operator matrix
- Ex: Consider the following operators, which measure the spin in the x, y, and z directions:

$$S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- Each matrix has the same eigenvalues, $\pm\frac{\hbar}{2}$, corresponding to spin-up and spin-down in each of the three directions. These are the only possible outcomes when measuring the spin of a particle

Observables are Eigenvalues of the Operator (Cont.)

- Note the expectation value could be different than the eigenvalues of the operator since it is an expected, or *average* measurement
- Note that the spin matrices minus the factor of $\frac{\hbar}{2}$ for the Pauli matrices (σ_x, σ_y, and σ_z), a computational basis for 2x2 matrices. These three matrices will appear many times throughout this course.

The Role of Eigenvectors

- If you measure a system and get an observable (eigenvalue) then you know that the system has collapsed into the state represented by the corresponding eigenvector.
  - Remember that eigenvalues and eigenvectors come in pairs.

$$A\vec{x} = \lambda\vec{x}$$

The Role of Eigenvectors (Cont.)

- Example: Consider the operator to determine the spin of a particle in the z-direction:

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- It has two eigenvalues: $\pm\frac{\hbar}{2}$. The positive eigenvalue corresponds to the eigenvector $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and the negative eigenvalue corresponds to the eigenvector $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.
- If you measure the spin in the z direction and get $+\frac{\hbar}{2}$ as your observable, then you can be certain you collapsed your state into $|0\rangle$.

Outer Products

- An outer product takes two vectors and creates a matrix (an inner product takes two vectors and creates a scalar).
- Consider the following two vectors of length 3:

$$|x\rangle = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \quad |y\rangle = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix}$$

- The outer product between these two vectors, represented as $|x\rangle\langle y|$ is

$$|x\rangle\langle y| = \begin{bmatrix} x_0 y_0^* & x_0 y_1^* & x_0 y_2^* \\ x_1 y_0^* & x_1 y_1^* & x_1 y_2^* \\ x_2 y_0^* & x_2 y_1^* & x_2 y_2^* \end{bmatrix}$$

Projection Operators

- A useful application of the outer product is in the construction of projection operators.
- Consider the computational basis states for vectors of length 2 defined in previous slides. We can construct the following projection operators, typically denoted as $\hat{P}$ and $\hat{Q}$:

$$\hat{P} = |0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad \hat{Q} = |1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

- The projection operator *projects* out a specific component of a of a state related to the basis state that was used to the projection operator.
- Example: Using $|\psi\rangle$ define previously, find $\hat{P}|\psi\rangle$ and $\hat{Q}|\psi\rangle$.

Further Generalizations to Extract Probabilities

- Consider a generic state $|\psi_0\rangle = \begin{bmatrix} c_0 \\ c_1 \end{bmatrix}$:

$$\hat{P}|\psi_0\rangle = \hat{P}\begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \hat{P}(\begin{bmatrix} c_0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ c_1 \end{bmatrix})$$

$$= \hat{P}(c_0\begin{bmatrix} 1 \\ 0 \end{bmatrix} + c_1\begin{bmatrix} 0 \\ 1 \end{bmatrix}) = \hat{P}(c_0|0\rangle + c_1|1\rangle)$$

$$= c_0\hat{P}|0\rangle + c_1\hat{P}\rangle = c_0\hat{P}|0\rangle = c_0|0\rangle$$

Further Generalizations to Extract Probabilities (Cont.)

Now consider that

$$\langle 0|\hat{P}|\psi_0\rangle = \langle 0|c_0|0\rangle = c_0$$

and

$$\langle 0|\hat{P}|\psi_0\rangle = \langle 0|0\rangle\langle 0|\psi_0 = \langle 0|\psi_0\rangle = c_0$$

- Note that P($|0\rangle$) $= |c_0|^2$
- The probability of obtaining an observable corresponding to basis state $|i\rangle$ when measuring $|\psi\rangle$ is $|\langle i|\psi\rangle|^2$.

Time-Independent Schr0dinger's Equation

- An important equation in quantum mechanics is known as the *time-independent Schrodinger's equation* which gives the energy of a system using the *Hamiltonian* operator.

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

- Note that the time-independent Schrodinger's equation is an eigenvalue problem.
- An important consequence of Schrodinger's equation is that if $|\psi\rangle$ is a solution then so is $a|\psi\rangle$ is a is a complex constant.
  - Normalizing a state does not change the system. *Always normalize states before using them!*

Entanglement is Represented as a Tensor Product

- Entanglement between two states is represented with a tensor product, which will result in a vector longer than the vectors of the entangled states.
- Consider the two states:

$$|x\rangle = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} \quad |y\rangle = \begin{bmatrix} y_0 \\ y_1 \end{bmatrix}$$

- If $|x\rangle$ and $|y\rangle$ become entangled, then we can represent the entangled state as the tensor product between the two states:

$$|x\rangle \otimes |y\rangle = \begin{bmatrix} x_0 y_0 \\ x_o y_1 \\ x_1 y_0 \\ x_1 y_1 \end{bmatrix}$$

Example 1

You may solve the following example by hand or use an online linear algebra calculator like Wolfram Alpha.

Consider a three-dimensional vector space spanned by an orthonormal basis $|1\rangle$, $|2\rangle$, and $|3\rangle$. States $|\alpha\rangle$ and $|\beta\rangle$ are given by:

$$|\alpha\rangle = i|1\rangle - 2|2\rangle - i|3\rangle, \quad |\beta\rangle = i|1\rangle + 2|3\rangle$$

- Construct $\langle\alpha|$ and $\langle\beta|$ in terms of $\langle 1|$, $\langle 2|$, and $\langle 3|$.
- Find $\langle\alpha|\beta\rangle$ and $\langle\beta|\alpha\rangle$ and confirm that $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$. **Hints**: What property should the coefficients of $|\alpha\rangle$ and $|\beta\rangle$ have before you start this problem? You do not need to know $|1\rangle$, $|2\rangle$, or $|3\rangle$ but you do need to know the properties of an orthonormal basis.

Example 2

You may solve the following example by hand or use an online linear algebra calculator like Wolfram Alpha.

The Hamiltonian for a certain three-level system is represented by the matrix

$$H = \hbar\omega \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

Two other observables, A and B, are represented by the matrices

$$A = \lambda \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad B = \mu \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

where ω, λ, and μ are positive, real numbers.

Example 2 (Cont.)

- What are the possible energies of this three-level system. Consider the following state:

$$|\psi\rangle = a \begin{bmatrix} -i \\ 3 \\ 2i \end{bmatrix}.$$

- Find a (i.e. normalize the state).
- Compute $\langle\psi|A|\psi\rangle$ and $\langle\psi|B|\psi\rangle$. Are these numbers observables or averages?
- What is the probability that, when measuring the energy of $|\psi\rangle$, you obtain $\hbar\omega$?

Example 3

You may solve the following example by hand or use an online linear algebra calculator like Wolfram Alpha.

Suppose a particle is in the state

$$|\psi\rangle = \frac{1}{\sqrt{6}} \begin{bmatrix} 1+i \\ 2 \end{bmatrix}$$

What are the probabilities of getting $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$, if you measure S_z and S_x?

Example 4

You may solve the following example by hand or use an online linear algebra calculator like Wolfram Alpha

An electron is in the state

$$|\psi\rangle = A \begin{bmatrix} 3i \\ 4 \end{bmatrix}$$

- Determine the normalization constant A.
- Find the expectation values of S_x, S_y, and S_z.