Day 2: Basics of Quantum Mechanics

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1 Axioms of Quantum Mechanics

1.1 States are Vectors

We can represent the state of a quantum system (the system is whatever we're looking at, for example a single electron in a box) as a vector of complex numbers. The system is parametrized by one or more variables, such as position of the electron in the box. The state of the system is then given by the values of all such variables. The space of all possible such vectors is called a *Hilbert space*, and is denoted by $\mathcal{H}$. The simplest example is a single spin σ, which can either point up or down. Since there are two possible states, the vector describing the system has two entries, which we will call "up" $\sigma = |+\rangle$ and down $\sigma = |-\rangle$.

It is convenient to represent vectors in the same way you may know from geometry, as brackets with entries for each dimension. We identify:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

State-vectors $\boldsymbol{a}, \boldsymbol{b} \in \mathcal{H}$ for a quantum mechanical system can be added together, with prefixes of complex numbers $c_{1,2} \in \mathbb{C}$:

$$c_1 \cdot \boldsymbol{a} + c_2 \cdot \boldsymbol{b}$$

They have a scalar product (with a_i and b_i being the entries of the vectors, numbered from 1 to N):

$$\boldsymbol{a} \cdot \boldsymbol{b} = \sum_i a_\iota^* \cdot b_\iota$$

A convenient notation is the bra-ket notation, where we write a vector as the *ket* $|v\rangle \in \mathcal{H}$, and the *conjugate* of the vector as the *bra* $\langle v| \in \mathcal{H}$. Taking the conjugate of a vector is what we do when we want to calculate the scalar product:

$$\langle a|b\rangle = \sum_i a_\iota^* \cdot b_\iota.$$

The scalar product fulfils a few properties that uniquely define it:

1.1.1 Properties of the Scalar product

1. It is *sesquilinear*. We denote the sum of two vectors inside the same bra/ket as $\langle a + b| \in \mathcal{H}$, and multiplication with a complex number $c_1 \in \mathbb{C}$ is written as $|c_1 \cdot a\rangle = c_1 |a\rangle$.

   $$\langle a + c_1 \cdot b|c\rangle = \langle a|c\rangle + c_1^* \langle b|c\rangle \text{ and } \langle a|c_1 \cdot b + c\rangle = \langle a|b\rangle + c_1 \langle a|c\rangle$$

   Note that pulling a complex number out of a bra will turn it into its complex conjugate! That is why it is only sesquilinear, not fully linear.

2. It is *hermitian*. That means that exchanging which vector is the bra and which is the ket will give the complex conjugate of the scalar product:

$$\langle a|b\rangle = \langle b|a\rangle^*$$

3. It is positive definite. That means the scalar product of a vector $|a\rangle \in \mathcal{H}$ with itself will always be positive, unless the vector is zero, in which case it is zero.

$$\langle a|a\rangle > 0 \quad \text{for } a \neq 0 \text{ and } \langle 0|0\rangle = 0.$$

1.1.2 The norm of a state

The norm of any quantum state $|v\rangle \in \mathcal{H}$ is given by the square root of its scalar product with itself:

$$\|v\| = \sqrt{\langle v|v\rangle}$$

In quantum mechanics, usually we assume that states are *normalised*. This means that the norm (or length) of the state vector is 1.

1.1.3 Orthogonality

We call two states $|v_1\rangle, |v_2\rangle \in \mathcal{H}$ *orthogonal* if their scalar product is zero: $\langle v_1|v_2\rangle = 0$.

1.1.4 Exercises

Question 1. In the Julia Notebook, implement a function which takes two spin-states and returns the scalar product.

Question 2. In the Julia Notebook, implement a function which takes two vectors as arguments and returns *true* if they are orthogonal, and *false* if they are not orthogonal.

Question 3. In the Julia Notebook, implement a function which takes one spin state, and returns its norm.

Question 4. In the Julia Notebook, implement a function which takes a vector, and returns the normalised version of this vector.

Question 5. Keep working through the notebook!

2 Observables as Hermitian Matrices

Observables are properties of a system which can be measured (observed). Examples include the momentum $\boldsymbol{p}$, the Energy E, position $\boldsymbol{x}$ and the spin σ. In Quantum mechanics the observables are defined through Hermitian matrices. Matrices in general can be thought of as defining linear transformation. They can be written as

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

in the case of a 2-dimensional vector space. For N-dimensional vector-spaces we have NxN matrices. (In general matrices can also have different lengths and widths, e.g. MxN matrices, but in quantum mechanics, all Matrices are square)

The product of a matrix and a vector is defined as

$$A|v\rangle = \sum_{j=1}^{N} a_{i,j} \cdot v_j$$

This means each entry from the first row of the matrix is multiplied by the corresponding entry of the vector. Their sum is the first entry of the new vector. Then the same is repeated for the second, third, ..., Nth row.

2.1 Definition of Hermitian Matrices

1. Hermitian matrices are square

2. Exchanging the indices for the entries of the matrix gives the complex conjugate:

$$a_{i,j} = a_{j,i}^*$$

If you prefer to think about the matrix as written out with rows and collumns, mirroring it along the diagonal will give the complex conjugate of the entries:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{12}^* & a_{22} \end{pmatrix}$$

2.2 Important properties

In general, when we multiply a matrix with a vector, we get a completely different vector, that points in a different direction. However, there is a set of special vectors, the so-called eigenvectors. Each hermitian matrix of size NxN has N unique eigenvectors.

Multiplying an eigenvector $|v_e\rangle$ with the corresponding matrix A will return the same vector, scaled by a number called the *eigenvalue* E.

$$A|v_e\rangle = E|v_e\rangle$$

The eigenvectors of a hermitian matrix are all orthogonal (not generally true for different matrices!) and therefore form a *basis* of the vectorspace $\mathcal{H}$. A basis is a collection of vectors $\{|v_1\rangle, \ldots, |v_N\rangle\}$, such that any vector $|a\rangle$ can be written as a linear combination of them:

$$|a\rangle = \sum_{i=1}^{N} c_i |v_i\rangle$$

Question 6. Work through the Chapter "The Second Axiom: Observables are Hermitian Matrices" in the Julia Notebook.

3 Measurements

Saying observables are represented by hermitian matrices is all well and good, but what does it mean? What happens when we try to measure the observable? It turns out that when measuring an observable, it is only possible to find the states which are eigenvectors of the hermitian matrix associated with that observeable. If the system is in a different state, it will *collapse* into one of the eigenstates (states which are eigenvectors). The outcome of the measurement (the measured value) is the eigenvalue E associated with the eigenstate $|v_e\rangle$.

This is the so-called wavefunction collapse, which is the source of many philosphical debates about the true nature of quantum mechanics. For our purposes, its not that important to know about, but if your interested, you can start here: https://en.wikipedia.org/wiki/Wave_function_collapse

The outcome of the measurement is determined probabilistically; The probability P to measure any particular eigenvalue E of an eigenstate $|v_e\rangle$ is given by the norm of the scalar product between the pre-measurement state $|\Psi\rangle$ and that eigenstate.

$$P(E) = ||\langle v_e|\Psi\rangle||^2$$

Question 7. Work through the Julia notebook chapter "The Third Axiom: Measurements".

4 The Time Evolution

The *time evolution* of any quantum system is determined by the *Schrödinger equation*. When we say time evolution what we mean is this:

Imagine you know the state of the system at time $t=0$, e.g. a spin which is in the state $|+\rangle$. What state will it be in time $t=1s$? or $t=2s$? This is determined by the time evolution: How the state changes over time. (In the Julia notebook, you will calculate the time evolution for a spin state such as $|+\rangle$.)

In quantum systems, the time dependent state $|\Psi(t)\rangle$ is described by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H\,|\Psi(t)\rangle$$

Here the left side is the derivative with respect to time, and the right hand-side is a matrix-multiplication of the matrix H and the state $|\Psi(t)\rangle$. After yesterday, we already know how to solve this kind of equation for real or complex number H, and it turns out that a matrix is not so different.

Deriving the solution of the time-dependent Schrödinger equation is left as an exercise to the reader, but analogous to yesterday we write it as

$$|\Psi(t)\rangle = \exp\left(\frac{-i\cdot t\cdot H}{\hbar}\right)|\Psi(0)\rangle$$

Here the exponential function exp when applied to a matrix is again a matrix itself. The way to calculate it involves the Taylor expansion of the exponential function, however, in order to understand this, you first need to understand how to multiply matrices.

In the index notation introduced earlier, multiplying two matrices A and B takes this form:

$$(A\cdot B)_{i,j} = \sum_k a_{i,k}\cdot b_{k,j}$$

Imagining this in the notation with rows and columns, the first row of the first matrix is multiplied element-wise with the first columns of the second matrix; This is the first entry of the new matrix. The one goes through all combinations of rows and columns to get the further entries, so the second row multiplied with the third column is the element with indices (2,3) of the new matrix.

$$A\cdot B = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}\,b_{11} + a_{12}\,b_{21} & a_{11}\,b_{12} + a_{12}\,b_{22} \\ a_{21}\,b_{11} + a_{21}\,b_{21} & a_{21}\,b_{12} + a_{22}\,b_{22} \end{pmatrix}$$

The exponential of a matrix A is then given by:

$$\exp(A) = \sum_{n=1}^{\infty} \frac{1}{n!} A^n$$

Things to note:

1. The eigenvectors of the exponentiated matrix and the original hermitian matrix are the same. (Why?)

2. For some matrices, the matrix exponential does not exist; However, for hermitian matrices, it always exists.

3. In general, the identity $\exp(A+B) = \exp(A)\exp(B)$ for matrices A, B does NOT hold for matrix exponentials.

Question 8. Go to the Julia notebook and finish it!