# Quantum Mechanics

## 1 Mathematical Foundations

In Quantum mechanics, we work with complex vector spaces (more percisely Hilbert spaces) where the elements $|A\rangle$ are called *kets*. We additionally require linearity for this space.

Each of our kets has a dual called bra $\langle A|$. It serves as a column vector of the ket vector and is complex conjugated. An important thing to remember is that the dual to $z|A\rangle$ is $\langle A|\overline{z}$.

The scalar product is called inner product and is written as $\langle B \mid K\rangle$. The result is a complex number. Also: $\langle B \mid A\rangle = \overline{\langle A \mid B\rangle}$. Let us introduce some terms.

- Normalized Vector: $\langle A \mid A\rangle = 1$.
- Orthagonal Vectors: $\langle A \mid B\rangle = 0$.

When using an *orthonormal* basis, the ket $|A\rangle$ can be represented as $|A\rangle = \sum_i \alpha_i |i\rangle$, where $|i\rangle$ are the base kets. To calculate $\alpha_i$ we do the following:

$$\alpha_j = \langle j \mid A\rangle = \sum_i \alpha_i \langle j \mid i\rangle.$$

This works because $\langle j \mid i\rangle$ acts as *Kroenecker Delta* $\delta_{ij}$

We will also define the *outer product* of two kets $|A\rangle$ and $|B\rangle$ as $|A\rangle\langle B|$. It is a matrix with the elements $A_i B_j$. If we have the special case of $|A\rangle = |B\rangle$, we get the *projection operator* $|A\rangle\langle A|$. Applying it to a ket $|C\rangle$ gives us the projection of $|C\rangle$ onto $|A\rangle$. (i.e. $|A\rangle\langle A||C\rangle$) Adding all the projection operators of an orthonormal basis gives us the *identity operator* $I$.

We define the *Expectation Value* $\langle L\rangle$ as the weighted sum $\sum_i \lambda_i P(\lambda_i)$. Further we define the *statistical correlation* of two probability distributions $P(\lambda_i)$ and $P(\mu_i)$ as $\langle AB\rangle - \langle A\rangle\langle B\rangle$. It is non-zero if the two observables are correlated and zero if they are not. One can also say that if $P(a,b) = P(a)P(b)$, then the observables are uncorrelated.

## 2 Matrices

For a Matrix $M$ we define the Hermitian Conjugation $M^\dagger$ as the complex conjugate of the transpose of $M$ (i.e. $M^\dagger = \overline{M^T}$). A matrix is called *Hermitian* if $M = M^\dagger$.

If we have $M|A\rangle = |B\rangle$, we have $\langle A|M^\dagger = \langle B|$.

> The eigenvectors of a Hermitian matrix form an orthogonal basis.

A matrix is called *unitary* if $U^\dagger U = I$. This means that the inverse of $U$ is $U^\dagger$.

The quantity $LM - ML$ is called the *commutator* of $L$ and $M$ and is denoted by $[L, M]$. By definition, $[L, M] = -[M, L]$ and $[L, M] = 0$ if $L$ and $M$ commute.

We define the *trace* of a matrix $M$ as the sum of its diagonal elements. If we have a hermitian matrix $H$ it's trace is further equal to the sum of its eigenvalues. Using the trace, the expectation value of an observable $L$ can be written as $\langle L\rangle = \mathrm{Tr}(L\rho)$, where $\rho$ is the density matrix of the system, where the density matrix is defined as $\rho = \sum_i P(\lambda_i)|\lambda_i\rangle\langle\lambda_i|$.

## 3 Tensor Products

Taking the Tensor product $\otimes$ can be used in quantum mechanics to combine two systems. For details see section 10. Let's look at Tensor product for two two 2x2 matrices $A$ and $B$. In standard notation, we have $A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix}$ or

$$A \otimes B = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}.$$

This special form of the tensor product for Matrices is called the *Kronecker Product*. In general if you have a *m*x*n* and a *p*x*q* matrix, the resulting matrix will be *mp*x*nq*. For vectors, just set $n$ or $q$ to 1.

## 4 Quantum States

Let's look at spin. We can conclude we have 2 dimesions. Now let's arbitrairly make up $|u\rangle$ and down $|d\rangle$ our base kets. Every state $|A\rangle$ is of the form $|A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$. Here $\alpha_u \cdot \overline{\alpha_u}$ is the probability to find the up state and likewise for $\alpha_d \cdot \overline{\alpha_d}$.

For left-right spin we just have a diffrent base looking like:

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle \text{ and } |l\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{1}{\sqrt{2}}|d\rangle$$

And for in-out spin:

$$|i\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{i}{\sqrt{2}}|d\rangle \text{ and } |o\rangle = \frac{1}{\sqrt{2}}|u\rangle - \frac{i}{\sqrt{2}}|d\rangle$$

We could also write spin states as column vectors with $|u\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|d\rangle = \begin{pmatrix}0\\1\end{pmatrix}$

## 5 Observables

A observable is a thing you can measure. For example $\sigma_z$, the z component of the spin. Observables are represented by hermitian matrices. The eigenvalues of these matrices form the possible outcomes of a measurement where the corresponding eigenvectors are the state the system collapses to after the measurement. If $|A\rangle$ is the state vector and $M$ the observable, the probability to measure the eigenvalue $\lambda_i$ is $\langle A \,|\, i\rangle\langle i \,|\, A\rangle$.

For our spin example, one can show that for the z component of the spin, we have the matrix representation $\sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$. As we can see the eigenvalues are 1 and -1 with the eigenvectors $|u\rangle$ and $|d\rangle$ respectively. We can further find the matrices in x and y direction. Together, they form the *Pauli Matrices*.

**Pauli Matrices**

$$\sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}, \sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}, \sigma_y = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}$$

One can also use these matrices to measure spin along any direction. If we measure spin along the direction $\vec{n} = (n_x, n_y, n_z)$, we can use the matrix representation $\sigma_n = n_x\sigma_x + n_y\sigma_y + n_z\sigma_z$.

Using the Pauli matrices, its also possible to write down all 2x2 Hermitian matrices. They are of the form $A = a_0 I + a_x\sigma_x + a_y\sigma_y + a_z\sigma_z$, where $I$ is the identity matrix.

Lastly, notice that there is a direction, that if we measure our spin in, we already know the outcome.

## 6 Time and Change

When we have two identical systems, and we have them at the same state at some point in time, both their past and future states are the same. Distinctions are conserved. This is called *unitary evolution*.

Consider a closed system at time $t$, namely $|\Psi(t)\rangle$. We can define some operator $U(t)$ such that $|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$. This operator is called the *time development operator*. We can use it to calculate the state of the system at any time $t$ and find the probabilities of outcomes in later experiments.

Our operator needs to satisfy some properties, firstly: Conservation of destinction. If we have two states $|\Psi\rangle$ and $|\Phi\rangle$, and $\langle\Psi(0) \,|\, \Phi(0)\rangle = 0$, then $\langle\Psi(t) \,|\, \Phi(t)\rangle = 0$. We also require that the operator is linear. From this we can see, that $U(t)$ is unitary.

## 7 Schrödingers Equation

The time dependent Schrödinger equation is given by

**Time Dependent Schrödinger Equation**

$$\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = -iH|\Psi(t)\rangle.$$

This equation describes how the state of a system evolves over time. The Hamiltonian $H$ is the observable that corresponds to the total energy of the system.

So now, how do we calculate the expectation value of an observable $A$ at time $t$? We could use the formula from the beginning, however for an observable $L$ we can also use the formula $\langle L\rangle = \langle\Psi(t)|L|\Psi(t)\rangle$.

We can now derive, how the expectation value of an observable changes over time. We find that

$$\frac{d}{dt}\langle\Psi(t)|L|\Psi(t)\rangle = \frac{i}{\hbar}\langle\Psi(t)|[HL - LH]|\Psi(t)\rangle$$

or in simple terms

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle[H, L]\rangle. = -\frac{i}{\hbar}\langle[L, H]\rangle$$

We can now talk about conserved quantities. If $[H, L] = 0$, then $\langle L\rangle$ is conserved. We can follow that even $[H, L^n] = 0$ for all $n$. If we now let $L$ be the Hamiltonian, we find that the energy is conserved. :)

From the time dependent Schrödinger equation we can derive the time independent Schrödinger equation. If we let the observable values of energy be $E_j$ with the corresponding eigenvectors $|E_j\rangle$, we have

**Time Independent Schrödinger Equation**

$$H|E_j\rangle = E_j|E_j\rangle.$$

This equation can be used to find the eigenvalues and corresponding eigenvectors of the Hamiltonian. Using the information of the time independent Schrödinger equation, we can also solve the time dependent Schrödinger equation. We can

also describe a state $|\Psi(t)\rangle$ as a linear combination of the eigenvectors of the Hamiltonian. It can be shown, that every coefficient $\alpha_j$ is of the form

$$\alpha_j = \alpha_j(0)e^{-iE_jt/\hbar}.$$

This equation holds, as long as the Hamiltonian is time independent. From here we can now easily derive the probabilities at some time $t$.

As a last comment. The wave function $|\Psi(t)\rangle$ collapses when it is measured. That means, that all the randomness about the given observable is gone. This is called the *collapse of the wave function.*

## 8 Wave function

Suppose the basis vectors of some quantum system to be $|a, b, \ldots\rangle$ with the corresponding eigenvalues $a, b, \ldots$. Consider an arbitrary state $|\Psi\rangle$. We can write it as $|\Psi\rangle = \sum_{a,b,\ldots} \psi(a, b, \ldots)|a, b, \ldots\rangle$. The quantities $\psi(a, b, \ldots)$ are just some coefficients. Where each of them can be found by $\psi(a, b, \ldots) = \langle a, b, \ldots \,|\, \Psi\rangle$. This set of coefficients $\psi(a, b, \ldots)$ is called the wave function of the system in the basis denoted by the observables $A, B, \ldots$.

Again probabilities for some state $|x\rangle$ is give by $\psi(x)\overline{\psi(x)}$ and the sum over all probabilities is equal to 1.

## 9 Uncertainty

Consider two observables $L$ and $M$. This can for example be two Qubits of which we each measure the spin in z direction. If we let $\lambda_i$ and $\mu_i$ be the eigenvalues of $L$ and $M$ respectively, we can find that in order to measure both observables at the same time, we need to have that the observables commute and vice versa. If the observables do not commute, we in general cannot have unambiguous values for both observables at the same time. We can now proof that we cannot have knowledge about spin in more than one direction at the same time.

Let's try and quantify uncertainty. Lets take an observable $A$ with eigenvalues $a$. For some state $|\Psi\rangle$, there is a probability distribution funtion with $\langle A\rangle = \sum_i a_i P(a_i)$. The variance of $A$ is given by

$$(\Delta A)^2 = \langle (A - \langle A\rangle)^2\rangle.$$

If the expectation value of an observable $A$ is 0, then the variance of $A$ is given by

$$(\Delta A)^2 = \langle A^2\rangle.$$

Now, let $|\Psi\rangle$ be an arbitrary state and let $A$ and $B$ be two observables. Now, define $|X\rangle = A|\Psi\rangle$ and $|Y\rangle = iB|\Psi\rangle$. Plugging this into the Cauchy-Schwarz inequality, we find that

$$2\sqrt{\langle A^2\rangle\langle B^2\rangle} \geq |\langle [A, B]\rangle|.$$

With some theorems about commutators, we can now derive the *Uncertainty Principle.*

For two observables $A$ and $B$, acting on a state $|\Psi\rangle$ we have

$$(\Delta A)(\Delta B) \geq \frac{1}{2}|\langle [A, B]\rangle|.$$

## 10 Entanglement

Consider two systems $A$ and $B$. Further let the space of states be $S_A$ and $S_B$. Our goal is now to a single composite system $AB$. It can be shown that this is done by taking the tensor product of the two spaces $S_A \otimes S_B$. This will result in new basis kets $|ab\rangle$. Where the number of them is the product of the number of basis kets of $A$ and $B$. A combined state could be written as $|a_i\rangle \otimes |b_j\rangle$. Typically the simpler version $|a_ib_j\rangle$ is used. However it is important that despite it being tempting to use this as a double index, it is not. $|a_ib_j\rangle$ is a single state of a combined system! Therefore, $\langle a_ib_j \,|\, a_kb_l\rangle = \delta_{ik}\delta_{jl}$. And thus we can write for a state $|\Psi\rangle$ of the combined system $|\Psi\rangle = \sum_{i,j} \psi(i, j)|a_ib_j\rangle$.

Let us return to two single spins. Let's call the spin of system $A$ $\sigma$ and the spin of system $B$ $\tau$, where $\sigma$ has components $\sigma_x, \sigma_y, \sigma_z$ and $\tau$ has components $\tau_x, \tau_y, \tau_z$. If we just consider spin in $z$ direction for both systems, we can write the combined state as

$$|\Psi\rangle = \alpha|uu\rangle + \beta|ud\rangle + \gamma|du\rangle + \delta|dd\rangle.$$

Let us first look at the special case of *Product States*. Here we require our initial spins to be independent of each other. So the result of system $B$ does not depend in any way on the result of system $A$ and vice versa. So for system A we have $|\Psi_A\rangle = \alpha_u|u\rangle + \alpha_d|d\rangle$ and for system B we have $|\Psi_B\rangle = \beta_u|u\rangle + \beta_d|d\rangle$. We also require noralziation of each state. The combined state is then $|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$. Expanding this we see that $|\Psi\rangle =$

$\alpha_u\beta_u|uu\rangle + \alpha_u\beta_d|ud\rangle + \alpha_d\beta_u|du\rangle + \alpha_d\beta_d|dd\rangle$. $|\Psi\rangle$ is called the product state.

Most states of a tensor product space are however not product states. These are called *Entangled States*. The most general vector in a composite space of our spin system is given by $|\Psi\rangle = \psi_{uu}|uu\rangle + \psi_{ud}|ud\rangle + \psi_{du}|du\rangle + \psi_{dd}|dd\rangle$. Where $\psi_{ij}$ are the complex coefficients of the state. Here the normalization condition is $\sum_{i,j} |\psi_{ij}|^2 = 1$. Suddenly we have two more degrees of freedom when not working with product states. This is called *Entanglement*.

Some systems can be more entangled than others. A maximally entangled state is both, a complete description of the system, such that no more can be known about it and at the same time, nothing is known about the individual systems. To see this, we have to ask ourselves, how the observables $\sigma_i$ and $\tau_j$ are represented in the tensor product states. If we apply for example $\sigma_y$ to system $A$ this should just ignore system $B$. Also to apply them we technically need to use $\sigma_z = \sigma_z \otimes I$ and $\tau_z = I \otimes \tau_z$ to make dimensions match.

From only one system we remember that $\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1$ holds for one direction when measuring spin. For a product state, the same thing still holds. However, consider the state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle)$. We can show that $\langle\sigma_x\rangle = \langle\sigma_y\rangle = \langle\sigma_z\rangle = 0$. The same thing of course goes for $\tau$. So despite us knowing exactly what the state is, we have expectation value of 0 for all directions. We clearly cannot say anything about whether the spin is +1 or -1. This raises the question: Is there more to know? The answer is no.

Suppose we have an observable $A$ for system $A$ and $B$ for system $B$. The correlation $C(A, B)$ is defined as $C(A, B) = \langle AB\rangle - \langle A\rangle\langle B\rangle$. If this quantity is not equal to zero, the two states in the systems must be entangled. Another test comes from the density matrix. Using a state $|\Psi\rangle$, which is a product state of $|\Psi_A\rangle$ and $|\Psi_B\rangle$, we know, the wave function is of the form $\psi(a, b) = \psi_A(a)\psi_B(b)$. The density matrix is then equal to $\rho_{a'a} = \overline{\psi_A(a)}\psi_A(a')\sum_b \overline{\psi_B(b)}\psi_B(b)$. If we note that the state of system B is normalized, we can see that the density matrix of system A reduces to $\rho_A(a', a) = \overline{\psi_A(a)}\psi_A(a')$. Now only for a product state, this density matrix has exactly one nonzero eigenvalue, which is exactly one.

For the opposite case of a maximally entangled state, if we have dimension $N_A$, the density matrix of system A is given by $\rho_A(a', a) = \frac{1}{N_A}\delta_{a'a}$. Which tells us that all eigenvalues are equal to $\frac{1}{N_A}$ and like that nothing can be said about the state of system A.

## 11 Continuous Variables

If we, for example, consider the position of a particle along the $x$-axis, we no longer only have 2 possible states. In fact we have uncountable infinitely many. Luckily, a vector is just a function so let's see the implications of this.

Consider some real value $x$ and some function $\psi(x)$. For operators, let's start with a simple example, the "multiply by $k$" operator. This operator is defined as $K\psi(x) = k\psi(x)$. We can also define the "differentiate" operator as $D\psi(x) = \frac{d\psi(x)}{dx}$. To show if some operator is Hermitian, we can sandwich the operator between a ket and a bra and need the relation $\langle\Psi|L|\Phi\rangle = \langle\Phi|L|\Psi\rangle$. In the case of $K$ we see that it is Hermitian, whilst $D$ is not. However since $D$ is anti-Hermitian ($D^\dagger = -D$) we can just multiply by $i$ or $-i$ to get a Hermitian operator. Thus, $-i\hbar D$ is Hermitian.

## 12 Heisenberg Uncertainty

To measure the position of a particle, we can use a hermitian operator $X$ of the form $X|\Psi\rangle = x_0|\Psi\rangle$. The wave function thus becomes $x\psi(x) = x_0\psi(x)$. Now this is interesting because we get $(x - x_0)\psi(x) = 0$. So either $x = x_0$ or $\psi(x) = 0$ Now, no ordinary, continuous function can do that. But there is the Dirac delta function... So for every real number $x_0$ there exists a corresponding eigenvector, sometimes also called *Eigenfunction*.

The momentum operator $P$ is defined as $-i\hbar D$ where $D$ is the differential operator from before. Again, applied to the wave function we get $P\psi(x) = -i\hbar\frac{d\psi(x)}{dx}$. Reformulating this and solving a differential equation we find $\psi_p(x) = Ae^{\frac{ipx}{\hbar}}$. The constant $A$ is found by normalization. In total we find that $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}$.

Now amazingly, we can notice, that the eigenfunctions of $P$ have the term $e^{\frac{ipx}{\hbar}}$ in them. This is very similar to wave equations. The wavelength then is given by $\lambda = \frac{2\pi\hbar}{p}$.

Now, if we look at uncertainty, we can see that the commutor $[X, P] = XP - PX$ is equal to $i\hbar$. This means that we cannot measure both position and momentum at the same time. More percisely, $\Delta X\Delta P \geq \frac{\hbar}{2}$.