QUANTUM SYSTEMS AND WAVE FUNCTIONS FOR MATHEMATICIANS

JINKUN HAN

Contents

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1. Introduction

We start with the physical model of photon polarization as a concrete model of the more abstract concept of single qubit systems. We then introduce the vector representation (linear algebra), Bloch's sphere representation (geometry), and the wave function representation (probability theory) of single qubit systems.

We then delve into wave functions, starting with the physical motivation behind wave functions, namely wave function as a representation of a state of a quantum system. Then, we introduce the mathematical insight of wave functions. After our discussion of a toy model, a discretized space that operates on the quantum scale, we then travel to the continuous space. In the continuum, we use Fourier transform to explore how a particle's position and momentum are derived (from the wave function) and measured. From the relationship between position and momentum arises the famous Heisenberg uncertainty principle.

This talk assumes basic knowledge of linear algebra (vector space, basis, orthonormality, inner product), analysis (convergence, Fourier transform, square integrability), and probability theory (probability density).

2. A Physical Model: photon polarization

(Experimental set-up: explained during talk).

2.1. Dirac's Notation for Arbitrary Polarization.

$$|v\rangle = a\,|\uparrow\rangle + b\,|\rightarrow\rangle,$$

where a, b are non-zero amplitude coefficients.

2.2. QM Significance of Photon Polarization.

- Each possible state of polarization of the photon is represented by a unit vector;
- photon's interaction with the polaroid is always probabilistic;
- photon polarization is a specific example of a qubit;
- a qubit has multiple possible states. More generally, a qubit is any quantum mechanical system that can be modeled by a 2-dimensional complex vector space.

3. Single Qubit System

3.1. States of a Qubit. A single qubit can be viewed as a state space, whose elements are the set of all possible states of the qubit. More particularly:

- such space has the standard basis defined as $\{|0\rangle, |1\rangle\}$;
- each element (state) of such state space is denoted as:

  $$a\,|0\rangle + b\,|1\rangle,$$

  where $a, b \in \mathbb{C}$ such that $|a|^2 + |b|^2 = 1$;

- if you are not familiar with Dirac's notation (e.g. $\langle\alpha|\beta\rangle$), think alternatively in terms of matrices:

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

so that:

$$|v\rangle := a\,|0\rangle + b\,|1\rangle = \begin{pmatrix}a\\b\end{pmatrix}.$$

3.2. **Bloch Sphere.** The Bloch Sphere is a way to geometrically represent a qubit. It becomes useful if one wishes to illustrate single-qubit quantum transformations. The construction of the Bloch Sphere representation of a qubit is as follows:

Construction of Bloch Sphere

Step 1 Construct a 1-1 correspondence between each quantum state $|v\rangle$ of the qubit and $\alpha \in \mathbb{C}$, where:

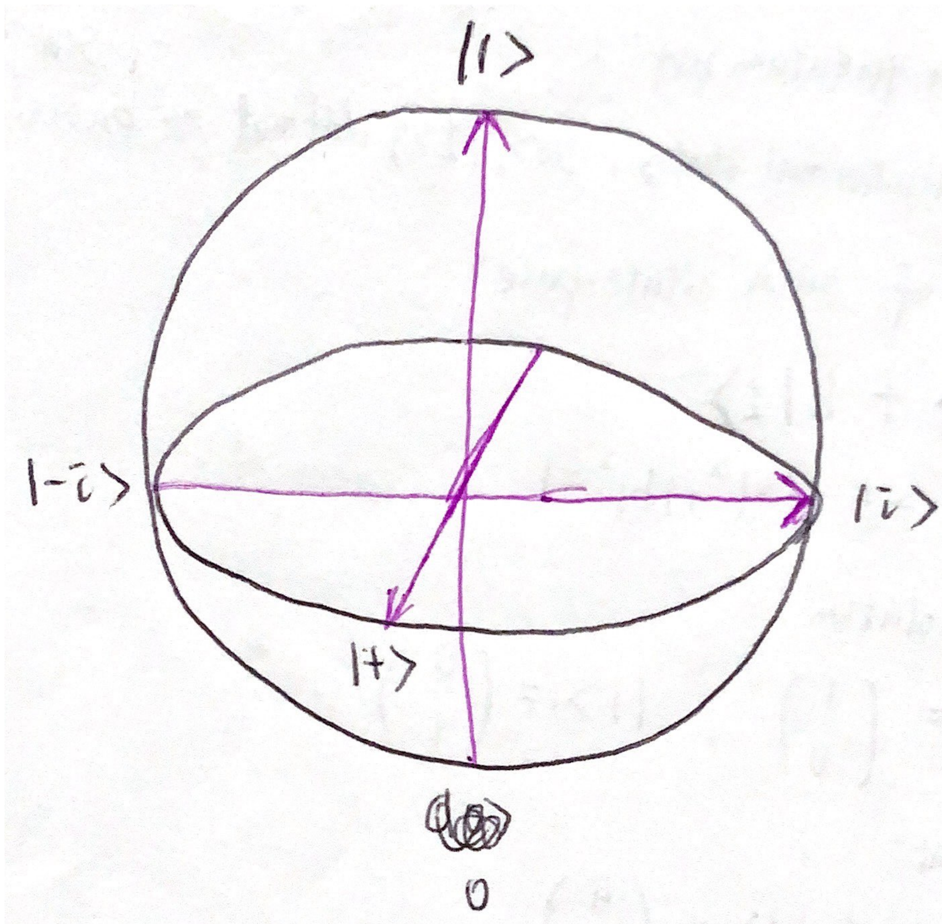
$$|v\rangle = a\,|0\rangle + b\,|1\rangle$$
$$\alpha = \frac{b}{a},$$

with consideration of the special case when $a = 0$:

$$\infty \leftrightarrow |1\rangle.$$

Step 2 For each $\alpha \in \mathbb{C}$, there exists $s, t \in \mathbb{R}$ s.t. $\alpha = s + it$. Now construct a 1-1 correspondence between each $\alpha = \langle s, t\rangle$ and a point on the unit sphere. The projection is defined as follows:

$$\langle s, t\rangle \mapsto \{\frac{2s}{|\alpha|^2+1}, \frac{2t}{|\alpha|^2+1}, \frac{1-|\alpha|^2}{|\alpha|^2+1}\}.$$



Remark 3.1. The antipodal points on the Bloch sphere correspond to pairs of orthonormal basis of the single-qubit system.

3.3. **Wave Functions.** Another way to represent each state of a single-bit system (or a 2- dimensional quantum system) is via wave functions. For now, you may think of wave functions as identity cards that encode specific information assigned to each quantum state. Moreover, wave functions are (time dependent) solutions to the time dependent Schrödinger equation. In the literature, wave functions are denoted as $\psi(x, t)$, with x denoting the position of the particle, t highlighting the time dependent nature of the function.

4. Wave Function

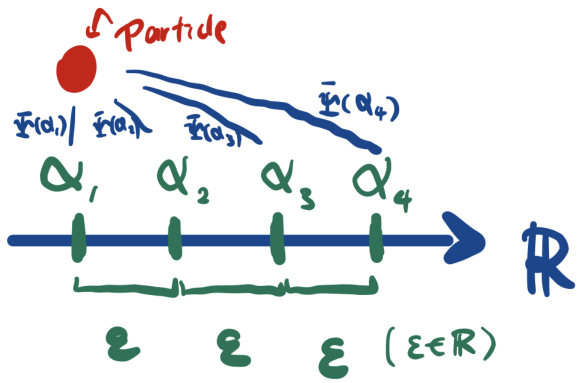
4.1. **Classical vs. Quantum.** As opposed to quantum mechanics, we refer to Newtonian mechanics as classical. In the classical sense, a particle is completely described by its position and momentum in time. In the quantum sense, a state of a particle (or in other words, a quantum system), may be represented by a complex function $\psi(x, t)$, also known as the wave function. Its physical significance will be discussed in the below sections. For the sake of clarity, in this talk we only consider the case of a quantum particle moving in the 1-dimension.

Though the function $\psi(x, t)$ does not encode information about the state's momentum directly, one may use the tool of Fourier transform to "extract" information about momentum from the wave function. Unfortunately, the full measurement of position and momentum of a quantum state may never be obtained simultaneously. This fact can be more rigorously formulated as Heisenberg's uncertainty principle (1927).

4.2. **A Probabilistic Interpretation.** By Born's probabilistic interpretation of quantum theory (1926), the outcome of an experiment may only be predicted in the probabilistic sense instead of the deterministic sense of Newtonian mechanics. In terms of bigger picture, one can construct the probability density function of finding the particle's position from $\psi(x, t)$. **The probability of the outcome of an experiment is encoded in $\psi(x, t)$.**

In the ensuing sections, we mainly focus on the mathematical aspect of wave functions. We use probability theory (section 4.5) to explore the probabilistic significance of wave functions and linear algebra (section 4.4) to explore how wave functions are elements of a vector space, which corresponds to a quantum system.

4.3. **Toy Model: Discretized Space.** Before we go to the continuous space, we start with a toy model, the discretized space:



[A particle moving along $\mathbb{R}$, with possible places $\alpha_1, \ldots, \alpha_4$]

Suppose we have a particle on the real number line, such that the particle might end up at four possible positions $\alpha_1, \alpha_2, \alpha_3, \alpha_4$. Moreover, the distance between each position is ϵ. By the probabilistic interpretation of quantum theory, the position of the particle can only be known in terms of probability. Mathematically, for all $\alpha_i, i = \{1, 2, 3, 4\}$, the probability of finding the particle at α_i is :

$$|\Psi(\alpha_i, t)|^2 \epsilon,$$

where $\Psi(\alpha_i, t)$ is the wave function corresponding to each α_i.

As mentioned earlier, each state of a quantum system may be encoded in a corresponding wave function. Thus, one may naturally think about expressing a system's information via wave functions. This is indeed possible: we can encode the above discretized space using a four dimensional complex vector. The rigorousness of such vector representation will be discussed in section 4.4.

Encoding Information Using Wave Functions (toy model version)

We define the toy model as a one dimensional discretized space (a real number line) such that a particle may have a finite number of positions denoted as α_i($i = 1, 2, .., n$). The wave function corresponding to each α_i is denoted as $\Psi(\alpha_i, t)$, then:

(1) The probability of finding such particle at α_i is:
$$|\Psi(\alpha_i, t)|^2\epsilon,$$
and to make notation clearer, define:
$$\psi_i = \sqrt{\epsilon}\Psi(\alpha_i, t),$$
so that the probability distribution of the position of the particle is $|\psi_i|^2$. Then it follows that:
$$\sum_i |\psi_i|^2 = 1,$$
and (the linear algebra aspect will be explained in section 4.4):
$$\langle\psi|\psi\rangle = \sum_i |\psi_i|^2.$$

(2) **State Vector**
We now see how exactly the toy model is encoded by wave functions. The system is encoded in a $n-$ dimensional complex vector:
$$|\Psi(t)\rangle = (\psi_1, ..., \psi_n).$$

Example 4.1. Say we have a particle that has equally spaced possible positions $\{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$. What is the state vector representing the particle ending up at position α_3?

4.4. **Wave Functions Live in $\mathcal{H}$.** We may now extend our toy model to the continuum. For the toy model introduced in section 4.3., notice that the state vector representing the system lives in a finite dimension. Now extend the space to an infinite dimensional vector space. In other words, we are still considering one particle moving along the real axis, but now the particle may end up at infinite number of positions. We still consider wave function $\psi : \mathbb{R} \to \mathbb{C}$.

We may now define the sufficient mathematical scheme, in terms of linear algebra, to describe how each ψ belongs to a vector space that corresponds to a quantum system. Later in section 4.5, we use probability theory to explore the information encoded in ψ. Now, we define the type of space that we deal with in quantum mechanics, the Hilbert spaces.

Definition 4.2. Hilbert space
A Hilbert space is a real or complex vector space equipped with an inner product $\langle \cdot, \cdot \rangle$, such that it is complete in the norm defined as:

$$||\cdot|| = \sqrt{\langle \cdot, \cdot \rangle}.$$

In this talk we consider wave functions that belong to the Hilbert space $L^2(\mathbb{R})$ (the space of square integrable functions). The proof for $L^2(\mathbb{R})$ being a Hilbert space is left to the readers to verify.

Definition 4.3. Inner product in Dirac's notation
In Dirac's notation, given a vector space V equipped with an inner product $\langle \cdot, \cdot \rangle$, then for vectors $|\alpha\rangle, |\beta\rangle \in V$ chosen arbitrarily:

$$\langle \alpha | \beta \rangle = \langle \alpha, \beta \rangle.$$

Wave Functions Live in a Unique Hilbert Space $\mathcal{H}$

You might ask:"why do wave functions live in a Hilbert space?" For now, just take this fact as an axiom of quantum mechanics.

(1) Wave functions belong to a unique Hilbert space $\mathcal{H}$ (linearity is implied) such that given $\psi_1(x), \psi_2(x) \in \mathcal{H}, \alpha, \beta \in \mathbb{C}$:

$$\alpha\psi_1(x) + \beta\psi_2(x) \in \mathcal{H}.$$

(2) The inner product associated with $\mathcal{H}$ is defined as:

$$\langle \psi_1 | \psi_2 \rangle = \int_{-\infty}^{+\infty} \overline{\psi_1(x)} \psi_2(x) dx.$$

(3) For all $\psi(x) \in \mathcal{H}$:

$$\langle \psi | \psi \rangle = ||\psi||^2 = \int_{-\infty}^{+\infty} \overline{\psi(x)} \psi(x) dx = \int_{-\infty}^{+\infty} |\psi(x)|^2 dx < \infty,$$

and due to (3), we say that wave functions live in the Hilbert space of square integrable functions, denoted $L^2(\mathbb{R})$.

4.5. **Probabilistic Approach to Wave Functions.** Recall that we consider a particle moving along $\mathbb{R}$ whose wave functions is defined as:

$$\psi : \mathbb{R} \to \mathbb{C},$$

such that the probability density of such particle being at position x is

$$|\psi(x)|^2.$$

Then, the probability of the particle being in $I \subset \mathbb{R}$ is defined as:

$$P\{x | x \in I \subset \mathbb{R}\} = \int_I |\psi(x)|^2 dx.$$

Moreover:

$$\int_{\mathbb{R}} |\psi(x)|^2 dx = 1,$$

which, from the physical point of view, is interpreted as the probability of the particle ending up at different positions on $\mathbb{R}$ must add up to 1. We then conclude that in general:

Normalization Condition for Wave Functions $\psi(x)$

All $\psi(x)$ must be normalizable, i.e.:

$$\int_{-\infty}^{+\infty} |\psi(x)| dx = 1.$$

Example 4.4. Normalizing a function
Given the function $f(x) = e^{-\frac{x^2}{2}}$, notice that:

$$\int_{-\infty}^{+\infty} e^{-\frac{x^2}{2}} dx = \sqrt{\pi}.$$

How can you modify $f(x)$ so that you get a new normalized function $f(x)$? What is your normalization factor? What can you say about the general pattern for normalizing a function (given that it is normalizable)?

4.6. **Deriving Momentum.** Notice that in the quantum mechanical sense, the parity that we have in the classical sense between position and momentum of a particle is broken. However, it is still possible to extract information about a particle's momentum from the wave functions. This section assumes basic knowledge of Fourier transform.

We start with a physical motivation:

De Broglie's Hypothesis (1924)

Given a particle such that its wave function has spatial frequency k (where $k \in \mathbb{Z}$), then its momentum p can be expressed as:

$$p = \hbar k,$$

where $\hbar$ is the reduced Plank constant.

Putting on the physicist's hat, if we attempt to recover the form of wave function $\psi(x)$ from de Broglie's hypothesis, we may guess that given k which represents the angular frequency, then:

$$\psi(x) = e^{ikx}?$$

But notice that $e^{ikx} \notin L^2$ (Why?). Thus, we may carry out more careful derivations. For the sake of clarity, we consider a particle moving on a circle and restrict the wave function to be 2π periodic. Then by the normalization requirement of wave functions, we expect $\psi(x,t)$ ($\in \mathrm{L}^2([0, 2\pi])$) to be:

$$\int_0^{2\pi} |\psi(x)|^2 dx = 1.$$

To satisfy the above condition, we may modify our original guess for $\psi(x) = e^{ikx}$ to be the normalized function (check this):

$$\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}, \; \psi \in L^2,$$

and by de Broglie's hypothesis, such particle has the momentum $p = \hbar k$ with probability 1, which is a nonrandom, deterministic measurement. We are, of course, not satisfied with the guess of wave function being $\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, as it does not match up to the probabilistic interpretation of quantum mechanics: it is impossible to know the exact momentum of a particle with probability 1.

Example 4.5. What is k?
Given a wave function for a 1-dimensional traveling wave:

$$f(x,t) = A\cos(\square x - \square t + \phi),$$

in which $\square$ should k be filled in?
Answer: the equation is:

$$f(x,t) = A\cos(kx - \omega t + \phi),$$

where:

k :=spatial angular frequency, i.e. the number of oscillations of the wave per unit space;

ω :=number of oscillations of the wave per unit time such that $T_{\text{period}} = 2\pi\omega$;

A :=amplitude;

ϕ :=the phase constant.

It is reasonable to conclude that for the limited case of a particle moving on a circle, its associated state space is the Hilbert space $L^2([0, 2\pi])$ equipped with an orthonormal basis (check this) defined in terms of functions $\{\frac{e^{ikx}}{\sqrt{2\pi}}\}_{k\in\mathbb{Z}}$. Thus, we may further modify our guess for wave function of such particle into a linear combination of the orthonormal basis:

$$\psi(x) = \sum_{k=-\infty}^{+\infty} a_k e^{ikx}. \tag{1}$$

Now we have a model of wave function that encodes the particle's momentum in the probabilistic sense. That is, every measurement gives momentum $p = \hbar k$, for some $k \in \mathbb{Z}$, with probability $|a_k|^2$.

Now, instead of considering a particle on a circle (see equation (1)), we consider a particle moving along $\mathbb{R}$. Recall that we first proposed the candidate $e^{ikx} (k \in \mathbb{Z})$ for wave function. However, we were not satisfied with e^{ikx} being not square integrable. Thus, we use Fourier transform to construct a square integrable wave function as a linear combination (of functions of the form e^{ikx}) in the continuous sense, i.e. an integral. As an analogy to (1), we define:

Constructing the Momentum Expression $\hat{\psi}(k)$ of a Particle

(1)
$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx} \hat{\psi}(k) dk,$$
where $\hat{\psi}(k)$ is the Fourier transform of ψ:
$$\hat{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx} \psi(x) dx.$$

(2) The associated Fourier transform operator $\mathcal{F}$ (i.e. imagine a function with input $\psi(k)$, output $\hat{\psi}(k)$) that maps from $L^2(\mathbb{R})$ to $L^2(\mathbb{R})$.

(3) (The Plancherel theorem)
$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_{-\infty}^{+\infty} |\hat{\psi}(k)|^2 dk = 1.$$

To rigorously provide a support for facts (1),(2),(3) stated above, we state the below proposition and theorem. Fact (2) directly follows from the below proposition, which is an extension of the result proven in the Schwarz space. This is because the Schwarz space is dense in $L^2(\mathbb{R}^n)$ and the Bounded Linear Theorem allows us to carry out such extension.

Proposition 4.1. *Given that $\psi \in L^2(\mathbb{R}^n)$, then $\hat{\psi} \in L^2(\mathbb{R}^n)$.*

Fact (1) and fact (3) follow from the below theorem:

Theorem 4.6. *The Fourier transform on $L^2(\mathbb{R})$*
Given the Fourier transform on $L^2(\mathbb{R}^n)$, $\mathcal{F} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, then:

(1) *$\mathcal{F}$ is defined as:*
$$\mathcal{F}(\psi)(k) = \frac{1}{2\pi^{\frac{n}{2}}} \lim_{A\to\infty} \int_{|x|\leqslant A} e^{-ikx} \psi(x) dx.$$

(2) *The Fourier inversion, denoted as $\mathcal{F}^{-1}$, is computed as:*
$$(\mathcal{F}^{-1} g)(x) = \frac{1}{2\pi^{\frac{n}{2}}} \lim_{A\to\infty} \int_{|x|\leqslant A} e^{ikx} g(k) dk.$$

(3) *The Plancherel theorem:*
$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_{-\infty}^{+\infty} |\hat{\psi}(k)|^2 dk. \tag{2}$$

It is worthwhile to notice that for the sake of presenting a big picture of the representation of the momentum function and its relation with the position function, many details of the Fourier transform has been swept under the rug. Moreover, if you are not satisfied with the explanation for the term e^{ikx} in the above expression, you may consult the formal explanation for such term, which involves solving the time independent Schrödinger equation.

In brief, the main take away from this section is :

Relation Between Position and Momentum

The probability density of the momentum of a particle is obtained via carrying out Fourier transform on the probability density of the position of the particle.

More insights could be obtained from the study of the relationship between the position and the momentum of a particle. For example, the uncertainty principle postulated by Heisenberg in 1927 is an intriguing result.

4.7. **A Quick Taste of the Heisenberg Uncertainty Principle.** As concluded in section 4.6., one may define the position and momentum of a particle using Fourier transform. However, both values cannot be measured simultaneously in the quantum mechanical sense (when the scale is smaller than h, the Planck constant). Such observation is formulated into the Heisenberg uncertainty principle:

Uncertainty Principle Stated in the Brief Way

If one measures the position and momentum of a particle on the quantum scale simultaneously, then:

$$\Delta x \cdot \Delta p \geqslant \frac{\hbar}{2},$$

where $\Delta x, \Delta p$ correspond to the precision of the measurement of the position and momentum of the particle.

There exist(s) more rigorous derivation(s) of the uncertainty principle. However, due to space and time limitation, we only cover the general take of the principle.

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