Quantum mechanics with real vectors

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Introduction

Quantum mechanics is usually formulated with a wave function which requires complex numbers, spin vectors which require Pauli matrices, operators which are needed to determine outcome probabilities and a Hamiltonian operator which determines the time evolution. I will examine how much of quantum mechanics can actually be done with *simple real vectors* from high-school, the usual dot product and a rotation of vectors alone, without using any of the previously mentioned mathematical objects. This reduced complexity will reveal a “geometric quantum mechanics” with a geometric interpretation and intuition.

While I assume that the overall computational cost does not decrease (and neither increases), this simpler representation may form a more intuitive way to think about interpretations of quantum mechanics.

This document will be extended with future topics (e.g. about what makes

quantum different from classical, time evolution calculations, other derivations, …). Come back if you are interested.

You may email suggestions to this email.

Wave function as a real vector

To transform a wave function to a real vector we use the density matrix for a pure state. We assume than whole system is considered and the density matrix can describe all outcomes. The operation that we commonly will apply to the density matrix is $P = \mathrm{Tr}(\rho A^\dagger)$ for some matrix A. It can be identified with an inner product in a vector space as follows:

$$P = \mathrm{Tr}(\rho A^\dagger) = \sum_{ij} \rho_{ij} A^\dagger_{ji} = \sum_{ij} \rho_{ij} A^*_{ij}$$

If we identify the wave function with a column vector $\Psi = (\rho_{11}, \rho_{12}, ...)$ and the other matrix with $A = (A_{11}, A_{12}, ...)$ we already get vectors in a complex vector space. This means introducing new basis vectors $e_i = |a\rangle\langle b|$ where i iterates over all (a, b) pairs.

The expression P becomes a dot product $P = \Psi \cdot A$. However, if all our matrices are Hermitian matrices $H_{ij} = H^*_{ji}$, we can continue and create a real vector space, due to the redundancy of the matrix values opposite of the diagonal.

$$\begin{aligned}
P &= \sum_i \rho_{ii} A_{ii} + \sum_{i<j} \left(\rho_{ij} A^*_{ij} + \rho_{ji} A^*_{ji}\right) \\
&= \sum_i \rho_{ii} A_{ii} + \sum_{i<j} \left(\rho_{ij} A^*_{ij} + \rho^*_{ij} A_{ij}\right) \\
&= \sum_i \rho_{ii} A_{ii} + \sum_{i<j} 2\Re(\rho_{ij} A^*_{ij}) \\
&= \sum_i \rho_{ii} A_{ii} + \sum_{i<j} 2\left(\Re(\rho_{ij})\Re(A_{ij}) + \Im(\rho_{ij})\Im(A_{ij})\right)
\end{aligned}$$

Therefore we can just stack the diagonal values and the real and imaginary parts of the off-diagonal values into an n^2-dimensional real column vector to do the same calculation with a dot product only.

$$\boxed{\Psi = \left(\rho_{11}, \rho_{22}, \dots, \rho_{nn}, \sqrt{2}\Re(\rho_{12}), \sqrt{2}\Im(\rho_{12}), \sqrt{2}\Re(\rho_{13}), \sqrt{2}\Im(\rho_{13}), ...\right)}$$

Usually you would want to rotate this to a new basis. In particular, it is convenient to rotate the first component into a constant vector $\sum \rho_{ii}$.

This is the recipe to convert density matrices and other matrices to the real vectors. Any matrix can be converted this way and the expression P becomes a simple dot product

$$P = \Psi \cdot A$$

It can be more revealing to rotate these vector into a new basis, which would still preserve the inner product outcome. The main feature of all of this is that we are preserving the inner product structure.

The probability to measure a certain eigenvector $|\lambda\rangle$ of an observable can be calculated by using $A = |\lambda\rangle\langle\lambda|$ in our expression which is like an observable with eigenvalue 1 for our desired eigenvector and 0 for all other orthogonal vectors. Therefore converting this the same way into a real vector $\Lambda = |\lambda\rangle\langle\lambda|$ we can write for the probability of measuring a quantum state in another measurement state

$$\boxed{P(\lambda) = \Psi \cdot \Lambda}$$

This equation has a much more natural and geometrically interpretable form than $|\langle\psi|\lambda\rangle|^2$. Note that it calculates the measurement probabilities, whereas the measurement outcomes (eigenvalues) are treated separately, unlike in usual quantum mechanics where the eigenstates and eigenvalues are "packed" together into an observable operator. Later we will see that other needed quantum mechanic operations are simply rotations of these real vectors.

Quantum postulates

Let us look how the postulates of quantum mechanics look with this alternative geometric formalism of quantum mechanics. The following postulates are usually stated for quantum mechanics (R.L.Jaffe 1996, MIT lecture handout)

1. At each instant the state of is system is completely represented by a ket vector $|\psi\rangle$ (in complex vector space)
2. Every observable is described by an operator that acts on the kets
3. The only possible result of a measurement is one of the eigenvalues of the corresponding operator
4. The probability of obtaining a value λ with the eigenstate $|\lambda\rangle$ is $P = |\langle\lambda|\psi\rangle|^2$
5. Immediately after the observable has yielded a value λ, the state of the system is the normalized eigenstate $|\lambda\rangle$

6. The evolution of the system is described by $|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$ for some unitary operator U.

In the alternative formalism introduced here we instead have

1. At each instant the state of is system is completely represented by a vector Ψ (in **real** vector space)
2. Every observable is described by a **vector** that can be **dotted with the state vector**.
3. The only possible result of a measurement is the values that you **independently assign to the observable vectors**.
4. The probability of obtaining a value λ with the eigenstate Λ is the **dot product** $P = \Psi \cdot \Lambda$
5. Immediately after the observable has yielded a value λ, the state of the system is the normalized eigenstate Λ
6. The evolution of the system is described by $\Psi(t) = U\Psi(0)U^\dagger$ for some **rotation** U where the geometric algebra product is used.

We see that overall fewer mathematical concepts are needed in the alternative formalism. The only drawback is, that to conveniently do rotations in arbitrary dimensions we will employ geometric algebra which extends vector spaces with a new type of vector-vector multiplication. (I'll work it out when I have some time)

One interesting point for the interpretation of quantum mechanics is that postulate (4) is like looking up the coefficient of the whole vector in a new basis. A vague idea is that that no collapse is happening at all and we are just looking at a particular basis.

Derivation of the formalism from principles

Here I show a partial derivation of the the postulates in the alternative formalism from basic principles. With some more principles maybe a theorem like Gleason's theorem can be derived, showing that the real vector formalism is the unique mathematical way to satisfy all principles.

We start with the principles

1. After measuring an outcome Λ, the probability of measuring this outcome again right after is 1.
2. After measuring an outcome Λ, the probability of measuring some other "orthogonal" outcomes right after is 0. They constitute disjoint events.
3. Considering all orthogonal, possible outcomes, the summed probabilities must add up to 1 as they are disjoint events.

In equations this would be

$$P(i \to j) = \delta_{ij}$$
$$\sum_j P(i \to j) = 1$$

This can easily be modeled mathematically with an inner product on vectors:

$$P(i \to j) = \psi_i \cdot \phi_j$$

and orthonormal vectors

$$\boxed{\psi_i \cdot \psi_j = \delta_{ij}}$$

form the disjoint event outcomes. With postulating more principles, this could be a unique way. Since we already know that this formalism is identical to the density matrix formalism, the mathematics is correct.

Note that ψ_i and ϕ_j are not necessarily from the same basis vector set. Different orthonormal bases can be chosen, but in any case we require

$$\boxed{\psi \cdot \psi = 1}$$

For the second equation, which due to linearity translates to $\psi_i \cdot \left(\sum_j \phi_j\right) = 1$, we require that we **only consider basis vector sets which all lie in a particular plane**

$$\boxed{\psi \cdot D = 1}$$

where D (diagonal) is some free-to-choose vector of length $\sqrt{n}$ and all *allowed* orthonormal bases need to satisfy $\sum_i \psi_i = D$. We could always choose D to be along our first basis vector of the vector space.

Actually, vectors satisfying $\psi \cdot \psi = 1$ form pure states, and convex combinations $\Psi = \sum \alpha_i \psi_i$ where $\sum \alpha_i = 1$, $\Psi \cdot \Psi < 1$, $\Psi \cdot D = 1$ can be thought of as mixed states.

The equations in this section correspond to Tr$(\rho) = 1$ and Tr$(\rho^2) = 1$ in quantum mechanics. I could imagine operations like traceing out states correspond to basic vector space operations.

Deriving the spin-1/2 states from geometric principles

We can use the derived conditions to guess the spin-1/2 eigenstate in our real vector space, without any knowledge of Pauli matrices or complex numbers. It could also be derived more rigorously or from the above density matrix conversion.

What do we need? An electron spin is some kind of “two-valuedness” and we need 3 symmetrically related axis, because we can measure it in 3 dimensions. Symmetry of space requires the symmetry of our geometrical states.

A single two-valued measurement means no more than we have two orthonormal vectors in our real vector space. We need to add two additional two-valued ways to measure, which means introducing two more pairs of orthonormal vectors. Apart from the symmetrical relation amongst these basis pairs, we always require the condition $\psi \cdot D = 1$ meaning that all basis sets have to sum to the same hypercube diagonal, or equivalently they lie in the same plane. For just two pairs this is easily visualized since our vector space is real:

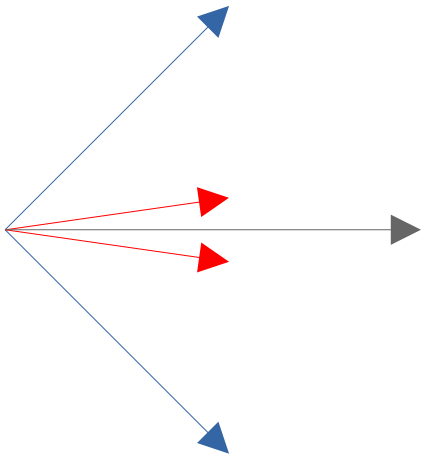

Figure 1: spins

where the blue arrows represent the basis of measurements in z-direction and the red arrows represent the basis of measurements in x-direction and are thought to be out-of-plane. The common diagonal is gray and is also perpendicular to the plane in which all basis vectors have to lay. However, due to being length 1 and being restricted to a plane, these basis vectors can only trace out a circle when rotated. Since we rather need a sphere to model all directions, we will require one more pair of basis vector which do not fit into 3-dimensional space anymore.

Mathematically, the easiest way to satisfy all requirements is to use the unnormalized pairs

$$e_0 \pm e_1, e_0 \pm e_2, e_0 \pm e_3$$

where e_i are an orthonormal basis in 4 dimensions. This is what it mean to have a two-valued measurement in 3 symmetric directions.

Combining the components and normalizing, we can identify the vector for a

single spin in direction $\hat{n}$ with the state vector

$$\Psi_n = \frac{1}{\sqrt{2}}(e_0 + \hat{n})$$

You would get the same with the above method of converting density matrices, if you additionally apply a rotation.

Comparing this to the conventional $\rho = \frac{1}{2}(I + \vec{\sigma} \cdot \hat{n})$ we see that it is similar, but apparently Pauli matrices and complex numbers are not needed anymore. The reason is probably that in quantum mechanics there is a asymmetry between wave function and observable operator, and moreover the observable has the outcomes already mixed in. Avoiding these two entanglements seems to simplify the mathematics.

As usual we can calculate the correct probability of measuring a given state in another measurement direction

$$\Psi_{n_1} \cdot \Psi_{n_2} = \frac{1}{2}(e_0 + \hat{n}_1) \cdot (e_0 + \hat{n}_2) = \frac{1}{2}(1 + \cos\theta) = \cos^2\frac{\theta}{2}$$

Multiply spin-1/2 state and Bell inequality

For 2 spins the state vector would probably be the tensor product of two spin vectors

$$\Psi = \frac{1}{\sqrt{2}}(e_0 + \hat{n}) \otimes \frac{1}{\sqrt{2}}(e_0 + \hat{n}) = (e_0 + \hat{n}_1 + \hat{n}_2 + e_8 n_{1x} n_{2x} + e_9 n_{1x} n_{2y} + \cdots)$$

where currently normalization and coefficients are missing.

However, with the tools of linear algebra we do not need to worry about components representations. Instead we can calculate the components in any basis as shown above and rotate those for our considered vectors into a smaller subspace. Let us do that for the states relevant in a demonstration of the Bell inequality.

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Multiplying a state by an operator

We still need to determine what an operator does to a state in our representation. For this we write

$$|\phi\rangle = M|\psi\rangle = \sum_{ij} |b_i\rangle\langle b_j|M_{ij} \sum_k \psi_k |b_k\rangle = \sum_{ij} |b_i\rangle M_{ij}\psi_j$$

$$\begin{aligned}
\rho &= |\phi\rangle\langle\phi| \\
&= \sum_{ij} |b_i\rangle M_{ij}\psi_j \sum_{kl} \langle b_k| M^*_{lk}\psi^*_l \\
&= \sum_{ijkl} |b_i\rangle\langle b_k| M_{ij}M^*_{lk}\psi^*_l\psi_j \\
&= \sum_{ik} |b_i\rangle\langle b_k| \sum_{jl} M_{ij}M^*_{lk}\psi^*_l\psi_j \\
&= \sum_{ik} B_{ik} \left(\sum_{jl} B_{jl}M_{ij}M^*_{lk} \right) \cdot \left(\sum_{jl} B_{jl}\psi^*_l\psi_j \right)
\end{aligned}$$

With this we could already do calculation in the real vector notation as it only requires the dot product between vector. However, later I will try to show that for unitary matrices this is related to $\rho = r\Psi r$ with geometric algebra.

Time evolution

I will try to show that time evolution will be a rotation of vectors

$$\frac{\partial \rho}{\partial t} = H\Psi H$$

in real vector space.

What makes quantum mechanics different from classical mechanics?

Work in progress.

The question is why quantum mechanics isn't even more natural than classical mechanics when it satisfies such fundamental principles. The first guess is that with a large n everything becomes classical and quantum mechanics is only weird, because it is the only few, discrete outcome theory, that satisfies our basic principles.