Quantum Mechanics

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I am interested in understanding the general framework, not so much in performing concrete calculations. We start by handing down a theory from God, if we have time we will try and figure out some of the motivations.

1 The Experimental Origins

[Hal13] has a very nice first chapter on the experiments that lead to Quantum mechanics that we will summarise here.

- **1804 - (L) Young:** The double slit experiment for light shows that it interferes.
- **1818 - (L) Arago:** Light shined at an opaque disc has a bright spot in the center of the shadow. Implies that the light is diffracting around the edge of the disc.
- **1888 - (L/E) Johannes Rydberg:** When a hydrogen tube has a current run accross it, the light emitted, when it is passed through a prism, splits into a discrete number of colors.
- **1905 - (L/E) Einstein:** The photoelectric effect is observed. When the intensity of light is increased the energy of the electrons released doesnt change, although the number does.
- **1909 - (L) Taylor:** Reduced intensity double slit experiment for light. Attempting to simulate light going through "one at a time", shows the same interference pattern.
- **1925 - 1927 - (E) David & Germer:** Electrons shot at reflective crystal plate produce a diffraction pattern similar to those of an x-ray in the reflection.
- **1961 - (E) Jonsson:** An electron double slit experiment is performed, with the same interference patter as light.
- **1989 - (E) Tonomura:** Electron single slit experiment is performed. The long term statistical patern matches that of light.

The key steps in the theory were made in 1865 when Maxwell produced a theory of EM radiation that predicted that the speed of EM waves matches that of light, 1900 when Planks theory predicts that EM should be quantise, 1924 when De Broglie provided a theory of electrons in the hydrogen atom based on the assumption that they were waves and finally 1926 when Schrodinger provided a more or less modern theory of QM.

2 A Framework

In classical mechanics the only intrinsic property of a particle is its position. The goal of mechanics is to solve for the position of the particle at a given time, this is a single point in (say) $\mathbb{R}^4$. In QM the same role is filled by the wave function, roughly describing a probability distribution. Unlike classical mechanics however a particle has another intrinsic property, known as spin. Thus a single particle is completely described only by an element in (say)

$$\mathcal{H} \;:=\; L^2(\mathbb{R}^4) \otimes V_{\text{spin}}$$

To clarify a few maters of notation; L^2 is functions that land in $\mathbb{C}$ and V_{spin} is some finite dimensional $\mathbb{C}$ vector space. Thus we can see that to describe a particle we need much more data. One simplifying observation is that [Ree, II.4]

$$L^2(X) \otimes \mathbb{C}^n \cong \left(L^2(X)\right)^{\oplus n}$$

Thus we can think of our states as n-tuples of L^2 functions. I think that Physicists call these spinors.

In classical mechanics we have Newtons laws or the Euler-Lagrange equations that give the fundamental differential equation that the position of our particle must obey. In QW we have the Schrodinger equation, that a state $\Psi \in \mathcal{H}$ must satisfy

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

where H is an operator on $\mathcal{H}$ that is dependent on the physical situation. Now it is clear that if Ψ is a solution to this equation then so is $c\Psi$ for any complex number c.

If $\Psi = \begin{bmatrix}\psi_1 & \cdots & \psi_n\end{bmatrix}^t$ then we *interpret*

$$\sum_{i=1}^{n} |\psi_i|^2 : \mathbb{R}^4 \to \mathbb{R}$$

as the probability distribution function for a particles location at a given time, we can say that it is a probability distribution because by our scale invariance we can always normalise our solution. If consider only $|\psi_i|^2$ then this is giving the probability that the particle is at a certain place *and in the spin state* i, if we integrate this function over all space we get the probability that it is in the given spin state at a given time.

Given this interpretation we can ask what the expected position is at any time, which taking the expected value of our pdf is given by

$$\langle x \rangle = \int x \begin{bmatrix}|\psi_1|^2 & \cdots & |\psi_n|^2\end{bmatrix}^t = \int x\Psi^*(x,t)\Psi(x,t)dx$$

where the asterix denote the conjugate transpose of our vector. Note that we are integrating component wise, so we get a vector where the entries are the expected position given it is in that spin state. In classical mechanics all observable values are expressible in terms of the momentum and position. If $Q(x,p)$ is a physical quantity of classical mechanics then we define its quantum mechanical version via the substitution $\hat{Q} = Q(x, -i\frac{\partial}{\partial x})$. This has the expected value given by

$$\langle \hat{Q} \rangle = \int \Psi^*[Q(x, -i\frac{\partial}{\partial x})](\Psi)dx.$$

The assumptions of QM are then that If you measure an observable $Q(x,p)$ on a particle in a state $\Psi(x,t)$ (a vector) you must get one of the eigen-values of $\hat{Q}(x,-i\frac{d}{dx})$. If the spectrum is discrete the probability of getting the particular eigenvalue q_n of eigen function f_n is $|\langle f_n|\Psi\rangle|^2 = \sum_i |\langle f_n|\psi_i\rangle|^2$. Note here that the operator coming from a classical quantity is acting component wise. There is another option of more general operators on $\mathcal{H}$ that act in more complicated ways, in which case the statement is the same.

Remark. Note that there may be solutions to the equations that have infinite integral or zero integral, which then cannot be normalised, **we reject them as non-physical** because of our interpretation.

Remark. Note that what we have said so far makes sense in any paradigm or ontology and moreover is empirically testable. If I claim some distribution for the result of an experiment given some initial condition you need only do the experiment many times to verify my prediction. This is therefore a statistical theory so far, we have not introduced any actual measurements or woo woo collapse of wave functions.

Remark. What does $\hat{Q} = Q(x,-i\frac{\partial}{\partial x})$ actually mean. This process is referred to by physicist as "quantizing". First we must assume something about our classical quantities Q, namely that they are analytic or smooth or something. We conflate them with a power series in x and p. Once this is done, we can see it as an element of say $\mathbb{C}[[x,p]]$. Now we can compose some morphisms to get an element in $\mathbb{C}[[x,-i\frac{\partial}{\partial x}]]$ and finally the relevant ring of operators.

This works when the operators commute or when they dont interact. But what about if the observable is of the form ab such that the pair of quantities quantum mechanical operators dont commute, that is $AB \neq BA$. In this case there are lots of things that can be done. [Hal13, Def 13.1] has a nice summary. The idea is to choose an ordering or take an average of the difference orders.

3 Spin Independent Hamiltonians

In the Schrodinger equation

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

the operator H is called the Hamiltonian. The simplest case is when the Hamiltonian does not depend on the spin state. In this case we can write it as a Kronecker product

$$H = H_{L^2} \otimes I_{V_{\text{spin}}}$$

which as a matrix is then just diagonal with the Hamiltonian H_{L^2} on the diagonals, thus it acts component wise on the tuple of functions. In this setting the most common Hamiltonian for the L^2 part is given by

$$-\frac{1}{2m}\nabla^2 + V.$$

Here V is some operator that will depend on the given situation. In this situation because the operator acts component wise, we can reduce the analysis to essentially assuming that V_{spin} is one dimensional or otherwise just not there in the Hilbert space tensor. Thus ignoring spin we have the basic case of the Schrodinger equation given by

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2m}\nabla^2\Psi + V\Psi.$$

4 Time Independent Schrodinger Equation in One Dimension

From [GS18]. Continuing our assumption that the Hamiltonian is of the above form (spin independent and given by some Laplacian) Here we make two assumptions on the form of V, first that as an operator it is just multiplication by some smooth function. The second is that that smooth function, which we also denote $V \in L^2(\mathbb{R}^4)$, is independent of time, that is a function only on $\mathbb{R}^3$, the spacial coordinates. Finally to simplify again we will pretend that our dynamics are on a line, that is we reduce $\mathbb{R}^4$ to $\mathbb{R}^2$.

To summarise the setup then, we are looking for functions $\Psi \in L^2(\mathbb{R}^2)$ that satisfy the differential equation

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

First we look for separable solutions, that is solutions of the form $\Psi(x,t) = \psi(x)\varphi(t)$. Under these assumptions we can separate the Schrodinger equation into a LHS that depends only on time and a RHS that depends only on space:

$$E \; := \; i\frac{1}{\varphi}\frac{d\varphi}{dt} = -\frac{1}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x)$$

E is called the "separation constant", this is because by solving $E = LHS$ and $E = RHS$ we have separated the Schrodinger equation into two ODEs:

$$E = i\frac{1}{\varphi}\frac{d\varphi}{dt}, \quad E = -\frac{1}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V(x)$$

Note that E must be a constant because on one hand it has no time dependence and on the other it has no space dependence. It can be complex constant a priori, this will depend on the Hamiltonian, as E will be the eigen-value of that operator. For this reason we often will assume things like the Hamiltonian having real eigen-values. The first equation is easily solved to give

$$\varphi(t) = \exp(-iEt)$$

with the dependence on E. The other equation cannot be solved without further assumptions on V, it is called the time independent Schrodinger equation. If we were to find ψ under these extra assumptions then the solution would have many nice properties

- They are so called stationary states because although the wave equation depends on time the probability density does not
$$|\Psi(x,t)|^2 = |\psi(x)|^2$$
- It follows from this that the expected values of our physical quantities are also time independent, in particular $\langle x \rangle$ is a constant and so $\langle p \rangle$ is zero. On average nothing happens, the state is stationary!
- One operator of x, p from classical mechanics is the so called total energy, or Hamiltonian
$$H(x,p) = \frac{p^2}{2m} + V(x)$$
if we naively substitute $-i\frac{\partial}{\partial x}$ for p then we get the so called Hamiltonian operator of the system, $\hat{H}$. Using this notation the time independent Schrodinger equation can be written
$$\hat{H}\psi = E\psi$$
so we see that the stationary states are eigenvectors of eigenvalue E for $\hat{H}$.

- Using this eigenvalue formula it is easy to calculate that

  $$\langle \hat{H} \rangle = E, \sigma_{\hat{H}} = 0$$

  and so any measurement of this variable is *certain* to always return the same value. This also makes clear the connection between E, the separation constant and energy, E is the expected value and certain value of the Hamiltonian which is the classical total energy of the system.

- Finally the general solution to the Schrodinger equation, where we still assume V is time independent, is given by linear combinations of the solutions to the time independent Schrodinger equation (iff). Thus if we have all the separable solutions $\Psi_k(x,t) = \psi_k e^{-iE_k t}$ we know that you are a solution iff you are of the following form

  $$\Psi(x,t) = \sum_{k \geq 1} c_k \psi_k e^{-iE_k t}$$

  The required constants may be solved for given some initial conditions.

5 Representation Theory

Here are a few places that representation theory comes up. First we are applying operators on $L^2(X)$, if H is such an operator then naturally we are dealing with a representation of the group $\langle H \rangle$ generated by that operator or whats the same is looking at $L^2(X)$ as a module over the algebra $\mathbb{C}\langle H \rangle$. Then we want to diagonalise this representation to see how the operator acts more simply. This would correspond exactly to finding the eigenvectors and values, thus the possible observables for an operator are the basis for this representation. By [Hal13, Prop 14.7] in this sense the position and momentum operators are irriducible. The Stone-Von Neuman theorem gives sufficient conditions for these representations to be (unitarily) equivalent.

Other representations enter the scene when we begin to talk about systems with symmetry. First consider a compact (this is sufficient but not necissary) group G acting on $\mathbb{R}^n$, then there is an induced action on $L^2(\mathbb{R}^n)$ given by $g.f(x) = f(g^{-1}x)$. Then [Bou04, Chapter VII, §2.2 and §2.4 (Remark 3)] we have a bijection between G invariant functions and functions on $L^2(\mathbb{R}^n/G)$. Moreover this bijection when the homogeneous spaces are given the induced measures of [Bou04, Prop 5.] becomes an isometry, one can verify this directly through the formula for the integral on the quotient. The point is that

$$L^2(X)/G \cong L^2(X/G).$$

Thus we can litterally think of a symmetry of our space, that is the action on X as a symmetry of the distributions that we might consider. Thats why [Hal13] ”symmetry is encoded is usually through a unitary action of the group on the relevant Hilbert space”.

Now recall that in this setting our representations are on a Hilbert space of functions. Moreover we have identified functions up to scaling by a constant, because we only want those that form probability distributions. This means that the representations that we consider are ”projective”, defined as a homomorphism from G to $U(\mathcal{H})/U(1)$.

So consider a unitary representation of a compact Lie group G on our Hilbert space $\mathcal{H}$. Then there is (several) a natural representation on the set of operators between this Hilbert space that we denote $\Gamma(\mathcal{H})$, which is given by

$$(g.Q)\psi \;\; := \;\; g.\big(Q(g^{-1}.\psi)\big)$$

or in less detail simply $g.Q = gQg^{-1}$. One reason that this representation is chosen is that it preserves the spectrum of Q and the other is that it satisfies the identity (just sub the definition into the RHS)

$$g.(Q\psi) = (g.Q)g.\psi$$

This identity *makes sense physically*, for instance rotating the measured state (LHS) is the same as rotating the state and measuring with a *rotated* apparatus (RHS). Now under these hypothesis we can consider the expectation value. By assumption the representation is by unitary operators and so they preserve the L^2 inner products. If we look at expected values we get

$$\begin{aligned} \langle (g.Q)(\psi) \rangle &= \langle \psi, gQg^{-1}\psi \rangle \\ &= \langle g.g^{-1}.\psi, gQg^{-1}\psi \rangle \\ &= \langle g^{-1}.\psi, Qg^{-1}\psi \rangle \end{aligned}$$

So the expected value of the "rotated" operator is the same as if we didnt rotate the operator and we "put the vector back", i.e. rotated it back. So this all makes good sense, any unitary representation on the Hilbert space interacts with all the observables in this way. So if your Hilbert space happens to have one of these representations then your physics has some symmetry in this sense.

One often considers the *stronger* condition that the representation commutes with some operator, i.e. we have that

$$g.Q(\psi) = Q(g.\psi)$$

if this is the case then we see that

$$\begin{aligned} \langle (g.Q)(\psi) \rangle &= \langle g^{-1}.\psi, Qg^{-1}\psi \rangle \\ &= \langle g^{-1}.\psi, g^{-1}.Q(\psi) \rangle \\ &= \langle \psi, Q(\psi) \rangle \\ &= \langle Q \rangle \end{aligned}$$

the expectation value not only transforms nicely but is actually *invariant*. I dont think that the converse, invariant implies commutes, is true in general, but certainly commuting is sufficient for this invariance. Note that commuting with one observable implies nothing about the others.

Remark. A symmetry is often defined as a representation that commutes with the Hamiltonian operator in particular. One perspective on this is that the Hamiltonian is the time evolution operator and therefore commuting with it says if you apply the symmetry and then evolve the system its the same as evolving then applying the symmetry.

References

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