Crash Course on Quantum Mechanics, Part I

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Abstract

What is the physical motivation for a theory like quantum mechanics? Starting with this question we will explore the basics of understanding the structure of the theory in comparison to classical mechanics, specifically discussing what a wavefunction is and how the state of a particle evolves based on the behavior of the wavefunction.

1. Experimental Motivation

Why was it the case that physics demanded a new theory vastly different from classical mechanics? In attempting to answer this question we want to study the *Stern-Gerlach* experiment and why it required a probabilistic approach to particle theory rather than the deterministic physics governed by Newton's laws. This very particular experiment involves the simple setup of sending a beam of silver atoms through an inhomogeneous[1] magnetic field and reading in which direction a particle gets deflected. More specifically, assume that we have a Stern-Gerlach machine for each direction of space which when receiving a beam of particles will filter them out based upon the direction they get deflected. Visually we have the following setup:

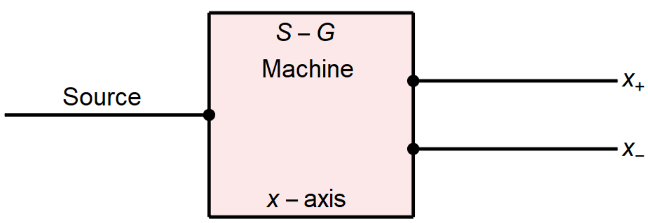

Fig. 1: Stern-Garlach machine along x-axis

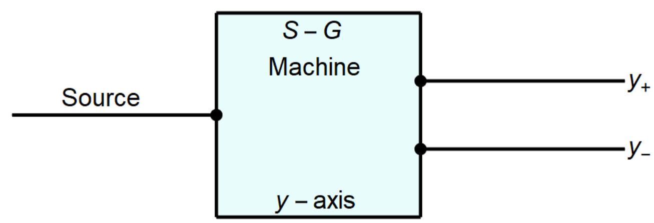

Fig. 2: Stern-Garlach machine along y-axis

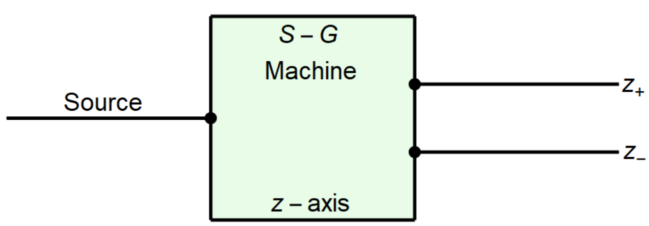

Fig. 3: Stern-Garlach machine along z-axis

When dealing with a single machine the experimental result aligns with the intuitive expectation in that we expect half of the particles to be pointing in the positive direction and the other half in the negative direction. What about using one machine after the other?

[1]The *inhomogeneous* aspect references that if we think of a particle as a classical magnetic dipole, then the forces exerted on opposite ends of the dipole by the magnetic field are not exactly equal, so as to produce a net force that deflects the particle's trajectory.

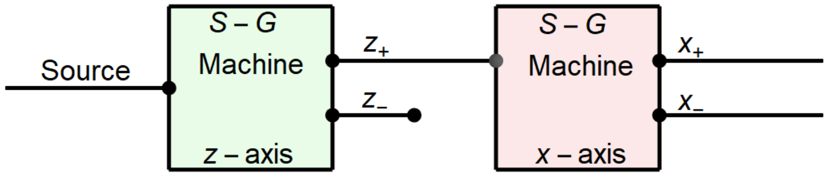

Fig. 4: Measurement along z-axis followed by measurement along x-axis

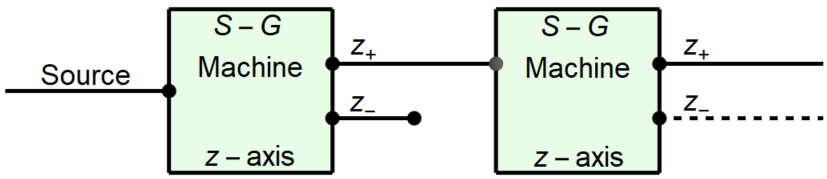

Fig. 5: Measurement along z-axis followed by measurement along z-axis

In the first scenario when measuring the deflection along the x-axis after having measured for the z-axis we find that the result is exactly as expected in that a positive (equivalent if negative) measurement along the z-axis will still produce on average half going positive and the other half going negative along the x-axis. Thus, the alternation of two different Stern-Gerlach machines yields nothing surprising.

Similarly, in the second scenario when measuring the deflection along the z-axis after having already measured it we find that a repeated measurement yields the exact same result. In other words, if the first measurement was positive (negative), then the second one is also positive (negative). By this point one might wonder how complicated the setup of the experiment has to be in order to produce some really unexpected behavior, but as it turns out three Stern-Gerlach machines are enough. Consider the following setup:

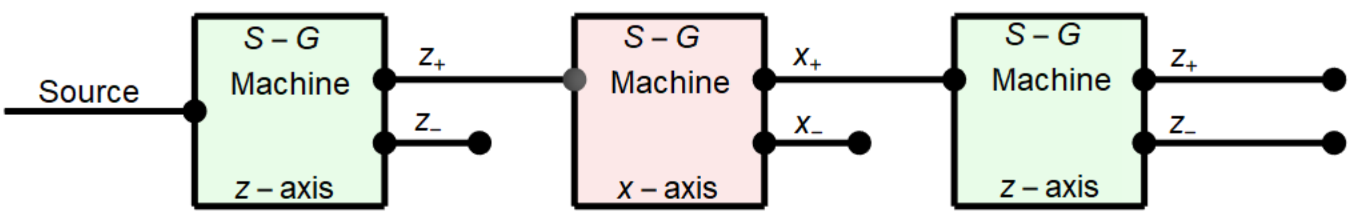

Fig. 6: Measurement along z-axis, then followed by measurement along z-axis, with a final measurement along z-axis

where we pass a particle through three Stern-Gerlach machines that measure along the directions of the z-axis, then x-axis, and finally the z-axis again. If we suppose that the first machine reads positive along the z-axis and the second machine reads positive along the x-axis, then we expect the third machine to read strictly positive along the z-axis since we have already made the measurement. As it turns out, experimentally this is not what occurs and that half the time the third machine will actually read negative. This result is very unexpected because it implies that the measurements along the z and x-axes are somehow *incompatible* with one another.

The Stern-Gerlach experiment alone implies that the expected result under the deterministic world governed by Newtonian mechanics does align with what we experience in the real world. Combining this with the fact that we cannot deterministically figure out whether the third machine will read positive or negative truly motivates that we require a non-deterministic theory of physics to model the probabilistic results.

2. Schrödinger Equation

In the case of classical mechanics the evolution of a state representing some particle is governed by Newton's second law:

$$F = ma = m\ddot{x}$$

where m and $x(t)$ are the mass and position of the particle. Solving this differential equation for a given (conservative) force will provide the equation(s) of motion whose solution will model the trajectory a particle travels along. When it comes to the study of quantum mechanics on the other hand the evolution of a state $\Psi(x,t)$ representing a single particle, sometimes also denoted as $|\Psi\rangle$ in *bra-ket notation*, is governed by the Schrödinger equation:

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

for $\hbar$ Planck's reduced constant, m the mass of the particle, V the potential, and Ψ the *wavefunction* of the particle. At this point it is not obvious what the exact connection between the wavefunction and the particle exactly is, but determining its behavior will provide us with information about the particle. With all of this in mind we can see that the setup is not too different from classical mechanics in that we have a differential equation modeling some property associated to the particle and that everything depends upon the choice of potential V where $F = -V$ in the classical case.
Knowing by now that we are building towards a non-deterministic theory of physics we introduce the statistical interpretation of the wavefunction, otherwise known as *Born's Rule*.

Definition 2.1 (Born's Rule)**.** The probability of finding the particle in the region $[a,b]$ at time t is given by:

$$\int_a^b |\Psi(x,t)|^2 \, \mathrm{d}x$$

It is worth pointing that in the Schrödinger equation there shows up the imaginary constant $i = \sqrt{-1}$ which never made an appearance in classical mechanics in such a fashion. Hence, in general $\Psi(x,t)$ is considered to be a complex-valued function which is why only $|\Psi(x,t)|^2 = \Psi^*\Psi$ can have a physical connection to the particle, namely being identified as the probability density function of the position of the particle. Furthermore, to ensure that this interpretation makes sense from a probabilistic point of view we have to impose a normalization constraint.

Definition 2.2 (Normalization)**.** The probability of finding the particle anywhere at time t is given by:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x = 1$$

In other words, there is a 100% chance of finding the particle somewhere.

3. Separation of Variables

Prior to jumping into solving the Schrödinger equation we must first introduce a standard process that is used to *separate* the time and space components of the wavefunction. More specifically, assume that $\Psi(x,t) = \psi(x)\varphi(t)$ and plug it into the *time-dependent* Schrödinger equation to attain:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}(\psi\varphi) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(\psi\varphi) + V(\psi\varphi) \\ i\hbar(\psi\varphi') &= -\frac{\hbar^2}{2m}(\psi''\varphi) + V(\psi\varphi) \\ i\hbar\frac{\varphi'}{\varphi} &= -\frac{\hbar^2}{2m}\frac{\psi''}{\psi} + V \end{aligned}$$

We typically take the case that the potential is independent of the time, i.e. $V = V(x)$, so as to be able to state that the left-hand side consists of a function of t strictly while the right-hand consists of a function of x strictly. The only manner in which this equality can hold then is if both sides are equal to the same constant E, thereby giving the two differential equations:

$$i\hbar\frac{\varphi'}{\varphi} = E \quad \text{and} \quad E = -\frac{\hbar^2}{2m}\frac{\psi''}{\psi} + V$$

The first of these equations can be solved to yield $\varphi(t) = e^{-\frac{iEt}{\hbar}}$ and reorganizing the second equation gives us what is commonly known as the *time-independent* Schrödinger equation:

$$E\psi = -\frac{\hbar^2}{2m}\psi'' + V\psi$$

States that satisfy such separation are known as *stationary states* having the interesting property that:

$$|\Psi|^2 = \Psi^*\Psi = (\psi^*\varphi^*)(\varphi\psi) = \psi^*\psi = |\psi|^2$$

Thus, the *phase factor* φ plays no role when it comes to calculating the probabilities of stationary states.