Quantum Dynamics and QuTiP

October 21, 2024

1 Introduction

In the 19th and 20th century several experimental results and phenomena which were not explainable by classical mechanics or electrodynamics. Some examples are the Stern Gerlach experiment, blackbody radiation, photoelectric effect, double slit experiment, atomic spectra, specific heats of solids etc. Over a span of 3 decades several renowned physicists and mathematicians made their contributions to a theory which explains the mechanics at the subatomic scale, which we now call Quantum Mechanics.

In the talk we started with the postulates of quantum mechanics which are a culmination of all these developments.

A good reference for delving into the history of QM is the three volume series "Constructing Quantum Mechanics" by Anthony Duncan and Michel Janssen.

2 The Postulates

2.1 Postulate 1: The State of a Quantum System

The state of a quantum system is completely described by a state vector, often referred to as a wavefunction, denoted as $|\psi\rangle$. This state vector resides in a complex Hilbert space, a mathematical structure that provides the necessary framework for describing quantum states. The wavefunction encodes all possible information about the system.
In general, the wavefunction is a superposition of the basis states of the system, i.e.,

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle$$

where $|\phi_i\rangle$ are the orthonormal basis states of the system and c_i are complex coefficients. The probabilities of outcomes are related to the magnitudes of these coefficients.

2.2 Postulate 2: Observables and Operators

Every measurable quantity in quantum mechanics, known as an observable, is represented by a Hermitian operator $\hat{O}$ that acts on the state vectors in the Hilbert space. The eigenvalues of these operators correspond to the possible outcomes of measurements.

2.3 Postulate 3: Measurement and the Collapse of the Wavefunction

Upon measurement of an observable O, the quantum system collapses into one of the eigenstates $|\phi_i\rangle$ of the operator associated with O. Before the measurement, the system can exist in a superposition of different states, but after the measurement, the system is found in the eigenstate corresponding to the measured eigenvalue.
Mathematically, if the system was initially in the state $|\psi\rangle$, the probability of collapsing to the eigenstate $|\phi_i\rangle$ is:

$$P(\lambda_i) = |\langle\phi_i|\psi\rangle|^2$$

where λ_i is the eigenvalue corresponding to ϕ_i and it will be the observed value upon measurement.

2.4 Postulate 4: Time Evolution of Quantum States

Usually this is the postulate were the Schrodinger equation is introduced. The time evolution of a quantum state is said to by governed by the Schrödinger equation. The change of the state vector $|\psi(t)\rangle$ over time is determined by the Hamiltonian operator $\hat{H}$, which corresponds to the total energy of the system. The time-dependent Schrödinger equation is:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

where $\hbar$ is the reduced Planck's constant, and $\hat{H}$ is the Hamiltonian operator of the system.

We will instead discuss an **equivalent** but **more insightful** version of this:
The time evolution of a *closed* system is described by a *unitary transformation*:

$$|\Psi(t)\rangle = U(t, t_0)|\Psi(t_0)\rangle, \quad \forall t, t_0$$

where unitary means that:

$$U^\dagger(t, t_0)U(t, t_0) = \mathbb{1} \quad (\textit{identity operator})$$

We will deal with this more in the upcoming sections and try to develop a deeper understanding of the **dynamics** of closed quantum systems.

2.5 Postulate 5: Composite Systems and Tensor Products

If two or more quantum systems are considered together, the state space of the composite system is the tensor product of the state spaces of the individual systems. If system A is described by a state vector $|\psi_A\rangle$ and system B is described by $|\psi_B\rangle$, then the combined state of the two systems is:

$$|\psi_{\text{AB}}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$$

This postulate is essential in describing entangled states, where the states of two subsystems are not independent, and the measurement of one affects the state of the other.

3 Measurement and Expectation Value

To makes sense of the probability of observing a particular eigenvalue upon measurement we introduce the concept of a ***pure ensemble***. A set consisting of a large number of "virtual" copies of a pure state. The probability of collapsing into a particular eigenstate represents the proportion of states that collapse into that eigenstate when all the constituent states in the ensemble are measured.

Given these probabilities we can calculate the expectation value of an observable A.

$$\langle A\rangle = E[A] = \sum_i a_i P(a_i)$$

where $\{a_i\}$ are the eigenvalues of A for a state ψ
We use postulate 3 to simplify this.

$$\langle A\rangle = \sum_i a_i \,|\langle a_i|\psi\rangle|^2$$

where $\{|a_i\rangle\}$ are the corresponding eigenvectors of A.
we also expand the mod-squared:

$$\langle A\rangle = \sum_i a_i \;|\psi\rangle\,(\langle a_i|\psi\rangle)^* = \sum_i a_i \;\langle a_i|\psi\rangle\,\langle\psi|a_i\rangle$$

we use a Kronecker delta (equal to 1 if indices are equal, else 0) to rewrite $\langle\psi|a_i\rangle$:

$$\langle\psi|a_i\rangle = \sum_j \langle\psi|a_j\rangle\,\delta_{ji}$$

this makes our expression a double summation:

$$\langle A\rangle = \sum_j\sum_i a_i\,\langle a_i|\psi\rangle\,\langle\psi|a_j\rangle\,\delta_{ji}$$

using the fact that the eigenvectors of A are orthonormal we rewrite the δ_{ji} as $\langle a_j|a_i\rangle$:

$$\langle A\rangle = \sum_j \sum_i a_i \langle a_i|\psi\rangle \langle\psi|a_j\rangle \langle a_j|a_i\rangle$$

rearranging this we get:

$$\langle A\rangle = \sum_j \sum_i \langle a_i|\psi\rangle \langle\psi|a_j\rangle \langle a_j| a_i |a_i\rangle$$

we know $a_i |a_i\rangle = A |a_i\rangle$:

$$\langle A\rangle = \sum_j \sum_i \langle a_i|\psi\rangle \langle\psi|a_j\rangle \langle a_j| A |a_i\rangle$$

pulling the a_i inside the inner product $\langle a_j|a_i\rangle$ we get:

$$\langle A\rangle = \sum_j \sum_i \langle\psi|a_j\rangle \langle a_j| A |a_i\rangle \langle a_i|\psi\rangle$$

we pull the summations inside:

$$\langle A\rangle = \langle\psi| \left(\sum_j |a_j\rangle \langle a_j|\right) A \left(\sum_i |a_i\rangle \langle a_i|\right) |\psi\rangle$$

By the completeness relation both the summation are equal to identity operator, hence we get:

$$\boxed{\langle A\rangle = \langle\psi| A |\psi\rangle}$$

4 Schrödinger Picture

The state space of quantum mechanics, the Hilbert space $\mathcal{H}$, is best thought of as a space with time-independent basis vectors. In the Schrödinger picture of the dynamics, the state of a quantum system depends on time. Time is treated as a parameter, and at different times the system is represented by different states in the Hilbert space. We write the state vector as:

$$|\Psi(t)\rangle$$

which is a vector whose components along the basis vectors of $\mathcal{H}$ are time-dependent. If we denote the basis vectors as $|u_i\rangle$, then:

$$|\Psi(t)\rangle = \sum_i |u_i\rangle c_i(t)$$

where the $c_i(t)$ are functions of time. Since a state must be normalized, $|\Psi(t)\rangle$ is a unit vector whose tip sweeps a trajectory in $\mathcal{H}$ as a function of time.

4.1 Unitary Time Evolution

We declare that for any quantum system, there is a unitary operator $U(t, t_0)$ such that for any state $|\Psi(t_0)\rangle$ of the system at time t_0, the state at time t is given by:

$$|\Psi(t)\rangle = U(t, t_0) |\Psi(t_0)\rangle , \quad \forall t, t_0 \tag{1}$$

This operator U generates time evolution for all possible states at time t_0, and is independent of the particular state $|\Psi(t_0)\rangle$. The unitarity of U ensures the conservation of the norm of the state:

$$\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(t_0)| U^\dagger(t, t_0)U(t, t_0) |\Psi(t_0)\rangle = \langle\Psi(t_0)| \mathbb{1} |\Psi(t_0)\rangle = \langle\Psi(t_0)|\Psi(t_0)\rangle$$

The following properties of the unitary operator $U(t, t_0)$ can be easily verfied using Eq (1):

- **No time evolution at $t = t_0$:** $U(t_0, t_0) = 1$.
- **Composition of time evolution:** Time evolution from t_0 to t_2 can be decomposed into two steps:

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$$

- **Inverses:** The inverse of $U(t, t_0)$ is given by (put $t_2 = t_0$ in the above equation):

$$U(t_0, t) = U^{-1}(t, t_0) = U^\dagger(t, t_0)$$

4.2 Unitary Time Evolution leads to Schrödinger Equation

The time evolution of states has been specified in terms of a unitary operator U assumed known. We now ask the 'reverse engineering' question: What kind of differential equation do the states satisfy for which the solution is unitary time evolution? The answer is simple and satisfying: a Schrödinger equation.

To obtain this result, we take the time derivative of the equation

$$|\Psi(t)\rangle = U(t,t_0)\,|\Psi(t_0)\rangle$$

to find

$$\frac{\partial}{\partial t}\,|\Psi(t)\rangle = \frac{\partial U(t,t_0)}{\partial t}\,|\Psi(t_0)\rangle\,.$$

We want the right-hand side to involve the ket $|\Psi(t)\rangle$, so we write

$$\frac{\partial}{\partial t}\,|\Psi(t)\rangle = \frac{\partial U(t,t_0)}{\partial t}U^\dagger(t,t_0)\,|\Psi(t)\rangle\,.$$

This now looks like a differential equation for the state $|\Psi(t)\rangle$. Let us introduce a name for the operator acting on the state in the right-hand side:

$$\frac{\partial}{\partial t}\,|\Psi(t)\rangle = \Lambda(t,t_0)\,|\Psi(t)\rangle\,,$$

where

$$\Lambda(t,t_0) = \frac{\partial U(t,t_0)}{\partial t}U^\dagger(t,t_0).$$

The operator $\Lambda(t,t_0)$ has units of **inverse time**. Note also that

$$\Lambda^\dagger(t,t_0) = U(t,t_0)\frac{\partial U^\dagger(t,t_0)}{\partial t}.$$

We now want to prove two important facts about $\Lambda(t)$:

1. $\Lambda(t,t_0)$ is anti-Hermitian. To prove this, begin with the equation

   $$U(t,t_0)U^\dagger(t,t_0) = 1$$

   and take a derivative with respect to time to find

   $$\frac{\partial U(t,t_0)}{\partial t}U^\dagger(t,t_0) + U(t,t_0)\frac{\partial U^\dagger(t,t_0)}{\partial t} = 0.$$

   From this, we have

   $$\Lambda(t,t_0) + \Lambda^\dagger(t,t_0) = 0,$$

   proving that $\Lambda(t,t_0)$ is indeed anti-Hermitian.

2. $\Lambda(t,t_0)$ is actually independent of t_0. To prove this, we show that $\Lambda(t,t_0)$ is actually equal to $\Lambda(t,t_1)$ for any other time $t_1 \neq t_0$. This implies that $\Lambda(t,t_0)$ does not depend on t_0.

   This is important because in the differential equation for the time evolution of the state,

   $$\frac{\partial}{\partial t}\,|\Psi(t)\rangle = \Lambda(t,t_0)\,|\Psi(t)\rangle\,,$$

   t_0 appears nowhere except in Λ.

   To prove the claim, we start with the definition of $\Lambda(t,t_0)$:

   $$\Lambda(t,t_0) = \frac{\partial U(t,t_0)}{\partial t}.$$

   We insert the identity operator between the two factors:

   $$\Lambda(t,t_0) = \frac{\partial U(t,t_0)}{\partial t}\left(U^\dagger(t_1,t_0)U(t_1,t_0)\right)U^\dagger(t,t_0).$$

   We can pull $U(t_1,t_0)$ inside the derivative as it is independent of t:

   $$\Lambda(t,t_0) = \frac{\partial\left(U(t,t_0)U^\dagger(t_1,t_0)\right)}{\partial t}U^(t_1,t_0)U^\dagger(t,t_0).$$

Then we use inverse property:

$$\Lambda(t,t_0) = \frac{\partial\left(U(t,t_0)U(t_0,t_1)\right)}{\partial t}U(t_1,t_0)U^\dagger(t,t_0).$$

We then use the composition property:

$$\Lambda(t,t_0) = \frac{\partial U(t,t_1)}{\partial t}U(t_1,t_0)U^\dagger(t,t_0).$$

we again use the inverse property:

$$\Lambda(t,t_0) = \frac{\partial U(t,t_1)}{\partial t}U(t_1,t_0)U(t_0,t).$$

And then the composition property:

$$\Lambda(t,t_0) = \frac{\partial U(t,t_1)}{\partial t}U(t_1,t)$$

which using the inverse simplifies to:

$$\Lambda(t,t_0) = \frac{\partial U(t,t_1)}{\partial t}U^\dagger(t,t_1), = \Lambda(t,t_1)$$

so:

$$\Lambda(t,t_0) = \Lambda(t,t_1).$$

Thus, $\Lambda(t)$ is independent of t_0.

It follows that we can write $\Lambda(t) \equiv \Lambda(t,t_0)$, and thus the equation becomes:

$$\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \Lambda(t)\left|\Psi(t)\right\rangle.$$

Multiplying both side by $i\hbar$ we get:

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = i\hbar\Lambda(t)\left|\Psi(t)\right\rangle.$$

The operator $i\hbar\Lambda(t)$ is hermitian ($\Lambda(t)$ is anti-hermitian) and has units of energy, we identity this as the Hamiltonian operator (it is hermitian so it is an observable and it has units of energy):

$$H(t) = i\hbar\Lambda(t),$$

leading to the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H(t)\left|\Psi(t)\right\rangle.$$

This is our main result. Unitary time evolution implies this equation.

4.3 Time Evolution of Expectation Values

Let us see how expectation values evolve in time. Expectation value for an observable A as we showed can be found using:

$$\langle A\rangle = \left\langle\psi(t)\right| A\left|\psi(t)\right\rangle$$

We differentiate with respect to time:

$$\frac{d\langle A\rangle}{dt} = \frac{d\left\langle\psi(t)\right| A\left|\psi(t)\right\rangle}{dt}$$

We assume the observable (operator) does not have any explicit time dependence:

$$\frac{d\langle A\rangle}{dt} = \frac{\partial\left\langle\psi(t)\right|}{\partial t}A\left|\psi(t)\right\rangle + \left\langle\psi(t)\right| A\frac{\partial\left|\psi(t)\right\rangle}{\partial t} + \left\langle\psi(t)\right|\frac{\partial A}{\partial t}\left|\psi(t)\right\rangle$$

The last term is just the expectation of $\frac{\partial A}{\partial t}$. Using the Schrödinger Equation we get:

$$\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar}\left\langle\psi(t)\right| HA\left|\psi(t)\right\rangle + \left(\frac{-i}{\hbar}\right)\left\langle\psi(t)\right| AH\left|\psi(t)\right\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

Simplifying this we get:

$$\frac{d\langle A\rangle}{dt} = \left(\frac{-i}{\hbar}\right) \langle\psi(t)| \left(AH - HA\right) |\psi(t)\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

The operator in the middle is the commutator of A and H written as $[A, H]$. This gives us:

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar} \langle\psi(t)| [A, H] |\psi(t)\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

Rewriting the first term as an expectation value, we get the *Generalized Ehrenfest Theorem*:

$$\boxed{\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle[A, H]\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle}$$

4.4 Time Independent Hamiltonian

When the hamiltonian is independent of time we can find the unitary time evolution operator (propagator). In this case:

$$i\hbar\frac{dU(t, t_0)}{dt} = HU(t, t_0),$$

is structurally of the form

$$\frac{dU(t)}{dt} = KU(t),$$

where $K = -\frac{i}{\hbar}H$ is a time-independent matrix. This is similar to the ordinary differential equation

$$\frac{du}{dt} = ku(t),$$

which has the solution:

$$u(t) = e^{kt}u(0).$$

By analogy, for the matrix case, we claim the following will satisfy the equation:

$$U(t, t_0) = e^{Kt}U_0.$$

The proof is left as an exercise. Using the fact that $U(t_0, t_0) = \mathbb{1}$ we find that $U_0 = exp\left(\frac{iHt_0}{\hbar}\right)$, so the solution becomes:

$$U(t, t_0) = exp\left(-\frac{iH(t - t_0)}{\hbar}\right).$$

This is the solution for the time evolution operator in the case where H is time-independent.

5 Heisenberg Picture

The idea here is to confine the dynamical evolution to the operators. We will incorporate the time dependence of the states into the operators. Since the objects we usually calculate are time-dependent expectation values of operators, this approach turns to be quite effective.

We will define time-dependent Heisenberg operators starting from Schrodinger operators.

In fact, to any Schrodinger operator we can associate its corresponding Heisenberg operator.

Schrodinger operators come in two types, time independent ones and time dependent ones. For each of those types of operators we will associate Heisenberg operators.

5.1 Heisenberg Operators

Let us consider a Schrödinger operator $\hat{A}_S$, with the subscript S for Schrödinger. This operator may or may not have time dependence. We now examine a matrix element of $\hat{A}_S$ between time-dependent states $|\alpha, t\rangle$ and $|\beta, t\rangle$, and use the time-evolution operator to convert the states to time $t = 0$:

$$\langle\alpha, t| \hat{A}_S |\beta, t\rangle = \langle\alpha, 0| U^\dagger(t, 0)\hat{A}_S U(t, 0) |\beta, 0\rangle . \tag{2}$$

We define the Heisenberg operator $\hat{A}_H(t)$ associated with $\hat{A}_S$ as:

$$\boxed{\hat{A}_H(t) = U^\dagger(t, 0)\hat{A}_S U(t, 0).}$$

Let us consider a number of important consequences of this definition:

1. At $t = 0$, the Heisenberg operator becomes equal to the Schrödinger operator:

$$\hat{A}_H(0) = \hat{A}_S.$$

2. The Heisenberg operator associated with the identity operator is the identity operator:

$$\mathbb{1}_H = U^\dagger(t,0)\mathbb{1}U(t,0) = \mathbb{1}.$$

3. The Heisenberg operator associated with the product of Schrödinger operators is equal to the product of the corresponding Heisenberg operators:

$$\hat{C}_S = \hat{A}_S\hat{B}_S \quad \Rightarrow \quad \hat{C}_H(t) = \hat{A}_H(t)\hat{B}_H(t).$$

Indeed,

$$\hat{C}_H(t) = U^\dagger(t,0)\hat{C}_S U(t,0) = U^\dagger(t,0)\hat{A}_S\hat{B}_S U(t,0),$$

which simplifies to:

$$\hat{C}_H(t) = U^\dagger(t,0)\hat{A}_S U(t,0)U^\dagger(t,0)\hat{B}_S U(t,0) = \hat{A}_H(t)\hat{B}_H(t).$$

4. It also follows that if we have a commutator of Schrödinger operators, the corresponding Heisenberg operators satisfy the same commutation relations:

$$[\hat{A}_S, \hat{B}_S] = \hat{C}_S \quad \Rightarrow \quad [\hat{A}_H(t), \hat{B}_H(t)] = \hat{C}_H(t).$$

Since $\mathbb{1}_H = \mathbb{1}$, this implies that, for example:

$$[\hat{x}, \hat{p}] = i\hbar\mathbb{1} \quad \Rightarrow \quad [\hat{x}_H(t), \hat{p}_H(t)] = i\hbar\mathbb{1}.$$

5. **Schrödinger and Heisenberg Hamiltonians:** Assume we have a Schrödinger Hamiltonian that depends on some Schrödinger momenta and position operators $\hat{p}$ and $\hat{x}$, as in $\hat{H}_S(\hat{p}, \hat{x}; t)$. Since the $\hat{x}$ and $\hat{p}$ in $\hat{H}_S$ appear in products, property 3 implies that the associated Heisenberg Hamiltonian $\hat{H}_H(t)$ takes the same form, with $\hat{x}$ and $\hat{p}$ replaced by their Heisenberg counterparts:

$$\hat{H}_H(t) = \hat{H}_S(\hat{p}_H(t), \hat{x}_H(t); t).$$

6. **Equality of Hamiltonians:** Under some circumstances, the Heisenberg Hamiltonian is equal to the Schrödinger Hamiltonian. Recall the definition:

$$\hat{H}_H(t) = U^\dagger(t,0)\hat{H}_S(t)U(t,0).$$

Assume now that $[\hat{H}_S(t), \hat{H}_S(t')] = 0$. Then, since $\hat{H}_S$ commutes both with $U(t,0)$ and $U^\dagger(t,0)$, we find:

$$\hat{H}_H(t) = \hat{H}_S(t).$$

This means that if we take $\hat{x}_H(t)$ and $\hat{p}_H(t)$ and plug them into the Hamiltonian, the result is the same as if we had simply plugged in $\hat{x}$ and $\hat{p}$.

7. **Equality of operators:** If a Schrödinger operator $\hat{A}_S$ commutes with the Hamiltonian $\hat{H}_S(t)$ for all times, then $\hat{A}_S$ commutes with $U(t,0)$. It follows that $\hat{A}_H(t) = \hat{A}_S$; that is, the Heisenberg operator is equal to the Schrödinger operator.

8. **Equality of Expectation Value:** By putting $|\alpha, t\rangle = |\beta, t\rangle = |\psi, t\rangle$ in Eq (2). We get that the expectation value of A_S and $A_H(t)$ is the same.

$$\boxed{\langle A_S\rangle = \langle A_H(t)\rangle}$$

5.2 Heisenberg Equation of Motion

We can calculate the Heisenberg operator associated with a Schrödinger one using the definition:

$$\hat{A}_H(t) = U^\dagger(t,0)\hat{A}_S U(t,0).$$

Alternatively, Heisenberg operators satisfy a differential equation: the Heisenberg equation of motion. This equation resembles the equations of motion for classical dynamical variables.

To determine the equation of motion for Heisenberg operators, we take time derivatives of the definition. We start with the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}_S(t)\left|\psi(t)\right\rangle,$$

Rewriting $|\psi(t)\rangle$ as $U(t,t_0)\,|\psi(t_0)\rangle$ we get:

$$i\hbar\frac{\partial}{\partial t}\left(U(t,t_0)\left|\psi(t_0)\right\rangle\right) = \hat{H}_S(t)U(t,t_0)\left|\psi(t_0)\right\rangle$$

Dropping the $|\psi(t_0)\rangle$ we get:

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = \hat{H}_S(t)U(t,t_0)$$

and by taking the adjoint we get:

$$i\hbar\frac{\partial}{\partial t}U^\dagger(t,t_0) = -U^\dagger(t,t_0)\hat{H}_S(t),$$

We will use the above two equation below.
We can now calculate:

$$i\hbar\frac{d}{dt}\hat{A}_H(t) = \left(i\hbar\frac{\partial U^\dagger(t,0)}{\partial t}\right)\hat{A}_S U(t,0) + U^\dagger(t,0)\left(i\hbar\frac{\partial \hat{A}_S}{\partial t}\right)U(t,0) + U^\dagger(t,0)\hat{A}_S\left(i\hbar\frac{\partial U(t,0)}{\partial t}\right).$$

The middle term is the Heisenberg operator form of $\frac{\partial \hat{A}_S}{\partial t}$, which we represent as $\left(\frac{\partial \hat{A}_S}{\partial t}\right)_H$, multiplied by $i\hbar$. For the other two terms we use the above two equations to get:

$$i\hbar\frac{d}{dt}\hat{A}_H(t) = \left(-U^\dagger(t,t_0)\hat{H}_S(t)\hat{A}_S U(t,t_0) + U^\dagger(t,t_0)\hat{A}_S\hat{H}_S(t)U(t,t_0)\right) + i\hbar\left(\frac{\partial \hat{A}_S}{\partial t}\right)_H$$

Which gives us:

$$i\hbar\frac{d}{dt}\hat{A}_H(t) = U^\dagger(t,t_0)[\hat{A}_S(t),\hat{H}_S(t)]U(t,t_0) + i\hbar\left(\frac{\partial \hat{A}_S(t)}{\partial t}\right)_H.$$

Recognizing the first time as the Heisenberg operator corresponding to the commutator and using point (4) from the list of properties of Heisenberg operators, we get the Heisenberg equation of motion:

$$\boxed{i\hbar\frac{d}{dt}\hat{A}_H(t) = [\hat{A}_H(t),\hat{H}_H(t)] + i\hbar\frac{\partial \hat{A}_S(t)}{\partial t}}$$

5.3 Time Evolution of Expectation Values

In Heisenberg picture the expression similar to that in Schrodinger dynamics. We obtain it by multiplying the Heisenberg equation of motion by $\langle\psi(t_0)|$ on the left and $|\psi(t_0)\rangle$ on the right.

$$\frac{d\langle A_H(t)\rangle}{dt} = \frac{1}{i\hbar}\langle[A_H(t),H_H(t)]\rangle + \left\langle\left(\frac{\partial A_S}{\partial t}\right)_H\right\rangle$$

6 An Example: Larmor Precession

Larmor Precession is the precession of magnetic moment of an object in an magnetic field. We will take the example of an electron in a magnetic field. The magnetic moment of an electron comes form the intrinsic angular moment it has due to its spin. It is a purely quantum mechanical phenomena explained by Dirac Equation (a relativistic quantum wave equation that describes the behaviour of spin-1/2 particles). The only takeaway we need is that spin angular momentum (S) is an observable and the electron spin is a 2-dimensional system (two basis states).

Pauli Matrices are 2x2 matrices that pop up in various places in the study of 2-dimensional systems in QM. The three Pauli matrices are:

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

6.1 The Hamiltonian

The classically hamiltonian for a particle with magnetic moment in a external magnetic field is given by:

$$H = \vec{\mu} \cdot \vec{B}$$

where

$$\vec{\mu} = \frac{-q}{2m} \vec{L}$$

In quantum mechanics the spin angular momentum and hence the magnetic moment is quantized and can take only two values for the case of the electron. These states are called up spin ($|\uparrow\rangle$) and down spin ($|\downarrow\rangle$) states (these are the eigenstates of S). The value of the spin angular moment is $+\hbar/2$ and $-\hbar/2$ respectively (these are the eigenvalues). Magnetic moment is given by:

$$\vec{\mu} = -g \frac{e}{2m} \vec{S}$$

where g is called the g-factor. Let

$$|\vec{\mu}| = \mu = g \frac{e}{2m} \left(\frac{\hbar}{2} \right)$$

We consider the case where magnetic field is along z direction. And electron spin aligns with the magnetic field.

$$H = \mu \, B \, cos\theta$$

where $B = |\vec{B}|$ and θ is the angle between magnetic moment and field. In our case for spin-up state $\theta = 0°$ and for the spin-down state $\theta = 180°$. The up and down sates are the eigenvectors for the hamiltonian and μB and $-\mu B$ are the corresponding eigenvalues. Hence H can be written as:

$$H = \mu B \left(|\uparrow\rangle \langle\uparrow| - |\downarrow\rangle \langle\downarrow| \right)$$

We simplify our notation by using $|\uparrow\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\downarrow\rangle = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. We get:

$$H = \mu B \left(|0\rangle \langle 0| - |1\rangle \langle 1| \right)$$

$$H = \mu B \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} \right)$$

$$H = \mu B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \mu B \sigma_z$$

6.2 Time Evolution Operator

Let's find the propagator $U(t, t_0)$ for this Hamiltonian. The Hamiltonian is time-independent we use the results from section 4.4 to find U.

$$U(t, t_0) = exp \left(-\frac{iH(t - t_0)}{\hbar} \right)$$

This can expanded using the Maclaurin series:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

We get:

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-iH(t-t_0)}{\hbar}\right)^n$$

Plugging in our Hamiltonian we get:

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i\mu B\sigma_z(t-t_0)}{\hbar}\right)^n$$

A property of the Pauli matrices is that they are their own inverses, so:

$$\sigma_z^2 = \mathbb{1}$$

So all even powers in the series give $\mathbb{1}$ while the odd powers give σ_z. Let $\theta = \frac{\mu B(t-t_0)}{\hbar}$ and we get:

$$\begin{aligned} U(t,t_0) &= \mathbb{1} - i\theta\sigma_z - \frac{\theta^2\mathbb{1}}{2!} + i\frac{\theta^3\sigma_z}{3!}\dots \\ &= \mathbb{1}\left(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \dots\right) - i\sigma_z\left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \dots\right) \\ &= \mathbb{1}cos(\theta) - i\sigma_z sin(\theta) \end{aligned}$$

We take a **simplified case** where $t_0 = 0$ and $\frac{\mu B}{\hbar} = 1$, we get (dropping the $\mathbb{1}$, it is implied from the expression):

$$U(t,0) = cos(t) - i\,\sigma_z sin(t)$$

6.3 Schrodinger Picture Solution

We use our simplified case described above. We use the state $|\psi(0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$ as our initial state.

We find $|\psi(t)\rangle$ using the time evolution operator $U(t,0)$.

$$\begin{aligned} |\psi(t)\rangle &= U(t,0)|\psi\rangle \\ &= (cos(t) - i\,\sigma_z sin(t))|\psi(0)\rangle \\ &= cos(t)|\psi(0)\rangle - i\,sin(t)\sigma_z|\psi(0)\rangle \end{aligned}$$

$$\sigma_z|\psi(0)\rangle = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1/\sqrt{2}\\ 1/\sqrt{2}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(cos(t)\begin{pmatrix}1\\ 1\end{pmatrix} - i\,sin(t)\begin{pmatrix}1\\ -1\end{pmatrix}\right)$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}cos(t) - isin(t)\\ cos(t) + isin(t)\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-it}\\ e^{it}\end{pmatrix} = \frac{1}{\sqrt{2}}e^{-it}\begin{pmatrix}1\\ e^{2it}\end{pmatrix}$$

Ignoring the global phase (e^{-it}) as it contributes nothing physically, we get:

$$\boxed{|\psi(t)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}e^{2it}|1\rangle}$$

Let us now compute expectation values of the Pauli matrices, starting with σ_z:

$$\begin{aligned} \langle\sigma_z\rangle &= \langle\psi(t)|\,\sigma_z\,|\psi(t)\rangle \\ &= \left(\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}e^{-2it}\langle 1|\right)\sigma_z\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}e^{2it}|1\rangle\right) \end{aligned}$$

We know $\sigma_z|0\rangle = |0\rangle$ and $\sigma_z|1\rangle = -|1\rangle$, hence:

$$\langle\sigma_z\rangle = \left(\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}e^{-2it}\langle 1|\right)\left(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}e^{2it}|1\rangle\right)$$

$|0\rangle$ and $|1\rangle$ are orthonormal so:

$$\langle\sigma_z\rangle = \frac{1}{2} - \frac{1}{2}e^{-2it}e^{2it}$$

Hence:

$$\boxed{\langle\sigma_z\rangle = 0}$$

For σ_y we have:

$$\begin{aligned}\langle \sigma_y \rangle &= \langle \psi(t) | \, \sigma_y \, | \psi(t) \rangle \\ &= \left(\frac{1}{\sqrt{2}} \langle 0 | + \frac{1}{\sqrt{2}} e^{-2it} \langle 1 | \right) \sigma_y \left(\frac{1}{\sqrt{2}} | 0 \rangle + \frac{1}{\sqrt{2}} e^{2it} | 1 \rangle \right)\end{aligned}$$

We know $\sigma_y |0\rangle = i |1\rangle$ and $\sigma_y |1\rangle = -i |0\rangle$, hence:

$$\langle \sigma_y \rangle = \left(\frac{1}{\sqrt{2}} \langle 0 | + \frac{1}{\sqrt{2}} e^{-2it} \langle 1 | \right) \left(\frac{i}{\sqrt{2}} | 1 \rangle - \frac{i}{\sqrt{2}} e^{2it} | 0 \rangle \right)$$

$|0\rangle$ and $|1\rangle$ are orthonormal so:

$$\begin{aligned}\langle \sigma_y \rangle &= -\frac{i}{2} e^{2it} + \frac{i}{2} e^{-2it} \\ &= \frac{1}{2} e^{i(2t-\pi/2)} + \frac{1}{2} e^{-i(2t-\pi/2)} \\ &= cos(2t - \frac{\pi}{2})\end{aligned}$$

Hence:

$$\boxed{\langle \sigma_y \rangle = sin(2t)}$$

For σ_x we have:

$$\begin{aligned}\langle \sigma_x \rangle &= \langle \psi(t) | \, \sigma_x \, | \psi(t) \rangle \\ &= \left(\frac{1}{\sqrt{2}} \langle 0 | + \frac{1}{\sqrt{2}} e^{-2it} \langle 1 | \right) \sigma_x \left(\frac{1}{\sqrt{2}} | 0 \rangle + \frac{1}{\sqrt{2}} e^{2it} | 1 \rangle \right)\end{aligned}$$

We know $\sigma_x |0\rangle = |1\rangle$ and $\sigma_x |1\rangle = |0\rangle$, hence:

$$\langle \sigma_x \rangle = \left(\frac{1}{\sqrt{2}} \langle 0 | + \frac{1}{\sqrt{2}} e^{-2it} \langle 1 | \right) \left(\frac{1}{\sqrt{2}} | 1 \rangle + \frac{1}{\sqrt{2}} e^{2it} | 0 \rangle \right)$$

$|0\rangle$ and $|1\rangle$ are orthonormal so:

$$\langle \sigma_x \rangle = \frac{1}{2} e^{2it} + \frac{1}{2} e^{-2it}$$

Hence:

$$\boxed{\langle \sigma_x \rangle = cos(2t)}$$

6.4 Heisenberg Picture Solution

We find the Heisenberg operators corresponding to the Pauli Matrices:

$$\boxed{(\sigma_z)_H = \sigma_z}$$

$$\begin{aligned}(\sigma_z)_H &= U^\dagger(t,0)\sigma_z U(t,0) \\ &= (cos(t) + i\,\sigma_z sin(t))\,\sigma_z\,(cos(t) - i\,\sigma_z sin(t)) \\ &= (cos(t) + i\,\sigma_z sin(t))\,(\sigma_z cos(t) - i\,sin(t)) \quad (using\ (\sigma_z)^2 = \mathbb{1}) \\ &= \sigma_z cos^2(t) + i\,sin(t)cos(t) - i\,sin(t)cos(t) + \sigma_z sin^2(t)\end{aligned}$$

Hence:

$$\boxed{(\sigma_z)_H = \sigma_z}$$

Alternatively we can say σ_z commutes with our Hamiltonian and hence it commutes with U and the result is therefore trivial.

For σ_y:

$$\begin{aligned}
(\sigma_y)_H &= U^\dagger(t,0)\sigma_y U(t,0) \\
&= (cos(t) + i\,\sigma_z sin(t))\,\sigma_y\,(cos(t) - i\,\sigma_z sin(t)) \\
&= (cos(t) + i\,\sigma_z sin(t))\,(\sigma_y cos(t) - i\,\sigma_y\sigma_z sin(t)) \\
&= \sigma_y cos^2(t) + i\,\sigma_z\sigma_y sin(t)cos(t) - i\,\sigma_y\sigma_z sin(t)cos(t) + \sigma_z\sigma_y\sigma_z sin^2(t) \\
&= \sigma_y cos^2(t) + i\,[\sigma_z, \sigma_y] sin(t)cos(t) + \sigma_z\sigma_y\sigma_z sin^2(t)
\end{aligned}$$

By writing out each Pauli matrix and using basic matrix multiplication we find

$$\boxed{(\sigma_y)_H = \sigma_y cos(2t) + \sigma_x sin(2t)}$$

Similarly for σ_x we get:

$$\boxed{(\sigma_x)_H = \sigma_x cos(2t) - \sigma_y sin(2t)}$$

We now find the expectation values.

Before that we see the **initial** expectation value of the Pauli matrices:

$$\begin{aligned}
\langle\psi(0)|\,\sigma_z\,|\psi(0)\rangle &= \frac{1}{2}\left(\left(\langle 0| + \langle 1|\right)\sigma_z\left(|0\rangle + |1\rangle\right)\right) \\
&= \frac{1}{2}\left(\left(\langle 0| + \langle 1|\right)\left(|0\rangle - |1\rangle\right)\right) \\
&= 0
\end{aligned}$$

$$\begin{aligned}
\langle\psi(0)|\,\sigma_y\,|\psi(0)\rangle &= \frac{1}{2}\left(\left(\langle 0| + \langle 1|\right)\sigma_y\left(|0\rangle + |1\rangle\right)\right) \\
&= \frac{1}{2}\left(\left(\langle 0| + \langle 1|\right)\left(i\,|1\rangle - i\,|0\rangle\right)\right) \\
&= 0
\end{aligned}$$

$$\begin{aligned}
\langle\psi(0)|\,\sigma_x\,|\psi(0)\rangle &= \frac{1}{2}\left(\left(\langle 0| + \langle 1|\right)\sigma_x\left(|0\rangle + |1\rangle\right)\right) \\
&= \frac{1}{2}\left(\left(\langle 0| + \langle 1|\right)\left(|1\rangle + |0\rangle\right)\right) \\
&= 1
\end{aligned}$$

We will use these results to find the expectation values, starting with σ_z:

$$\begin{aligned}
\langle\sigma_z\rangle &= \langle(\sigma_z)_H\rangle \\
&= \langle\psi(0)|\,(\sigma_z)_H\,|\psi(0)\rangle \\
&= \langle\psi(0)|\,\sigma_z\,|\psi(0)\rangle \\
&= 0
\end{aligned}$$

Hence:

$$\boxed{\langle\sigma_z\rangle = 0}$$

For σ_y:

$$\begin{aligned}
\langle \sigma_y \rangle &= \langle (\sigma_y)_H \rangle \\
&= \langle \psi(0)| \, (\sigma_y)_H \, |\psi(0)\rangle \\
&= \langle \psi(0)| \, (\sigma_y cos(2t) + \sigma_x sin(2t)) \, |\psi(0)\rangle \\
&= \langle \psi(0)| \, \sigma_y \, |\psi(0)\rangle \, cos(2t) + \langle \psi(0)| \, \sigma_x \, |\psi(0)\rangle \, sin(2t)
\end{aligned}$$

Hence:

$$\boxed{\langle \sigma_y \rangle = sin(2t)}$$

For σ_x:

$$\begin{aligned}
\langle \sigma_x \rangle &= \langle (\sigma_x)_H \rangle \\
&= \langle \psi(0)| \, (\sigma_x)_H \, |\psi(0)\rangle \\
&= \langle \psi(0)| \, (\sigma_x cos(2t) - \sigma_y sin(2t)) \, |\psi(0)\rangle \\
&= \langle \psi(0)| \, \sigma_x \, |\psi(0)\rangle \, cos(2t) - \langle \psi(0)| \, \sigma_y \, |\psi(0)\rangle \, sin(2t)
\end{aligned}$$

Hence:

$$\boxed{\langle \sigma_x \rangle = cos(2t)}$$

These results match with the Schrodinger Picture solutions.

We simulate this exact system in QuTiP and plot the expectation of the Pauli matrices.

To Learn more about QuTiP refer to https://qutip.org/index.html