Quantum Mechanics

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Operators in QM

- ✓ So far we have described the states of a physical system by vectors belonging to a complex vector space.

Insufficient to fully describe the properties of a physical system

- ✓ **How the state of a system evolves in time ?**
- ✓ **How to represent fundamental physical quantities such as position, momentum or energy ?**

  - ➢ It requires further developments in the mathematics of vector spaces.

  - ✓ Involve the introduction a new mathematical entity known as an **operator**.

It's role is to 'operate' on state vectors and map them into other state vectors

<u>Operators play many different roles in quantum mechanics !!</u>

- ✓ The evolution of the state of a system in time !
- ✓ The creation or destruction of particles !
- ✓ Represent the observable properties of a system (x, p , E e.t.c.).

Operators in QM: Definition

- ✓ It is needed to introduce the mathematical notion of an operator into quantum mechanics !

  - ➢ The system will evolve in time i.e. its state will be time dependent

✓ The changes in a state can be brought about by various processes !!

- ➢ It is possible to describe a physical process by an exhaustive list of all the changes that it induces on every state of the system.

  - ✓ The state of a system in quantum mechanics is represented by a vector !

- ➢ We can prepare a table of all possible before and after states.

  - ✓ A mathematical device can then be constructed which represents this list of before and after states.

Operator

The operator representing the physical process is a mathematical object that acts on the state of a system and maps this state into some other state in accordance with the exhaustive list proposed above.

$$\hat{Q}\,\psi = \chi$$

Operators in QM: Types

- It is well motivated to introduce the idea of an operator as something that acts to change the state of a quantum system !

- ✓ However, there are many operators that arise in quantum mechanics, which can act on a state vector to map it into another state vector, do not represent a physical process acting on the system.

- ✓ In fact, the operators that represent such physical processes as the evolution of the system in time, are one kind of operator important in quantum mechanics known as **unitary operators**.

- ✓ Another very important kind of operator, which represents the physically observable properties of a system, such as momentum or energy, is known as **Hermitian operator** ! → Not an actual physical process

❖ Hermitian operators represent observables of a system !!

❖ Unitary operators represent possible actions performed on a system !!

Operators in QM: Hermitian

Postulate 4

- ✓ Every dynamical variable in classical mechanics can be replaced by **operator** which will act on the wave function .

- ✓ An operator is merely the mathematical rule used to describe a certain mathematical operation.

- ✓ For each dynamical variable, x, there exist an expectation value $< x >$

- ✓ Real world, measurable observables needs to be **real** values !

What makes for real expectation value ?

<Q> = $\int_{-\infty}^{\infty} dx\, \psi^* \,\hat{Q}\, \psi = < Q >^* = \int_{-\infty}^{\infty} dx\, \psi^* \,\hat{Q}^*\, \psi$

$\boxed{Q = Q^*}$ ⇒ **Hermitian operator**

More general definition for an operator to be Hermitian $\int_{-\infty}^{\infty} dx\, \psi_1{}^* \,\hat{Q}\, \psi_2 = \int_{-\infty}^{\infty} dx\, \psi_2{}^* \,\hat{Q}^*\, \psi_1$

Eigenvalues are real and their **eigen functions** are orthonormal!

$\hat{Q}\,\psi = \lambda\, \psi$

Operators in QM: Properties !

- ✓ Most operators in quantum mechanics have a very important property: they are linear or, at worst, anti-linear.

$$\hat{T}\,(c_1\,\psi_1 + c_2\,\psi_2) = c_1^{\,*}(\,\hat{T}\,\psi_1) + c_2^{\,*}(\hat{T}\,\psi_2)$$

$$\hat{A}\,(c_1\,\psi_1 + \,c_2\,\psi_2\,) = \;c_1(\,\hat{A}\,\psi_1) + \,c_2\,(\hat{A}\,\psi_2)$$

- ✓ Equality of Operators : If $\hat{A}\,\psi = \hat{B}\,\psi$ then $\hat{A} = \hat{B}$!!
- ✓ The Unit Operator and the Zero Operator : $\hat{1}\,\psi = \psi$ & $\hat{0}\,\psi = 0$
- ✓ Addition of Operators: $(\,\hat{A} + \hat{B}\,)\,\psi = \hat{A}\,\psi + \hat{B}\,\psi$
- ✓ Multiplication of an Operator by a Complex Number : $\hat{A}\,(\lambda\,\psi) = \lambda\,(\hat{A}\,\psi)$
- ✓ Multiplication of Operators : $\hat{A}\,\{\,\hat{B}\,\psi\,\} = \hat{A}\,\hat{B}\,\psi$

Commutator

- ✓ Commutators : In general, $\hat{A}\,\hat{B} \neq \hat{B}\,\hat{A}$

The difference $\hat{A}\,\hat{B} - \hat{B}\,\hat{A} = [\,\hat{A}, \hat{B}\,]$

- ➢ If the commutator vanishes, the operators are said to commute.

Two observable properties of a system can be known simultaneously with precision !

Time evolution

Let us define an operator U(t +Δ t, t) such that

$$\psi(t+\Delta t) = U(t+\Delta t, t)\,\psi(t)$$

Now as $\Delta t \to 0$, $U(t+\Delta t, t) = \hat{\mathbb{1}}$

$\Downarrow$

identity

We can expand around this, to obtain

$$U(t+\Delta t, t) = \hat{\mathbb{1}} - \frac{i}{\hbar}\hat{H}\Delta t + \cdots$$

generator

$$\therefore \lim_{\Delta t \to 0} \frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} = -\frac{i}{\hbar}\hat{H}\psi(t)$$

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

Hence $\psi(t) = e^{-\frac{i\hat{H}t}{\hbar}}\psi(0)$

$$= e^{-\frac{iEt}{\hbar}}\psi(0)$$