Quantum Mechanics

Soumitra Nandi

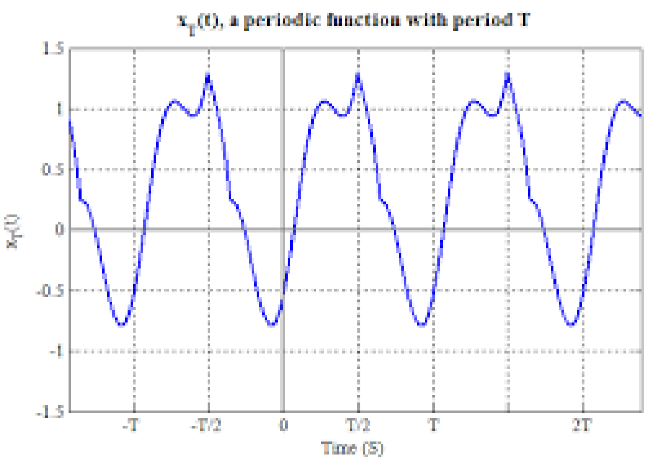
PH101, Lec-6

Short introduction to Fourier series expansion

Fourier series

- ✓ A graph of periodic function f(x) that has period L exhibits the same pattern every L units along the x-axis, so that f(x+L) = f(x) for every value of x.

- ✓ If we know what the function looks like over one complete period, we can thus sketch a graph of the function over a wider interval of x !



Fourier methods give us a set of powerful tools for representing any periodic function as a sum of sines and cosines.

✓ The Fourier series of a function, f(x), with period 2L =>

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left(a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right)$$

Fourier analysing a signal, we can immediately tell which harmonics are the important ones.

✓ The note that we get when a flute is played is made up from the sum of many pure tones !

Few standard integrals

$$\int_0^L \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}dx = \begin{cases} 0 & \text{if } m = n = 0 \\ \frac{L}{2}\delta_{mn} & \text{otherwise} \end{cases}$$

$$\int_0^L \cos\frac{n\pi x}{L}\cos\frac{m\pi x}{L}dx = \begin{cases} L & \text{if } m = n = 0 \\ \frac{L}{2}\delta_{mn} & \text{otherwise} \end{cases}$$

$$\int_{-L}^L \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}dx = \begin{cases} 0 & \text{if } m = n = 0 \\ L\delta_{mn} & \text{otherwise} \end{cases}$$

$$\int_{-L}^L \cos\frac{n\pi x}{L}\cos\frac{m\pi x}{L}dx = \begin{cases} 2L & \text{if } m = n = 0 \\ L\delta_{mn} & \text{otherwise} \end{cases}$$

$$\int_{-L}^L \sin\frac{n\pi x}{L}\cos\frac{m\pi x}{L}dx = 0$$

$$\int_{-L}^L e^{i(n-m)\pi x/L}dx = 2L\delta_{nm}$$

Fourier series

The Fourier expansion of f(x) for the interval [-π , π] :

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos nx + b_n \sin nx$$

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin nx\, dx$$

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\, dx \qquad a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos nx\, dx$$

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left(a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right)$$

Complex representation

$$f(x) = \sum_{n=-\infty}^{\infty} c_n\, e^{\frac{in\pi x}{L}}$$

The exponentials are orthogonal and normalized over the interval

$$\frac{1}{2L}\int_{-L}^{L} e^{\frac{in\pi x}{L}}\, e^{\frac{-im\pi x}{L}}\, dx = \delta_{nm}$$

$$c_n = \frac{1}{2L}\int_{-L}^{L} f(x)\, e^{\frac{-in\pi x}{L}}\, dx$$

Wave number $k = \frac{n\pi}{L}$

As L → ∝, k can take on any value

Our sum over n becomes an integral over k

dk = $\frac{\pi}{L}$ **dn ,**

We define **A(k) =** $\sqrt{\frac{2}{\pi}}\, L\, c_n$

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)e^{ikx}dk$$

$$A(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx$$

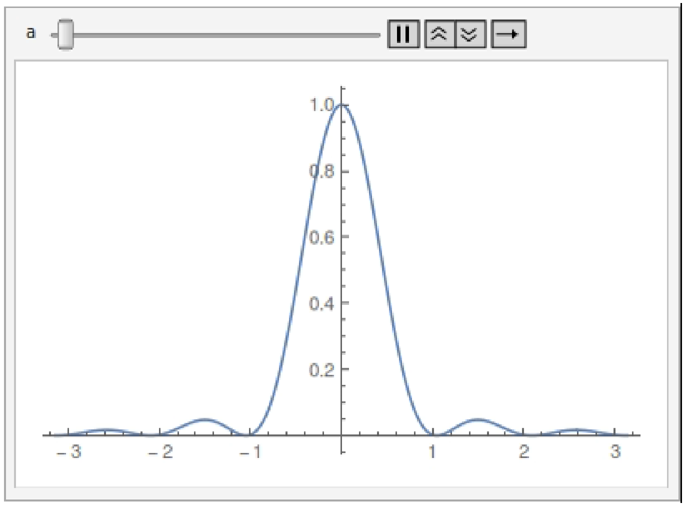
Square Wave packet

$$A(k) = \frac{1}{\sqrt{a}} \quad \text{for } k_0 - \frac{a}{2} < k < k_0 + \frac{a}{2}$$

= 0 elsewhere

width $\Delta k = a$

$P(x) \propto \sin^2(a\,x/2)/(ax)^2$



Normalization

$$\int_{-\infty}^{\infty} |A(k)|^2 dk = \frac{1}{a} \int_{k_0-\frac{a}{2}}^{k_0+\frac{a}{2}} dk \quad = \frac{1}{a} a = 1$$

Fourier Transformation

$$f(x) \quad = \quad \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{a}} \int_{k_0-\frac{a}{2}}^{k_0+\frac{a}{2}} e^{ikx} dk \quad = \quad \frac{1}{\sqrt{2\pi a}} \frac{1}{ix} \left[e^{ikx}\right]_{k_0-\frac{a}{2}}^{k_0+\frac{a}{2}} = \sqrt{\frac{a}{2\pi}} e^{ik_0 x} \frac{2\sin\left(\frac{ax}{2}\right)}{ax}$$

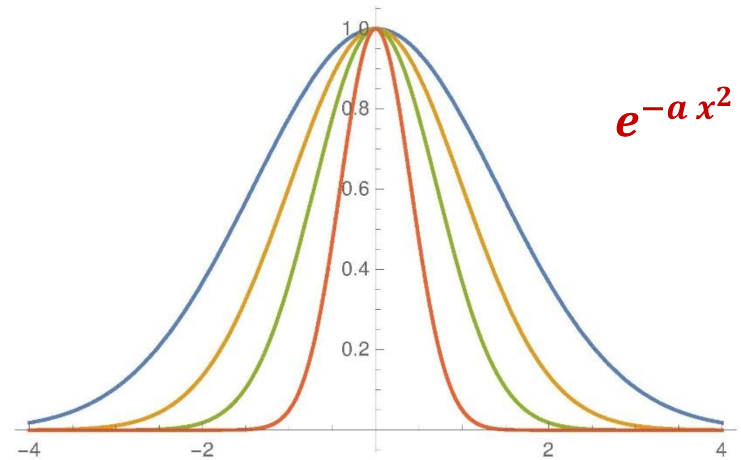
width $\Delta x = 4\pi/a$

Uncertainty relation: $\Delta x\, \Delta k = 4\,\pi$

Gaussian wave packet

A Gaussian packet: $A(k) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha(k-k_0)^2}$

$$|A(k)|^2 = P(k) = \sqrt{\frac{2\alpha}{\pi}} e^{-2\alpha(k-k_0)^2}$$



Normalization

$$\sigma_k = \frac{1}{\sqrt{4\alpha}}$$

$$\int_{-\infty}^{\infty} |A(k)|^2 dk = \sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-2\alpha(k-k_0)^2} dk$$

$$= \sqrt{\frac{2\alpha}{\pi}} \sqrt{\frac{\pi}{2\alpha}} = 1$$

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-X)^2}{2\sigma^2}}$$

Standard Gaussian distribtuion

Fourier Transformation

$$f(x) = \frac{1}{\sqrt{2\pi}} \left(\frac{2\alpha}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\alpha(k-k_0)^2} e^{ikx} dk \;=\; \left(\frac{1}{2\pi\alpha}\right)^{1/4} e^{ik_0 x} e^{-\frac{x^2}{4\alpha}}$$

$$\sigma_x = \sqrt{\alpha}$$

Check the Normalization

$$\text{P(x)} = |f(x)|^2 = \frac{1}{\sqrt{2\pi\alpha}}\, e^{-\frac{x^2}{2\alpha}}$$

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \sqrt{\frac{1}{2\pi\alpha}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\alpha}} dx = \sqrt{\frac{1}{2\pi\alpha}} \sqrt{2\alpha\pi} = 1$$

$$\sigma_x \sigma_k = \frac{1}{2}$$

Uncertainty relation

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

Operators play many different roles in quantum mechanics !!

- ✓ 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.

➢ 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 $<\hat{x}>$
- ✓ Real world, measurable observables needs to be **real** values !

What makes for real expectation value ?

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

$Q = Q^*$ ⇒ **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 : $\hat{A}\,\{\,\hat{B}\,\psi\,\} = \hat{A}\,\hat{B}\,\psi$
- ✓ Commutators : In general, $\hat{A}\,\hat{B} \neq \hat{B}\,\hat{A}$

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

Commutator

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

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