PHY 712 Quantum Mechanics
12-12:50 PM MWF Olin 103

Plan for Lecture 4:
Reading: Skim chapters #2 & #3 and start reading #4 in Shankar

1. **Mathematical formalisms that can represent quantum phenomena**
2. **State vector**
3. **Physical variables and their representations**

PHY 741 Quantum Mechanics

MWF 12 PM - 12:50 PM | OPL 103 | http://www.wfu.edu/~natalie/f17phy741/

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Course schedule

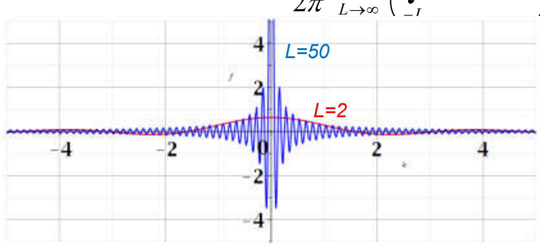
(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/28/2017	Chap. 1	Review of basic principles	#1	9/6/2017
2	Wed, 8/30/2017	Chap. 1	Linear vector spaces	#2	9/6/2017
3	Fri, 9/01/2017	Chap. 1	Linear vector spaces	#3	9/6/2017
4	Mon, 9/04/2017	Chap. 4	Principles of Quantum Mechanics	#4	9/8/2017
5	Wed, 9/06/2017				
6	Fri, 9/08/2017				
7	Mon, 9/11/2017				
8	Wed, 9/13/2017				

Dirac delta functions

$$\delta(k-k') \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(k-k')x}dx$$

$$= \frac{1}{2\pi}\lim_{L\to\infty}\left(\int_{-L}^{L} e^{i(k-k')x}dx\right)$$

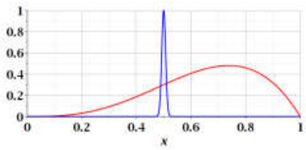


Properties of the Dirac delta function

$$\delta(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases}$$

$$\int_{-\epsilon}^{\epsilon} \delta(x)dx = 1$$

$$\int_{-\infty}^{\infty} G(x)\delta(x)dx = G(0)$$



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Properties of the Dirac delta function -- continued

$$\int_{-\infty}^{\infty} G(x)\delta(f(x))dx = \int_{-\infty}^{\infty} G(x)\delta(f(x))\frac{df}{df}dx$$

$$\int_{-\infty}^{\infty} G(x)\frac{\delta(f(x))}{df/dx}df = \sum_i \frac{G(x_i)}{\left|\frac{df}{dx}\right|_{f(x_i)=0}}$$

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Properties of the Dirac delta function -- continued

$$\int_{-\infty}^{\infty} G(x)\delta'(x)dx = -\left.\frac{dG(x)}{dx}\right|_{x=0}$$

Details:

$$\int_{-\infty}^{\infty} G(x)\frac{d\delta(x)}{dx}dx = \int_{-\infty}^{\infty} \frac{d\left(G(x)\delta(x)\right)}{dx}dx - \int_{-\infty}^{\infty} \frac{dG(x)}{dx}\delta(x)dx$$

=0 provided that
G(∞) is well-behaved

Note: Shankar has minus sign issue….

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Material to skim:

2

Review of Classical Mechanics

In this chapter we will develop the Lagrangian and Hamiltonian formulations of mechanics starting from Newton's laws. These subsequent reformulations of mechanics bring with them a great deal of elegance and computational ease. But our principal interest in them stems from the fact that they are the ideal springboards from which to make the leap to quantum mechanics. The passage from the Lagrangian formulation to quantum mechanics was carried out by Feynman in this path integral formalism. A more common route to quantum mechanics, which we will follow for the most part, has as its starting point the Hamiltonian formulation, and it was discovered mainly by Schrödinger, Heisenberg, Dirac, and Born.

It should be emphasized, and it will soon become apparent, that all three formulations of mechanics are essentially the same theory, in that their domains of validity and predictions are identical. Nonetheless, in a given context, one or the other may be more inviting for conceptual, computational, or simply aesthetic reasons.

2.1. The Principle of Least Action and Lagrangian Mechanics

Material to skim:

3

All Is Not Well with Classical Mechanics

It was mentioned in the Prelude that as we keep expanding our domain of observations we must constantly check to see if the existing laws of physics continue to explain the new phenomena, and that, if they do not, we must try to find new laws that do. In this chapter you will get acquainted with experiments that betray the inadequacy of the classical scheme. The experiments to be described were never performed exactly as described here, but they contain the essential features of the actual experiments that were performed (in the first quarter of this century) with none of their inessential complications.

3.1. Particles and Waves in Classical Physics

Start reading Chapter 4 in Shankar

Mathematical formalisms that can describe quantum phenomena --

Classical Mechanics	Quantum Mechanics
I. The state of a particle at any given time is specified by the two variables $x(t)$ and $p(t)$, i.e., as a point in a two-dimensional phase space.	I. The state of the particle is represented by a vector $\|\psi(t)\rangle$ in a Hilbert space.

Classical Mechanics

II. Every dynamical variable ω is a function of x and p: $\omega = \omega(x, p)$.

Quantum Mechanics

II. The independent variables x and p of classical mechanics are represented by Hermitian operators X and P with the following matrix elements in the eigenbasis of X‡

$$\langle x|X|x'\rangle = x\delta(x-x')$$
$$\langle x|P|x'\rangle = -i\hbar\delta'(x-x')$$

The operators corresponding to dependent variables $\omega(x, p)$ are given Hermitian operators

$$\Omega(X, P) = \omega(x \to X, p \to P)§$$

Classical Mechanics

III. If the particle is in a state given by x and p, the measurement‖ of the variable ω will yield a value $\omega(x, p)$. The state will remain unaffected.

Quantum Mechanics

III. If the particle is in a state $|\psi\rangle$, measurement‖ of the variable (corresponding to) Ω will yield one of the eigenvalues ω with probability $P(\omega) \propto |\langle\omega|\psi\rangle|^2$. The state of the system will change from $|\psi\rangle$ to $|\omega\rangle$ as a result of the measurement.

Classical Mechanics

IV. The state variables change with time according to Hamilton's equations:

$$\dot{x} = \frac{\partial \mathscr{H}}{\partial p}$$
$$\dot{p} = -\frac{\partial \mathscr{H}}{\partial x}$$

Quantum Mechanics

IV. The state vector $|\psi(t)\rangle$ obeys the *Schrödinger equation*

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

where $H(X, P) = \mathscr{H}(x \to X, p \to P)$ is the quantum Hamiltonian operator and $\mathscr{H}$ is the Hamiltonian for the corresponding classical problem.

Expectation values

For an operator $\mathbf{O}$ and a system in a state $|\psi\rangle$:

$$\langle \mathbf{O} \rangle = \langle \psi | \mathbf{O} | \psi \rangle$$

Uncertainty values

For an operator $\mathbf{O}$ and a system in a state $|\psi\rangle$:

$$\langle \Delta\mathbf{O} \rangle = \left(\langle \psi | \left(\mathbf{O} - \langle \mathbf{O} \rangle \right)^2 | \psi \rangle \right)^{1/2}$$

Consider the following example of the four 2-dimensional operators:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}$$

Eigenvectors of σ_z and σ^2:

$$|\psi_\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\psi_\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Expectation values:

$$\langle \psi_\downarrow | \sigma_x | \psi_\downarrow \rangle = 0 \quad \langle \psi_\downarrow | \sigma_y | \psi_\downarrow \rangle = 0 \quad \langle \psi_\downarrow | \sigma_z | \psi_\downarrow \rangle = -1 \quad \langle \psi_\downarrow | \sigma^2 | \psi_\downarrow \rangle = 3$$

$$\langle \psi_\uparrow | \sigma_x | \psi_\uparrow \rangle = 0 \quad \langle \psi_\uparrow | \sigma_y | \psi_\uparrow \rangle = 0 \quad \langle \psi_\uparrow | \sigma_z | \psi_\uparrow \rangle = +1 \quad \langle \psi_\uparrow | \sigma^2 | \psi_\uparrow \rangle = 3$$

Uncertainty values:

$$\langle \psi_\downarrow | \Delta\sigma_x | \psi_\downarrow \rangle = 1 \quad \langle \psi_\downarrow | \Delta\sigma_y | \psi_\downarrow \rangle = 1 \quad \langle \psi_\downarrow | \Delta\sigma_z | \psi_\downarrow \rangle = 0 \quad \langle \psi_\downarrow | \Delta\sigma^2 | \psi_\downarrow \rangle = 0$$

$$\langle \psi_\uparrow | \Delta\sigma_x | \psi_\uparrow \rangle = 1 \quad \langle \psi_\uparrow | \Delta\sigma_y | \psi_\uparrow \rangle = 1 \quad \langle \psi_\uparrow | \Delta\sigma_z | \psi_\uparrow \rangle = 0 \quad \langle \psi_\uparrow | \Delta\sigma^2 | \psi_\uparrow \rangle = 0$$

Further considerations --

Consider the following example of the four 2-dimensional operators:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}$$

Eigenvectors of σ_x:

$$|\psi_{x1}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad |\psi_{x2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Expectation values:

$$\langle \psi_{x1} | \sigma_x | \psi_{x1} \rangle = -1 \quad \langle \psi_{x1} | \sigma_y | \psi_{x1} \rangle = 0 \quad \langle \psi_{x1} | \sigma_z | \psi_{x1} \rangle = 0 \quad \langle \psi_{x1} | \sigma^2 | \psi_{x1} \rangle = 3$$

$$\langle \psi_{x2} | \sigma_x | \psi_{x2} \rangle = +1 \quad \langle \psi_{x2} | \sigma_y | \psi_{x2} \rangle = 0 \quad \langle \psi_{x2} | \sigma_z | \psi_{x2} \rangle = 0 \quad \langle \psi_{x2} | \sigma^2 | \psi_{x2} \rangle = 3$$

Uncertainty values:

$$\langle \psi_{x1} | \Delta\sigma_x | \psi_{x1} \rangle = 0 \quad \langle \psi_{x1} | \Delta\sigma_y | \psi_{x1} \rangle = 1 \quad \langle \psi_{x1} | \Delta\sigma_z | \psi_{x1} \rangle = 1 \quad \langle \psi_{x1} | \Delta\sigma^2 | \psi_{x1} \rangle = 0$$

$$\langle \psi_{x2} | \Delta\sigma_x | \psi_{x2} \rangle = 0 \quad \langle \psi_{x2} | \Delta\sigma_y | \psi_{x2} \rangle = 1 \quad \langle \psi_{x2} | \Delta\sigma_z | \psi_{x2} \rangle = 1 \quad \langle \psi_{x2} | \Delta\sigma^2 | \psi_{x2} \rangle = 0$$

Time evolution

Suppose that the Hamiltonian for this system has the form:

$$H = \sigma_z B = \begin{pmatrix} -B & 0 \\ 0 & B \end{pmatrix} \quad \text{where } B \text{ is a constant}$$

Schroedinger equation:

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

Note that if $|\psi(t=0)\rangle = |\psi_\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, then $|\psi(t)\rangle = e^{iBt/\hbar}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Note that if $|\psi(t=0)\rangle = |\psi_\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, then $|\psi(t)\rangle = e^{-iBt/\hbar}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Note that if $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, then $|\psi(t)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{iBt/\hbar} \\ e^{-iBt/\hbar} \end{pmatrix}$

Time evolution -- continued

Note that if $|\psi(t=0)\rangle = |\psi_\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, then $|\psi(t)\rangle = e^{iBt/\hbar}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\Rightarrow \langle H \rangle = \langle \psi(t)|B|\psi(t)\rangle = -B$$

Note that if $|\psi(t=0)\rangle = |\psi_\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, then $|\psi(t)\rangle = e^{-iBt/\hbar}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\Rightarrow \langle H \rangle = \langle \psi(t)|H|\psi(t)\rangle = B$$

Note that if $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, then $|\psi(t)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{iBt/\hbar} \\ e^{-iBt/\hbar} \end{pmatrix}$

$$\Rightarrow \langle H \rangle = \langle \psi(t)|H|\psi(t)\rangle = 0$$

Time evolution -- continued

Note that if $|\psi(t=0)\rangle = |\psi_\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, then $|\psi(t)\rangle = e^{iBt/\hbar}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\Rightarrow \langle \sigma_x \rangle = \langle \psi(t)|\sigma_x|\psi(t)\rangle = 0$$

Note that if $|\psi(t=0)\rangle = |\psi_\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, then $|\psi(t)\rangle = e^{-iBt/\hbar}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\Rightarrow \langle \sigma_x \rangle = \langle \psi(t)|\sigma_x|\psi(t)\rangle = 0$$

Note that if $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, then $|\psi(t)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{iBt/\hbar} \\ e^{-iBt/\hbar} \end{pmatrix}$

$$\Rightarrow \langle \sigma_x \rangle = \langle \psi(t)|\sigma_x|\psi(t)\rangle = \cos(2Bt/\hbar)$$

Other examples

Suppose we have a state vector which is a continuous function of x:

$$|\psi(x)\rangle = \frac{1}{\left(\pi\Lambda^2\right)^{1/4}} e^{-(x-a)^2/(2\Lambda^2)}$$

$$\langle x\rangle = \langle\psi(x)|x|\psi(x)\rangle = \frac{1}{\left(\pi\Lambda^2\right)^{1/2}} \int_{-\infty}^{\infty} x e^{-(x-a)^2/(\Lambda^2)} dx = a$$

$$\langle x^2\rangle = \langle\psi(x)|x^2|\psi(x)\rangle = \frac{1}{\left(\pi\Lambda^2\right)^{1/2}} \int_{-\infty}^{\infty} x^2 e^{-(x-a)^2/(\Lambda^2)} dx = a^2 + \frac{\Lambda^2}{2}$$

$$\langle \Delta x\rangle = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{\Lambda}{\sqrt{2}}$$

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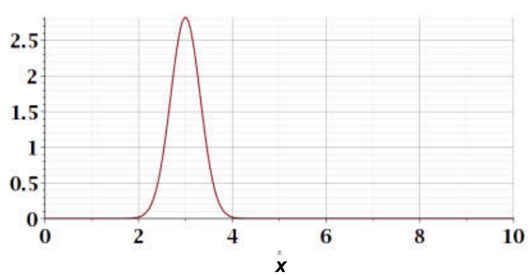
$$P(x) = \frac{1}{\left(\pi\Lambda^2\right)^{1/2}} e^{-(x-a)^2/(\Lambda^2)}$$



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Example continued

$$|\psi(x)\rangle = \frac{1}{\left(\pi\Lambda^2\right)^{1/4}} e^{-(x-a)^2/(2\Lambda^2)}$$

Expectation value and uncertainty of momentum

$$\langle p\rangle = \langle\psi(x)|p|\psi(x)\rangle = \langle\psi(x)|-i\hbar\frac{d}{dx}|\psi(x)\rangle = 0$$

$$\langle p^2\rangle = \langle\psi(x)|p^2|\psi(x)\rangle = \langle\psi(x)|-\hbar^2\frac{d^2}{dx^2}|\psi(x)\rangle = \frac{\hbar^2}{2\Lambda^2}$$

$$\langle \Delta p\rangle = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{\hbar}{\sqrt{2}\Lambda}$$

Note that:

$$\langle \Delta x\rangle\langle \Delta p\rangle = \frac{\Lambda}{\sqrt{2}}\frac{\hbar}{\sqrt{2}\Lambda} = \frac{\hbar}{2}$$

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