Sept 4, 2014

P423: Quantum Mechanics II

Lecture 1: Intro and review of the postulates of Quantum Mechanics

ELL 160

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Course website: www.web.uvic.ca/~rdesousa/teaching/P423/Phys423.html
See syllabus and all online materials/rules.

- Homeworks and solutions posted online

→ A1 already posted, due Friday Sept 12 at 6pm in dropbox at the following (Labelled "P423").
(all assignments due Friday @ 6pm)

Office hours: Thursdays 3:00 – 4:00 pm

Textbook: "Introduction to quantum mechanics", David J. Griffiths, 2nd Ed.

Midterm exam: Oct. 9th in Class

→ Take a photo of the Class

Classical Mechanics

In Classical mechanics, the state of any physical system is determined by the position $\vec{r}=(x,y,z)$ and velocity $\vec{v} = \frac{d\vec{r}}{dt} = (\dot{x},\dot{y},\dot{z})$ of its points or particles.

We can introduce generalized coordinates $q_i(t)$ and their velocities $\dot{q}_i(t)$ to describe the system. Specifying $q_i(t_0)$ and $\dot{q}_i(t_0)$ at any given time t_0 enables the calculation for all times t of all future $q_i(t)$ and $\dot{q}_i(t)$. For this we need is the Lagrangian $L(q_i, \dot{q}_i)$.
The motion of the system is determined by the path that minimizes the action $S = \int dt\, L \Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$.
Define the Canonical momentum p_i as

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

The $q_i(t)$ and $p_i(t)$ are called the fundamental dynamical variables. All physical quantities associated to the system (observables such as energy, angular momentum, etc) can be expressed as a func of them. The total energy or Hamiltonian func is given by

$$H(p_i, q_i, t) = \sum_i p_i \dot{q}_i - L,$$

and the motion of the system is determined by solving the Hamilton's eqns of motion (equivalent to Lagrange):

$$\begin{cases} \dot{q}_i = \dfrac{\partial H}{\partial p_i} \\ \dot{p}_i = -\dfrac{\partial H}{\partial q_i} \end{cases}$$

For example, single particle in 3d: $H = \frac{(\vec{p})^2}{2m} + V(\vec{q})$

$$\Rightarrow \begin{cases} \dot{\vec{q}} = \dfrac{\partial H}{\partial \vec{p}} = \dfrac{\vec{p}}{m} \\ \dot{\vec{p}} = -\dfrac{\partial H}{\partial \vec{q}} = -\dfrac{\partial V}{\partial \vec{q}} \end{cases}$$

Let's talk a bit more about the action $S = \int_{t_i}^{t_f} L\,dt$. Instead of fixing the endpoints $\delta q(t_f) = \delta q(t_i) = 0$ let us allow the final endpoint to be arbitrary, so that we can think of $S = S(q, t)$ where we made $t_f \to t$.

In that case:

$$\delta S = \int_{t_0}^{t} dt \left(\frac{\partial L}{\partial q}\,\delta q + \underbrace{\frac{\partial L}{\partial \dot q}\,\delta \dot q}_{\text{integrate by parts}} \right) = \frac{\partial L}{\partial \dot q}\,\delta q \Big|_{t_0}^{t} + \underbrace{\int_{t_0}^{t} dt \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\right)\right)}_{=0}$$

Assume $\delta q(t_0) = 0$ but $\delta q(t)$ arbitrary: $\boxed{\delta S = p\,\delta q}$

Thus, $\boxed{\frac{\partial S}{\partial q_i} = p_i}$. Moreover, $\underbrace{\frac{dS}{dt}}_{=L} = \frac{\partial S}{\partial t} + \sum_i \underbrace{\frac{\partial S}{\partial q_i}}_{=p_i} \dot q_i$,

so $\frac{\partial S}{\partial t} = L - \sum_i p_i \dot q_i = -H$.

$$\Rightarrow \boxed{\frac{\partial S}{\partial t} = -H} //.$$

Poisson bracket in CM: For an observable $A(q_i, p_i)$:

$$\frac{dA}{dt} = \{A, H\} + \frac{\partial A}{\partial t}$$

$$\{A, B\} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right)$$

e.g. $\{q_i, p_j\} = \delta_{ij}$

Therefore, summarizing CM:

(i) The state of the system at any t is defined by specifying $\vec q(t)$ and $\vec p(t)$

(ii) The value of all observables is completely defined at any t once the state is known.

(iii) Time evolution uniquely determined for all t once the state at t_0 is known

$\mapsto$ Deep Philosophical consequence: Determinism, no free will! (Date joke – No matter what you will do, she will say no, or yes!)

This classical description is not correct. Particularly, it fails miserably at small energies and length scales.

The formulation of QM answers the following questions:

- How is the state of a system described?

- Given that state, how can we predict the results of measurements of various physical quantities (observables)?

- How can the state of a system at arbitrary time t be found when the one at t_0 is known?

Postulates of Quantum Mechanics

I) At time t_0, the state of a system is defined by specifying a ket $|\psi(t_0)\rangle$ belonging to the vector space $\mathcal{E}$.

▶ Superposition principle: Linear combinations such as $|\psi\rangle = \underbrace{\alpha |\varphi_1\rangle + \beta |\varphi_2\rangle}_{\text{complex numbers.}}$ are allowed states.

"Hot application": How about storing / processing information with "quantum bits" = qubits like $\alpha|0\rangle + \beta|1\rangle$ instead of the usual 0's and 1's? Quantum Computation is an active area of research that I work on.

II) Every measurable physical quantity A is described by an operator $\hat{A}$ acting on $\mathcal{E}$; this operator is called an <u>observable</u>.

→ Note how different QM is from CM:
- States are vectors in an abstract linear algebra sense.
- Observables are operators acting on this space.

III) The only possible result of the measurement of a physical quantity A is one of the eigenvalues of the corresponding operator $\hat{A}$.

▶ Since all A is always real, $\hat{A}$ is by definition Hermitian, $\hat{A} = \hat{A}^\dagger$.
If the spectrum of $\hat{A}$ is discrete, the results that can be obtained by measuring A are <u>quantized</u>.

For the case of a discrete nondegenerate spectrum:

IV) When A is measured on a system in the normalized state $|\psi\rangle$, the probability $P(a_n)$ of obtaining a_n is $P(a_n) = |\langle u_n|\psi\rangle|^2$, where $|u_n\rangle$ is the normalized eigenvector of $\hat{A}$ associated with the eigenvalue a_n, $\hat{A}|u_n\rangle = a_n|u_n\rangle$.

For discrete degenerate: $P(a_n) = \sum_{i=1}^{g_n} |\langle u_n^i|\psi\rangle|^2$ where $\{|u_n^i\rangle, i=1,\dots,g_n\}$ forms a basis of the space $\hat{A}|\psi\rangle = a_n|\psi\rangle$

For continuous spectrum $\hat{A}|u_\alpha\rangle = \alpha|u_\alpha\rangle$, the probability of measuring $\alpha \in [\alpha, \alpha+d\alpha]$ is $\underbrace{|\langle u_\alpha|\psi\rangle|^2}_{\text{Prob. density}} d\alpha$

Example: Consider a basis for localized particles in 3d $\{|\vec{r}\rangle\}$. The quantity

$\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$ is called "wave func" and

gives a "coordinate representation" of any state $|\psi\rangle$ in that basis $\{|\vec{r}\rangle\}$. Quantum particles are described by the complex matter wave $\psi(\vec{r})$,
and the probability of measuring a particle localized at $\vec{r}$ (i.e. at the state $|\vec{r}\rangle$) is

$|\langle\vec{r}|\psi\rangle|^2 = |\psi(\vec{r})|^2$.

V) If the measurement of A in the system state $|\psi\rangle$ gives the result a_n, the state of the system immediately after the measurement is the normalized projection of $|\psi\rangle$ onto the subspace associated with a_n: $|\psi\rangle \xrightarrow{\text{Measurement outcome } a_n} \dfrac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_n|\psi\rangle}}$ where e.g. $\hat{P}_n = |u_n\rangle\langle u_n|$ for nondegenerate discrete spectra.

Connection with CM and the introduction of $\hbar$

The passage of QM into CM requires taking a limit where particles propagating as waves start propagating along well defined paths, with the spread of the waves going to zero.

We can think of this limit as analogous to the transition between wave optics and geometrical (or ray) optics. Wave optics the electromagnetic waves are described as $\vec{E}$ and $\vec{B}$ vectors that satisfy Maxwell's eqns; on the other hand in ray optics light propagates along well defined paths.

This limit occurs when $\lambda \to 0$ (wavelength) (high energy light), or when the waves can be described by

$$\psi = a\, e^{i\phi} \quad , \text{ with } \phi \text{ varying rapidly over } \vec{r}\ , \ \phi >> 1 .$$

Let's assume that in the classical limit the QM wave fn assumes such a form.

In ray optics the direction of light propagation can be determined by Fermat's principle: That rays of light take the path of least (or maximum) length, such that $\int_{\vec{x}_i}^{\vec{x}_f} |d\vec{\ell}|$ is an extremum. But from wave optics the phase is given by

$$\phi = \int_{\vec{x}_i}^{\vec{x}_f} \vec{k}\cdot d\vec{\ell} = k \int_{\vec{x}_i}^{\vec{x}_f} |d\vec{\ell}| \quad (\text{In the ray limit } \vec{k} \parallel d\vec{\ell}).$$

Hence Fermat's principle is equivalent of saying that the phase is an extremum, $\delta\phi = 0$.

In CM we have a similar principle in that paths minimize the action $S = \int_i^f L\, dt$. Extending this analogy we can propose

$$\phi = \text{Constant} \times S = \frac{1}{\hbar} S$$

for the quasiclassical phase. We introduced a constant $\hbar$ with dimensions of action $= Et = xp$. Note the parallel with λ in that when $\hbar \to 0$ we get the classical limit (just as $\lambda \to 0$ gives the ray limit of optics).

Thus

$$\boxed{\psi_{\text{classical limit}}(\vec{q},t) \approx \underset{\substack{\uparrow \\ \text{varies slowly}}}{a}\; e^{\frac{i}{\hbar} \underset{\substack{\downarrow \\ \text{varies rapidly}}}{S(\vec{q},t)}}}$$

Now assuming $a(t)$ varies much slower than $S(t)$:

$$\frac{\partial \psi_{class}}{\partial t} \approx \frac{i}{\hbar} \underbrace{\frac{\partial S}{\partial t}}_{=-H} \psi_{class} = \frac{1}{i\hbar} H \psi_{class}$$

VI) The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger eqn

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \, , \quad \text{where } H \text{ is the Hamiltonian fnc in operator form.}$$

But how to represent momentum? Use $\vec{p} = \frac{\partial S}{\partial \vec{q}} = \vec{\nabla}_q S$:

$$\vec{p}\, \psi_{class} = (\vec{\nabla}_q S)\, \psi_{class} = \frac{\hbar}{i} \left(\frac{i}{\hbar} \vec{\nabla}_q S \right) \psi_{class} = \left(\frac{\hbar}{i} \vec{\nabla}_q \right) \psi_{class}$$

the canonical momentum $\vec{p} = \frac{\partial L}{\partial \dot{q}} \to \hat{\vec{p}} = \frac{\hbar}{i} \vec{\nabla}_q$ in the "coordinate representation". In particular, the eigenstates of
very important!
momentums are $\psi_{\vec{p}}(\vec{r}) \propto e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$, and the wave fnc in momentum space is

$$\varphi(\vec{p}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r \, \psi(\vec{r}, t)\, e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \, , \quad \text{or in } d=1$$

$$\varphi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \, \psi(x, t)\, e^{-\frac{i}{\hbar} p x} \, ,$$

with $|\varphi(p,t)|^2$ the probability density for measurement of momentum.

One final comment about the Quantum to Classical correspondence: Because the commutator $[x, p] = xp - px = i\hbar$ and the Poisson bracket $\{x, p\} = 1$ we have

$$\{\ ,\ \}_{class.} \to \frac{1}{i\hbar} [\ ,\ ]_{quantum}$$