Chapter One: Physics 660
History and Introduction

* History:
  a. experimental background:
    - Light: wave or particle?
    - Wave: continuous object e.g. Newton
    - Particle: discrete

  Clouds for classical physics:
  1. Black-body radiation: Plank

\[ \varepsilon_\nu = \frac{8\pi\hbar \nu^3}{c^2} \frac{1}{e^{\hbar \nu/kT} - 1} \]

* Energy is counted discretely!! (hv)
* Different statistics (boson)

A perfect fit!!
II: Photoelectric effect (Einstein)

\[ E_V = E_e - E_c \]

Classical view: more light (increasing intensity of light), larger \( E_e \), therefore for any voltage, one expects electron at detector as soon as enough intensity of light.

Experimental facts: no electron escapes unless frequency of light:

\[ E_V = h \nu - E_c \]

III: Specific heat: Einstein, Debye: (low temperature)

Classical: specific heat is determined by degrees of freedom, \( C_V = \frac{3}{2} k \bar{T} \)

Experiment: \( C_V \propto T^3 \)
Einstein: discrete energy: \( h \nu \)
Suggestion:

1. At low temperature, the classical physics fails for light; Maxwell theory is not valid in many cases. Light is more like particle.

microscopic physics

a. Electron (charge \(-1\)), mass \(\neq 0\), a good particle:

\[ \lambda = \frac{\hbar}{p} \]

\[
\uparrow \rightarrow \downarrow \ 	ext{d} \lambda
\]

Electron beam

Interferences pattern observed

\[ \text{Electron is wave} \]

b. Stability of an atom

\[ e^- \] electromagnetic radiation

\[ N^+ \] unstable?
Bohr–Sommerfeld quantization.
\[ \oint p \, dc = 2\pi n \]

The stability of atom can also be explained by Heisenberg Uncertainty principles:
\[ \Delta x \cdot \Delta p \geq \hbar \]

Energy Conservation + Uncertainty Principle

\[ \rightarrow \text{atom is stable} \]

No quantum mechanics, No life!!

*Modern Quantum Mechanics:
Builder: Bohr → Heisenberg → Pauli → Schrödinger
\[ \rightarrow \text{Dirac} \rightarrow \text{Born} \ldots \]

A complete and consistent theory of microscopic world!!

Einstein - Bohr debate
a. New development of quantum mechanics  
   1. Quantum computing & information motivation: Control quantum effect  
      1) Quantum bit \( \Rightarrow \) qubit  
      2) Quantum Computer: big challenge

b. Nanotechnology: quantum effect becomes important!

c. Advanced materials:  
   macroscopic quantum effect:  
      1) magnetism  
      2) Superconductor  
      3) Phase transition  
      4) Quantum Hall effect

d. Low dimension and low temperature physics

e. Others: biology \( \Rightarrow \) quantum mechanics?
Classical vs. quantum:

* Planck constant $\hbar$ (a label for $\hbar$)
* Uncertainty Principle $\Delta x \Delta p \geq \frac{\hbar}{4}$
* Wave function $\Psi$
* Quantized energy
* Superposition $\Psi = d\Psi_1 + \beta\Psi_2$
* Probability $|\Psi|^2$
* Complex Algebra $\Psi$
* $[x, p] = i\hbar$
* Identical particles
* Spin

{ Fermion

vs. Boson

Fermi statistics, Boson statistics
Difference between Undergraduate Q.M. and Graduate Q.M.

1. Deeper Understanding
2. Advanced Math Tools
3. New Concepts & Application

Requirement: 1. Differential Equations
2. Linear Algebra
3. Basic Concepts of Quantum Mechanics
Chapter Two. Review of Classical Dynamics

a. In classical dynamics, there are two fundamental objects: Particle, \(\text{Wave} \rightarrow \text{field} \)

- Particle: Newton’s law: \(\vec{F} = ma = m \frac{d^2\vec{x}}{dt^2}\)
- Wave, field: Maxwell equation:
  \[
  \begin{align*}
  \nabla \cdot \vec{B} &= 0 \\
  \nabla \times \vec{B} &= \frac{\partial \vec{E}}{\partial t} \\
  \nabla \cdot \vec{E} &= \rho \\
  \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t}
  \end{align*}
  \]

b. Equivalent description: Unification of Maxwell and Newton

4. Principle of least action:

\[
S = \int_{t_i}^{t_f} L(x, \dot{x}) \, dt
\]

How to determine the path
\[\leftrightarrow \text{Least action}\]

\[L = T - V; \] (\(T\): kinetic energy, \(V\): potential energy)
Least action: The value of $S$ is a minimum if $F$ is a functional of path $X(t)$:

$$F[x(t)]$$

Let: $x_0(t)$ is a minimum.

$$F[x_0(t)]$$

Consider: $x(t) = x_0(t) + \eta(t)$

($\eta(t)$ is a perturbation)

$$F[x(t)] = F[x_0(t) + \eta(t)]$$

$$= F[x_0(t)] + \int_{t_i}^{t_f} \frac{\partial F}{\partial x(t')} |_{x(t') = x_0(t')} \eta(t') \, dt'$$

$$+ O(\eta^2)$$

Minimum: \[\frac{\partial F}{\partial x(t')} |_{x(t') = x_0(t')} = 0\]

Now for: $S[x(t), x'(t)]$, let: $x_0(t)$ is the minimum path: $x(t) = x_0(t) + \eta(t)$

$$S[x(t), x'(t)] = S_0 + 8S + O(\eta^2)$$

$$8S = 0 = \int_{t_i}^{t_f} \frac{\partial F}{\partial x(t')} |_{x(t') = x_0(t')} \eta(t') \, dt'$$
\[ + \int_{t_i}^{t_f} \frac{\dot{\eta}}{\dot{x}(G')} \bigg|_{x(G')} \eta(G') \, dt' \]

Assume \( t_f, t_i \) is fixed, i.e. \( \eta(t_f) = \eta(t_i) = 0 \)

\[
\int_{t_i}^{t_f} \frac{\dot{\eta}}{\dot{x}(G')} \bigg|_{x(G')} \eta(G') \, dt' \\
= \eta(G') \left. \frac{\partial x}{\partial x(G')} \right|_{x(G')} \bigg|_{t_i}^{t_f} - \int_{t_i}^{t_f} \frac{\partial \dot{x}}{\partial x(G')} \bigg|_{x(G')} \eta(G') \, dt'
\]

\( \leq 0 \)

\[ \Rightarrow \int_{t_i}^{t_f} \left( \frac{\partial x}{\partial x(G')} \bigg|_{x(G')} - \frac{d}{dt} \frac{\partial \dot{x}}{\partial x(G')} \bigg|_{x(G')} \right) \eta(G') \, dt' = 0 \]

\[ \Rightarrow \frac{\partial x}{\partial x} - \frac{d}{dt} \frac{\partial \dot{x}}{\partial x} = 0 \text{ for classical path} \]

For a single particle: \( L = \frac{1}{2}m \dot{x}^2 - V(x) \)

Check: \( m \frac{d^2}{dt^2} x = -\frac{dV}{dx} = F \) (Newton's law)

Canonical momentum conjugate to \( x \):

\( p = \frac{\partial H}{\partial \dot{x}} = m \dot{x}, \quad F = \frac{\partial H}{\partial x} \)
Extension to many dimensions:

\[ \{ x_1, \ldots, x_N \} : \quad p_i = \frac{\partial H}{\partial x_i} \]

\[ \frac{dx_i}{dt} = \frac{d}{dt} \frac{\partial H}{\partial x_i} \]

\*: Hamiltonian formulation

Legendre transformation

Lagrangian \( L \) is a function of \( x, \dot{x} \) \( \leftrightarrow p \)

Hamiltonian \( H \) is a function of \( x, p \)

\[ p_i = \frac{\partial H}{\partial x_i} \quad \leftrightarrow \quad \dot{x}_i = \frac{\partial H}{\partial p_i} \]

\[ H(x, p) = \dot{x} \cdot p - L(x, \dot{x}(p)) \]

Check:

\[ \frac{\partial H}{\partial p} = \dot{x} + p \cdot \frac{\partial \dot{x}(p)}{\partial p} - \frac{\partial H}{\partial x} \frac{\partial \dot{x}}{\partial p} = \dot{x} + p \cdot \frac{\partial \dot{x}(p)}{\partial p} - p \frac{\partial ^2 \dot{x}}{\partial p^2} = \dot{x} \]

Dynamics:

\[ \dot{x} = \frac{\partial H}{\partial p} \]

\[ \frac{\partial H}{\partial x} = -\frac{\partial H}{\partial \dot{x}} = p \]

Thus,

\[ \left( \begin{array}{c} \dot{x} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial x} \end{array} \right) \rightarrow \text{Hamiltonian} \]
for single particle:
\[ H = \frac{p^2}{2m} + V(x) \quad \text{(total energy)} \]

The dynamical equation is not symmetric to \( x, p \). In order to achieve a symmetric formulation, we introduce Poisson Bracket:

\[ \{ f, g \} = \frac{\partial f}{\partial x} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial x} \]

if there is many degrees:
\[ \{ f, g \} = \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x_i} \]

Now, if \( f \) is independent of \( p_i \):
\[ \{ f, g \} = \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial p_i} \]

\( f \) is independent of \( x_i \):
\[ \{ f, g \} = -\frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x_i} \]

\[ x_i = \frac{\partial H}{\partial p_i} = \{ x_i, H \} \]
\[ \{ p_i, H \} = -\frac{\partial H}{\partial x_i} = \{ p_i, H \} \]
for any function: \( W(x, p) \) no explicit dependent

\[
\frac{dw}{dt} = \frac{\partial w}{\partial x} \dot{x} + \frac{\partial w}{\partial p} \dot{p} = \frac{\partial w}{\partial x} \frac{dx}{dt} \frac{\dot{x}}{p} - \frac{\partial w}{\partial p} \frac{dx}{dt} \frac{\dot{p}}{\partial x} = \{w, H\}
\]

\( \star \): Jacobi-Hamiltonian equation:

\[
S = \int_{t_i}^{t_f} L(x, \dot{x}) \, dt
\]

Let's consider: \( S \) as function of \( t_f \) too.

\[
S[x(t_f), t] = \int_{t_i}^{t_f} L(x, \dot{x}) \, dt,
\]

\( x(t_f) = x_0(t_f) + x(t_f) \), \( x(t_i) = 0 \)

\[
\delta S = S[x(t_f) + \delta x(t_f), t] - S[x(t_f), t] = \delta S
\]

\[
\delta S = \int_{t_i}^{t_f} \left( \frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right) \, dt
\]

\[
+ \frac{\partial L}{\partial x} x \bigg|_{t_i}^{t_f} \delta x(t_f) = \frac{\partial L}{\partial \dot{x}} \delta \dot{x}(t_i) = \frac{\partial L}{\partial \dot{x}} \delta \dot{x}(t_i)
\]

\[
\Rightarrow: \frac{\partial L}{\partial \dot{x}} = \frac{\partial S}{\partial \dot{x}(t_f)} = p
\]
So: \( p = \frac{\partial S}{\partial x(t)} \) : momentum as a derivative of action

\[
\frac{dS}{dt} = \frac{\partial S}{\partial x(t)} \dot{x} + \frac{\partial S}{\partial t} = p \dot{x} + \frac{\partial S}{\partial t}
\]

\[
\frac{dS}{dt} = \frac{d}{dt} \int_{t_i}^{t_f} L \, dt = L
\]

\[
\frac{\partial S}{\partial t} = - (p \dot{x} - L) = -H(p, x, t)
\]

\[
= -H\left(\frac{\partial S}{\partial x}, x, t\right)
\]

\( \Rightarrow \) **Jacobi - Hamilton equation**

For single particle:

\[
\frac{\partial S}{\partial t} = -\frac{1}{2m} \left(\frac{\partial S}{\partial x}\right)^2 - V(x)
\]

Higher dimension:

\[
\frac{\partial S}{\partial t} = -\frac{1}{2m} \sum_i \left(\frac{\partial S}{\partial x_i}\right)^2 + V(x)
\]

Example: if \( H \) is time independent, particle with energy \( E \):

\[
\frac{\partial S}{\partial t} = -E, \quad S_0: S = S_0(x) - Et
\]

\[
\frac{1}{2m} \left(\nabla S_0\right)^2 = V(x) - E \quad \text{or} \quad (\nabla S_0)^2 = 2mCE - V(x))
\*: Note: every formulation in classical dynamics will be useful in quantum mechanics

\[ \mathcal{H} \rightarrow \text{Schrödinger equation} \]

\[ \mathcal{A}, \mathcal{S} \rightarrow \text{Path integral formulation} \]

\[ \text{Jacobi-Hamiltonian} \rightarrow \text{Quantum equivalence when } (\hbar = 0) \]

C: Canonical transformation

\*: Coordinate transformation,

\[ \{x_i, \ldots, x_N\} \rightarrow \{\bar{x}_i, \ldots, \bar{x}_N\} \]

\[ \bar{x}_i = x_i [x_1, \ldots, x_N] \]

\[ \frac{\partial}{\partial \bar{x}_i} = \frac{\partial}{\partial x_j} \frac{\partial x_j}{\partial \bar{x}_i} = \frac{\partial^2}{\partial x_j \partial \bar{x}_i} = \frac{\partial^2}{\partial x_j \partial x_i} \]

\[ L(x_i, \dot{x}_i) \rightarrow \bar{L}(\bar{x}_i, \dot{\bar{x}}_i) \]

One can define: \[ \bar{p}_i = \frac{\partial L}{\partial \dot{\bar{x}}_i} \]

all of our formulation will be held.

\*: Canonical transformation
mixing between $x$, $p$

$x \rightarrow \bar{x}$ \hspace{1cm} $\bar{x} \{x_1, \ldots, x_n, p_1, \ldots, p_m\}$

$p \rightarrow \bar{p}$ \hspace{1cm} $\bar{p} \{x_1, \ldots, x_n, p_1, \ldots, p_m\}$

Such transformation has to satisfy some condition in order to keep our formulism

$x_j = \{x_j, H\}$, $p_j = \{p_j, H\}$

$\bar{x}_j = \{\bar{x}_j, H\}$, $\bar{p}_j = \{\bar{p}_j, H\}$ \hspace{1cm} (1)

What's the condition for transformation if (1) is valid?

$\bar{x}_j = -\frac{\partial H}{\partial \bar{p}_j}$

$\dot{x}_j = \frac{\partial \bar{x}_j}{\partial x_i} \dot{x}_i + \sum_i \frac{\partial \bar{x}_j}{\partial p_i} \dot{p}_i$ \hspace{1cm} (2)

$\dot{x}_i = -\frac{\partial H}{\partial p_i} = \frac{1}{2} \frac{\partial \bar{x}_j}{\partial x_i} \dot{x}_j + \sum_j \frac{\partial \bar{x}_j}{\partial x_i} \dot{x}_j$ \hspace{1cm} (3)

$\dot{p}_i = \frac{\partial H}{\partial x_i} = -\frac{1}{2} \frac{\partial \bar{x}_j}{\partial p_j} \dot{x}_j + \sum_j \frac{\partial \bar{x}_j}{\partial x_i} \dot{x}_j$ \hspace{1cm} (4)
Plug 0 to 0:
\[ \dot{x}_j = \frac{\hbar}{i \hbar} \{ \overline{x}_j, x_\nu \} + \sum \frac{\hbar}{\hbar \overline{p}_i} \{ \overline{x}_j, \overline{p}_i \} \]

\{ \} is the standard poisson bracket.

Similarly:
\[ \dot{\overline{p}}_j = \frac{\hbar}{i \hbar} \{ \overline{p}_j, x_\nu \} + \sum \frac{\hbar}{\hbar \overline{p}_i} \{ \overline{p}_j, \overline{p}_i \} \]

So:
\[ \dot{x}_j = \frac{\hbar}{\hbar \overline{p}_j} \Rightarrow \{ x_j, x_\nu \} = 0 \]
\[ \dot{\overline{p}}_j = -\frac{\hbar}{\hbar \overline{x}_j} \Rightarrow \{ \overline{p}_j, \overline{p}_i \} = 0 \]

\[ \Rightarrow \{ \overline{x}_\nu, \overline{p}_j \} = \delta_{ij} \]
\[ \overline{x}_\nu, \overline{z}_j \text{ independent. (Canonical Condition)} \]
d: Symmetry and Conservation

* Consider: a transformation (canonical)
  \[ x \rightarrow O(x), \quad p \rightarrow O(p) \]
  if: \( H(x, p) = H(O(x), O(p)) \)

We say that the system is invariant under operation \( O \), or \( H \) has a symmetry

Example:

\[ H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) \]

\[
\begin{align*}
  O(x) &= x \cos \theta - y \sin \theta \\
  O(y) &= y \cos \theta + x \sin \theta
\end{align*}
\]

the same for \( p \)

\[ H(O(x), O(p)) = H(x, p) \]

\rightarrow Rotation symmetry in two dimension

* Generator of the transformation:
  Consider: \( \theta \rightarrow \text{infinitesimal small} \)
  \[
  \begin{align*}
    O(x) &= x - y \theta \\
    O(y) &= y + x \theta
  \end{align*}
  \]
or: \[
\begin{align*}
\delta x &= -y_0 \\
\delta y &= x_0
\end{align*}
\]
the same for \( \delta p \)

Let's assume: \[
\begin{align*}
\delta x &= 0 \frac{\partial g}{\partial px} \\
\delta y &= 0 \frac{\partial g}{\partial py} \\
\delta px &= -0 \frac{\partial g}{\partial x} \\
\delta py &= -0 \frac{\partial g}{\partial y}
\end{align*}
\]

In our case: the explicit form of \( g \)

is: \( g(x, p) = xp - yp x \)

g is called the generator of the symmetry

\[ H(x, p) = H(0(x), 0(p)) \]

\[ = H(x + \delta x, p + \delta p) \]

\[ = H(x, p) + \frac{\partial H}{\partial x} \delta x + \frac{\partial H}{\partial p} \delta p \]

\[ = H(x, p) + \frac{\partial H}{\partial x} \left( \frac{\partial g}{\partial x} \delta x + \frac{\partial g}{\partial p} \delta p \right) \]

\[ \Rightarrow \left[ \frac{\partial H}{\partial x} \frac{\partial g}{\partial x} - \frac{\partial H}{\partial p} \frac{\partial g}{\partial p} \right] = 0 \]

\[ \Rightarrow \{ g, H \} = 0 \]
$g$ is conserved: $\dot{g} = \{g, H\} = 0$

$g$ is time independent!

for any system, a symmetry means a conservation.

Note: * We will see many symmetries in quantum mechanics

* The rule holds for quantum mechanics too.

* Symmetry $\Rightarrow$ good quantum number

* Symmetry determines the form of Hamiltonian

* Symmetry $\Rightarrow$ selection rules