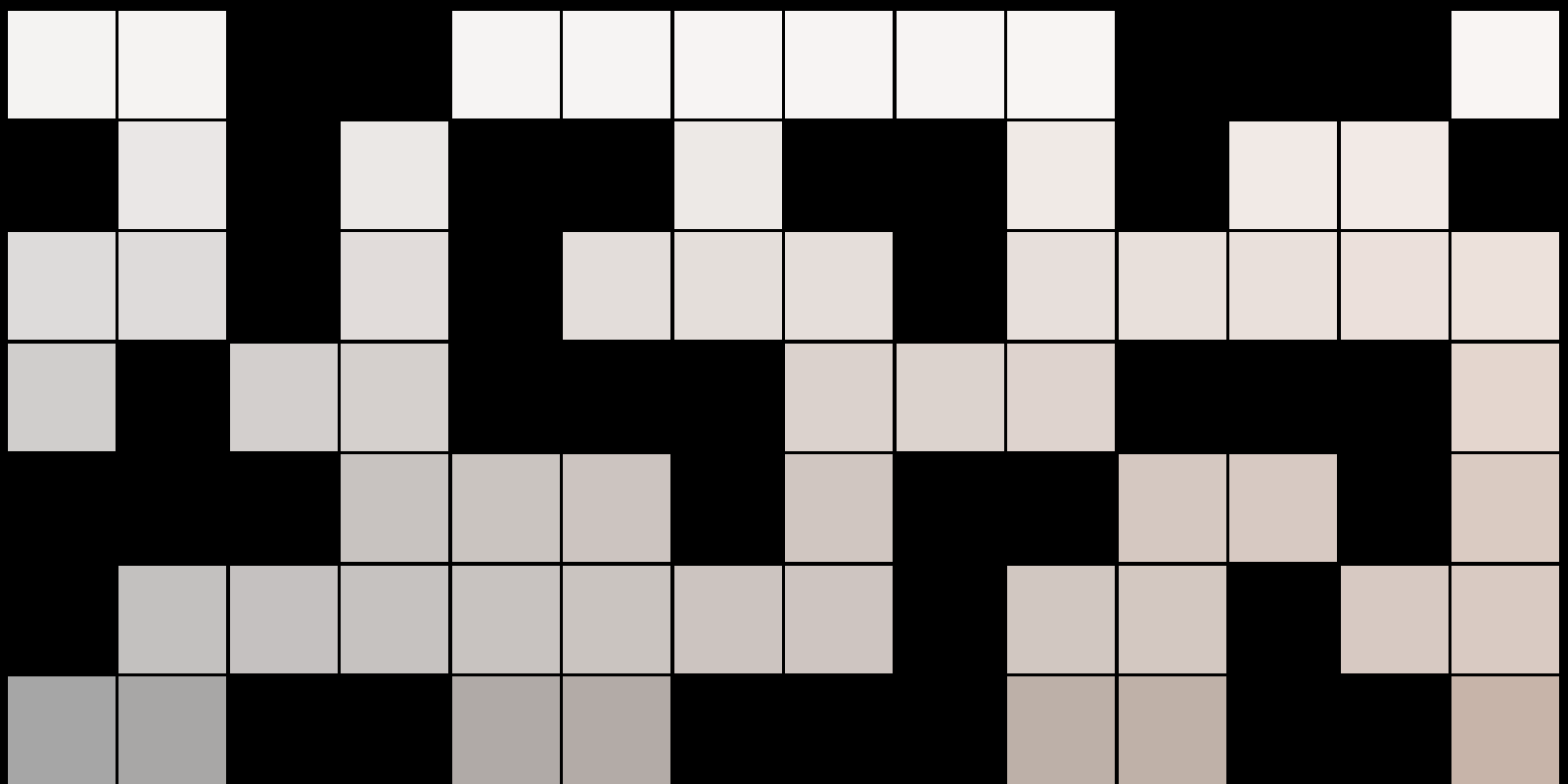


Particle Physics

Review for Particle Physics

Name:

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Mathematical Remarks

1.1 Functional Derivative

1.1.1 Definition

Consider a quantity I defined as follows:

$$I := \int_A^B dx F(x) \quad (1.1)$$

Notice that I is not really a function of x , but if you had to say, it is more a "function" of F - may be $F(x) = e^x$, or $F(x) = ax^2 + bx + c$, or, etc. So, to denote the dependence of I on the function F , we write

$$I[f] := \int_A^B dx F(x) \quad (1.2)$$

This is called a **(linear) functional**. Now, imagine that F is a function of f , for example, $F[f] = f(x)^2$. By chain rule, a small change in F , denoted as δF , can be expressed as:

$$\delta F[f] = F[f + \delta f] - F[f] \quad (1.3)$$

$$= \frac{\partial F}{\partial f} \delta f \quad (1.4)$$

so, similarly,

$$\delta I[F] = I[F + \delta F] - I[F] \quad (1.5)$$

$$= \int_A^B dx \delta F[f] \quad (1.6)$$

$$= \int_A^B dx \frac{\partial F}{\partial f} \delta f \quad (1.7)$$

Then, the **functional derivative** of I with respect to f , $\frac{\delta I}{\delta f}$, is defined as follows:

Definition 1.1: Functional Derivative

If a function $\phi(x)$ exists, such that

$$\delta I = \int_A^B dx \phi(x) \delta f(x), \quad (1.8)$$

we say that $\phi(x)$ is the **functional derivative** of I with respect to f , and denote it as

$$\frac{\delta I}{\delta f(x)} := \phi(x) \iff \delta I := \int_B^A dx \frac{\delta I}{\delta f(x)} \delta f(x). \quad (1.9)$$

Immediatly, by comparing Eq.(1.9) and Eq.(1.7), we see the following relation:

Theorem 1.1.1 Functional-density relation

For a quantity $I[F]$ and its density $F[f(x)]$, the functional derivative satisfies the following relation:

$$I = \int_A^B dx F[f(x)] \implies \frac{\delta I}{\delta f(x)} = \frac{\partial F[f(x)]}{\partial f(x)} \quad (1.10)$$

1.1.2 Two function case

Consider a case where I is the functional of F , which is also a functional of f and g :

$$I[F[f, g]] = \int_B^A dx F[f(x), g(x)] \quad (1.11)$$

Or more generally, if a function $D(x)$ satisfies the following Now, let us add some small change of f , δf :

$$I[F[f + \delta f, g]] = \int_B^A dx F[f(x) + \delta f(x), g(x)] \quad (1.12)$$

$$= \int_B^A dx F[f, g] + \frac{\partial F}{\partial f} \delta f \quad (1.13)$$

and similarly, by adding δg ,

$$I[F[f, g + \delta g]] = \int_B^A dx F[f(x), g(x) + \delta g(x)] \quad (1.14)$$

$$= \int_B^A dx F[f, g] + \frac{\partial F}{\partial g} \delta g \quad (1.15)$$

Combining these two, we have

$$I[F[f + \delta f, g + \delta g]] = \int_B^A dx F[f(x) + \delta f(x), g(x) + \delta g(x)] \quad (1.16)$$

$$= \int_B^A dx F[f, g] + \frac{\partial F}{\partial f} \delta f + \frac{\partial F}{\partial g} \delta g \quad (1.17)$$

$$\implies I[F[f + \delta f, g + \delta g]] - I[F[f, g]] = \int_B^A dx \frac{\partial F}{\partial f} \delta f + \frac{\partial F}{\partial g} \delta g \quad (1.18)$$

In this case, we just like our normal derivative, we should denote the LHS as:

$$\delta I := \int_B^A dx \frac{\partial F}{\partial f} \delta f + \frac{\partial F}{\partial g} \delta g \quad (1.19)$$

or alternatively,

$$\delta I := \int_B^A dx \frac{\delta I}{\delta f} \delta f + \frac{\delta I}{\delta g} \delta g \quad (1.20)$$

1.1.3 Euler-Lagrange Equation

For the two function case, especially consider that $g = \frac{df}{dx}$, and let us see what happens. Specifically, let us set that $\delta f(A) = \delta f(B) = 0$. Then, we have:

$$\frac{\delta I}{\delta g} \delta g = \frac{\delta I}{\delta \frac{df}{dx}} \delta \frac{df}{dx} \quad (1.21)$$

we can change the order of the derivative:

$$= \frac{\delta I}{\delta \frac{df}{dx}} \frac{d \delta f}{dx} \quad (1.22)$$

from the differentiation of a product, we have

$$= \frac{d}{dx} \left(\frac{\delta I}{\delta \left(\frac{df}{dx} \right)} \delta f \right) - \frac{d}{dx} \frac{\delta I}{\delta \left(\frac{df}{dx} \right)} \delta f \quad (1.23)$$

Now, substituting this to the two function case, we get:

$$\delta I = \int_B^A dx \left[\left(\frac{\delta I}{\delta f} - \frac{d}{dx} \frac{\delta I}{\delta \left(\frac{df}{dx} \right)} \right) \delta f + \frac{d}{dx} \left(\frac{\delta I}{\delta \left(\frac{df}{dx} \right)} \delta f \right) \right] \quad (1.24)$$

the total derivative term is zero, since $\delta f(A) = \delta f(B) = 0$. Thus, we have

$$\delta I = \int_B^A dx \left(\frac{\delta I}{\delta f} - \frac{d}{dx} \frac{\delta I}{\delta \left(\frac{df}{dx} \right)} \right) \delta f \quad (1.25)$$

and since $I = \int_B^A dx F[f(x), g(x)]$, we can say that

$$\frac{\partial F}{\partial f} = \frac{\delta I}{\delta f}, \quad \frac{\partial F}{\partial g} = \frac{\delta I}{\delta g} \quad (1.26)$$

Then

$$\delta I = \int_B^A dx \left(\frac{\partial F}{\partial f} - \frac{d}{dx} \frac{\partial F}{\partial \left(\frac{df}{dx}\right)} \right) \delta f \quad (1.27)$$

And if we somehow want to find a minimum of I , we can set $\delta I = 0$:

$$\implies \frac{\partial F}{\partial f} - \frac{d}{dx} \frac{\partial F}{\partial \left(\frac{df}{dx}\right)} = 0 \quad (1.28)$$

This is called the **Euler-Lagrange equation**.

Theorem 1.1.2 Euler-Lagrange Equation

For a functional $I\left[F\left(f, \frac{df}{dx}\right)\right]$ to be stationary, ($\delta I = 0$), the **Euler-Lagrange equation** must be satisfied:

$$\delta I\left[F\left(f, \frac{df}{dx}\right)\right] \iff \frac{\partial F}{\partial f} - \frac{d}{dx} \left(\frac{\partial F}{\partial \left(\frac{df}{dx}\right)} \right) = 0 \quad (1.29)$$

1.1.4 Important Property

In general, consider that the functional F is a function of $f_1(t), f_2(t), \dots, f_n(t)$:

$$F[f_1, f_2, \dots, f_n] \implies \delta F = \sum_{j=1}^n \frac{\delta F}{\delta f_j(t)} \delta f_j(t) \quad (1.30)$$

If $F = f_i$, we expect that

$$\frac{\delta f_i}{\delta f_i} = 1 \implies \delta f_i = \sum_{j=1}^n \frac{\delta f_i}{\delta f_j} \delta f_j \implies \frac{\delta f_i}{\delta f_j} = \delta_{ij} \quad (1.31)$$

Similarly, consider a continous case where F is a function of $f(x)$;

$$F[f(x, t)] \implies \delta F = \int_A^B dx' \frac{\delta F}{\delta f(x', t)} \delta f(x', t) \quad (1.32)$$

Note the distinction between the variable x and the integration variable x' . This is because x is an "index" of $f(t)$: $f_i \rightarrow f(x)$. Then, if we set $F = f(x)$, we expect that

$$\frac{\delta f(x, t)}{\delta f(x, t)} = 1 \implies \delta f(x, t) = \int_A^B dx' \frac{\delta f(x, t)}{\delta f(x', t)} \delta f(x', t) \quad (1.33)$$

Comparing with this with the definition of **Dirac delta function**:

Definition 1.2: Dirac Delta Function

The **Dirac delta function** $\delta(x)$ is defined as a function that satisfies the following property:

$$\int dx' \delta(x' - x) \varphi(x') = \varphi(x), \quad \forall \varphi(x') \in C^\infty \quad (1.34)$$

we have

Theorem 1.1.3 Property of Functional Derivative

For a functional $f_i(t)$ or $f(x, t)$, the functional derivative satisfies the following property:

$$\frac{\delta f_i(t)}{\delta f_j(t)} = \delta_{ij}, \quad \text{or} \quad \frac{\delta f(x, t)}{\delta f(x', t)} = \delta(x - x') \quad (1.35)$$

1.1.5 In a n-dimensional space

In the previous discussions, we have considered the functional I as an integral on 1D space represented by x . Here, we aim to generalize the discussion to n -dimensional space, e.g. \mathbb{R}^n . For \mathbb{R}^n , let us define a functional I and functional derivative as follows:

Definition 1.3: Functional on \mathbb{R}^n

A quantity $I \in \mathbb{R}$ defined on $V \subset \mathbb{R}^n$ is called a **(linear) functional** if it can be expressed as follows:

$$I[f_i] := \int_{x \in V} d^n x F(f_i(x)) = \int_V d^n x F(f_i(x)), \quad i \in \mathbb{N} \quad (1.36)$$

Definition 1.4: Functional Derivative on \mathbb{R}^n

The **functional derivative** of a functional $I[f_i]$ with respect to $f_i(x)$ is defined as follows:

$$\frac{\delta I[f_j]}{\delta f_i(x)} := \phi_i(x) \stackrel{\text{def}}{\iff} \delta I = \int_V d^n x' \frac{\delta I[f_j]}{\delta f_i(x')} \delta f_i(x') \quad (1.37)$$

where $\phi_i(x)$ is a function of x .

Then, the variation of the functional δI can be expressed as:

$$\delta I = \delta \int_V d^n x' F(f_j(x')) = \int_V d^n x' \delta F(f_j(x')) = \int_V d^n x' \sum_j \frac{\partial F}{\partial f_j(x')} \delta f_j(x') \quad (1.38)$$

Now,

$$\delta f_j(x') = \int_V d^n x \delta^n(x - x') \delta f_j(x) \quad (1.39)$$

$$= \int_V d^n x \sum_i \delta_{ij} \delta^n(x - x') \delta f_i(x) \quad (1.40)$$

$$\implies \frac{\delta f_j(x')}{\delta f_i(x)} = \delta_{ij} \delta^n(x - x') \quad (1.41)$$

so,

$$\frac{\delta I}{\delta f_i(x)} = \int_V d^n x' \frac{\partial F}{\partial f_i(x')} \delta(x - x') = \frac{\partial F}{\partial f_i(x)} \quad (1.42)$$

thus we see that the functional-density relation still holds:

Theorem 1.1.4 Functional-density relation

For a quantity $I[F]$ and its density $F[f_i(x)]$, the functional derivative satisfies the following relation:

$$I = \int_V d^n x F[f_j(x)] \implies \frac{\delta I[f_j]}{\delta f_i(x)} = \frac{\partial F[f_j]}{\partial f_i(x)} \quad (1.43)$$

[1]

1.2 Derivative by Derivative

1.2.1 An Interesting Problem

Question 1: Derivative by derivative

What would the following operator mean?

$$\frac{d}{d \frac{d}{dx}} \quad (1.44)$$

Let us define a differential operator D :

Definition 1.5: Mysterious Operator

The operator D is defined as the derivative of the derivative with respect to x :

$$D := \frac{d}{dx} \quad (1.45)$$

Now let us actually apply D to some functions:

Example 1.2.1 (A power function)

Let us apply $\frac{d}{dx}$ to a power function $f(x) = x^n$, $n \in \mathbb{Z}^+$:

$$Df(x) = \frac{d}{dx}x^n = nx^{n-1} = \frac{n}{x}x^n \implies D = \frac{n}{x} \quad (1.46)$$

Then,

$$\frac{d}{dD}f(x) = \frac{d}{dD}\left(\frac{n}{D}\right)^n = n^n \cdot (-n) \cdot D^{-n-1} = -\left(\frac{n}{D}\right)^{n+1} = -x^{n+1} \quad (1.47)$$

Example 1.2.2 (Exponential Function)

Let us apply $\frac{d}{dx}$ to the exponential function $f(x) = e^{\alpha x}$:

$$\frac{df}{dx} = \frac{d}{dx}e^{\alpha x} = \alpha f(x) \implies \frac{d}{dx} = \alpha \quad (1.48)$$

$$\implies Df(x) = \frac{de^{\alpha x}}{d\alpha} = xe^{\alpha x} \quad (1.49)$$

An important property of this operator is in the commutator with the x operator:

Definition 1.6: x operator

The x operator is defined as the operator that maps a function f to the function $x \cdot f$:

$$x : f \mapsto x \cdot f \quad (1.50)$$

Definition 1.7: Commutator

For two operators $A : f \mapsto Af$ and $B : f \mapsto Bf$, the commutator is defined as:

$$[A, B] := AB - BA \quad (1.51)$$

Then the commutator of the x operator and the D operator is given by:

$$[x, D] = xD - Dx \quad (1.52)$$

applying this to a function $f(x)$, we have:

$$[x, D]f(x) = xDf(x) - D(xf(x)) \quad (1.53)$$

$$= xDf(x) - Dx f(x) - xDf(x) \quad (1.54)$$

$$= -Df(x) = -1 \cdot f(x) \quad (1.55)$$

$$\implies [x, D] = -1 \quad (1.56)$$

and notice since both x and D are just linear operators, if we define $x = \frac{d}{dD}$, then we have:

$$[x, D] f(D) = \frac{d}{dD} D f(D) - D \frac{d}{dD} f(D) \quad (1.57)$$

$$= f(D) + D \frac{df}{dD} - D \frac{df}{dD} \quad (1.58)$$

$$= f(D) \quad (1.59)$$

so in general,

$$\left[\omega, \frac{d}{d\omega} \right] = -1 \quad (1.60)$$

Note the bi-linearity of the commutator:

Theorem 1.2.1 Bi-linearity of Commutator

For $\alpha, \beta \in \mathbb{C}$ and operators A, B , the commutator satisfies:

$$[\alpha A, \beta B] = \alpha \beta [A, B] \quad (1.61)$$

This immediately leads to:

Principle 1.1: Canonical Commutation Relation

For the x operator and the D operator, the commutation relation is given by:

$$[x, -i\hbar D] = i\hbar = \left[x, -i\hbar \frac{\partial}{\partial x} \right] = \left[i\hbar \frac{\partial}{\partial p}, p \right] \quad (1.62)$$

Let us remark on other properties:

Theorem 1.2.2 Commutator of General Function

For a general function $f(x)$, the commutator with the D operator is given by:

$$[D, f(x)] = \frac{df(x)}{dx} \quad (1.63)$$

Proof: Consider functions $f(x)$ and $g(x)$, then:

$$[D, f(x)] g(x) = D f(x) g(x) - f(x) D g(x) \quad (1.64)$$

$$= \frac{df(x)}{dx} g(x) + f(x) \frac{dg(x)}{dx} - f(x) \frac{dg(x)}{dx} \quad (1.65)$$

$$= \frac{df(x)}{dx} g(x) \quad (1.66)$$

$$\implies [D, f(x)] = \frac{df(x)}{dx} \quad (1.67)$$

□

Theorem 1.2.3 Commutator of General Operator

For a general operator F that is a function of D , the commutator with the x operator is given by:

$$[F(D), x] = \frac{dF(D)}{dD} \quad (1.68)$$

Proof: Assume that F is a function of D , and we can write it as a Taylor series:

$$F(D) = \sum_{n=0}^{\infty} a_n D^n \quad (1.69)$$

Then,

$$[F, x] = Fx - xF \quad (1.70)$$

$$= \sum_{n=0}^{\infty} a_n D^n x - x \sum_{n=0}^{\infty} a_n D^n \quad (1.71)$$

$$= \sum_{n=0}^{\infty} a_n (D^n x - x D^n) \quad (1.72)$$

$$= \sum_{n=0}^{\infty} a_n n D^{n-1} = \frac{dF}{dD} \quad (1.73)$$

□

Finally, let us comment on the relationship with the **shift operator**:

Definition 1.8: Shift Operator

The **shift operator** S_a is defined as the operator that shifts a function by a constant a :

$$S_a[f](x) := f(x + a) \quad (1.74)$$

The commutator of the shift operator and the x operator is given by:

$$[S_a, x] f(x) = S_a[xf(x)] - xS_a[f(x)] \quad (1.75)$$

$$= (x + a)f(x + a) - xf(x + a) \quad (1.76)$$

$$= af(x + a) = aS_a[f(x)] \quad (1.77)$$

Thus,

Theorem 1.2.4 Commutator of Shift Operator and x

The commutator of the shift operator S_a and the x operator is given by:

$$[S_a, x] = aS_a \implies S_a = e^{aD} \quad (1.78)$$

Analytical Mechanics

2.1 Lagrange Formalism

2.1.1 Quick Recap: Newtonian Mechanics

In Newtonian mechanics, the motion of a particle is described through a few important quantities: for a particle of (inertial) mass m , position \vec{r} , we have

$$\text{velocity : } \vec{v} = \frac{d\vec{r}}{dt} \quad (2.1)$$

$$\text{acceleration : } \vec{a} = \frac{d\vec{v}}{dt} = \frac{d^2\vec{r}}{dt^2} \quad (2.2)$$

$$\text{momentum : } \vec{p} = m\vec{v} = m \frac{d\vec{r}}{dt} \quad (2.3)$$

and the relations between these quantities, in the presence of external forces $\vec{F}_{\text{ext}}^{(i)}$ acting on the particle, are given by *Newton's second law*:

$$\frac{d\vec{p}}{dt} = m \frac{d^2\vec{r}}{dt^2} = \sum_i \vec{F}_{\text{ext}}^{(i)} \quad (2.4)$$

The work done by such forces is given by

$$W_{\text{total}} = \sum_i \int_l d\vec{x} \cdot \vec{F}_{\text{ext}}^{(i)}, \quad \text{where } l \text{ is the path of the particle.} \quad (2.5)$$

This is the energy change of the particle through the motion:

$$W_{\text{total}} = \sum_i \int_l d\vec{x} \cdot \vec{F}_{\text{ext}}^{(i)} \quad (2.6)$$

$$= \int_{t_i}^{t_f} dt \vec{v} \cdot m \frac{d\vec{v}}{dt} \quad (2.7)$$

$$= \int_{t_i}^{t_f} dt \frac{m}{2} \frac{d}{dt} \vec{v}^2 \quad (2.8)$$

$$= \frac{m}{2} \vec{v}_f^2 - \frac{m}{2} \vec{v}_i^2 \quad (2.9)$$

meaning that $m\vec{v}^2/2$ is the energy due to the motion of the particle: the **kinetic energy** T :

$$T = \frac{m}{2}\vec{v}^2 \quad (2.10)$$

Now, often, the external force acting on the particle is due to a potential V :

$$\vec{F}_{\text{ext}} = -\nabla V \quad (2.11)$$

For example, for a 1D spring, the potential is given by

Example 2.1.1 (1D spring/ Harmonic potential)

$$V = \frac{1}{2}kx^2 \implies F_{\text{ext}} = -kx \quad (2.12)$$

or the electrostatic potential:

Example 2.1.2 (Electrostatic potential)

$$V = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r} \implies F_{\text{ext}} = -\nabla V = -\frac{q_1 q_2}{4\pi\epsilon_0 r^2} \hat{r} \quad (2.13)$$

Now, for a particle whose the external forces are given by a potential:

$$m \frac{d^2 \vec{r}}{dt^2} = -\nabla V \iff -m \frac{d^2 \vec{r}}{dt^2} - \nabla V = 0 \quad (2.14)$$

This looks as if the forces $-\nabla V$ and $m\ddot{\vec{r}}$ are in equilibrium. So, if we move a particle by an infinitesimal distance $\delta\vec{r}$, the total work done by these forces must be zero:

$$\left(-m \frac{d^2 \vec{r}}{dt^2} - \nabla V \right) \cdot \delta\vec{r} = 0 \quad (2.15)$$

at any time t . We want to apply this for entire path of the motion of the particle, from t_i to t_f . Then, the integral of this equation over the time interval $[t_i, t_f]$ gives

$$\delta I = \int_{t_i}^{t_f} dt \left(-m \frac{d^2 \vec{r}}{dt^2} - \nabla V \right) \cdot \delta\vec{r} = 0 \quad (2.16)$$

now, we can apply integration by parts:

$$\frac{d}{dt} [\dot{\vec{r}} \cdot \delta\vec{r}] = \ddot{\vec{r}} \cdot \delta\vec{r} + \dot{\vec{r}} \cdot \frac{d\delta\vec{r}}{dt} \quad (2.17)$$

$$= \ddot{\vec{r}} \cdot \delta\vec{r} + \dot{\vec{r}} \cdot \delta\dot{\vec{r}} \quad (2.18)$$

$$\iff -m\ddot{\vec{r}} = -\frac{d}{dt} (\dot{\vec{r}} \cdot \delta\vec{r}) + \dot{\vec{r}} \cdot \delta\dot{\vec{r}} \quad (2.19)$$

$$= -\frac{d}{dt} (m\dot{\vec{r}} \cdot \delta\vec{r}) + \delta \left(\frac{m}{2} \left(\frac{d\vec{r}}{dt} \right)^2 \right), \quad (2.20)$$

where we used the commutativity of $\frac{d(\cdot)}{dt}$ and $\delta(\cdot)$. Then the integral becomes

$$\delta I = \int_{t_i}^{t_f} dt \left(\delta \left[\frac{m}{2} \left(\frac{d\vec{r}}{dt} \right)^2 \right] - \delta V \right) \quad (2.21)$$

$$= \int_{t_i}^{t_f} dt (\delta T - \delta V) = 0 \quad (2.22)$$

$$\iff \delta I = \delta \int_{t_i}^{t_f} dt (T - V) = 0 \quad (2.23)$$

[2]

2.1.2 Lagrangian and Variational Principle

In Lagrangian mechanics, we will use a different approach to describe the motion of a particle than the Newtonian mechanics. Instead of using the usual Euclidean space, we will use a *configuration space* \mathcal{C} , which is the space of all possible positions of the particle. This space is spanned by the so-called **generalized coordinates** q_i , and their time derivatives (or generalized velocity) $\dot{q}_i := \frac{dq_i}{dt}$. Now, let us define quantities called the **Lagrangian** L and **action** S :

Definition 2.1: Lagrangian L and Action S

The Lagrangian L is defined as the difference between the kinetic energy T and potential energy V of a particle:

$$L := T - V, \quad S[L] := \int_{t_i}^{t_f} dt L \quad (2.24)$$

Now, **variation** of the action δS is given by

$$\delta S = \delta \int_{t_i}^{t_f} dt (T - V) \quad (2.25)$$

which is an identical expression to (2.23). So, we postulate that the motion of the particle is such that the action is stationary:

Principle 2.1: Variational Principle

The motion of a particle is such that the action S is stationary, i.e., $\delta S = 0$.

$$\delta S = \delta \int_{t_i}^{t_f} dt L(q_i(t), \dot{q}_i(t), t) = 0 \quad (2.26)$$

As to show why this maybe useful, let us compare between Eq. (2.16):

$$\delta I = \delta S[L] = \int_{t_i}^{t_f} dt \left(-m \frac{d^2 \vec{r}}{dt^2} - \nabla V \right) \cdot \delta \vec{r} = 0 \quad (2.27)$$

and Eq. (1.27):

$$\delta I = \delta S[f] = \int_B dx \left(\frac{\partial F}{\partial f} - \frac{d}{dx} \frac{\partial F}{\partial \frac{df}{dx}} \right) \delta f = 0 \quad (2.28)$$

which immediately gives that the EoM is the Euler-Lagrange equation, if we set $F = L(q_i, \dot{q}_i, t)$:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = 0 \iff m \frac{d^2 \vec{r}}{dt^2} = -\nabla V \quad (2.29)$$

The generalization to multiple particles is straightforward:

$$L = \sum_n \frac{m_n}{2} \dot{\vec{r}}_n^2 - V(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \quad (2.30)$$

The Euler-Lagrange equation is given by

$$\frac{\partial L}{\partial \vec{r}_i^{(N)}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\vec{r}}_i^{(N)}} \right) = 0 \quad (2.31)$$

2.1.3 Harmonic Oscillator

Let us consider a particle of mass m in a 1D harmonic potential:

$$V = \frac{1}{2} k x^2 \implies F_{\text{ext}} = -\nabla V = -kx \quad (2.32)$$

then the Lagrangian is given by

$$L = T - V = \frac{m}{2} \dot{x}^2 - \frac{1}{2} k x^2 \quad (2.33)$$

The Euler-Lagrange equation yields

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) = 0 \implies \frac{\partial L}{\partial x} = -kx, \quad \frac{\partial L}{\partial \dot{x}} = m\dot{x} \quad (2.34)$$

$$\implies -kx - \frac{d}{dt}(m\dot{x}) = 0 \quad (2.35)$$

$$\implies m \frac{d^2 x}{dt^2} = -kx \quad (2.36)$$

which is the equation of motion of a harmonic oscillator in Newtonian mechanics. Here, notice that

$$\frac{\partial L}{\partial x} = -kx = -\nabla V = F_{\text{ext}} \quad (2.37)$$

and

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x} = p \quad (2.38)$$

these derivatives of the Lagrangian are the **generalized force** and **conjugate momentum**, respectively.

$$\frac{\partial L}{\partial q} = F_g, \quad \frac{\partial L}{\partial \dot{q}} = p_g \quad (2.39)$$

2.2 Hamiltonian Formalism

2.2.1 Legendre Transform

Consider a function $f(x, y)$. The total differential of f is given by

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy \quad (2.40)$$

Often we want to find another function g such that

$$g = p \cdot y - f(x, y) \quad (2.41)$$

and the total differential of g is given by

$$dg = \frac{\partial g}{\partial p} dp + \frac{\partial g}{\partial y} dy - df \quad (2.42)$$

$$= y dp + p dy - \frac{\partial f}{\partial x} dx - \frac{\partial f}{\partial y} dy \quad (2.43)$$

$$= y dp - \frac{\partial f}{\partial x} dx + \left(p - \frac{\partial f}{\partial y} \right) dy \quad (2.44)$$

for this function g to be a function of x and p , we need to have

$$p = \frac{\partial f}{\partial y}, \quad \frac{\partial g}{\partial x} = -\frac{\partial f}{\partial x}. \quad (2.45)$$

This is called the **Legendre transform** of f .

Definition 2.2: Legendre transform (Analytical Mechanics)

The Legendre transform of a function $f(x, y)$ is defined as

$$g(p, x) = p \cdot y - f(x, y) \quad (2.46)$$

where

$$p = \frac{\partial f}{\partial y}, \quad \frac{\partial g}{\partial x} = -\frac{\partial f}{\partial x} \quad (2.47)$$

[3]

2.2.2 Hamiltonian and Canonical Equations

Now, we define Hamiltonian $H = H(q, p)$ as the Legendre transform of Lagrangian $L = L(q, \dot{q})$:

Definition 2.3: Hamiltonian H

The Hamiltonian $H(q, p)$ is defined as the Legendre transform of the Lagrangian $L(q, \dot{q})$ ($\dot{q} \rightarrow p$):

$$H(q, p) = p \cdot \dot{q} - L(q, \dot{q}) \quad (2.48)$$

where

$$p = \frac{\partial L}{\partial \dot{q}}, \quad \frac{\partial H}{\partial q} = -\frac{\partial L}{\partial q} \quad (2.49)$$

Note:

In Lagrange formalism, generalized coordinate span the configuration space, while in Hamilton formalism, generalized coordinates and **generalized momenta** or **conjugate momenta** span the **phase space**.

This is actually a physically intuitive quantity. Since p is defined as the derivative of Lagrangian L :

$$p = \frac{\partial L}{\partial \dot{q}} \quad (2.50)$$

$$= \frac{\partial}{\partial \dot{q}} \left(\frac{1}{2} m \dot{q}^2 - V(q) \right) = m \dot{q} \quad (2.51)$$

and we can rewrite the Hamiltonian as

$$H(q, p) = p \cdot \dot{q} - L(q, \dot{q}) \quad (2.52)$$

$$= m \cdot \dot{q}^2 - \left(\frac{1}{2} m \dot{q}^2 - V(q) \right) \quad (2.53)$$

$$= \frac{1}{2} m \dot{q}^2 + V(q) = T + V \quad (2.54)$$

This is the total energy of the system, for the case of non-velocity dependent potential $V(q)$.

This relation is useful because we can obtain Lagrangian L from the Hamiltonian H as well:

$$L(q, \dot{q}) = \dot{q} \cdot p - H(q, p) \implies \dot{q} = \frac{\partial H}{\partial p} \quad (2.55)$$

and the Euler-Lagrange equation can be rewritten in terms of Hamiltonian:

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = 0 \quad (2.56)$$

$$\implies -\frac{\partial H}{\partial q} - \frac{d}{dt}(p) = 0 \iff \dot{p} = -\frac{\partial H}{\partial q} \quad (2.57)$$

These two equations are called the **canonical equations** or **Hamilton's equations**:

Theorem 2.2.1 Canonical Equations

The relationship between a mechanical variable q and its canonical conjugate variable p is given by the canonical equations:

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q} \quad (2.58)$$

For multiple degrees of freedom, we can write the Hamiltonian as

$$H(\{q_i\}, \{p_i\}, t) = \sum_i p_i \dot{q}_i - L(\{q_i\}, \{\dot{q}_i\}, t) \quad (2.59)$$

and the canonical equations as

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad (2.60)$$

where

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \quad \frac{\partial H}{\partial q_i} = -\frac{\partial L}{\partial q_i} \quad (2.61)$$

2.2.3 Poisson Bracket

Now, consider how a physical quantity $X(q_i, p_i, t)$ changes with time:

$$\frac{dX(q_i, p_i, t)}{dt} = \frac{\partial X}{\partial t} + \frac{\partial X}{\partial q_i} \dot{q}_i + \frac{\partial X}{\partial p_i} \dot{p}_i \quad (2.62)$$

from the canonical equations, the second part becomes:

$$\frac{\partial X}{\partial q_i} \dot{q}_i + \frac{\partial X}{\partial p_i} \dot{p}_i = \frac{\partial X}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial X}{\partial p_i} \frac{\partial H}{\partial q_i} \quad (2.63)$$

Since this term only depend on X and H , given q_i and p_i , we can define a new quantity called the **Poisson bracket**:

Definition 2.4: Poisson Bracket

The Poisson bracket of two physical quantities A and B is defined as

$$\{A, B\} := \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right) \quad (2.64)$$

If a physical quantity X does not explicitly depend on time, we can rewrite the time derivative as:

$$\frac{dX(q_i, p_i)}{dt} = \{X, H\} \quad (2.65)$$

Now, what happens if X happens to be q_i or p_i ? A physical quantity q_i or p_i can be written as a function of q_i and p_i - simply as itself (noting that no explicit time dependence is present):

$$q_i(q_i, p_i) = q_i, \quad p_i(q_i, p_i) = p_i \quad (2.66)$$

Then, the Poisson bracket of q_i and H is given by

$$\{q_i, H\} = \sum_j \left(\frac{\partial q_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial q_i}{\partial p_j} \frac{\partial H}{\partial q_j} \right) \quad (2.67)$$

$$= \sum_j \left(\delta_{ij} \frac{\partial H}{\partial p_j} - 0 \right) = \frac{\partial H}{\partial p_i} \quad (2.68)$$

where Eq. (1.31) is used. Similarly, the Poisson bracket of p_i and H is given by

$$\{p_i, H\} = \sum_j \left(\frac{\partial p_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial p_i}{\partial p_j} \frac{\partial H}{\partial q_j} \right) \quad (2.69)$$

$$= \sum_j \left(0 - \delta_{ij} \frac{\partial H}{\partial q_j} \right) = - \frac{\partial H}{\partial q_i} \quad (2.70)$$

Thus, we can rewrite the canonical equations in terms of Poisson bracket:

Theorem 2.2.2 Canonical Equations with Poisson Bracket

The canonical equations can be rewritten in terms of Poisson bracket as follows:

$$\dot{q}_i = \{q_i, H\}, \quad \dot{p}_i = \{p_i, H\} \quad (2.71)$$

Finally, note that the Poisson bracket of q_i and p_j gives:

$$\{q_i, p_j\} = \sum_k \frac{\partial q_i}{\partial q_k} \frac{\partial p_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k} \frac{\partial p_j}{\partial q_k} \quad (2.72)$$

$$= \sum_k \delta_{ik} \delta_{jk} - 0 = \delta_{ij} \quad (2.73)$$

Theorem 2.2.3 Canonical Conjugate Relation in Analytical Mechanics

The Poisson bracket of the generalized coordinate q_i and its conjugate momentum p_j is given by

$$\{q_i, p_j\} = \delta_{ij} \quad (2.74)$$

2.3 Symmetry of a System

2.4 Summary

Lagrangian and action integral are defined as follows:

$$L := \sum T - V, \quad S[L] := \int_{t_i}^{t_f} dt L(q_i, \dot{q}_i, t) \quad (2.75)$$

we define the Hamiltonian as the Legendre transform of the Lagrangian:

$$H(q_i, p_i, t) := \sum_i p_i \cdot \dot{q}_i - L(q_i, \dot{q}_i, t) \quad (2.76)$$

The action integral is stationary under the variation of the path:

$$\delta S = \delta \int_{t_i}^{t_f} dt L(q_i, \dot{q}_i, t) = \delta \int_{t_i}^{t_f} dt \sum_i p_i \cdot \dot{q}_i - H(q_i, \dot{q}_i, t) = 0 \quad (2.77)$$

In the **Variational Principle**, we postulate that the motion of a particle is such that the action is stationary, yielding the Euler-Lagrange equation or Hamilton's equations:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = 0 \quad (2.78)$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad (2.79)$$

Physics of Fields

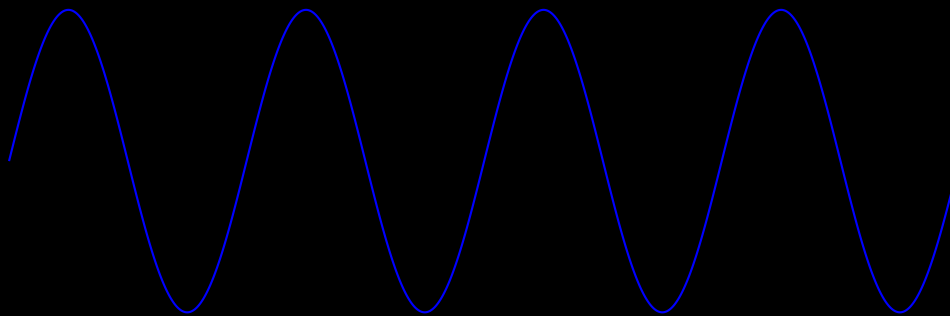
3.1 Introduction: 1D String

3.1.1 Newtonian Derivation

Now let us consider the motion of 1D wave on a very long string.

- Tension: T
- Line density (mass per unit length): μ

Notice, that any point on the string is not moving in x direction, otherwise the string itself will be moving. Also, if we produce a "uniform" wave, then at all points on the string, the wave will have the same amplitude A , wavelength λ , and frequency f and velocity v . This means



that we can choose convenient point on the string, and calculate A , λ , f , and v , then the same values will be valid for all points on the string. For a moving wave, a stationary point of view is not very useful, so we will use a moving point of view: the Lagrange description in fluid mechanics.

Consider moving in the x direction, at the same constant velocity v , as the wave. Then, our new x coordinate is given by the Galilean transformation:

Definition 3.1: Galilean Transformation

The **Galilean transformation** is a transformation of coordinates from a stationary observer to a moving observer with constant velocity v .

$$\xi = x - vt \quad (3.1)$$

where ξ is the new coordinate, x is the old coordinate, v is the velocity of the observer, and t is time.

In this new perspective, we do not have to worry about the motion of the wave, since we are moving with the wave. In short, the wave is stationary in the new coordinate system. This means that vertical displacement of the wave at a point ξ only depends on the ξ coordinate, and not on time:

$$\psi(x, t) = \psi(\xi) \quad (3.2)$$

and any point on the string seems to move at velocity $-v$.

Then immediately,

$$\frac{\partial \psi(\xi)}{\partial x} = \frac{\partial \psi(\xi)}{\partial \xi} \frac{\partial \xi}{\partial x} = \frac{\partial \psi(\xi)}{\partial \xi}, \quad (3.3)$$

$$\frac{\partial \psi(\xi)}{\partial t} = \frac{\partial \psi(\xi)}{\partial \xi} \frac{\partial \xi}{\partial t} = -v \frac{\partial \psi(\xi)}{\partial \xi} \quad (3.4)$$

$$\Rightarrow \frac{\partial^2 \psi(\xi)}{\partial x^2} = \frac{\partial^2 \psi(\xi)}{\partial \xi^2}, \quad \frac{\partial^2 \psi(\xi)}{\partial t^2} = v^2 \frac{\partial^2 \psi(\xi)}{\partial \xi^2} \quad (3.5)$$

$$\Rightarrow \frac{\partial^2 \psi(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi(x, t)}{\partial t^2} \quad (3.6)$$

we obtain the wave equation, but we should find its physical meaning.

Theorem 3.1.1 Wave Equation in 1D

The wave equation in 1D is given by:

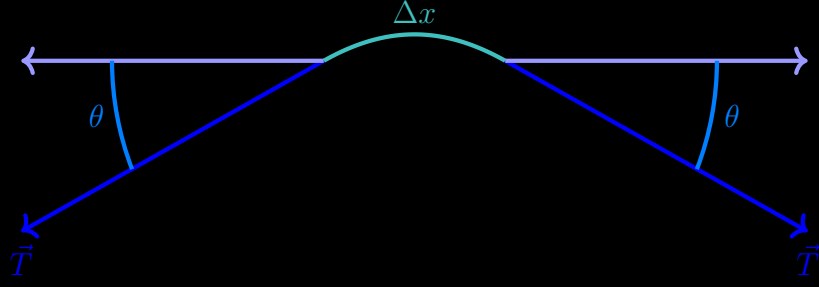
$$\frac{\partial^2 \psi(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi(x, t)}{\partial t^2} \quad (3.7)$$

where $\psi(x, t)$ is the vertical displacement of the wave at point x and time t , and v is the velocity of the wave.

Now, let us focus on one of the peaks of the wave, at the point ξ_0 . The tension on the string at ξ_0 cancels out horizontally, but adds vertically:

$$F_x = T \cos \theta - T \cos \theta = 0 \quad (3.8)$$

$$F_y = F_{-y} + F_{+y} = -T \partial_x \psi \left(\xi_0 + \frac{\Delta x}{2} \right) + T \partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) \quad (3.9)$$



Thus the equation of motion for the infinitesimal segment of the string at ξ_0 is given by:

$$\vec{F} = m\ddot{\vec{r}} \iff T\left(\partial_x\psi\left(\xi_0 + \frac{\Delta x}{2}\right) - \partial_x\psi\left(\xi_0 - \frac{\Delta x}{2}\right)\right) = \mu\Delta x \partial_t^2\psi(\xi_0) \quad (3.10)$$

by rearranging,

$$\frac{1}{\Delta x}\left(\partial_x\psi\left(\xi_0 + \frac{\Delta x}{2}\right) - \partial_x\psi\left(\xi_0 - \frac{\Delta x}{2}\right)\right) = \frac{\mu}{T} \partial_t^2\psi(\xi_0) \quad (3.11)$$

as $\Delta x \rightarrow 0$, LHS becomes the derivative of the first derivative:

$$\partial_x^2\psi(\xi_0) = \frac{\mu}{T} \partial_t^2\psi(\xi_0) \quad (3.12)$$

Now, note that the infinitesimal section experiences force in y direction, while it moves in x direction, This is equivalent to a circular motion with radius $r = \psi(\xi_0)$:

$$F_c = \frac{mv^2}{r} = \frac{\mu\Delta x v^2}{\psi(\xi_0)} = F_y \quad (3.13)$$

In this limit of $\Delta x \rightarrow 0$, $\Delta x = 2\psi(\xi_0)\theta$,

$$\implies 2\theta\mu v^2 = 2T \sin \theta \approx 2T\theta \quad (3.14)$$

$$\implies v^2 = \frac{T}{\mu} \quad (3.15)$$

Thus, the wave equation can be written as:

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2\psi(x,t)}{\partial t^2}, \quad \text{where } v = \sqrt{\frac{T}{\mu}} \quad (3.16)$$

3.2 Lagrange Formalism

3.2.1 Potential and Momentum Density

Now, notice that the force on the infinitesimal section is given by

$$\dot{p} = \mu \partial_t^2 \psi \Delta x \quad (3.17)$$

since the extension of the string in $\Delta x/2$ is given by

$$\Delta l - \frac{\Delta x}{2} = \frac{\Delta x}{2} \sqrt{1 + \left[\partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) \right]^2} - \frac{\Delta x}{2} \quad (3.18)$$

$$\approx \frac{\Delta x}{2} \partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) \quad (3.19)$$

The force on the infinitesimal section due to the extension is then given by

$$F = -k \left(\Delta l - \frac{\Delta x}{2} \right) = -k \frac{\Delta x}{2} \partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) = -T \partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) \quad (3.20)$$

$$\Rightarrow V = \frac{k}{2} \left(\Delta l - \frac{\Delta x}{2} \right)^2 = \frac{k}{2} \left(\frac{\Delta x}{2} \partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) \right)^2 = \frac{T}{2} \frac{\Delta x}{2} \left(\partial_x \psi \left(\xi_0 - \frac{\Delta x}{2} \right) \right)^2 \quad (3.21)$$

We should define these quantity as the potential energy density and the momentum density:

Definition 3.2: Momentum and Potential Energy Density

The **momentum density** and **potential energy density** is defined as the momentum and potential energy per unit length of the string:

$$\pi = \mu \partial_t \psi, \quad \tilde{V} = \frac{T}{2} (\partial_x \psi)^2 \quad (3.22)$$

Now, since we have defined our potential energy (density) and momentum (density), we can write the Lagrangian:

$$L = T - V \quad (3.23)$$

$$= \int dx \tilde{T} - \int dx \tilde{V} \quad (3.24)$$

$$= \int dx \frac{\mu}{2} (\partial_t \psi)^2 - \frac{T}{2} (\partial_x \psi)^2 \quad (3.25)$$

thus we should define the Lagrangian density \mathcal{L} as:

Definition 3.3: Lagrangian Density for 1D String

The **Lagrangian density** is defined as the Lagrangian per unit length of the string:

$$\mathcal{L}[\partial_x \psi, \partial_t \psi] = \frac{\mu}{2} (\partial_t \psi)^2 - \frac{T}{2} (\partial_x \psi)^2 \quad (3.26)$$

Then the Euler-Lagrange equation for the Lagrangian density \mathcal{L} is given by:

$$\partial_t \left(\frac{\partial \mathcal{L}}{\partial (\partial_t \psi)} \right) + \partial_x \left(\frac{\partial \mathcal{L}}{\partial (\partial_x \psi)} \right) = \frac{\partial \mathcal{L}}{\partial \psi} \quad (3.27)$$

$$\implies \partial_t (\mu \partial_t \psi) + \partial_x (-T \partial_x \psi) = 0 \quad (3.28)$$

$$\implies \mu \partial_t^2 \psi - T \partial_x^2 \psi = 0 \quad (3.29)$$

$$\implies \partial_x^2 \psi = \frac{\mu}{T} \partial_t^2 \psi \quad (3.30)$$

which is the wave equation in 1D. Notice that our mechanical variable is now the field $\psi(x, t)$ and its derivatives, rather than the position of a particle or the velocity of a particle.

3.2.2 Generalization to General Field

Now, we would like to apply Lagrange formalism to a general field $\psi(\vec{x}, t)$. We can define the Lagrangian density for a general field $\psi(\vec{x}, t)$ as:

Definition 3.4: Lagrangian Density of a Field

The **Lagrangian density** of a field $\psi(\vec{x}, t)$ is defined such that the Lagrangian is given by the integral of the Lagrangian density over the whole space:

$$L[\psi, \partial_t \psi, \partial_i \psi] = \int d\vec{x} \mathcal{L}(\psi, \partial_\mu \psi) \quad (3.31)$$

where for $\mu = 0, 1, 2, 3$, $x^{0,1,2,3} = (t, \vec{x})$

$$\partial_\mu \psi := \frac{\partial \psi}{\partial x^\mu} = \left(\frac{\partial \psi}{\partial t}, \frac{\partial \psi}{\partial x^1}, \frac{\partial \psi}{\partial x^2}, \frac{\partial \psi}{\partial x^3} \right) \quad (3.32)$$

Definition 3.5: Action of a Field

The **action** of a field $\psi(\vec{x}, t)$ is defined as the integral of the Lagrangian over time:

$$S[\psi] = \int dt L[\psi, \partial_t \psi, \partial_i \psi] = \int dt \int d^3 \vec{x} \mathcal{L}(\psi, \partial_\mu \psi) \quad (3.33)$$

where \mathcal{L} is the Lagrangian density of the field $\psi(\vec{x}, t)$.

and the stationary point of the action is given by:

$$\delta S[\mathcal{L}] = 0 \implies \int dt \int d^3\vec{x} \frac{\partial \mathcal{L}}{\partial \psi} \delta\psi + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \delta(\partial_\mu \psi) = 0 \quad (3.34)$$

where $\delta\psi = 0$ at the boundary of the integration region. The second term can be integrated by parts:

$$\int dt \int d^3\vec{x} \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \delta(\partial_\mu \psi) = \int dt \int d^3\vec{x} \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \partial_\mu(\delta\psi) \quad (3.35)$$

$$= \int dt \int d^3\vec{x} \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \delta\psi \right) - \int dt \int d^3\vec{x} \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right) \delta\psi \quad (3.36)$$

Since $\delta\psi = 0$ at the boundary of the integration region, the first term vanishes:

$$= - \int dt \int d^3\vec{x} \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right) \delta\psi \quad (3.37)$$

Thus, the stationary point of the action is given by:

$$\int dt \int d^3\vec{x} \left(\frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right) \right) \delta\psi = 0 \quad (3.38)$$

Since time and space are arbitrary, the integrand must be zero:

$$\frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right) = 0 \iff \partial_t \left(\frac{\partial \mathcal{L}}{\partial(\partial_t \psi)} \right) + \sum_i \partial_i \left(\frac{\partial \mathcal{L}}{\partial(\partial_i \psi)} \right) = \frac{\partial \mathcal{L}}{\partial \psi} \quad (3.39)$$

This is the **Euler-Lagrange equation** for a field $\psi(\vec{x}, t)$:

Theorem 3.2.1 Euler-Lagrange Equation for a Field

The **Euler-Lagrange equation** for a field $\psi(\vec{x}, t)$ is given by:

$$\frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right) = 0 \quad (3.40)$$

where \mathcal{L} is the Lagrangian density of the field $\psi(\vec{x}, t)$.

Additionally, we define the **canonical conjugate field** $\pi(\vec{x}, t)$ as:

Definition 3.6: Canonical Conjugate Field

The **canonical conjugate field** or **canonical momentum density** $\pi(\vec{x}, t)$ is defined as the derivative of the Lagrangian density with respect to the time derivative of the field ψ :

$$\pi(\vec{x}, t) := \frac{\partial \mathcal{L}}{\partial(\partial_t \psi(\vec{x}, t))} \quad (3.41)$$

3.3 Hamilton Formalism

3.3.1 Legendre Transformation

Now, remember that we obtained the **Hamiltonian** H of the system through the **Legendre transformation** of the Lagrangian L :

$$H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i) \quad (3.42)$$

where i represents each degree of freedom of the system.

In the field, the degree of freedom is infinite - each indexed by the spatial position \vec{x} , then,

Definition 3.7: Hamiltonian of a Field

The **Hamiltonian** of a field $\psi(\vec{x}, t)$ (whose canonical conjugate field is $\pi(\vec{x}, t)$) is defined as

$$H[\psi, \partial_i \psi, \pi] = \int d^3 \vec{x} \left[\pi \cdot \partial_t \psi \right] - L = \int d^3 \vec{x} \left[\pi \cdot \partial_t \psi - \mathcal{L} \right] \quad (3.43)$$

thus, we should define the **Hamiltonian density** \mathcal{H} as:

Definition 3.8: Hamiltonian Density

Hamiltonian density \mathcal{H} is defined as the Hamiltonian per unit volume of the field:

$$\mathcal{H}(\psi, \partial_i \psi, \pi, t) = \pi \cdot \partial_t \psi - \mathcal{L}(\psi, \partial_i \psi, \partial_t \psi, t) \quad (3.44)$$

which satisfies:

$$\int d^3 \vec{x} \mathcal{H}(\psi, \partial_i \psi, \pi, t) = H[\psi, \partial_i \psi, \pi, t] \quad (3.45)$$

which makes the Hamiltonian H a functional of the field ψ , its spatial derivatives $\partial_i \psi$, and the conjugate field π .

Note:

Similarly to the discrete case, we can write the Lagrangian density \mathcal{L} in terms of the Hamiltonian density \mathcal{H} :

$$\mathcal{L}[\psi(\vec{x}, t), \pi(\vec{x}, t)] = \pi \cdot \partial_t \psi - \mathcal{H}[\psi(\vec{x}, t), \pi(\vec{x}, t)] \quad (3.46)$$

where

$$\partial_t \psi = \frac{\partial \mathcal{H}[\psi, \pi]}{\partial \pi} \quad (3.47)$$

3.3.2 Canonical Equations of Fields

We are also interested in the **canonical equations** of fields, which are derived from the variational principle:

$$\delta S = 0 \iff \delta \int dt \int d^3 \vec{x} \mathcal{L} = \delta \int dt \int d^3 \vec{x} \pi \cdot \partial_t \psi - \mathcal{H} \quad (3.48)$$

The variation on this integral can be expanded as follows:

$$\delta S = \int dt \int d^3 \vec{x} \delta \pi \partial_t \psi + \pi \delta(\partial_t \psi) - \delta \mathcal{H} \quad (3.49)$$

$$= \int dt \int d^3 \vec{x} \delta \pi \partial_t \psi + \pi \partial_t(\delta \psi) - \frac{\partial \mathcal{H}}{\partial \psi} \delta \psi - \frac{\partial \mathcal{H}}{\partial \pi} \delta \pi - \frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \delta(\partial_i \psi) \quad (3.50)$$

$$= \int dt \int d^3 \vec{x} \left(\partial_t \psi - \frac{\partial \mathcal{H}}{\partial \pi} \right) \delta \pi + \left(\pi \partial_t(\delta \psi) - \frac{\partial \mathcal{H}}{\partial \psi} \delta \psi - \frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \partial_i(\delta \psi) \right) \quad (3.51)$$

the $\delta \psi$ term can be integrated by parts:

$$\int dt \int d^3 \vec{x} \pi \partial_t(\delta \psi) - \frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \partial_i(\delta \psi) \quad (3.52)$$

$$= \int dt \int d^3 \vec{x} \partial_t(\pi \delta \psi) - \int dt \int d^3 \vec{x} \partial_t \pi \cdot \delta \psi \quad (3.53)$$

$$\begin{aligned} & - \int dt \int d^3 \vec{x} \partial_i \left(\frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \delta \psi \right) + \int dt \int d^3 \vec{x} \partial_i \left(\frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \right) \delta \psi \\ & = \int d^3 \vec{x} [\pi \delta \psi]_{\text{boundary}} - \int dt \int d^3 \vec{x} \partial_t \pi \delta \psi \\ & \quad - \int dt \int_{\text{boundary}} dS \frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \delta \psi + \int dt \int d^3 \vec{x} \partial_i \left(\frac{\partial \mathcal{H}}{\partial(\partial_i \psi)} \right) \delta \psi \end{aligned} \quad (3.54)$$

the boundary terms vanish, so we end up with:

$$\int dt \int d^3\vec{x} \pi \partial_t(\delta\psi) - \frac{\partial\mathcal{H}}{\partial(\partial_i\psi)} \partial_i(\delta\psi) = - \int dt \int d^3\vec{x} \partial_t\pi \delta\psi + \int dt \int d^3\vec{x} \partial_i \left(\frac{\partial\mathcal{H}}{\partial(\partial_i\psi)} \right) \delta\psi \quad (3.55)$$

$$= - \int dt \int d^3\vec{x} \left[\partial_t\pi - \nabla \cdot \left(\frac{\partial\mathcal{H}}{\partial(\nabla\psi)} \right) \right] \delta\psi \quad (3.56)$$

and thus the variation of the action becomes:

$$\delta S = \int dt \int d^3\vec{x} \left(\partial_t\psi - \frac{\partial\mathcal{H}}{\partial\pi} \right) \delta\pi - \left(\partial_t\pi - \nabla \cdot \left(\frac{\partial\mathcal{H}}{\partial(\nabla\psi)} \right) \right) \delta\psi \quad (3.57)$$

for the action to be stationary, the integrand must vanish:

$$\begin{cases} \partial_t\psi - \frac{\partial\mathcal{H}}{\partial\pi} \\ \partial_t\pi + \frac{\partial\mathcal{H}}{\partial\psi} - \partial_i \left(\frac{\partial\mathcal{H}}{\partial(\partial_i\psi)} \right) \end{cases} = 0 \iff \begin{cases} \frac{\partial\psi(\vec{x},t)}{\partial t} = \frac{\partial\mathcal{H}[\psi,\pi]}{\partial\pi} \\ \frac{\partial\pi(\vec{x},t)}{\partial t} = -\frac{\partial\mathcal{H}[\psi,\pi]}{\partial\psi} + \partial_i \left(\frac{\partial\mathcal{H}}{\partial(\partial_i\psi)} \right) \end{cases} \quad (3.58)$$

Thus we have the **canonical equations of fields**:

Theorem 3.3.1 Canonical Equations of Fields

The variational principle in Hamilton formalism leads to the **canonical equations of fields**:

$$\frac{\partial\psi(\vec{x},t)}{\partial t} = \frac{\partial\mathcal{H}(\psi, \partial_i\psi, \pi)}{\partial\pi}, \quad \frac{\partial\pi(\vec{x},t)}{\partial t} = -\frac{\partial\mathcal{H}(\psi, \partial_i\psi, \pi)}{\partial\psi} + \partial_i \left(\frac{\partial\mathcal{H}(\psi, \partial_i\psi, \pi)}{\partial(\partial_i\psi)} \right) \quad (3.59)$$

Corollary 3.3.1 Canonical Equations of Fields using H

Using Theorem 1.1.1, the **canonical equations of fields** can be re-written using the Hamiltonian H instead of the Hamiltonian density \mathcal{H} :

$$\frac{\partial\psi(\vec{x},t)}{\partial t} = \frac{\delta H[\psi,\pi]}{\delta\pi}, \quad \frac{\partial\pi(\vec{x},t)}{\partial t} = -\frac{\delta H[\psi,\pi]}{\delta\psi} \quad (3.60)$$

3.3.3 Poisson Bracket

In the discrete case, the time evolution of a physical quantity $X(q_i, p_i, t)$, \dot{X} can be written as:

$$\dot{X} = \frac{dX}{dt} = \frac{\partial X}{\partial t} + \sum_i \left(\frac{\partial X}{\partial q_i} \dot{q}_i + \frac{\partial X}{\partial p_i} \dot{p}_i \right) = \frac{\partial X}{\partial t} + \{X, H\} \quad (3.61)$$

In the continuous case, a physical quantity X should be an integral of "density" \tilde{X} over

some volume:

$$X = \int_V d^3 \vec{x}' \tilde{X}(\vec{x}', t) \quad (3.62)$$

and assume that \tilde{X} is a function of the field $\psi(\vec{x}, t)$ and its conjugate field $\pi(\vec{x}, t)$ (which makes X a functional of the fields):

$$\implies X[\psi, \pi, t] = \int_V d^3 \vec{x}' \tilde{X}(\psi(\vec{x}', t), \pi(\vec{x}', t), t) \quad (3.63)$$

Then the time evolution of X can be written as:

$$\frac{dX[\psi, \pi, t]}{dt} = \frac{d}{dt} \int_V d^3 \vec{x}' \tilde{X}(\psi(\vec{x}', t), \pi(\vec{x}', t), t) = \int_V d^3 \vec{x}' \frac{d\tilde{X}(\psi(\vec{x}', t), \pi(\vec{x}', t), t)}{dt} \quad (3.64)$$

$$= \int_V d^3 \vec{x}' \frac{\partial \tilde{X}(\psi, \pi, t)}{\partial t} + \frac{\partial \tilde{X}(\psi, \pi, t)}{\partial \psi} \partial_t \psi + \frac{\partial \tilde{X}(\psi, \pi, t)}{\partial \pi} \partial_t \pi \quad (3.65)$$

$$= \int_V d^3 \vec{x}' \frac{\partial \tilde{X}}{\partial t} + \int_V d^3 \vec{x}' \left(\frac{\partial \tilde{X}}{\partial \psi} \frac{\partial \mathcal{H}}{\partial \pi} - \frac{\partial \tilde{X}}{\partial \pi} \frac{\partial \mathcal{H}}{\partial \psi} \right) \quad (3.66)$$

Using Theorem 1.1.1, the partial derivatives can be replaced with functional derivatives:

$$\frac{\partial \tilde{X}}{\partial t} = \frac{\delta X}{\delta t}, \quad \frac{\partial \tilde{X}}{\partial \psi} = \frac{\delta H}{\delta \psi}, \quad \frac{\partial \tilde{X}}{\partial \pi} = \frac{\delta H}{\delta \pi} \quad (3.67)$$

Thus, we can write the time evolution of X as:

$$\frac{dX[\psi, \pi, t]}{dt} = \frac{\partial X[\psi, \pi, t]}{\partial t} + \int d^3 \vec{x}' \left(\frac{\delta X}{\delta \psi} \frac{\delta H}{\delta \pi} - \frac{\delta X}{\delta \pi} \frac{\delta H}{\delta \psi} \right) \quad (3.68)$$

If we were to write the coordinates explicitly,

$$\frac{dX[\psi, \pi, t]}{dt} = \frac{\partial X}{\partial t} + \int d^3 \vec{x}' \left(\frac{\delta X[\psi, \pi, t]}{\delta \psi(\vec{x}', t)} \frac{\delta H[\psi, \pi, t]}{\delta \pi(\vec{x}', t)} - \frac{X[\psi, \pi, t]}{\delta \pi(\vec{x}', t)} \frac{\delta H[\psi, \pi, t]}{\delta \psi(\vec{x}', t)} \right) \quad (3.69)$$

Comparing with the discrete case, we can define the **Poisson bracket** of two physical quantities X and Y as:

Definition 3.9: Poisson Bracket of a Field

The **Poisson bracket** of two physical quantities $X[\psi, \pi, t]$ and $Y[\psi, \pi, t]$ is defined as:

$$\{X, Y\} = \int d^3 \vec{x}' \left(\frac{\delta X}{\delta \psi(\vec{x}', t)} \frac{\delta Y}{\delta \pi(\vec{x}', t)} - \frac{\delta X}{\delta \pi(\vec{x}', t)} \frac{\delta Y}{\delta \psi(\vec{x}', t)} \right) \quad (3.70)$$

Theorem 3.3.2 Time Evolution of a Physical Quantity

The time evolution of a physical quantity $X[\psi, \pi, t]$ can be written as:

$$\frac{dX}{dt} = \frac{\partial X}{\partial t} + \{X, H\} \quad (3.71)$$

Theorem 3.3.3 Poisson Brackets of Fields

For ψ and its conjugate field π , the Poisson bracket satisfies the following properties:

$$\left\{ \psi(\vec{x}, t), \pi(\vec{x}', t) \right\} = \delta^3(\vec{x} - \vec{x}') \quad (3.72)$$

$$\left\{ \psi(\vec{x}, t), \psi(\vec{x}', t) \right\} = 0 \quad (3.73)$$

$$\left\{ \pi(\vec{x}, t), \pi(\vec{x}', t) \right\} = 0 \quad (3.74)$$

Quantum Mechanics

4.1 Hilbert Space in Quantum Mechanics

4.1.1 Hilbert Space

Definition 4.1: Hilbert Space

A **Hilbert space** is a complete inner product space, which is a vector space with an inner product that is complete with respect to the norm induced by the inner product. It is denoted as \mathcal{H} . We denote the basis vectors of the Hilbert space as $|i\rangle$, where i is an index.

Definition 4.2: (Hermitian) Inner Product and Norm

Inner product of a Hilbert space \mathcal{H} is a function $\mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$, that satisfies the following properties:

1. Conjugate symmetry

$$\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^* \quad (4.1)$$

2. Linearity

$$\langle \psi | (a|\varphi\rangle + b|\phi\rangle) = a\langle \psi | \varphi \rangle + b\langle \psi | \phi \rangle \quad (4.2)$$

3. Positivity

$$\langle \psi | \psi \rangle \geq 0, \langle \psi | \psi \rangle = 0 \iff |\psi\rangle = |0\rangle \quad (4.3)$$

where $|\psi\rangle, |\phi\rangle, |\varphi\rangle \in \mathcal{H}$ and $a, b \in \mathbb{C}$.

The **norm** of a vector $|\psi\rangle \in \mathcal{H}$ is defined as

$$\| |\psi\rangle \| := \sqrt{\langle \psi | \psi \rangle} \geq 0 \quad (4.4)$$

Definition 4.3: Completeness

A vector space is said to be **complete** if every Cauchy sequence in the space converges to a limit in the space:

$$\forall \epsilon > 0, \exists N \in \mathbb{N} : \forall m, n > N, \| |v_m\rangle - |v_n\rangle \| < \epsilon \quad (4.5)$$

where $|v_m\rangle, |v_n\rangle \in \mathcal{H}$ are vectors in the space. Colloquially, this property ensures that any sum (even uncountably infinite) of vectors in \mathcal{H} will still be in \mathcal{H} .

4.1.2 Basis Vectors and Completeness Relation

Definition 4.4: Basis Vectors

A set of vectors $\{|i\rangle\}$ in a Hilbert space \mathcal{H} is said to be a **basis** if it is a set of vectors that spans the space, satisfying the following conditions:

1. Linear Independence

$$\sum_i c_i |i\rangle = |0\rangle \iff c_i = 0 \quad \forall i \quad (4.6)$$

2. Completeness

$$\forall |\psi\rangle \in \mathcal{H}, \exists \{c_i\} \in \mathbb{C} \text{ s.t. } |\psi\rangle = \sum_i c_i |i\rangle \quad (4.7)$$

3. Orthogonality

$$\langle i | j \rangle = 0 \quad \forall i \neq j \quad (4.8)$$

Especially, if the basis vectors satisfy:

$$\langle i | j \rangle = \delta_{ij} \quad \forall i, j \quad (4.9)$$

then the basis is said to be **orthonormal**.

Theorem 4.1.1 Completeness Relation

The following relation holds for a complete set of orthonormal basis vectors $\{|i\rangle\}$ in a Hilbert space \mathcal{H} :

$$|\psi\rangle = \sum_i c_i |i\rangle \iff \sum_i |i\rangle \langle i| = \hat{\mathbf{I}} \quad (4.10)$$

Proof: • (\implies)

$$\sum_i |i\rangle \langle i|\psi\rangle = \sum_i c_i |i\rangle = |\psi\rangle, \quad c_i := \langle i|\psi\rangle \quad (4.11)$$

• (\impliedby)

$$|\psi\rangle = \hat{\mathbf{I}}|\psi\rangle = \sum_i |i\rangle \langle i|\psi\rangle = \sum_i c_i |i\rangle \quad (4.12)$$

□

4.2 Linear Algebra Approach

4.2.1 Basic Concepts

A formal mathematical description of quantum mechanics is essentially linear algebra in a Hilbert space. The "state" of quantum particle is represented by a vector $|\psi\rangle \in \mathcal{H}$: a Hilbert space.

Definition 4.5: Observable, Hermitian Operator

A physical quantity (**observable**) A is represented by a Hermitian (self-adjoint) operator \hat{A} acting on the state vector $|\psi\rangle$:

$$\hat{A} = \hat{A}^\dagger, \quad \hat{A}|a\rangle = a|a\rangle, \quad a \in \mathbb{R} \quad (4.13)$$

where \hat{A}^\dagger is **Hermitian conjugate** of \hat{A} , and $|a\rangle$ is an **eigenstate** of the operator \hat{A} with eigenvalue a .

and we postulate that the probability of finding the system in the state $|\phi\rangle$ from another state $|\psi\rangle$ is given by the inner product:

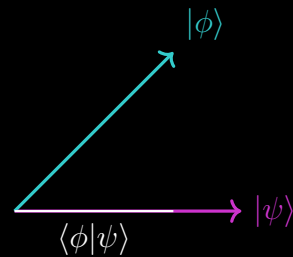
Principle 4.1: Born's Probability Interpretation

The probability of finding the system in the state $|\phi\rangle$ from another state $|\psi\rangle$ is given by:

$$P(\phi|\psi) = |\langle\phi|\psi\rangle|^2 \quad (4.14)$$

where $\langle\phi|\psi\rangle$ is the inner product of the two state vectors.

Intuitively, the inner product $\langle\phi|\psi\rangle$ indicates how "close" the two states $|\phi\rangle$ and $|\psi\rangle$ are: Note that the inner product is a complex number, and the probability is given by the square of the absolute value of the inner product.



4.2.2 Position and Momentum in Quantum Mechanics

The position and momentum of a particle are represented by operators \hat{x} and \hat{p} , and we impose the canonical commutation relation onto these operators:

Principle 4.2: Canonical commutation relation

The position and momentum operators satisfy the following commutation relation:

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij} \quad (4.15)$$

where \hbar is the reduced Planck's constant.

This implies that in the position basis, the momentum operator acts as a derivative operator (refer to Principle 1.2.1):

$$\hat{p}|x\rangle = -i\hbar \frac{\partial}{\partial x}|x\rangle \quad (4.16)$$

The eigenstates of \hat{x} and \hat{p} are denoted as $|x\rangle$ and $|p\rangle$, respectively, and they satisfy the completeness relation:

Principle 4.3: Completeness relation of Continuous Eigenbasis

for $|x\rangle$ and $|p\rangle$, the following completeness relation holds:

$$\langle x|x'\rangle = \delta(x - x'), \quad \langle p|p'\rangle = \delta(p - p') \quad (4.17)$$

$$\iff \int dx |x\rangle\langle x| = \hat{\mathbf{I}}, \quad \int dp |p\rangle\langle p| = \hat{\mathbf{I}} \quad (4.18)$$

Now, we can define the position and momentum wavefunctions $\psi(x), \psi(p)$, whose magnitude squared gives the probability density of finding the particle at a certain position x or momentum p :

Definition 4.6: Wavefunction

The **wavefunction** $\psi(x)$ of a quantum particle is defined as the inner product of the state vector $|\psi\rangle$ with the position eigenstate $|x\rangle$:

$$\psi(x) = \langle x|\psi\rangle \quad (4.19)$$

Colloquially, wavefunction represents the probability amplitude of finding the particle at position x in state $|\psi\rangle$.

Note:

We can equally define a wavefunction in the momentum basis:

$$\psi(p) = \langle p|\psi\rangle \quad (4.20)$$

in which the \hat{x} operator becomes a derivative operator w.r.t. p :

$$\hat{x}|p\rangle = i\hbar \frac{\partial}{\partial p}|p\rangle \quad (4.21)$$

4.2.3 Unitary Transformations: Shift Operator and Fourier Transform

Now, consider a shift operator $\hat{S}(a)$ that shifts the position eigenstate $|x\rangle$ by a constant a :

Definition 4.7: Shift Operator

The **shift operator** $\hat{S}(a)$ is defined as:

$$\hat{S}(a)|x\rangle = |x + a\rangle \quad (4.22)$$

From the discussion in Sec. 1.2,

Theorem 4.2.1 Commutator of Shift Operator

For operators satisfying the commutation relation $[\hat{D}, \hat{x}] = 1$,

$$[\hat{S}(a), \hat{x}] = a\hat{S}(a) \implies \hat{S}(a) = e^{a\hat{D}} \quad (4.23)$$

since $\hat{p} = -i\hbar\hat{D} \iff \hat{D} = \frac{\hat{p}}{-i\hbar}$, we can write the shift operator as:

$$\hat{S}(a) = e^{\frac{a\hat{p}}{-i\hbar}} = e^{i\frac{\hat{p}}{\hbar}a} \quad (4.24)$$

Definition 4.8: Fourier Transform in Quantum Mechanics

The position wavefunction $\langle x|\psi\rangle$ can be expanded in the momentum basis $|p\rangle$, by the **Fourier transform**:

$$\langle x|\psi\rangle = \int dp \langle x|p\rangle \langle p|\psi\rangle = \int \frac{dp}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x} \langle p|\psi\rangle \quad (4.25)$$

4.3 Harmonic Oscillator

5.1 Schrödinger Equation

5.1.1 Historical Background

In 1905, Albert Einstein found the photoelectric effect, suggesting that light has a particle like property, such as discrete energy [4]. Following this work, Arthur Compton in 1923 discovered the Compton effect, which is the scattering of X-rays by electrons, further supporting the particle nature of light and confirming the discrete momentum of photons [5]. Specifically, energy and momentum are each related to the frequency and wavelength of light, respectively, as follows:

Proposition 5.1.1 Planck-Einstein relation

For a photon with frequency ν and wave length λ , the energy E and momentum p are given by

$$E = h\nu, \quad p = \frac{h}{\lambda} = \frac{h\nu}{c} = \frac{E}{c}, \quad (5.1)$$

In 1925, Louis de Brogile posulated that other particles (or any matter) also have a wave-like property, and the energy-frequency/ momentum-wavelength relation is given by the Planck-Einstein relation Eq. (5.1) [6].

Then in 1913, Niels Bohr proposed a model of the hydrogen atom, which describes the electron as a particle orbiting the nucleus in discrete energy levels [7]. The implication of this model is that electrons have a fixed, discrete(quantized) angular momentum $\vec{L} := \vec{r} \times \vec{p}$. For a particle orbiting in a circular orbit, the angular momentum is given by

$$\vec{L} = rp = \frac{hr}{\lambda} \quad (5.2)$$

For the electron wave to be continous around the orbit of radius r , the wavelength must be an integer multiple of the circumference of the orbit:

$$\lambda = \frac{2\pi r}{n}, \quad n = 1, 2, 3, \dots \implies \vec{L} = n \frac{h}{2\pi} := n\hbar \quad (5.3)$$

5.1.2 Schrödinger Equation

Now, a classical wave obeys a wave equation:

$$\frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} - \nabla^2 \psi = 0 \quad (5.4)$$

but does the matter wave also obey wave equation?

Well, not a classical wave equation, but a quantum wave should follow a quantum wave equation, which must satisfy a few conditions that match with the physics as we know it:

- Planck-Einstein relation: $E = \hbar\omega$, $\vec{p} = \hbar\vec{k}$
- Energy equation: $E = T + V$
- For $V = V_0$, the solution must be a plane wave: $\psi(\vec{x}, t) = Ae^{i(\vec{k}\cdot\vec{x} - \omega t)}$ (i.e. constant momentum and constant energy).

The energy equation is given by

$$E = T + V = \frac{p^2}{2m} + V_0 \iff \hbar\omega = \frac{\hbar^2 \vec{k}^2}{2m} + V \quad (5.5)$$

If we multiply both sides by $\psi(\vec{x}, t)$, we get

$$\hbar\omega\psi(\vec{x}, t) = \frac{\hbar^2}{2m} \vec{k}^2 \psi(\vec{x}, t) + V\psi(\vec{x}, t) \quad (5.6)$$

For a plane wave solution,

$$\frac{\partial}{\partial t} \psi(\vec{x}, t) = -i\omega\psi(\vec{x}, t) \implies i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \hbar\omega\psi(\vec{x}, t) \quad (5.7)$$

$$\nabla^2 \psi(\vec{x}, t) = -\vec{k}^2 \psi(\vec{x}, t) \implies -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{x}, t) = \frac{\hbar^2 \vec{k}^2}{2m} \psi(\vec{x}, t) \quad (5.8)$$

Thus, we can write the wave equation as

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{x}, t) + V_0 \psi(\vec{x}, t) \quad (5.9)$$

And we postulate that for any potential $V(\vec{x})$, the wave equation is given by

Principle 5.1: Schrödinger Equation

The Schrödinger equation is given by

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{x}, t) + V(\vec{x})\psi(\vec{x}, t) \quad (5.10)$$

where $\psi(\vec{x}, t)$ is the wave function, $V(\vec{x})$ is the potential, and m is the mass of the particle.

5.2

Variational Principle in Fluid Mechanics

5.2.1

Overview: Cauchy's Equation of Motion

The equation of motion of a point mass is given by Newton's second law:

$$m \frac{d^2 \vec{r}}{dt^2} = \vec{F} \quad (5.11)$$

The equation of motion of a fluid (in general) is given by Cauchy's equation of motion:

$$\int_V \rho dV \frac{D\vec{u}}{Dt} = \oint_S dS \sigma \vec{n} + \int_V \rho dV \vec{F} \quad (5.12)$$

where

- V : Volume of the fluid
- S : Surface of V
- $\rho(\vec{r}, t)$: Density of the fluid at position \vec{r} and time t
- $\vec{u}(\vec{r}, t)$: Velocity of the fluid at position \vec{r} and time t
- \vec{n} : Normal vector of the surface S pointing outward
- $\sigma(\vec{r}, t)$: Stress tensor of the fluid
- \vec{F} : External force per unit volume acting on the infinitesimal volume dV of fluid

the stress tensor shows how the forces act on any surface within a fluid.

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \quad (5.13)$$

The Newtonian derivation of Cauchy's equation of motion is based on the conservation of the momentum of a fluid element:

$$\left(\frac{\partial p}{\partial t} + \Delta p \text{ flux per time} \right) = (\Delta p \text{ from the surface force}) + (\Delta p \text{ from the volume force}) \quad (5.14)$$

$$\implies \rho dV \frac{D\vec{u}}{Dt} = \nabla \cdot (\sigma \vec{n}) + \rho dV \vec{F} \quad (5.15)$$

[8]

5.2.2

Lagrange Derivative

Imagine that you want to measure the height of the water in a river at a certain point and time. Let us assume that you put a very light, small box with some measuring equipment on

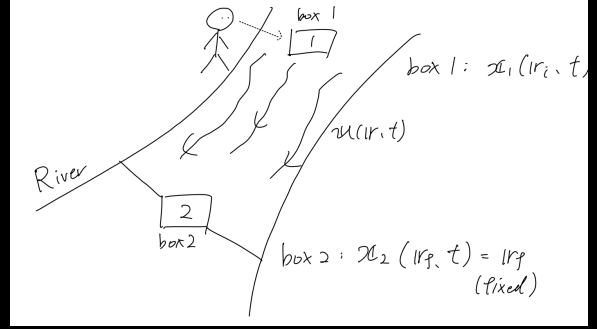
the water surface at some point \vec{r}_i at time t_i . Then we put another box at another point \vec{r}_f at the same time t_i , but we fix this box so that it does not move.

Since the water surface is not static, box 1 will be carried by the water flow. Let us denote the position of the box 1 at time t as $\vec{\xi}(\vec{r}_i, t; t_i)$, where the box 1 is placed at the point \vec{r}_i at time t_i .

Let us denote the height of the water surface at a point \vec{r} at time t by $X(\vec{r}, t)$. Then, we can write the height of the water surface at the positions of box 1 and 2 at time t as

$$X(\vec{\xi}, t) = X_1(t) \quad (5.16)$$

$$X(\vec{r}_f, t) = X_2(t) \quad (5.17)$$



Finally, assume that the box 1 will reach \vec{r}_f at time t_f .

Now, at initial time t_i , the change in height of the water surface is given by:

$$X(\vec{r}_f, t_i) - X(\vec{r}_i, t_i) = \nabla X(\vec{r}_i, t_i) \cdot (\vec{r}_f - \vec{r}_i) \quad (5.18)$$

$$= \nabla X(\vec{r}_i, t_i) \cdot \Delta \vec{r} \quad (5.19)$$

assuming that $\Delta \vec{r} := \vec{r}_f - \vec{r}_i$ is small enough. On the other hand, for box 2, the change in height of the water surface in a time interval $\Delta t = t_f - t_i$ is given by:

$$X(\vec{r}_f, t_f) - X(\vec{r}_f, t_i) = \frac{\partial X(\vec{r}_f, t_i)}{\partial t} \Delta t \quad (5.20)$$

Thus, the total change of X measured by box 1, during Δt , moving at the velocity \vec{u} is given by

$$X(\vec{r}_f, t_f) - X(\vec{r}_i, t_i) = X(\vec{r}_f, t_f) - \underbrace{X(\vec{r}_f, t_i) + X(\vec{r}_f, t_i)}_{=0} - X(\vec{r}_i, t_i) \quad (5.21)$$

$$= \frac{\partial X}{\partial t} \Delta t + \nabla X(\vec{r}_i, t_i) \cdot \Delta \vec{r} \quad (5.22)$$

Now, since $\vec{r}_i = \vec{\xi}(\vec{r}_i, t_i)$ and $\vec{r}_f = \vec{\xi}(\vec{r}_i, t_f)$, we can rewrite the equation above:

$$X(\vec{\xi}(\vec{r}_i, t_f), t_f) - X(\vec{\xi}(\vec{r}_i, t_i)) = \frac{\partial X}{\partial t} \Delta t + \nabla X(\vec{\xi}(\vec{r}_i, t_i)) \cdot \Delta \vec{\xi} \quad (5.23)$$

where $\Delta \vec{\xi} = \vec{\xi}(\vec{r}_i, t_f) - \vec{\xi}(\vec{r}_i, t_i)$.

Using $\Delta t = t_f - t_i$, we can rewrite the equation above as:

$$\frac{X(\vec{\xi} + \Delta \vec{\xi}, t_i + \Delta t) - X(\vec{\xi}, t_i)}{\Delta t} = \frac{\partial X}{\partial t} + \nabla X(\vec{\xi}, t_i) \cdot \frac{\Delta \vec{\xi}}{\Delta t} \quad (5.24)$$

$$(5.25)$$

Since the box 1 is a part of the fluid, the time derivative of $\vec{\xi}$ is the velocity of the fluid at the position $\vec{\xi}$:

$$\frac{\partial \vec{\xi}(\vec{r}_i, t)}{\partial t} = \vec{u}(\vec{\xi}, t) \quad (5.26)$$

Note:

In this derivative, we fix the starting position \vec{r}_i , we only care about the time evolution from the position \vec{r}_i . This is different from the total derivative, which takes into account a change in the starting position \vec{r}_i .

thus, by taking $\Delta t \rightarrow 0 (\implies \Delta x \rightarrow 0)$, we can rewrite the equation above as:

$$\frac{DX(\vec{\xi}, t_i)}{Dt} := \frac{\partial X(\vec{\xi}, t_i)}{\partial t} + \vec{u}(\vec{\xi}, t_i) \cdot \nabla X(\vec{\xi}, t_i) \quad (5.27)$$

where $\frac{D}{Dt}$ indicates that we are tracking the box 1 and its measurement of X . This is called the **Lagrange derivative**:

Definition 5.1: Lagrange Derivative

The Lagrange description in Eulerian perspective is given as the **Lagrange derivative**:

$$\frac{DX}{Dt} := \frac{\partial X}{\partial t} + \vec{u} \cdot \nabla X \quad (5.28)$$

which tracks the change of a physical quantity X with the flow.

Now, define a new quantity called the "position function" $\vec{x}(\vec{r}, t)$:

$$\vec{x}(\vec{r}, t) := \vec{r} \quad (5.29)$$

If we measure this position function at the box 1 at $t = t_i$,

$$\vec{x}(\vec{r}_i, t_i) = \vec{r}_i \quad (5.30)$$

and notice that tracking the position of box 1 is equivalent to observing the time-evolved position $\vec{\xi}(\vec{r}_i, t_i)$:

$$\frac{\partial \vec{\xi}}{\partial t} = \frac{D\vec{x}}{Dt} = \vec{u}(\vec{x}, t) \quad (5.31)$$

5.2.3 Derivation from Action Integral

In Newtonian mechanics, for a particle of mass m , the action integral S is given by:

$$S = \int dt L = \int dt m \mathcal{L}, \quad \mathcal{L} := \frac{L}{m} = \left[\frac{1}{2} \dot{\vec{x}}^2 - \tilde{V}(\vec{x}) \right] \quad (5.32)$$

where \mathcal{L} is the Lagrangian density, and

$$\tilde{V}(\vec{x}) = \frac{V(\vec{x})}{m} \quad (5.33)$$

by assuming a similar form of the Lagrangian density for a fluid, we can write the action integral for a fluid as:

$$S = \int dt L = \int dt \int_V \rho(\vec{x}, t) dV(\vec{x}, t) \mathcal{L}\left(\vec{x}, \frac{D\vec{x}}{Dt}\right) \quad (5.34)$$

where the Lagrangian density is

$$\mathcal{L}\left(\vec{x}(\vec{r}, t), \frac{D\vec{x}(\vec{r}, t)}{Dt}\right) = \frac{1}{2} \left(\frac{D\vec{x}(\vec{r}, t)}{Dt} \right)^2 - \tilde{V}(\vec{x}(\vec{r}, t)) + \frac{1}{\rho(\vec{r}, t)} \nabla \cdot \sigma(\vec{r}, t) \vec{x}(\vec{r}, t) \quad (5.35)$$

Then the Euler-Lagrange equation for this Lagrangian density is given by:

$$\frac{\partial \mathcal{L}}{\partial \vec{x}} - \frac{D}{Dt} \left(\frac{\partial \mathcal{L}}{\partial \left(\frac{D\vec{x}}{Dt} \right)} \right) = 0 \quad (5.36)$$

calculating the partial derivative gives:

$$\frac{\partial \mathcal{L}}{\partial \vec{x}} = \frac{1}{\rho} \nabla \cdot \sigma - \nabla \tilde{V}(\vec{x}) = \frac{1}{\rho} \nabla \cdot \sigma + \vec{F} \quad (5.37)$$

$$\frac{\partial \mathcal{L}}{\partial \left(\frac{D\vec{x}}{Dt} \right)} = \frac{D\vec{x}}{Dt} = \vec{u}(\vec{x}, t) \quad (5.38)$$

hence the Euler-Lagrange equation becomes:

$$\frac{D\vec{u}}{Dt} = \frac{1}{\rho} \nabla \cdot \sigma + \vec{F} \quad (5.39)$$

by integrating over the volume V , we get

$$\int_V \rho dV \frac{D\vec{u}}{Dt} = \int_V dV \nabla \cdot \sigma + \int_V \rho dV \vec{F} \quad (5.40)$$

$$\Rightarrow \int_V \rho dV \frac{D\vec{u}}{Dt} = \int_V ds \vec{n} \cdot \sigma + \int_V \rho dV \vec{F} \quad (5.41)$$

5.2.4 Hamilton Formalism

Similarly to the point mass case, we should define the momentum density $\vec{\pi}(\vec{r}, t)$ as the derivative of the Lagrangian density with respect to the velocity:

$$\vec{\pi}(\vec{r}, t) = \frac{\partial \mathcal{L}}{\partial \left(\frac{D\vec{x}}{Dt} \right)} \quad (5.42)$$

then the Hamiltonian density should be defined by the Legendre transformation:

$$\mathcal{H}(\vec{\pi}, \vec{x}) = \vec{\pi} \cdot \frac{D\vec{x}}{Dt} - \mathcal{L}\left(\vec{x}, \frac{D\vec{x}}{Dt}\right) \quad (5.43)$$

$$= \frac{1}{2} \left(\frac{D\vec{x}}{Dt} \right)^2 + \tilde{V}(\vec{x}) - \frac{1}{\rho} \nabla \cdot \sigma \vec{x} \quad (5.44)$$

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