4. Canonical Field Quantization for Bosons:

Motivation:

1 classical particle $\xrightarrow{\text{"first quantization"}}$ 1 quantum particle

1 quantum particle $\xrightarrow[\text{systematically derived via canonical field quantization}]{\text{"second quantization"}}$ arbitrary number of quantum particles

4.1 Action of Schrödinger Field:

Task: Schrödinger equation of motion $\longleftrightarrow$ action

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = \left\{-\frac{\hbar^2}{2m}\Delta + V_1(\vec{x})\right\}\psi(\vec{x},t) \qquad \Big| \cdot \delta\psi^*(\vec{x},t)$$

$$-i\hbar \frac{\partial \psi^*(\vec{x},t)}{\partial t} = \left\{-\frac{\hbar^2}{2m}\Delta + V_1(\vec{x})\right\}\psi^*(\vec{x},t) \qquad \Big| \cdot \delta\psi(\vec{x},t)$$

$$\int dt \int d^3x \left\{ i\hbar \left[\underbrace{\delta\psi^*(\vec{x},t)\frac{\partial\psi(\vec{x},t)}{\partial t} - \delta\psi(\vec{x},t)\frac{\partial\psi^*(\vec{x},t)}{\partial t}}_{1} \right] \right.$$
$$\left. + \frac{\hbar^2}{2m}\left[\underbrace{\delta\psi^*(\vec{x},t)\Delta\psi(\vec{x},t) + \delta\psi(\vec{x},t)\Delta\psi^*(\vec{x},t)}_{2}\right] - V_1(\vec{x})\underbrace{\left[\delta\psi^*(\vec{x},t)\psi(\vec{x},t) + \delta\psi(\vec{x},t)\psi^*(\vec{x},t)\right]}_{=\delta\left[\psi^*(\vec{x},t)\psi(\vec{x},t)\right]}\right\} = 0$$

1. partial integration: assume that variations of Schrödinger fields ψ, ψ^* vanish at integration boundary

$$\int dt \; (1) = \int dt \left\{ \delta\psi^*(\vec{x},t)\frac{\partial\psi(\vec{x},t)}{\partial t} + \underbrace{\left(\frac{\partial}{\partial t}\delta\psi(\vec{x},t)\right)}_{=\delta\frac{\partial}{\partial t}\psi(\vec{x},t)}\cdot\psi^*(\vec{x},t)\right\} = \delta\int dt \; \psi^*(\vec{x},t)\frac{\partial\psi(\vec{x},t)}{\partial t}$$

2. partial integration:

$$\int d^3x \; (2) = -\int d^3x \left\{ \underbrace{\vec{\nabla}\delta}_{=\delta\vec{\nabla}}\psi^*(\vec{x},t)\cdot\vec{\nabla}\psi(\vec{x},t) + \underbrace{\vec{\nabla}\delta}_{=\delta\vec{\nabla}}\psi(\vec{x},t)\cdot\vec{\nabla}\psi^*(\vec{x},t)\right\} = -\delta\int d^3x \, \vec{\nabla}\psi^*(\vec{x},t)\cdot\vec{\nabla}\psi(\vec{x},t)$$

$$\Rightarrow \quad \delta \mathcal{A}[\psi^*(\cdot,\cdot);\psi(\cdot,\cdot)] = 0$$ Hamilton principle of classical field theory

action

$$\mathcal{A} = \int dt \, L\left[\psi^*(\cdot,t), \frac{\partial\psi^*(\cdot,t)}{\partial t}; \psi(\cdot,t), \frac{\partial\psi(\cdot,t)}{\partial t}\right]$$

Lagrange function

$$L = \int d^3x \, \mathcal{L}\left(\psi^*(\vec{x},t), \vec{\nabla}\psi^*(\vec{x},t), \frac{\partial\psi^*(\vec{x},t)}{\partial t}; \psi(\vec{x},t), \vec{\nabla}\psi(\vec{x},t), \frac{\partial\psi(\vec{x},t)}{\partial t}\right)$$

Lagrange density

$$\mathcal{L} = i\hbar\,\psi^*(\vec{x},t)\frac{\partial\psi(\vec{x},t)}{\partial t} - \frac{\hbar^2}{2m}\vec{\nabla}\psi^*(\vec{x},t)\cdot\vec{\nabla}\psi(\vec{x},t) - V_1(\vec{x})\,\psi^*(\vec{x},t)\,\psi(\vec{x},t)$$

4.2 Functional Derivative: Definition

Overview:

$\frac{df(q)}{dq}$ total derivative for one variable

$\frac{\partial f(q_1,\dots,q_N)}{\partial q_j}$ partial derivative for finite number of variables

$\frac{\delta F[\phi(\cdot)]}{\delta\phi(x)}$ functional derivative for a continuum of variables

functional: mapping of a function to $\mathbb{R}(\mathbb{C})$

$$\frac{dq}{dq} = 1 \qquad \frac{\partial q_i}{\partial q_j} = \delta_{ij} \qquad \frac{\delta\phi(x)}{\delta\phi(y)} = \delta(x-y)$$

Partial derivatives:

$$df(q_1,\dots,q_N) = \sum_{j=1}^N \frac{\partial f(q_1,\dots,q_N)}{\partial q_j}\cdot dq_j$$

special case: $\delta q_j = \varepsilon\,\delta_{ij}$

$$f(q_1,\dots,q_i+\varepsilon,\dots,q_N) - f(q_1,\dots,q_i,\dots,q_N) = df(q_1,\dots,q_N) = \sum_{j=1}^N \frac{\partial f(q_1,\dots,q_N)}{\partial q_j}\varepsilon\,\delta_{ij} = \varepsilon\cdot\frac{\partial f(q_1,\dots,q_N)}{\partial q_i}$$

$$\Rightarrow \frac{\partial f(q_1,\dots,q_N)}{\partial q_i} = \lim_{\varepsilon\to 0}\frac{f(q_1,\dots,q_i+\varepsilon,\dots,q_N) - f(q_1,\dots,q_N)}{\varepsilon}$$

Functional derivatives:

$$\delta F[\phi(\cdot)] = \int dx \, \frac{\delta F[\phi(\cdot)]}{\delta\phi(x)}\,\delta\phi(x)$$

special case: $\delta\phi(x) = \varepsilon\,\delta(x-y)$

$$F[\phi(\cdot)+\varepsilon\,\delta(\cdot-y)] - F[\phi(\cdot)] = \delta F[\phi(\cdot)] = \int dx\,\frac{\delta F[\phi(\cdot)]}{\delta\phi(x)}\,\varepsilon\,\delta(x-y) = \varepsilon\,\frac{\delta F[\phi(\cdot)]}{\delta\phi(y)}$$

$$\Rightarrow \frac{\delta F[\phi(\cdot)]}{\delta\phi(y)} = \lim_{\varepsilon\to 0}\frac{F[\phi(\cdot)+\varepsilon\,\delta(\cdot-y)] - F[\phi(\cdot)]}{\varepsilon}$$

$\Rightarrow$ definition as limit of difference quotient

$\Rightarrow$ starting point to derive calculational rules

Consequences:

1) "Trivial" functional derivative:

$$\frac{\delta\phi(x)}{\delta\phi(y)} = \lim_{\varepsilon\to 0}\frac{\phi(x)+\varepsilon\,\delta(x-y)-\phi(x)}{\varepsilon} = \delta(x-y)$$

2) Product rule:

$$\frac{\delta\{F[\phi(\cdot)]\cdot G[\phi(\cdot)]\}}{\delta\phi(y)} = \lim_{\varepsilon\downarrow 0}\frac{1}{\varepsilon}\Big\{F[\phi(\cdot)+\varepsilon\,\delta(\cdot-y)]\,G[\phi(\cdot)+\varepsilon\,\delta(\cdot-y)]$$
$$- F[\phi(\cdot)]\,G[\phi(\cdot)+\varepsilon\,\delta(\cdot-y)] + F[\phi(\cdot)]\,G[\phi(\cdot)+\varepsilon\,\delta(\cdot-y)] - F[\phi(\cdot)]\cdot G[\phi(\cdot)]\Big\}$$
$$= \frac{\delta F[\phi(\cdot)]}{\delta\phi(y)}\,G[\phi(\cdot)] + F[\phi(\cdot)]\cdot\frac{\delta G[\phi(\cdot)]}{\delta\phi(y)}$$

3) Chain rule:

$$\frac{\delta f(\phi(x))}{\delta\phi(y)} = \frac{\partial f(\phi(x))}{\partial\phi(x)}\cdot\underbrace{\frac{\delta\phi(x)}{\delta\phi(y)}}_{=\delta(x-y)}$$

4.3 Functional Derivatives: Application:

$$[\hat a_{\vec x_n}\cdots\hat a_{\vec x_1},\hat a^+_{\vec x}]_- = \sum_{r=1}^{n}\delta(\vec x-\vec x_r)\,\hat a_{\vec x_n}\cdots\hat a_{\vec x_{r+1}}\hat a_{\vec x_{r-1}}\cdots\hat a_{\vec x_1}$$
$$= \frac{\delta}{\delta\hat a_{\vec x}}\,\hat a_{\vec x_n}\cdots\hat a_{\vec x_1}$$

generalized to arbitrary functional:

$$F[\hat a_\cdot] = \sum_{n=1}^{\infty}\int d^3x_1\cdots\int d^3x_n\,F_n(\vec x_1,\dots,\vec x_n)\,\hat a_{\vec x_n}\cdots\hat a_{\vec x_1}$$

$$[F[\hat a_\cdot],\hat a^+_{\vec x}]_- = \frac{\delta}{\delta\hat a_{\vec x}}F[\hat a_\cdot] \quad (1)$$

analogously: $[\hat a_{\vec x},F[\hat a^+_\cdot]]_- = \frac{\delta}{\hat a^+_{\vec x}}F[\hat a^+_\cdot] \quad (2)$

application: $[\hat a_{\vec x},\hat a^+_{\vec x'}]_- \overset{(1)}{=} \frac{\delta}{\delta\hat a_{\vec x'}}\hat a_{\vec x} \overset{(2)}{=} \frac{\delta}{\delta\hat a^+_{\vec x}}\hat a^+_{\vec x'} = \delta(\vec x-\vec x')$

further generalization to functional $F[\hat a^+_\cdot,\hat a_\cdot]$ with normal ordering

$$[F[\hat a^+_\cdot,\hat a_\cdot],\hat a^+_{\vec x}]_- = F[\hat a^+_\cdot,\hat a_\cdot]\underrightarrow{\frac{\delta}{\delta\hat a_{\vec x}}}$$

$$[\hat a_{\vec x},F[\hat a^+_\cdot,\hat a_\cdot]]_- = \underleftarrow{\frac{\delta}{\delta\hat a^+_{\vec x}}}F[\hat a^+_\cdot,\hat a_\cdot]$$

application:

$$[\hat a^+_{\vec x},\hat a^+_{\vec x'}]_- = \hat a^+_{\vec x}\frac{\delta}{\delta\hat a_{\vec x'}} = 0,\qquad [\hat a_{\vec x},\hat a_{\vec x'}]_- = \overrightarrow{\frac{\delta}{\delta\hat a^+_{\vec x}}}\,\hat a_{\vec x'} = 0$$

Extension from Schrödinger to Heisenberg picture

$$[F[\hat\psi^+(\cdot,\cdot),\hat\psi(\cdot,\cdot)],\hat\psi^+(\vec x,t)]_- = F[\hat\psi^+(\cdot,\cdot),\psi(\cdot,\cdot)]\frac{\delta}{\delta\hat\psi(\vec x,t)}$$

$$[\hat\psi(\vec x,t),F[\hat\psi^+(\cdot,\cdot),\psi(\cdot,\cdot)]]_- = \frac{\delta}{\delta\hat\psi^+(\vec x,t)}F[\hat\psi^+(\cdot,\cdot),\psi(\cdot,\cdot)]$$

Heisenberg equations:

$$i\hbar\frac{\partial}{\partial t}\hat\psi(\vec x,t) = [\hat\psi(\vec x,t),\hat H_H(t)]_- = \frac{\delta}{\delta\hat\psi^+(\vec x,t)}\hat H_H(t)$$

$$i\hbar\frac{\partial}{\partial t}\hat\psi^+(\vec x,t) = [\hat\psi^+(\vec x,t),\hat H_H(t)]_- = -\hat H_H(t)\frac{\delta}{\delta\hat\psi(\vec x,t)}$$

ABC-rules <=> functional derivatives (normal ordered)

4.4 Euler-Lagrange Equations:

$$\delta\mathcal A = \int dt\int d^3x\Big\{\underbrace{\frac{\delta\mathcal A}{\delta\psi^*(\vec x,t)}\,\delta\psi^*(\vec x,t) + \frac{\delta\mathcal A}{\delta\psi(\vec x,t)}\cdot\delta\psi(\vec x,t)}_{\text{arbitrary}}\Big\} \overset{!}{=} 0 \Rightarrow \begin{cases}\frac{\delta\mathcal A}{\delta\psi^*(\vec x,t)} = 0\\ \frac{\delta\mathcal A}{\delta\psi(\vec x,t)} = 0\end{cases}$$

$$\mathcal A = \int dt'\,L\Big[\psi^*(\cdot,t'),\frac{\partial\psi^*(\cdot,t')}{\partial t'};\ \psi(\cdot,t'),\frac{\partial\psi(\cdot,t')}{\partial t'}\Big]$$

$$\frac{\delta\mathcal A}{\delta\psi^*(\vec x,t)} = \int d^3x\Big\{\frac{\delta L}{\delta\psi^*(\vec x,t')}\cdot\underbrace{\frac{\delta\psi^*(\vec x,t')}{\delta\psi^*(\vec x,t)}}_{=\delta(t-t')} + \frac{\delta L}{\delta\frac{\partial\psi^*(\vec x,t')}{\partial t'}}\cdot\underbrace{\frac{\delta\frac{\partial\psi^*(\vec x,t')}{\partial t'}}{\delta\psi^*(\vec x,t)}}_{\frac{\partial}{\partial t'}\frac{\delta\psi^*(\vec x,t')}{\delta\psi(\vec x,t)}}\Big\}$$

partial integration:

$$= \int d^3x \left\{ \frac{\delta L}{\delta \psi^*(\vec{x},t')} - \frac{\partial}{\partial t'} \frac{\delta L}{\delta \frac{\partial \psi^*(\vec{x},t')}{\partial t'}} \right\} \underbrace{\frac{\partial \psi^*(\vec{x},t')}{\delta \psi^*(\vec{x},t)}}_{=\delta(t-t')} = \frac{\delta L}{\delta \psi^*(\vec{x},t)} - \frac{\partial}{\partial t} \frac{\delta L}{\delta \frac{\partial \psi^*(\vec{x},t)}{\partial t}} \doteq 0 \quad (1)$$

$$L = \int d^3x' \, \mathcal{L}\left(\psi^*(\vec{x}',t), \vec{\nabla}'\psi^*(\vec{x}',t), \frac{\partial \psi^*(\vec{x}',t)}{\partial t}; \psi(\vec{x}',t), \vec{\nabla}'\psi(\vec{x}',t), \frac{\partial \psi(\vec{x}',t)}{\partial t} \right)$$

$$\frac{\delta L}{\delta \psi^*(\vec{x},t)} = \frac{\partial \mathcal{L}}{\partial \psi^*(\vec{x},t)} - \vec{\nabla} \frac{\partial \mathcal{L}}{\partial \vec{\nabla}\psi^*(\vec{x},t)} \quad (2)$$

(1)+(2): Euler-Lagrange equation of field theory

$$\frac{\partial \mathcal{L}}{\partial \psi^*(\vec{x},t)} - \vec{\nabla} \frac{\partial \mathcal{L}}{\partial \vec{\nabla}\psi^*(\vec{x},t)} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi^*(\vec{x},t)}{\partial t}} = 0 \quad (3)$$

$$\frac{\partial \mathcal{L}}{\partial \psi(\vec{x},t)} - \vec{\nabla} \frac{\partial \mathcal{L}}{\partial \vec{\nabla}\psi(\vec{x},t)} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi(\vec{x},t)}{\partial t}} = 0 \quad (4)$$

$$\mathcal{L} = i\hbar \psi^* \frac{\partial \psi}{\partial t} - \frac{\hbar^2}{2m} \nabla\psi^* \nabla\psi - V_1 \psi^* \psi$$

$$\frac{\partial \mathcal{L}}{\partial \psi^*} = i\hbar \frac{\partial \psi}{\partial t} - V_1 \psi, \quad \frac{\partial \mathcal{L}}{\partial \nabla\psi^*} = -\frac{\hbar^2}{2m} \nabla\psi, \quad \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi^*}{\partial t}} = 0 \quad (5)$$

$$\frac{\partial \mathcal{L}}{\partial \psi} = -V_1 \psi^*, \quad \frac{\partial \mathcal{L}}{\partial \nabla\psi} = -\frac{\hbar^2}{2m} \nabla\psi^*, \quad \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi}{\partial t}} = i\hbar \psi^* \quad (6)$$

(5) in (3): $i\hbar \frac{\partial \psi}{\partial t} - V_1 \psi + \frac{\hbar^2}{2m} \Delta\psi = 0 \Rightarrow i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi + V_1 \psi$

(6) in (4): $-V_1 \psi^* + \frac{\hbar^2}{2m} \Delta\psi^* - i\hbar \frac{\partial \psi^*}{\partial t} = 0 \Rightarrow -i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi^* + V_1 \psi^*$

4.5 Hamilton Field Theory: canonical momentum fields

$$\pi^*(\vec{x},t) = \frac{\delta L}{\delta \frac{\partial \psi^*(\vec{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi^*(\vec{x},t)}{\partial t}} = 0$$

$$\pi(\vec{x},t) = \frac{\delta L}{\delta \frac{\partial \psi(\vec{x},t)}{\partial t}} = \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi(\vec{x},t)}{\partial t}} = i\hbar \psi^*(\vec{x},t)$$

Hamilton function via Legendre transformation:

$$H = \int d^3x \left\{ \underbrace{\cancel{\pi^*(\vec{x},t) \frac{\partial \psi^*(\vec{x},t)}{\partial t}}}_{=0} + \pi(\vec{x},t) \frac{\partial \psi(\vec{x},t)}{\partial t} \right\} - L$$

$$= \int d^3x \left\{ \cancel{\pi(\vec{x},t) \frac{\partial \psi(\vec{x},t)}{\partial t}} - \cancel{\pi(\vec{x},t) \frac{\partial \psi(\vec{x},t)}{\partial t}} + \frac{\hbar^2}{2m} \frac{1}{i\hbar} \vec{\nabla}\pi(\vec{x},t) \cdot \vec{\nabla}\psi(\vec{x},t) + V_1(\vec{x}) \frac{1}{i\hbar} \pi(\vec{x},t) \psi(\vec{x},t) \right\}$$

$$H = \int d^3x \, \mathcal{H}\left(\pi(\vec{x},t), \vec{\nabla}\pi(\vec{x},t); \psi(\vec{x},t), \vec{\nabla}\psi(\vec{x},t) \right)$$

Hamilton density

$$\mathcal{H} = \frac{\hbar}{2mi} \vec{\nabla}\pi \cdot \vec{\nabla}\psi + \frac{V_1}{i\hbar} \pi \cdot \psi$$

Hamilton equations of field theory? $A = A[\pi(\cdot,\cdot); \psi(\cdot,\cdot)]$

$$\delta A = \int dt \int d^3x \left\{ \frac{\delta A}{\delta \pi(\vec{x},t)} \delta\pi(\vec{x},t) + \frac{\delta A}{\delta \psi(\vec{x},t)} \delta\psi(\vec{x},t) \right\} = 0$$

Hamilton principle

$$\Rightarrow \frac{\delta A}{\delta \pi(\vec{x},t)} = 0, \quad \frac{\delta A}{\delta \psi(\vec{x},t)} = 0$$

$$A = \int dt \, L = \int dt \int d^3x \, \pi(\vec{x},t) \frac{\partial \psi(\vec{x},t)}{\partial t} - \int dt \, H[\pi(\cdot,t); \psi(\cdot,t)]$$

$$\frac{\delta A}{\delta \pi(\vec{x},t)} = \frac{\partial \psi(\vec{x},t)}{\partial t} - \frac{\delta H}{\delta \pi(\vec{x},t)} \qquad \left[\text{analogue: } \dot{q} = \frac{\partial H}{\partial p}\right]$$

$$\frac{\delta A}{\delta \psi(\vec{x},t)} = -\frac{\partial \pi(\vec{x},t)}{\partial t} - \frac{\delta H}{\delta \psi(\vec{x},t)} \qquad \left[\text{analogue: } \dot{p} = -\frac{\partial H}{\partial q}\right]$$

$$\frac{\delta H}{\delta \pi(\vec{x},t)} = \frac{\partial \mathcal{H}}{\partial \pi(\vec{x},t)} - \vec{\nabla} \frac{\partial \mathcal{H}}{\partial \vec{\nabla}\pi(\vec{x},t)}$$

$$\frac{\delta H}{\delta \psi(\vec{x},t)} = \frac{\partial \mathcal{H}}{\partial \psi(\vec{x},t)} - \vec{\nabla} \frac{\partial \mathcal{H}}{\partial \vec{\nabla}\psi(\vec{x},t)}$$

$$\frac{\partial \mathcal{H}}{\partial \pi} = \frac{V_1}{i\hbar} \psi, \quad \frac{\partial \mathcal{H}}{\partial \vec{\nabla}\pi} = \frac{\hbar}{2mi} \nabla\psi \Rightarrow \frac{\partial \psi}{\partial t} = \frac{\delta H}{\delta \pi} = \frac{V_1}{i\hbar} \psi - \frac{\hbar}{2mi} \Delta\psi$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi + V_1 \psi$$

$$\frac{\partial \mathcal{H}}{\partial \psi} = \frac{V_1}{i\hbar} \pi, \quad \frac{\partial \mathcal{H}}{\partial \vec{\nabla}\psi} = \frac{\hbar}{2mi} \nabla\pi \Rightarrow -\frac{\partial \pi}{\partial t} = \frac{V_1}{i\hbar} \pi - \frac{\hbar}{2mi} \Delta\pi$$

$$\pi = i\hbar \psi^* \Rightarrow -i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi^* + V_1 \psi^*$$