Mathematical preparations for QFT in curved space:

Plan today:
1. Functional derivatives $\frac{\delta F[g]}{\delta g(x)} = ?$
2. Example use 1: to make the QFT Schrödinger equation well defined.
3. Example use 2: to define the Functional Legendre transform.
4. Use both to obtain the Lagrangian formulation of QFT, which will be starting point for QFT on curved space.

Functional differentiation

Recall:

a) Differentiation of functions of one variable, $F(u)$:

$$\frac{dF(u)}{du} := \lim_{\varepsilon \to 0} \frac{F(u+\varepsilon) - F(u)}{\varepsilon}$$

b) Differentiation of functions of countably many variables, $F(\{u_j\}_{j=1}^{\infty})$:

$$\frac{\delta F(\{u_j\}_{j=1}^{\infty})}{\delta u_i} := \lim_{\varepsilon \to 0} \frac{F(u_1, \ldots, u_i+\varepsilon, \ldots) - F(u_1, \ldots, u_i, \ldots)}{\varepsilon}$$

$$= \lim_{\varepsilon \to 0} \frac{F(\{u_j\}_{j=1}^{\infty} + \varepsilon \delta u_j \delta u_{j+1} \cdots) - F(\{u_j\}_{j=1}^{\infty})}{\varepsilon}$$
**Definition:**

c.) Differentiation of functions of uncountably many variables, $F(\sum_{x \in \mathbb{R}} u(x)^2)$:

\[
\frac{\delta F(\sum_{x \in \mathbb{R}} u(x)^2)}{\delta u(y)} := \lim_{\varepsilon \to 0} \frac{F(\sum_{x \in \mathbb{R}} u(x)^2 + \varepsilon \delta(x-y)^2) - F(\sum_{x \in \mathbb{R}} u(x)^2)}{\varepsilon}
\]

→ Since $F$ is a "functional", i.e., is mapping functions to numbers

$F: u \to F[u] \in \mathbb{R}$

↑ function

short for $\{u(x) \}_{x \in \mathbb{R}}$

we call $\frac{\delta F}{\delta u(y)}$ a **functional derivative**.

**Example:**

$F[u] := \int_{\mathbb{R}} \cos(x) \, u(x)^2 \, dx$

Then:

\[
\frac{\delta F}{\delta u(y)} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[ \int_{\mathbb{R}} \cos(x) \left( u(x)^2 + \varepsilon \delta(x-y)^2 \right) - \int_{\mathbb{R}} \cos(x) \, u(x)^2 \, dx \right]
\]

Distribution theory would be needed. But it does not anymore

\[
= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_{\mathbb{R}} \cos(x) \left( u(x)^2 + \varepsilon \delta(x-y) \delta(x-y) + \varepsilon^2 \delta^2(x-y) - u(x)^2 \right) \, dx
\]

\[
= \lim_{\varepsilon \to 0} \frac{\varepsilon}{\varepsilon} \int_{\mathbb{R}} 2 \, u(x) \delta(x-y) \cos(x) \, dx
\]

\[
= 2 \cos(y) \, u(y)
\]
Similarly, one obtains: \[
\frac{\delta}{\delta u(x)} \int_{\mathbb{R}} f(y) u(x)^n \, dy = f(x) + u(x)^{n-1}
\]

- Functional derivatives act on polynomials (and suitable power series) in \(u\) by removing the integral and reducing the power in \(u\) by one, as expected from ordinary derivatives.

**Remark:**
- Worked with \(u(x)\).
- * Would obtain same result if we used any other continuous or discrete basis of \(L^2\).
- E.g., other basis (continuous): \(e^{ipx}\), i.e. use \(\hat{u}(p)\)
- E.g., other basis (countable): \(H_n(x) x^2\), i.e., use \(\hat{u}_n\)
- Hermite polynomials

- Functional differentiation is, up to basis change, usual differentiation.

**Note:** How can \(L^2[0,1]\) have countable basis? Recall: \(L^2[0,1]\) consists not of functions, but of equivalence classes of functions.

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**Example application 1:**

**Schrödinger equation of QFT now well defined:**

**QM:**
\[\hat{\Psi} = \hat{p} \hat{\Psi} + i \hat{\tau} \hat{\Psi} \quad \text{with} \quad \hat{\Psi}(x) \equiv \Psi(x, t)\]

**QFT:**
\[\hat{\phi}(x) = \frac{\hat{p}(x)}{\hat{m}} + i \frac{\hat{\tau}}{\hat{m}} \hat{\phi}(x) + W(\hat{\phi}(x)) \quad \text{with} \quad \hat{\phi}(x) \equiv \phi(x, t)\]

**Example:** \(W(\phi) = \frac{1}{4} \phi^4(x)\)

In general, \(W(\phi)\) also contains other fields.

**QM:**
Example of complete set of commuting s. adj. operators:
\[\{\hat{\xi}_j, \hat{\xi}^*_k\}_{j, k = 1}^3\]

**QFT:**
Example of complete set of commuting s. adj. operators:
\[\{\hat{\phi}(x)^2\}_{x \in \mathbb{R}^3}\]
QM: The joint eigenbases \( \{ |q_i, z_i^\mu\rangle \} \) of the \( \hat{q}_i, \hat{z}_i^\mu \) obeys:
\[
\hat{q}_i |q_i, z_i^\mu\rangle = q_i |q_i, z_i^\mu\rangle
\]

QFT: The joint eigenbases \( \{ |\psi(x)\rangle \} \) of the \( \hat{\psi}(x) \) obeys:
\[
\hat{\psi}(x) |\psi(x)\rangle = \psi(x) |\psi(x)\rangle
\]

QM: Wave function of a state \( |\psi(x)\rangle \in \mathcal{H} \) in position eigenbases:
\[
\psi(q, z^\mu, t) = \langle q, z^\mu | \Psi(x) \rangle \quad \text{(like } \psi(q) = \langle q | \Psi(x) \rangle \text{)}
\]

QFT: Wave functional of a state \( |\phi(x)\rangle \in \mathcal{F} \) in field eigenbases:
\[
\Psi[\phi(x)] = \langle \phi(x) | \Psi(x) \rangle
\]

Simplified notation:

QM: \( \psi(q, t) = \langle q | \Psi(x) \rangle \)

QFT: \( \Psi[\phi(t)] = \langle \phi(t) | \Psi(x) \rangle \)

QM: Representation of \( \hat{q}_i, \hat{p}_i \) obeying \( [\hat{q}_i, \hat{p}_j] = i \delta_{ij} \) in \( q \) eigenbases:
\[
\hat{q}_i : \psi(q, t) \rightarrow q_i \psi(q, t)
\]
\[
\hat{p}_i : \psi(q, t) \rightarrow -i \frac{\partial}{\partial q_i} \psi(q, t)
\]

QFT: Representation of \( \hat{\phi}(x), \hat{\pi}(x) \) obeying \( [\hat{\phi}(x), \hat{\pi}(y)] = i \delta(x-y) \) in \( \phi \) eigenbases:
\[
\hat{\phi}(x) : \Psi[\phi(t)] \rightarrow \phi(x) \Psi[\phi(t)]
\]
\[
\hat{\pi}(x) : \Psi[\phi(t)] \rightarrow -i \frac{\partial}{\partial \phi(x)} \Psi[\phi(t)]
\]

Exercise: Verify that \( \partial_t, \hat{\phi}(x) \) obey the CCRs.
QM: Schrödinger equation:

\[ i \frac{d}{dt} \Psi(q, t) = \sum_{j=1}^{n} \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial q_j^2} \Psi(q, t) + V(q, t) \Psi(q, t) \]

Recall: It is to be solved for all \( q \)

QFT: Schrödinger equation:

\[ i \frac{d}{dt} \Psi[\phi, t] = \left( \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial \phi(x)^2} + \frac{1}{2} \phi(x)(m^2 - \Delta)\phi(x) + W(\phi(x), t) \right) \Psi[\phi, t] \]

Recall: It is to be solved for all \( \phi \)

Remark: With \( W \) it can be solved only perturbatively.

Exercise: Set \( W = 0 \). Fourier transform to be variables in box regularization. Verify that the wave functional \( \Psi_0 \) of the vacuum state obtained before does obey the Schr. eqn.

Example application 2: The functional Legendre transform!

Motivation? We will need to determine in curved space:

What becomes of: \( \hat{\Pi}(x, \tau) = \hat{\phi}(x, \tau) \) ?

Problem? Time is proper coordinate in Hamiltonian formalism.

* But the formalism must be coordinate system independent to fit general relativity (G.R).

* Now, for example, \( \hat{\Pi}(x, \tau) = \frac{d}{d\tau} \hat{\phi}(x, \tau) \) is not the same as \( \hat{\Pi}(x, \tau) = \frac{d}{d\tau} \hat{\phi}(x, \tau) \) for arbitrary \( \tau(t) \):

\[ \hat{\Pi}(x, \tau) = \frac{d}{d\tau} \hat{\phi}(x, \tau(t)) = \frac{d}{d\tau} \hat{\phi}(x, \tau(t)) \frac{d\tau(t)}{dt} \neq \frac{d}{d\tau} \hat{\phi}(x, \tau) \]
Strategy: 1. Transform to coordinate-independent Lagrange formalism.
   2. Move from special to general relativity (GR).
   3. Transform GR result back to Hamilton formalism.
   4. Apply 2nd quantization.

SR, 1st Q Hamiltonian formalism \[\rightarrow\] Lagrange formalism

GR, 1st Q Hamiltonian formalism \[\rightarrow\] Lagrange formalism
\[\text{(as outlined already)}\]

GR, 2nd Q Hamiltonian formalism \[\rightarrow\] Lagrange formalism
\[\text{(both integral over)}\]

The Legendre transform (LT):

- Assume given a function, \( F(u) \).
- Define a new variable \( w(u) \):
  \[w(u) := \frac{dF}{du}\]  (I)
- Assume that (I) can be solved to obtain: \( u(w) \)
  (that's ok if \( F \) is convex, say \( F''(u) > 0 \) for all \( u \))
- The Legendre transform of \( F \) is a new function, \( G \), of \( w \):
  \[F(u) \xrightarrow{LT} G(w)\]
- Namely:
  \[G(w) := wu(w) - F(u(w))\]
Proposition:

\[(LT)^2 = \text{id}\]

Proof:

1. Define a new variable: \(v(w) := \frac{\partial G(w)}{\partial w}\)
2. In fact:

\[
v(w) = \frac{2}{\partial w} \left( w u(w) - F(u(w)) \right)
= u(w) + \frac{w \partial u(w)}{\partial w} - \frac{\partial F(u(w))}{\partial u(w)} \frac{\partial u(w)}{\partial w}
= u \quad \checkmark \]

Therefore \(LT^2\) yields \(F(u) \xrightarrow{LT} G(w) \xrightarrow{LT} H(v)\) with:

\[H = v w - G = v w - (wu - F) = F\]

Example:

* Consider \(f(x, y, z) := ax^2y\)

* Find \(LT\) with respect to \(y\) (i.e., while treating \(a, x\) as "spectator variables"):

\[f(x, y, z) \xrightarrow{LT} g(a, \beta, c)\]

* Define \(\beta(a, \beta, c) := \frac{\partial f}{\partial y} = ax^2\)

* Invert: \(b(a, \beta, c) = c \frac{\ln \frac{\beta}{a c}}{x^2}\)

* Legendre transform:

\[f(x, y, z) \xrightarrow{\text{LT}} g(a, \beta, c)\]

\[g(a, \beta, c) := \beta b(a, \beta, c) - f(a, b(a, \beta, c), c)\]

\[g(a, \beta, c) = \frac{\beta}{c} \ln \frac{\beta}{ac} - a \frac{\beta}{c} \ln \frac{\beta}{ac} = \frac{\beta}{c} \ln \frac{\beta}{ac} - \frac{\beta}{c}\]
Case of countably many variables:

- How to define
  \[ F(\xi u_j, \xi z) \xrightarrow{LT} G(\xi w_j, \xi z) \]

- Define: \[ w_j := \frac{\partial F}{\partial u_j} \]

- Assume we can invert to obtain:
  \[ u_j(\xi w, \xi z) \]

- Define:
  \[ G(\xi w, \xi z) := \sum_j w_j u_j(\xi w, \xi z) - F(\xi u_j(\xi w, \xi z), \xi z) \]
  (we may also allow for spectator variables)

Case of uncountably many variables:

- How to define
  \[ F[\xi u(x), \xi z_{x \in \mathbb{R}^n}] \xrightarrow{LT} G[\xi w(x), \xi z_{x \in \mathbb{R}^n}] \]

- Define: \[ w(x) := \frac{\delta F}{\delta u(x)} \]

- Assume we can solve to obtain:
  \[ u(x, \xi w(x), \xi z_{x \in \mathbb{R}^n}) \]

- Define:
  \[ G[\xi w(x), \xi z_{x \in \mathbb{R}^n}] := \int_{\mathbb{R}^n} w(x) u(x, \xi w(x), \xi z_{x \in \mathbb{R}^n}) dx - F[\xi u(x, \xi w(x)), \xi z_{x \in \mathbb{R}^n}] \]

- Note: We still have that \( LT \circ LT = id \).
Application to CM:

* Assume the Hamiltonian $H(q, p)$ is given.

* Hamilton equations for arbitrary $f(q, p)$:

$$\dot{f}(q, p) = \frac{\partial}{\partial q} f(q, p) H(q, p) + \frac{\partial}{\partial p} f(q, p) \dot{H}(q, p)$$

Recall, Poisson bracket $\{q, p\} = 1$

See my notes to denseg 893.

Dirac showed: Quantization consists in keeping the Poisson bracket definition and the Hamilton equations unchanged while allowing $q, p$ noncommutativity in such a way that the Poisson algebra structure stays. This fixes noncommutativity to be $\hat{q} \hat{p} = \frac{1}{i\hbar}$ and $\{q, p\} = \hbar$

* From this, one can prove the eqns of motion for $q, p$:

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

* Legendre transform:

$$H(q, p) \xrightarrow{LT} L(q, b) \quad (q \text{ is spectator})$$

* Example: $H(q, p) = \frac{p^2}{2} + V(q)$.

Then:

$$b = \frac{p}{q} \text{ and } \dot{q} = b$$

$$\Rightarrow L(q, b) = b p(q, b) - H(q, p(q, b)) = b p(q, q) - H(q, p(q, q)) = L(q, q)$$

Proposition:

The equations of motion (EoM) now take the form:

$$b = q \quad \text{ and } \quad \frac{\partial L}{\partial q} = \frac{d}{dt} \frac{db}{dt} \quad (Euler-Lagrange equation)$$

Proof: Exercise

Example:

$$H = \frac{q^2}{2m} + \frac{\omega^2 q^4}{2} \xrightarrow{LT} L[q, b] = \frac{1}{2} q^2 - \frac{\omega^2}{2} q^2$$

$$\hat{q} = \frac{e}{m}, \quad \hat{p} = -\omega^3 \hat{q} \quad \text{ and } \quad b = q$$
Application to CFT:

- Assume Hamiltonian $H(\phi, \pi)$ is given.
- Hamilton equation for arbitrary $f(\phi, \pi)$:
  \[
  \dot{f}(\phi, \pi, x, t) = \sum \frac{\delta f(\phi(x, t), \pi(x, t))}{\delta \phi(x, t)} \delta \phi(x, t)
  \]
  with:
  \[
  \delta \phi(x, t), \pi(x', t) \delta(x - x') = \delta^3(x - x')
  \]
- This yields the eqns of motion:
  \[
  \dot{\phi}(x, t) = \frac{\delta H}{\delta \pi(x, t)}, \quad \dot{\pi}(x, t) = -\frac{\delta H}{\delta \phi(x, t)} \quad (\text{EoM})
  \]
- Legendre Transform:
  \[H(\phi, \pi) \xrightarrow{\text{L.T.}} L(\phi, \pi)\]

Example: \[H = \int \frac{1}{2} \pi(x, t)^2 + V(\phi(x)) \, d^3x\]

\[S(x, t) := \frac{\delta H}{\delta \pi(x, t)} \quad \text{EoM}\]

Thus:

\[
L(\phi, \pi) = L(\phi, \pi(x, t)) = \int_{\mathbb{R}^3} f(x, t, \pi(\phi, \phi, x, t)) \, d^3x - H(\phi, \pi(\phi, x, t))
\]

Proposition: The eqns of motion (EoM) are equivalent to:

\[
\frac{\delta L}{\delta \phi(x, t)} = \frac{\partial}{\partial t} \left( \frac{\delta L}{\delta \pi(x, t)} \right) \quad \text{Exercise: Check}
\]

Enter Lagrange eqn.
Example:

\[ H(\phi, \pi) = \int_{\mathbb{R}^3} \left( \frac{\pi^2(x,t)}{2} + \frac{1}{2} \phi(x,t)(m^2 - \Delta) \phi(x,t) \right) d^3x \]

yields:

\[ \dot{\phi}(x,t) = \pi(x,t) \quad \ddot{\pi}(x,t) = -(m^2 - \Delta) \phi(x,t) \]

i.e.: \[ \ddot{\phi} - \Delta \phi + m^2 \phi = 0 \quad \text{K.C. eqn.} \]

After Legendre transform:

\[ L(\phi, \dot{\phi}) = \int_{\mathbb{R}^3} \left( \frac{\dot{\phi}(x,t)^2}{2} - \frac{1}{2} \phi(x,t)(m^2 - \Delta) \phi(x,t) \right) d^3x \]

yields directly:

\[ -(m^2 - \Delta) \phi + \dot{\phi}^2 = 0 \]

Remark: (see arxiv:0810.4293)

a) Solving a quantum theory is to do a Fourier transform.

b) The lowest order approximation is the Legendre transform.

c) The Legendre transform yields the solution to the classical theory.

a) Consider the path integral in QFT

(covers in detail later in this course)

\[ e^{-iW[\phi]} = \int \mathcal{D}[\phi] e^{i\int_{x} \phi(x) \bar{\psi}(x) dx} \]

\[ \Rightarrow e^{-iW[\phi]} \text{ is the Fourier transform of } e^{iS[\phi]} \]
b) The integrand contributes most, where it is stationary:

\[ e^{-iW[J]} = e^{-iS[\phi] - i\int J \phi \, dx} \]

for that \( \phi \) for which

\[ \frac{\delta}{\delta \phi} \left( iS[\phi] - i\int J \phi \, dx \right) = 0 \]

Condition of stationarity of the phase

i.e.

\[ W^{\text{approx}}[J] = \int J \phi \, dx - S'[\phi] \]

where \( \phi \) obeys

\[ \frac{\delta S}{\delta \phi} (x) = J(x) \]

i.e. \( W^{\text{approx}}[J] = \int J \phi[\phi] \, dx - S'[\phi][J] \) where \( \phi[J] \) follows from:

\[ \frac{\delta S}{\delta \phi} (x) = J(x) \]

i.e. it's the Legendre transform!

c) So what is knowing \( W^{\text{approx}}[J] \) good for?

Consider \( S^{\text{total}}[\phi] = S'[\phi] - \int J \phi \, dx \).

As a classical action, it describes a classical field \( \phi(x) \) driven by an external "driving force" \( J(x) \):

\[ \frac{\delta S^{\text{total}}}{\delta \phi} = 0 \quad \text{i.e.,} \quad \frac{\delta S'}{\delta \phi} (x) = J(x) \quad \text{(Eom)} \]

To solve the classical equations of motion (Eom) is to find the field \( \phi(x) \) for any given driving \( J(x) \).

This is what \( W^{\text{approx}}[J] \) provides:

\[ \phi(x) = \frac{\delta W^{\text{approx}}[J]}{\delta J(x)} \]

Because:

\[ (\text{Legendre transform})^2 = 1 \]