Lect 4

Last time

- $\overset{\dim \le n}{\text{isotropic}}$, $\overset{\dim \ge n}{\text{coisotropic}}$, $\overset{= n}{\text{Lagrangian}}$ submanifolds in sympl. manifolds

M_{2n} $\qquad \underline{\omega_x(T_x N)}$, $\underline{(T_x N)^{\perp}}$ in $\underline{T_x^* M}$

$N \subset M$

- Variational b.c.: boundary terms vanish if b. cond $\gamma(t_1) \in L_1$, $\gamma(t_2) \in L_2$ are such that

| HJ action $\omega = d\alpha$

$$\alpha|_{L_1} = \alpha|_{L_2} = 0$$

$\omega = d\alpha \Rightarrow$

$$\omega|_{L_1} = \omega|_{L_2} = 0$$

$\Rightarrow L_1, L_2$ - isotropic

dim balance $\Rightarrow$ L_1, L_2 - $\underline{\text{Lagrangian}}$

<u>Conclusion</u>: variational b.c.

are α-exact Lagrangian submanif.

$\alpha|_{L_1} = \alpha|_{L_2} = 0$, L_1 & L_2 -

- Lagrangian

- Giving properties of solutions to EL equations.
  - Lagr. action
  - HJ action

Lagrangian b.c. should come in a family

M

fibered by Lagr. submanifolds

Def. A variational b.c. is a fibration

$$\begin{array}{c} M_{2n} \\ \pi \big\downarrow \\ B_n \end{array}$$

$\leftarrow$ generic fiber is an α-exact Lagrangian submanifold

<u>Example</u>: $\mathcal{M} = T^*Q_n \leftarrow T_q^*Q_n$

$$\begin{array}{c} T^*Q_n \\ \downarrow \\ Q_n \end{array}$$

$\omega = d\alpha$,
locally
$\alpha = \sum_{i=1}^n p_i dq^i$, $\qquad \alpha\Big|_{T_q^*Q_n} = 0$

Lagrangian fibration by α-exact submanifolds.

- Quantization
  - deformation quantization (analytic def. quantization)
  - (formal deform. quantization $\mathbb{C}[[\hbar]]$)
  - <u>Examples</u>: ...

<u>Quantum algebra of observables</u>

- A family of associative algebras

- (deform. quantization of a classical alg. of observables / $\mathbb{C}$) $A_\hbar$
- $*$ - algebras
  - $(\lambda a)^* = \bar{\lambda} a^*$
  - $(ab)^* = b^* a^*$
- $*$ - representation of $A_\hbar$

$\pi : A_\hbar \longrightarrow End(H_\hbar)$

$H_\hbar$ - vector space with Hermitian structure $(\cdot , \cdot)$

$\pi(a^*) = \pi(a)^+$

Herm. conjugate

$(A^+ u, v) = (u, Av)$

<u>**Def.**</u> Observables, the space of observables = real vector space

(O_1, O_2, $aO_1 + bO_2$ is also observ.

of $a, b \in \mathbb{R}) \subset A_h$ of fixed points of $*$. $0^* = 0$.

State

Classically: a probabilistic state on (M_{2n}, ω) is a probability measure on M_{2n}.

$$\mu(M_{2n}) = 1, \quad \underset{U \subset M_{2n}}{\mu(U) \geq 0}$$

$$\mu(U) = \int_U d\mu \, ,$$

Expectation value of a classical observable f in the state μ:

$$\mathbb{E}_\mu(f) = \int_M f \, d\mu = \langle f \rangle_\mu$$

Quantum: A quantum state

is a linear map $\ell : A_h \to \mathbb{C}$

- $\ell(a) \in \mathbb{R}$, if $a^* = a$ (an observable)
- $\ell(a^* a) \geq 0$, ($= 0$ iff $a = 0$)
- $\ell(1) = 1$

<u>The density matrix construction</u>:

A_h, $\pi : A_h \to H$,

Assume we have a <u>trace class Hermitian operator</u> $\hat{\rho} : H \to H$

- $\hat{\rho} \geq 0$, ($\mathrm{spec}(\hat{\rho}) \geq 0$) $\hat{\rho}^{+} = \hat{\rho}$
- $\mathrm{tr}(\hat{\rho}) = 1$ (if discrete $\sum_i \lambda_i = 1$)

$0 \leq \lambda_i \leq 1$

such $\hat{\rho}$ is called a density matrix

Corresponding state $\varrho_{\hat{\rho}}$:

$$\boxed{\varrho_{\hat{\rho}}(a) = \mathrm{tr}_{\mathcal{H}}\left(\pi(a)\hat{\rho}\right)}$$

Examples :

(i) A_h - a matrix algebra
(f.d. QM $\to$ quantum inform)

H - f.dim. Hilbert space
(Hermitian)

(ii) $A_h = \mathrm{Diff}\left(-i\frac{\partial}{\partial q}, q\right)$

$\mathcal{H} = L^2(Q_n)$ assuming there is a volume form on Q_n or a density. ($\frac{1}{2}$- densities)
will return to this

Def. If $\hat{\rho}_\psi = P_\psi$, $\psi \in H, \|\psi\|=1$
$(\psi,\psi)=1$

$P_\psi(\varphi) = (\psi,\varphi)\,\psi$

it is called a <u>pure state</u>.

ψ and $e^{i\alpha}\psi$ correspond to the same density matrix $\Rightarrow$

Pure states $\longleftrightarrow$ H/S^1

<u>Assume H is finite dim</u> : $A = End(H)$

a – an observable, $a^* = a$,

$$a = \sum_i a_i P_{\varphi_i}, \quad \varphi_i \text{ - eigenvectors}$$

spectral decomp. of a

$$\langle a \rangle_{\hat{\rho}_\psi} = tr(\hat{\rho}_\psi a) = \sum_i a_i \, tr(P_\psi P_{\varphi_i})$$

$$= \boxed{\sum_i a_i |(\psi, \varphi_i)|^2}$$

$$\sum_i P_{\varphi_i} = 1 \Rightarrow \boxed{\sum_i |(\psi, \varphi_i)|^2 = 1}$$

Probabilistic interpretation:

$|(\psi, \varphi_i)|^2$ = the probab that the sytem being in a state P_φ will be observed with $a = a_i$

__Def.__ $\hat{\rho}$ is a mixed state if

$$\hat{\rho} = \sum_\alpha \rho_\alpha P_{\psi_\alpha}$$

for some ψ_α, $\sum_\alpha \rho_\alpha = 1$, $0 \leq \rho_\alpha \leq 1$

$$\mathbb{E}_{\hat{\rho}}(a) = tr(\hat{\rho} a) =$$

$$= \sum_{\alpha, i} \rho_\alpha a_i |(\psi_\alpha, \varphi_i)|^2$$

__Uncertainty principle__

$\hat{\rho}$ - a state on quantum algebra of observable $\mathcal{A}$. $\hat{\rho} : \mathcal{H} \circlearrowleft$ (density matrix)

$$\Delta_{\hat{\rho}}(a) = \mathbb{E}_{\hat{\rho}}\left(\left(a - \mathbb{E}_{\hat{\rho}}(a)\right)^2\right) \in \mathbb{R} \text{ if } a^* = a$$

The dispersion (variance) of a in a state ρ. (all quantum)

Thm. $a, b : H \circlearrowleft$ two observables

$$\boxed{\Delta_{\hat\rho}(a)^2 \, \Delta_{\hat\rho}(b)^2 \geq \frac{1}{4} \Delta_{\hat\rho}(i[a,b])^2}$$

$a^* = a$ $\quad$ $b^* = a$

$[a,b]^* =$
$= (ab - ba)^* =$
$= b^* a^* - a^* b^* =$
$= -[a^*, b^*] =$
$= -[a,b]$

Proof. H.W. hints:

1) assume $\hat\rho = P_\psi$

consider

$$((a + i\alpha b)\psi, (a + i b)\psi) \geq 0$$

quadratic in α $\Rightarrow$ discrim. ≤ 0

2) consider mixed states. ∎

Time evolution

1) of observables.

a - an observable

To define a time evolution of a quantum system we have to define the Hamiltonian of the quantum system.

$\boxed{\hat{H} : \mathcal{H} \to \mathcal{H}}$, Hermitical operator (an observable represented in $\mathcal{H}$)

$\hat{H}^* = \hat{H}$

Physical meaning = the energy operator (eigenvalues of $\hat{H}$ = energy levels)

Def. $a(t)$ = the time evolution of a

- $-i\hbar \dfrac{\partial a(t)}{\partial t} = [\hat{H}, a(t)]$
- $a(0) = a$

$$\boxed{a(t) = U_t \, a \, U_t^{-1}}, \quad U_t^* = U_t^{-1} \text{ unitary}$$

$U_t = e^{-i\frac{\hat{H}t}{\hbar}}$ = the time propagator of the system

The evolution of states:

$\hat{\rho}_t$ – the evolution of the density matrix $\hat{\rho}$

$$\mathrm{Tr}(\hat{\rho}_t a) \overset{\text{def}}{=} \mathrm{Tr}(\hat{\rho}\, a_t)$$

from here: $\mathrm{Tr}(\hat{\rho}\, a_t) = \mathrm{Tr}(\hat{\rho}\, U_t a U_t^{-1})$

$$= \mathrm{Tr}(U_t^{-1} \hat{\rho}\, U_t\, a)$$

$$\Rightarrow \boxed{\hat{\rho}_t = U_t^{-1} \hat{\rho}\, U_t}$$

<u>Semiclassical limit</u>:

$h \to 0$ (mathematically)

$h \ll$ characteristic scales of the system.

A_h = the quantum algebra of

observable quantizing $C^\infty(M_{2n})$

$$a *_\hbar b = a \cdot b + O(\hbar)$$

$\uparrow$ in $C^\infty(M_{2n})$ as $\hbar \to 0$

$$a *_\hbar b - b *_\hbar a = i\hbar \{a, b\} + O(\hbar^2)$$

Loosely : $\boxed{[a, b] = i\hbar \{a, b\} + O(\hbar^2)}$

Time evolution of elements of $A_\hbar$ (of observables)

$$a(t) = e^{-\frac{iHt}{\hbar}} a \, e^{\frac{iHt}{\hbar}}$$

$$\boxed{e^{B} A e^{-B} = \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{[B[B \cdots [B, A] \cdots]}_{n}}$$

(id. of formal power series in B)

Apply it to the case $A = a$,

$$B = -\frac{iHt}{\hbar}$$

$$\underbrace{[B[B\cdots[B,A]\cdots]}_{n} = \left(\frac{-it}{\hbar}\right)^n [H\cdots[H,a]\cdots]$$

$$\xrightarrow[\hbar\to 0]{} \left(\frac{-it}{\hbar}\right)^n (i\hbar)^n \{H_{cl}\}\cdots\{H_{cl},a_{cl}\}\cdots\} \, (1+O(\hbar))$$

$$\boxed{a(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\{H_{cl}\cdots\{H_{cl},a_{cl}\}\}(1+O(\hbar))}$$

$a = a_{cl}$ as an element of the algebra observables

$$a_{cl}(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\{H_{cl}\cdots\{H_{cl},a_{cl}\}\}$$

$$\Updownarrow$$

h.w.

$$\frac{d}{dt}a_{cl}(t) = \{H_{cl}, a_{cl}(t)\}$$

Hamilton equations for classical observables.

Quantum evol. $\xrightarrow[\hbar\to 0]{}$ Classical Hamilt evolution

Trace class: $\operatorname{Tr}(A) < \infty$

Quantum mechanics in $\mathbb{R}^n$

$$\hat{H} = H\left(-i\hbar\frac{\partial}{\partial q}, q\right)^{\text{symm.}} \leftarrow H(p,q) \leftarrow \text{symbol of}$$

differentual operator with smooth coefficients, Hermitian

$$\mathcal{H} = L_2(\mathbb{R}^n), \quad (\varphi,\psi) = \int_{\mathbb{R}^n} \overline{\varphi}(q)\psi(q)\,d^nq$$

Hermitian:

$$(H\varphi,\psi) = (\varphi, H\psi)$$

$$\left(-i\hbar\frac{\partial}{\partial q_j}\varphi, \psi\right) = \left(\varphi, -i\hbar\frac{\partial}{\partial q_j}\psi\right)$$

$f(q)\left(-i\hbar\frac{\partial}{\partial q_j}\right)$ is not Hermitian

$$\left(f(q)\left(-i\hbar\frac{\partial}{\partial q_j}\right)\right)^* = \left(-i\hbar\frac{\partial}{\partial q_j}\right)f(q) \neq$$

$$\neq f(q)\left(-i\hbar\frac{\partial}{\partial q_j}\right)$$

in order to have Hermitian we have to symmetrize (Weyl)

$H(p,q)$ = the symbol of the differential operator $H(-i\hbar\frac{\partial}{\partial q}, q)^{symm}$

$\uparrow$ Hermitian $\qquad \hat{H}_{Schr} = -\Delta + U(q)$

$\psi \in L^2(\mathbb{R}^n)$, $\quad (\psi,\psi) = \int_{\mathbb{R}^n} |\psi(q)|^2 d^n q$ finite

$\hat{\rho}_\psi$ - pure state with $(\psi,\psi)=1$.

$\hat{\rho}_\psi$ - the orthogonal projection in $L^2(\mathbb{R}^n)$ to ψ

$$A = A(-i\hbar\frac{\partial}{\partial q}, q)^{symm}$$

$$\mathbb{E}_{\hat{\rho}_\psi}(A) = Tr(\hat{\rho}_\psi A) = (A\psi, \psi)$$

$$= \int_{\mathbb{R}^n} \overline{\psi}(q)\, \overset{\text{symbol}}{A}(\underbrace{-i\hbar \tfrac{\partial}{\partial q}}_{\to 0}, q)\, \psi(q)\, d^n q$$

Take the limit $\hbar \to 0$, ψ is smooth

$$\mathbb{E}_{\hat{\rho}_\psi}(A) \xrightarrow{\hbar \to 0} \int_{\mathbb{R}^n} \overline{\psi}(q)\, A(0,q)\, \psi(q)\, d^n q$$

$$= \boxed{\int_{\mathbb{R}^n} A(0,q)\, |\psi(q)|^2\, d^n q}$$

a distrib. supported on $p=0$ with $\rho = |\psi|^2$

with $\boxed{\int_{\mathbb{R}^n} |\psi(q)|^2 dq = 1}$

Classical prob. state is a probab. measure on $\mathcal{M}_{2n} = \mathbb{R}^{2n} = \{(p,q)\}$ and if $A(p,q)$ – classical observable then

$$\langle A \rangle_\mu = \boxed{\int_{\mathbb{R}^{2n}} A(p,q)\, d\mu(p,q)}$$

Digression. $\mathbb{R}^N$, $\delta_{x_0}(y)$

$$\int_{\mathbb{R}^N} f(y)\,\delta_{x_0}(y)\,d^N y \overset{def}{=} f(x_0)$$

$S_k \subset \mathbb{R}^N$, contin. measure $d\mu_S$ on S

$d\mu_S =$

$= \rho(u)\,du_1 \dots du_k$

$\{u_i\}$ - local coord. on S.

Define $\delta_{(\rho)}$ - measure on $\mathbb{R}^n$ supported on S_k

$$\int_{\mathbb{R}^n} f(y)\,\underbrace{\delta_{(\rho)}(y)}_{\substack{\parallel \\ \int_S \delta_{x(u)}(y)\,\rho(x(u))\,d^k u}}\,d^N y \overset{def}{=} \int_{S_k} f(x(u))\,\rho(u)\,d^k u$$

$S_k \hookrightarrow \mathbb{R}^N$

$u \mapsto x(u)$

u - intrinsic coord.

<u>Conclusion</u>. as $h \to 0$

$$\mathbb{E}_{\hat{\rho}_\psi}(\hat{A}) \xrightarrow{h\to 0} \int_{\mathbb{R}^{2n}} A(p,q)\, \mu(p,q)\, d^n p\, d^n q$$

$$\mu(p,q) = \delta_0(p)\, |\psi(q)|^2$$ supported on $p=0$

$$\int_{U\subset\mathbb{R}^{2n}} \mu\, dp\, dq \geq 0$$

$$\int_{\mathbb{R}^{2n}} \mu\, dp\, dq = \int_{\mathbb{R}^n} |\psi|^2 d^n q = 1$$

$$-ih\frac{\partial}{\partial q_j}\psi(q) \to 0, \quad h\to 0$$

To change it assume:

$$\psi(q) = e^{\frac{i}{h}f(q)}\varphi(q)$$

f fixed, φ fixed ($h \to 0$)

$$-ih\frac{\partial}{\partial q_j}\underline{\psi(q)} \xrightarrow[h\to 0]{} \frac{\partial f}{\partial q_j}(q)\,\underline{\psi(q)},$$

asymptotically

H.W.

Show that

$$\mathbb{E}_{\rho_\psi}(A) \xrightarrow[h\to 0]{} \int_{\mathbb{R}^n} A\left(\frac{\partial f}{\partial q}, q\right) |\psi(q)|^2 \, d^n q$$

the probab. measure supported on $\mathcal{L}_f = \{(df(q), q)\} \in T^*\mathbb{R}^n = \mathbb{R}^{2n}$

H.W. Describe states which would converge as $h \to 0$ to

$$\int_{\mathbb{R}^{2n}} A(p,q)\, \rho(p,q)\, d^n p\, d^n q$$

smooth