Lecture 4

States in Hamiltonian mechanics

Def. A state on $C^\infty(M)$ is a probability measure on M.

Expectation value of $f \in C^\infty(M)$ on μ:

$$\langle f \rangle_\mu = \int_M f \, d\mu$$

Examples 1) State supported at $x_0 \in M$

For a subset $U \subset M$

$$\mu_{x_0}(U) = \begin{cases} 1, & x_0 \in U \\ 0, & x_0 \notin U \end{cases}$$

$$\langle f \rangle_{\mu_{x_0}} = f(x_0)$$

2) A state supported on $N \subset M$

with probability measure ν on N.

$$\langle f \rangle_{\nu_N} = \int_N f(x)\, d\nu$$

3) A state with density $\rho \in C^\infty(M_{2n})$. Given a density function, we can use the symplectic volume form to define the measure

For $U \subset M_{2n}$ with $\dim(U) = 2n$

$$\mu_\rho(U) = \int_U \rho(x) \wedge^n \omega_x$$

where $\rho(x) \geq 0$, $\int_M \rho(x) \wedge^n \omega_x = 1$.

Note that for such measure $\mu_\rho(U) = 0$ if $U \subset M$ with $\dim(U) < 2n$,

Time evolution of classical states

Let f_t be the evolution of the observable $f \in C^\infty(M_{2n})$,

$$f_t(x) = f(x(t))$$

where $x(t)$ is the flow line of the evolution vector field v_H passing through x at time t.

The evolution of a state μ is defined as

$$\langle f_t \rangle_\mu = \langle f \rangle_{\mu_t}$$

If $\langle f \rangle_\mu = \int_{M_{2n}} \rho(x) f(x) \wedge^n \omega$

then $\rho_t(x) = \rho(x(-t))$, i.e.

$$\frac{d\rho_t}{dt} = -\{H, \rho_t\}, \quad \rho_0 = \rho$$

Quantum states

Def. A state on a quantum algebra of observables is a normalize nonegative linear functional $\ell : A \to \mathbb{C}$, i.e.

- $\ell(a) \in \mathbb{R}$ if $a^* = a$, i.e. if a is an observable
- $\ell(a^* a) \geq 0$ and $\ell(a^* a) = 0$ iff $a = 0$
- $\ell(1) = 1$, normalization.

If $\pi : A \to \mathrm{End}(V)$ is a $*$-representation of the algebra of observables on can construct such functionals using density matrices.

<u>Def.</u> A Hermitian operator on a Hilbert space V is a <u>density matrix</u> if

- $\hat{\rho} \geq 0$
- $\mathrm{tr}(\hat{\rho}) = 1$

<u>Remark.</u> The last property assumes that $\hat{\rho}$ is a trace class operator, i.e. that $\mathrm{tr}(\hat{\rho})$

exists.

Now we can construct a state on the quantum algebra of observables A as

$$\ell_{\hat{\rho}}(a) = tr(\hat{\rho}\,\pi(a))$$

Clearly $\ell_{\hat{\rho}}(a) \in \mathbb{R}$ if $a^* = a$, $\ell_{\hat{\rho}}(aa^*) \geq 0$ and $\ell_{\hat{\rho}}(1) = 1$ and if $\ker(\pi) = \{0\}$ it satisfies the property $\ell_{\hat{\rho}}(aa^*) = 0$ iff $a = 0$.

Thus

<u>Proposition</u> A density matrix on a faithful representation ($\ker(\pi) = 0$) defines a state.

<u>Remark</u>. If $\ker(\pi) \neq 0$, $\ker(\pi) \subset A$ is a two sided ideal and $\hat{\rho}$ defines a state on $A/\ker(\pi)$.

Let $\psi \in V$, $\hat{\rho} = P_\psi$ be the orthogonal projection to ψ:

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

Here we assume that $(\psi, \psi) = 1$.

<u>Def.</u> The state P_ψ is the pure state corresponding to vector $\psi \in V$.

It is clear that pure state corresponding to ψ and $e^{i\alpha}\psi$ are the same. Thus we have a bijection

$$(\text{Pure states}) \longleftrightarrow V/S^1$$

Suppose that A is an observable acting on V, i.e. a Hermitian operator on V. If it has discrete spectrum we have the spectral decomposition

$$A = \sum_i a_i P_{\psi_i}$$

where a_i are eigenvalues and ψ_i are corresponding normalized eigenvectors.

For the identity operator we have:

$$I = \sum_i P_{\psi_i}$$

If ψ is a normalized vector,

$$1 = (\psi, \psi) = \sum_i (\psi, P_{\psi_i} \psi) = \sum_i |(\psi, \psi_i)|^2$$

Thus $|(\psi, \psi_i)|^2$ is a probability distribution on the set of eigenvalues of A.

For the expectation value of A in a pure state $\hat{\rho} = P_\psi$ we have:

$$\langle A \rangle_{P_\psi} = tr(\hat{\rho}_{P_\psi} A) = (\psi, A\psi) =$$

$$= \sum_i a_i |(\psi, \psi_i)|^2$$

Thus, this expectation value is the usual expectation value of eigenvalues with repect to the distribution $|(\psi, \psi_i)|^2$.

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

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

$0 \le \rho_\alpha \le 1$, $\sum_\alpha \rho_\alpha = 1$ and $\{\varphi_\alpha\}$ are independent

Remark. If the sum is infinite, it should converge in a proper sense.

Remark. We can alway apply an orthogonalization procedure and assume that $\{\varphi_\alpha\}$ are orthogonal.

For the expectation value of an observable we have

$$\langle A \rangle_{\hat{\rho}} = \sum_\alpha \rho_\alpha (\varphi_\alpha, A\varphi_\alpha) =$$

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

This means the observable A has the probability $tr(\hat{\rho} P_{\psi_i}) = \sum_\alpha \rho_\alpha |(\varphi_\alpha, \psi_i)|^2$ of having value a_i it the state $\hat{\rho}$. The probability to find the system in a pure state P_{φ_α} and for A to have value a_i is

$$p_\alpha |(\varphi_\alpha, \psi_i)|^2$$

<u>Uncertainty principle</u>

Let $\hat{\rho}$ be a density matrix and A be an observable. The dispersion, or variance, of the distribution of eigenvalues of A in the state $\hat{\rho}$ is

$$\Delta_{\hat{\rho}}(A) = \left\langle \left(A - \langle A \rangle_{\hat{\rho}}\right)^2 \right\rangle_{\hat{\rho}}$$

Now let and A and B be two observables.

<u>Theorem</u>

$$\Delta_{\hat{\rho}}(A)^2 \, \Delta_{\hat{\rho}}(B)^2 \geq \frac{1}{4} \Delta_{\hat{\rho}}\left(i[A,B]\right)^2$$

Proof (HW) 1) Prove it for a pure state P_ψ.

Consider

$$((A+iB\alpha)\psi, (A+iB\alpha)\psi)$$

It is nonnegative quadratic polynomial therefore its discriminant is nonpositive. This gives the inequality.

2) Extend it to mixed states. ∎

Matrix quantum mechanics

Quantum algebra of observables is a matrix algebra, say $N\times N$ complex matrices. In other words, we have N-dimensional Hermitian space V, $(\cdot,\cdot): V\otimes V \to \mathbb{C}$, with an orthonormal basis $\{e_i\}$, $(e_i, e_j) = \delta_{ij}$. Linear operators $A: V\to V$ are represented by matrices

$$A e_i = \sum_j A_i^j e_j$$

The $*$-operation is the Hermitian conjugation

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

$$(A^+)_i^j = \overline{A}_j^i$$

Time evolution

Time evolution in classical Hamiltonian mechanics is generated by the Hamiltonian function of the system. It also determins the evolution of classical states.

Similarly quantum evolution is determined by the choice of a special quantum observable, quantum Hamiltonian $\hat{H}$. We can assume that $\hat{H}$ is a Hermitian operator acting in the Hilbert space.

The Hamiltonian $\hat{H}$ from the physical point of view is the energy operator. Its eigenvalues, and more general, its spectrum are possible energy values of the system.

Def. The time evolution of an observable A in a quantum system with the Hamiltonian $\hat{H}$ is

$$A(t) = U_t A U_t^{-1}$$

where $U_t = \exp(-\frac{i}{\hbar}\hat{H}t)$ is the evolution operator.

Equivalently, the evolution can be thaugh of as a solution to the Cauchy problem:

$$i\hbar \frac{\partial A(t)}{\partial t} = [\hat{H}, A(t)], \quad A(0) = A$$

The evolution operator U_t is also known as time propagator.

The evolution of a state with density matrix $\hat{\rho}$ is defined as $\{\hat{\rho}_t\}_{t>0}$

$$\mathrm{Tr}(\hat{\rho}_t A) = \mathrm{Tr}(\hat{\rho} A(t))$$

i.e.

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

or $\hat{\rho}_t$ can be regarded as the solution to the Cauchy problem

$$-i\hbar \frac{\partial \hat{\rho}_t}{\partial t} = [\hat{H}, \hat{\rho}_t], \quad \hat{\rho}_0 = \hat{\rho}$$

Semiclassical limit

Mathematically, this is the limit $\hbar \to 0$.

In physics $\hbar$ is a fundamental constant and taking $\hbar \to 0$ means that

$h \ll$ characteristic scales of the system

Assume that the quantum algebra of observables is $C^\infty(M_{2n})$ with a $*$-product. Even more specifically $M_{2n} = T^*Q_n$ and

$$A_h = \mathrm{Diff}_h(Q_n)$$

is a quantization of $C^\infty_{pol}(T^*Q_n)$.

We have $*_h$ on $C^\infty_{pol}(T^*Q_n)$ and

$$a *_h b = ab + O(h)$$

$$a *_h b - b *_h a = ih\{a, b\} + O(h^2)$$

Let $\hat{H} = P(-ih\frac{\partial}{\partial q}, q)$, its <u>symbol</u> $H(p,q) \in C^\infty_{pol}(T^*Q_n)$ is the function

$$P(p,q)\Big|_{h=0}.$$

We will has $\hat{H}$ is the Weyl quantization of $H(p,q) = \sum_k p^k f_k(q)$ if

$$\hat{H} = \sum_k \frac{1}{2}\left(\hat{p}^k f(q) + f(q)\hat{p}^k\right)$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial q}.$$

Let $\hat{A}$ be an observable,

$$\hat{A}_t = e^{-i\frac{\hat{H}t}{\hbar}}\hat{A}e^{i\frac{\hat{H}t}{\hbar}}$$

be its time evolution. Let A and H be symbols of $\hat{A}$ and $\hat{H}$ respectively, $A, H \in$ $\in C^\infty_{pol}(T^*Q_n)$.

<u>Theorem</u>.

$$\hat{A}_t = \sum_{n\geq 0}^{\infty} \frac{t^n}{n!}\{H\{H\cdots\{H, A\}\cdots\} + O(\hbar)$$

as $\hbar \to 0$.

<u>Proof</u>. HW. First prove the identity

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

$\blacksquare$

HW. Prove that $A_t = \sum_{n=0}^{\infty} \frac{t^n}{n!} \{H \dots \{H, A\} \dots\}$

is the solution to the Cauchy problem

$$\frac{dA_t}{dt} = \{H, A_t\}, \quad A_0 = A$$

Thus for the evolution of observables we proved that

$$\text{Quantum evolution} \xrightarrow[\hbar \to 0]{} \text{Classical evolution}$$

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

Let $H(p,q) \in C^\infty_{pol}(T^*Q_n)$ and $\hat{H} =$
$= H(-i\hbar \frac{\partial}{\partial q}, q)^{symm}$ be its Weyl quantization.

$$V = L^2(\mathbb{R}^n), \quad (\varphi, \psi) = \int_{\mathbb{R}^n} \overline{\varphi}(q) \psi(q) \, d^n q$$

Let $\hat{A} = A(-i\hbar \frac{\partial}{\partial q}, q)^{symm}$ be the Weyl quantization of the classical observable $A(p,q)$.

Consider the limit $h \to 0$ in states of such system.

1) Let $\hat{\rho} = P_\psi$ be the density matrix of a pure state with $\psi \in V$.

$$\langle A \rangle = (\psi, \hat{A}\psi) = \int_{\mathbb{R}^n} \overline{\psi}(q)\, A\left(-ih\frac{\partial}{\partial q}, q\right)^{sym} \psi(q)\, d^n q$$

When $h \to 0$

$$\langle A \rangle_{P_\psi} \to \int_{\mathbb{R}^n} \overline{\psi}(q)\, A(0,q)\, \psi(q)\, d^n q =$$

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

Since ψ is normalized:

$$(\psi, \psi) = \int_{\mathbb{R}^n} |\psi(q)|^2 d^n q = 1$$

we have a probability distribution $|\psi(q)|^2 d^n q$ on $\mathbb{R}^n$. Thus $\hat{\rho} = P_\psi$ converges to the classical state with

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

with $\rho(p,q) = |\psi(q)|^2 \delta(p)$

i.e. we have a classical state supported on Lagrangian submanifold $\{(0,q)\} \subset$ $\subset T^* Q_n$ (zero section) with the density $|\psi(q)|^2 d^n q$ on the zero section.

2) Similarly if we assume

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

$$\langle \hat{A} \rangle_{P_\psi} \to \int_{\mathbb{R}^n} A\left(\frac{\partial f(q)}{\partial q}, q\right) |\varphi(q)|^2 d^n q$$

This is the state supporten on the section $\mathcal{L}_f = \{(df(q), q)\} \subset T^*Q_n$ with the density $|\varphi(q)|^2 d^n q$

3) HW construct a state supporten on the whole T^*Q_n (hint: take a superposition of above states).