QUANTUM FIELD THEORY

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1. Hamiltonian Mechanics

Newton's Second Law of Motion.

$$F = ma$$

We apply this to k particles with fixed positions $x_1, ..., x_k \in \mathbb{R}^3$. The j^{th} particle is acted on by the force $F_j(x_1, ..., x_k, t, ...)$. Let $x = (x_1, ..., x_k) \in \mathbb{R}^{3k}$, $F = (F_1, ..., F_k)$,

$$m = \begin{pmatrix} m_1 I_3 & & 0 \\ & \ddots & \\ 0 & & m_k I_3 \end{pmatrix}.$$

The differential initial value problem is

$$\begin{aligned} \frac{dx}{dt} &= v \\ m\frac{dv}{dt} &= F \\ x(0) &= x_0\ ,\ v(0) = v_0\ . \end{aligned}$$

This yields a unique solution.

Assume that F is autonomous (independent of t) and conservative ($\oint_C F \cdot dx = 0$ for every closed curve C). This implies

$$F = -\nabla V$$

for some potential function V. (Think of V as potential energy.) The total energy is

$$E = T + V$$

with T the kinetic energy

$$T = \frac{1}{2}\sum m_i |v_i|^2 .$$

The total energy is conserved because of the second law, because

$$\begin{aligned} \frac{dE}{dt} &= mv \cdot \frac{dv}{dt} + \nabla V \cdot \frac{dx}{dt} \\ &= (ma - F) \cdot v = 0. \end{aligned}$$

In Hamiltonian mechanics, momentum $p = mv$ is used instead of v as a primary object. The Hamiltonian is the total energy as a function of x and p:

$$H(x, p) = \frac{1}{2} m^{-1} p \cdot p + V(x) .$$

The second law of Newton is equivalent to Hamilton's Equations:

$$\begin{aligned}\frac{dx}{dt} &= \frac{\partial H}{\partial p} = \nabla_p H \\ \frac{dp}{dt} &= -\frac{\partial H}{\partial x} = -\nabla_x H.\end{aligned}$$

If $f = f(x, p)$, then

$$\begin{aligned}\frac{df}{dt} &= \nabla_x f \cdot \frac{dx}{dt} + \nabla_p f \cdot \frac{dp}{dt} \\ &= \{f, H\},\end{aligned}$$

where the Poisson bracket is

$$\{f, g\} = \nabla_x f \cdot \nabla_p g - \nabla_p f \cdot \nabla_x g.$$

Note that $\{x_i, x_j\} = \{p_i, p_j\} = 0$, and

$$\{x_i, p_j\} = \delta_{ij}.$$

The fundamental mathematical structure of Hamiltonian equations is a symplectic structure. Recall that a symplectic manifold is a C^∞ manifold M equiped with a differential 2-form Ω with the following properties:

$$\begin{aligned} d\Omega &= 0 \text{ (Ω is closed), and} \\ & \Omega \text{ is nondegenerate.}\end{aligned}$$

This means

$$\Omega(X, Y) = 0$$

for all vector fields Y implies that $X = 0$. Note that this implies M has even dimension. The smooth skew-symmetric map

$$\Omega : TM \times TM \to \mathbb{R}$$

satisfies

$$\Omega(X, Y) = -\Omega(Y, X).$$

In local coordinates $u_1, ..., u_p$ on M^p we have

$$\Omega = \sum_{i<j} a_{ij}(u) \ du_i \wedge du_j \ .$$

Nondegeneracy of Ω provides a canonical identification of 1-forms ω with vector fields X_ω via the equation

$$d\Omega(X_\omega, Y) = \omega(Y)$$

for all vector fields Y. In particular if $f \in C^\infty(M)$, let

$$X_f := X_{df} \quad ,$$

so that

$$\Omega(X_f, Y) = df(Y) = Yf.$$

The vector field X_f is called the **Hamiltonian vector field associated to** f.

The **Poisson bracket** $\{f, g\}$ of two functions $f, g \in C^\infty(M)$ is defined to be

$$\begin{aligned}\{f, g\} &= \Omega(X_f, X_g) \\ &= X_g f = -X_f g.\end{aligned}$$

Exercise: Check the Jacobi identity

$$\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0.$$

Note that $(C^\infty(M), \{\cdot\ ,\ \cdot\})$ is a(n infinite-dimensional) Lie algebra. There is a Lie algebra homomorphism

$$\begin{aligned} (C^\infty(M), \{\cdot\ ,\ \cdot\}) &\to (\Gamma(TM), -[\cdot\ ,\ \cdot]) \\ f &\mapsto X_f \\ X_{\{f,g\}}h &= -[X_f, X_g]\, h. \end{aligned}$$

Theorem 1.1. *(Darboux) If (M, Ω) is symplectic, for every $z \in M$, there exists a neighborhood U_z and local coordinates $x_1, ..., x_n, p_1, ..., p_n$ in U_p such that*

$$\Omega = \sum dx_i \wedge dp_i\ .$$

These coordinates are called ***canonical****, and the coordinates x_i and p_i are called* ***canonically conjugate****.*

In canonical coordinates,

$$\begin{aligned} X_f &= \sum \frac{\partial f}{\partial p_i}\frac{\partial}{\partial x_i} - \frac{\partial f}{\partial x_i}\frac{\partial}{\partial p_i} \\ \{f, g\} &= \sum \frac{\partial g}{\partial p_i}\frac{\partial f}{\partial x_i} - \frac{\partial g}{\partial x_i}\frac{\partial f}{\partial p_i}. \end{aligned}$$

A diffeomorphism $\phi : M \to M$ that preserves Ω is called a **symplectomorphism** or a **canonical transformation**. Suppose $\{\Phi_t : t \in \mathbb{R}\}$ is a one-parameter group of symplectomorphisms, then its infinitessimal generator is the vector field X defined by

$$Xf = \left.\frac{d}{dt}\right|_{t=0} f \circ \Phi_t\ .$$

Since Ω is preserved by Φ_t, then

$$0 = \lim_{t \to 0} \frac{\Phi_t^* \Omega - \Omega}{t} =: \mathcal{L}_X \Omega$$

($\mathcal{L}_X$ is the Lie derivative.) But Cartan's formula gives

$$\mathcal{L}_X \Omega = i_X(d\Omega) + d(i_X \Omega),$$

where the interior product is defined on forms by

$$i_X \alpha = \alpha(X, \cdot).$$

Then

$$\mathcal{L}_X \Omega = i_X(d\Omega) + d(i_X \Omega) = d(i_X \Omega).$$

If $\mathcal{L}_X \Omega = 0$, then $i_X \Omega$ is a closed one-form. Locally, this means that

$$\begin{aligned} i_X \Omega &= df \text{ (locally), i.e.} \\ X &= X_f\ . \end{aligned}$$

We have just proved:

Proposition 1.2. *Locally, Hamiltonian vector fields are precisely infinitessimal generators of canonical transformations.*

Example: N^n has cotangent bundle $T^*N \xrightarrow{\pi} N$. Then T^*N is canonically a symplectic manifold, as follows. Note that T^*N has a canonical one-form $\omega \in \Gamma(T^*(T^*N))$, defined as follows. For $v \in T_\phi(T^*N)$,

$$\omega(v) = \phi(\pi_* v).$$

The canonical symplectic form is

$$\Omega = d\omega.$$

In local coordinates in $U \subset N$, $\{x_1, ..., x_n\}$, T^*U has local coordinates $\{x_1, ..., x_n, dx_1, ..., dx_n\} = \{x_1, ..., x_n, p_1, ..., p_n\}$, and then

$$\omega = \sum p_j dx_j \ , \Omega = \sum dp_j \wedge dx_j \ .$$

Physics applications:

- The state of the system: positions x and momenta p of all particles.
- Configuration space: $N =$ manifold of all possible positions of particles.
- Position-velocity space is TN.
- Position-momentum state space is a symplectic manifold T^*N .
- Relation between TN and T^*N: $p = mv = (v, \cdot)_m$ (Riemannian metric). That is, $mv \cdot v$ is a positive definite quadratic form on $\mathbb{R}^{3k}$.

Continuing with the cotangent bundle. The Hamiltonian is a function on T^*N given by

$$H(\alpha) = \langle \alpha, \alpha \rangle_m + V(\pi(\alpha))$$

Note that $\langle \cdot \ , \ \cdot \rangle_m$ is a pointwise inner product. Here, $\alpha \in \Gamma(T^*N)$ and $\pi : T^*N \to N$. The Hamilton's equations (in canonical coordinates (q, p)) are

$$\begin{aligned} \frac{dq}{dt} &= \nabla_p H \\ \frac{dp}{dt} &= -\nabla_q H. \end{aligned}$$

One may think of this as follows. There is a diffeomorphism (Hamiltonian flow) $\phi_\tau : T^*N \to T^*N$ defined by $(q(t), p(t)) \to (q(t+\tau), p(t+\tau))$ through the solution to the Hamilton equations. The associated infinitessimal generator is the Hamiltonian vector field. That is, the equations say that the Hamiltonian field X_H satisfies

$$X_H = (\nabla_p H, -\nabla_q H).$$

Thus, time-translations are canonical transformations (preserve the symplectic form).

2. Noether's Theorem

Emi Noether proved the following result.

Theorem 2.1. *Suppose that $\{\psi_s : (M, \Omega) \to (M, \Omega)\}$ is a one-parameter group of canonical transformations, and suppose that the function H is invariant. Suppose X_f is a Hamiltonian vector field that is an infinitessimal generator of $\{\psi_s\}$ (so that $X_f H = 0$). Then*

$$0 = X_f H = -\{f, H\} = \frac{df(p(t), q(t))}{dt},$$

so f is a conserved quantity.

For example, if $N=\mathbb{R}^{3k}$ and ψ_s is spatial translation in the direction of a fixed unit vector $u\in\mathbb{R}^3$. Then

$$\psi_s(x,p)=(x_1+su,...,x_n+su),$$

which implies

$$\begin{aligned} X_f &= (u,...,u,0,...,0), \\ f(x,p) &= (p_1+...+p_n)\cdot u. \end{aligned}$$

(part of angular momentum is conserved).

3. Two-body Problem

Two interacting particles; $N=\mathbb{R}^6$.

$$H=\frac{|p_1|^2}{2m_1}+\frac{|p_2|^2}{2m_2}+V(x_1-x_2).$$

We let

$$M=m_1+m_2, m=\frac{m_1m_2}{m_1+m_2}.$$

The symplectic form is

$$\Omega=dx\wedge dp.$$

Then

$$\begin{aligned} X &= \frac{m_1x_1+m_2x_2}{m_1+m_2}, x=x_1-x_2, \\ P &= M\frac{dx}{dt}=p_1+p_2,\ p=m\frac{dx}{dt}=\frac{m_2p_1-m_1p_1}{m_1+m_2} \end{aligned}$$

The transformation

$$(x_1,x_2,p_1,p_2)\to(X,x,P,p)$$

is canonical, and

$$H=\frac{|P|^2}{2M}+\frac{|p|^2}{2m}+V(x)$$

The Hamilton equations are

$$\begin{aligned} \frac{dX}{dt} &= \frac{P}{M},\ \frac{dP}{dt}=0 \\ \frac{dx}{dt} &= \frac{p}{m},\ \frac{dp}{dt}=-\nabla V(x). \end{aligned}$$

The two-body problem turns into a one-body problem!

4. The one-dimensional harmonic oscillator

There is a point mass m attached to a spring, which is in turn attached to a wall. The force is given by

$$F = -kx.$$

We have

$$H(p,x) = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Then

$$\Omega = dx \wedge dp$$

is the symplectic = area form. Let

$$\widetilde{x} = (km)^{1/4}\, x, \widetilde{p} = \frac{p}{(km)^{1/4}}.$$

Then

$$H(\widetilde{x},\widetilde{p}) = \frac{\omega}{2}\left(\widetilde{p}^2 + \widetilde{x}^2\right),$$

with

$$\omega = \sqrt{\frac{k}{m}}.$$

We have polar coordinates:

$$\begin{aligned} (\widetilde{x},\widetilde{p}) &\mapsto (s,\theta) \\ s &= \frac{1}{2}r^2 = \frac{1}{2}\left(\widetilde{p}^2 + \widetilde{x}^2\right). \end{aligned}$$

Then

$$H(s,\theta) = \omega s.$$

The Hamilton equations are:

$$\begin{aligned} \frac{ds}{dt} &= 0 \\ \frac{d\theta}{dt} &= -\omega \end{aligned}$$

So s is constant, $\theta = \theta_0 - \omega t$.

In other words,

$$x(t) = \sqrt{\frac{2E}{\omega}}\cos(\omega t - \theta_0).$$

5. Lagrangian Mechanics

Hamiltonian mechanics does not generalize to include relativity, but the Lagrangian mechanics formulation does.

Given a system of particles moving in potential V, then Hamiltonian is

$$H(x,p) = \frac{1}{2}m^{-1}p\cdot p + V(x).$$

The simple Lagrangian is

$$\begin{aligned} L(x,v) &= mv\cdot v - H(x,mv) \\ &= \frac{1}{2}mv\cdot v - V(x). \end{aligned}$$

More intrinsically,

$$\begin{aligned} L &: TN \to \mathbb{R} \\ L(x,\xi) &= \langle j_m \xi, \xi \rangle - H(x, j_m \xi). \end{aligned}$$

Here, $j_m : TN \to T^*N$ is given via the metric, and $\langle \cdot\ ,\ \cdot \rangle$ is the natural pairing of TN and T^*N. Then the second law of Newton is

$$\frac{d}{dt}(\nabla_v L) = \nabla_x L.$$

This is the Euler-Lagrange equation (from variational calculus) for the variational problem.

Problem: Minimize the **action**

$$S(x) := \int_{t_0}^{t_1} L(x(t), x'(t))\ dt,$$

and this is a function of the path from $(t_0, x_0 = x(t_0))$ to $(t_1, x_1 = x(t_1))$ (both fixed). To find the minimum, we consider variations $x(t) + \delta x(t)$ with $\delta x(t_0) = \delta x(t_1) = 0$ and $S(x + \delta x) - S(x) = 0$ up to degree 1 in δx.

We get

$$\begin{aligned} S(x+\delta x) - S(x) &= \int_{t_0}^{t_1} L\left(x(t) + \delta x(t), x'(t) + (\delta x)'(t)\right)\ dt - \int_{t_0}^{t_1} L(x(t), x'(t))\ dt \\ &= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial v}(\delta x)' \right) dt + \text{higher order} \\ &= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial x} + \frac{d}{dt}\frac{\partial L}{\partial v} \right)(\delta x)\, dt + \text{higher order} \end{aligned}$$

If we force this to be zero up through first order for all such variations δx, we get

$$\begin{aligned} \frac{\partial L}{\partial x} + \frac{d}{dt}\frac{\partial L}{\partial v} &= 0, \text{ or} \\ \frac{d}{dt}(\nabla_v L) &= \nabla_x L. \end{aligned}$$

6. Example: derivation of wave equation

We will go from finite to infinite degrees of freedom. We have a long elastic rod or a long air column, and we want to study longitudinal vibrations. Divide the rod into little bits, and each bit for us is a small particle. Assume that the paticles are connected by springs and have mass Δm and separation Δx. Let $u_j =$ displacement of j^{th} particle from its rest position. The second law of Newton is

$$\Delta m \frac{d^2 u_j}{dt^2} = k(u_{j+1} - u_j) - k(u_j - u_{j-1}),$$

by Hooke's Law. Here, k is the spring constant, which depends on the average displacement Δx. In fact,

$$k(\Delta x) \cdot \Delta x \to Y,\ \Delta x \to 0.$$

We see

$$\frac{\Delta m}{\Delta x}\frac{d^2 u_j}{dt^2} = k\Delta x \frac{(u_{j+1} - 2u_j + u_{j-1})}{(\Delta x)^2}. \tag{6.1}$$

The Lagrangian is

$$\begin{aligned} L &= T - V \\ &= \left[\frac{1}{2} \sum \frac{\Delta m}{\Delta x} \left(\frac{du_j}{dt} \right)^2 - \frac{1}{2} \sum k \Delta x \left(\frac{u_{j+1} - u_j}{\Delta x} \right)^2 \right] \Delta x. \end{aligned}$$

Then we take the limit as $\Delta x \to 0$.

$$L = \frac{1}{2} \sum \mu \left(\frac{du_j}{dt} \right)^2 - \frac{1}{2} \sum Y \left(\frac{u_{j+1} - u_j}{\Delta x} \right),$$

where μ is the density, $k\Delta x \to Y =$ Young's modulus, and (6.1) becomes

$$\mu \frac{\partial^2 u}{\partial t^2} = Y \frac{\partial^2 u}{\partial x^2}.$$

Then the Lagrangian is

$$L = \int_a^b \frac{1}{2} \mu \left(\frac{\partial u}{\partial t} \right)^2 - \frac{1}{2} Y \left(\frac{\partial u}{\partial x} \right)^2 dx = \int_a^b \mathcal{L} \left(\nabla_t u, \nabla_x u \right) dx.$$

Here, $\mathcal{L}$ is the Lagrangian density.

7. Mathematical Framework of Quantum Mechanics

Given any physical system, there are *states* and *observables.* A state is a specific condition of a system at a given time. An observable is a physical quantity (eg position, velocity, etc.) that can be measured. The state space is the set of all possible states for a given system. In Hamiltonian mechanics, a state space is a symplectic manifold (M, Ω), and states are points of M. Observables are Borel-measurable functions $f : M \to \mathbb{R}$. Among all observables, there are True-False observables $f : M \to \{0, 1\}$. These are equivalent to the information in the set $\{x \in M : f(x) = 1\}$ (ie a Borel subset). True-False statements (with conjunctions or, and, not) correspond to (union, intersection, complement) — called Boolean algebra. In quantum mechanics, True-False statements do not form a Boolean algebra. In particular, the following law does not hold:

$$\begin{aligned} &(A \text{ or } B) \text{ and } C \text{ is not the same as} \\ &(A \text{ and } C) \text{ or } (B \text{ and } C)\ . \end{aligned}$$

Here is the examples. If an electron beam with two slits A and B is projected on a screen C. The first statement corresponds to an interference pattern. The second statement yields no interference pattern.

The quantum-mechanical model for states and observables is ; the state space is a projective Hilbert space denoted $\mathbb{P}\mathcal{H}$. ($\mathcal{H}$ is a complete inner product space, usually infinite-dimensional.) $\mathbb{P}\mathcal{H}$: we identify u with cu, for all scalars c (usually $\in \mathbb{C}^*$), $u \in \mathcal{H}$. Unit vectors are the *normalized states.* True-False statements or observables correspond to closed linear subspaces $V \subset \mathcal{H}$. So $\mathcal{H} = V \oplus V^\perp$. These closed linear subspaces are identified with orthogonal projectors onto V (P_V, where $P_V^2 = P_V, P_V^* = P_V$). The logical operations correspond to :

$$\begin{aligned} \text{and} &\leftrightarrow \cap \\ \text{or} &\leftrightarrow \text{closed linear span} \\ \text{not} &\leftrightarrow \text{orthogonal complement} \end{aligned}$$

If the system is in the state $u \in \mathcal{H}$ ($\|u\| = 1$), and P is a True-False question, then

$$u = u_0 + u_1,$$

where $u_0 \in \ker P$, $u_1 \in \text{Range}(P)$, We have $1 = \|u\|^2 = \|u_0\|^2 + \|u_1\|^2$. These components $\|u_j\|^2$ are the probabilities.

Example: True or False: Is the quantum-mechanical system which is in the state $v \in \mathcal{H}$ also in the state u? Answer: $P_u(\bullet) = \langle \bullet, u\rangle u$ is the projector. Note $P_u(u) = u$, $P_u(v) = \langle v, u\rangle u$. (answer is between yes and no) So a quantum mechanical particle can be in several states at the same time. (Note that question is a function.) The probability that the state v is also in the state u is $|\langle v, u\rangle|^2$. This is called *transitional probability* in physics.

What about a general observable? An observable $\mathcal{O}$ is given. Let E be a Borel subset of $\mathbb{R}$. The statement "observable $\mathcal{O}$ is in E" corresponds to $P(E)$ (projector). There are three properties of projectors:

(1) $P(\varnothing) = 0$
   $P(\mathbb{R}) = \mathbf{1}_{\mathcal{H}}$
(2) $P(E_1) P(E_2) = 0$ if $E_1 \cap E_2 = \varnothing$.
(3) $P(E_1) + P(E_2) = P(E_1 \sqcup E_2)$ (extend to countable disjoint unions)

These three things define a projection-valued measure. We could make a probability distribution out of it as follows.

$$P_u(E) = |\langle P(E) u, u\rangle|^2,$$

the probability that the state u has observable value E.

Big theorem (Spectral Theorem):

Theorem 7.1. *Projection-valued measures are in one-to-one correspondence with self-adjoint operators.*

Suppose A is a self-adjoint operator; then one may obtain $f(A)$ (for f a bounded Borel function) using the functional calculus. Then

$$P_A(E) := \chi_E(A).$$

On the other hand, given a projection-valued measure P, one may associate a linear operator by

$$A = \int_{-\infty}^{+\infty} t\, dP,$$
$$\langle Au, u\rangle = \int_{-\infty}^{+\infty} t\, d\langle Pu, u\rangle$$

This a Riemann sum $\sum t_k P([t_{k+1}, t_k])$. That's all, folks!

8. Unbounded self-adjoint operators

Let $(\mathcal{H}, \langle \bullet, \bullet\rangle)$ be a complex Hilbert space and $A : D_A \to \mathcal{H}$, with $D_A \subset \mathcal{H}$, be a linear operator. The domain D_A is a dense linear subspace of $\mathcal{H}$. For bounded A, $D_A = \mathcal{H}$.

The **spectrum** of A (denoted $\sigma(A)$) is defined as

$$\sigma(A) = \{\lambda \in \mathbb{C} : A - \lambda I \text{ is not invertible, bounded}\}.$$

That is, $\lambda \in \sigma(A)$ iff $(A-\lambda I)^{-1} : \mathcal{H} \to \mathcal{H}$ does not exist. We have $\overline{\sigma(A)} = \sigma(A)$. We say (A, D_A) is symmetric if $\langle Au, v\rangle = \langle u, Av\rangle$ for all $u, v \in D_A$. We say that (A, D_A) is self-adjoint if $A^* = A$, in particular $D_{A^*} = D_A$, $\sigma(A) \in \mathbb{R}$.

For bounded A, symmetric = self-adjoint, and $D_A = D_{A^*} = \mathcal{H}$. In quantum mechanics, observables correspond to projector=projection-valued measures P_E on $\mathbb{R}$, which correspond exactly to self-adjoint operators. Note that $\sigma(A)$ is the set of all allowed values of the observable A.

For example, $\mathcal{H} = \updownarrow^2(\mathbb{C}) = \left\{(z_1, ..., z_n, ...) : \sum |z_i|^2 < \infty\right\}$. Let

$$A = \begin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & 0 & \\ & & \ddots & & \\ & 0 & & \lambda_n & \\ & & & & \ddots \end{pmatrix}.$$

Then $\sigma(A) = \overline{\{\lambda_i : i = 1, 2, ...\}} = \{\text{eigenvalues}\} \cup \{\text{limit points of eigenvalues}\}$. Then $P_{(-\infty,\lambda]}$ =orthogon projection to eigenspaces to $\lambda_i \leq \lambda$. ("Fourier series" case). This is the case where the observable takes discrete values.

Another example: $\mathcal{H} = L^2(\mathbb{R})$ or $L^2[a, b]$.

$$\langle f, g\rangle = \int_{-\infty}^{\infty} f\overline{g}\, dx.$$

Let

$$(Af)(x) = a(x) f(x),$$

where $a(x)$ is a Borel measurable function. Then the spectrum of A is

$$\sigma(A) = \overline{\{a(x) : x \in \mathbb{R}\}}.$$

If $a(x)$ is nonconstant and continuous, then there are no eigenfunctions. In this case, we say that $\sigma(A)$ consists of continuous spectrum. Here the projection is

$$\begin{aligned} P_{(-\infty,\lambda]}(x) &= \chi_\lambda(x) \\ &= \begin{cases} 1, & a(x) \leq \lambda \\ 0, & a(x) > \lambda \end{cases} \end{aligned}$$

This corresponds to the case of "Fourier transform".

The example in quantum mechanics: A free quantum particle localized on the interval $[a, b]$. The state space $\mathcal{H} = L^2[a, b]$ (sort of – actually projectivized). Then $f \in \mathcal{H}$ implies that $|f|^2$ is the probability distribution for the location of the particle. The operator of note is classically **energy**. The observable is

$$A = -\frac{d^2}{dx^2}.$$

Observe that A is unbounded. We choose

$$D_A = ??$$

Then the adjoint operator would be defined using:

Lemma 8.1. *(Riesz Lemma)* $\mathcal{H}' = \mathcal{H}$.

That is, if $\updownarrow : \mathcal{H} \to \mathbb{C}$ is a linear bounded functional, then $\updownarrow(\bullet) = \langle \bullet, v \rangle$ for some $v \in \mathcal{H}$.
Now, given $A : D_A \to \mathcal{H}$, where D_A is dense in $\mathcal{H}$. The domain D_{A^*} is defined as

$$D_{A^*} = \{v \in \mathcal{H} : \langle A\bullet, v \rangle = \updownarrow_v(\bullet) : D_A \to \mathbb{C} \text{ is bounded}\}.$$

Extend $\updownarrow_v(\bullet) : D_A \to \mathbb{C}$ to $\mathcal{H} \to \mathbb{C}$. Then $\updownarrow_v(\bullet) = \langle \bullet, w \rangle$ for some w, by the Lemma. By definition,

$$A^* v = w.$$

Note that A is by definition self-adjoint if $D_{A^*} = D_A$ and $\langle Au, v \rangle = \langle u, Av \rangle$ for all $u, v \in D_A$.
(Bad) Examples:

(1) $A_1 = -\frac{d^2}{dx^2}$, $D_{A_1} = C_0^\infty[a,b]$. This is certainly symmetric, since

$$\langle -f'', g \rangle = \langle f, -g'' \rangle.$$

In particular, $D_{A_1^*} \supset D_{A_1}$. In fact,$D_{A_1^*} \supset C^\infty[a,b]$. The spectrum of A_1 is $\mathbb{C}$!!!!! The reason is that $(A_1 - \lambda I)$ cannot be invertible, since

$$\left\langle (A_1 - \lambda I) f, e^{kx} \right\rangle = 0,$$

if $k^2 = \lambda$. Not only that, there are no eigenfunctions! So D_{A_1} is too small.

(2) $A_2 = -\frac{d^2}{dx^2}$, $D_{A_2} = C^\infty[a,b]$. This operator is not even symmetric. The spectrum of this operator is again everything, and it consists entirely of eigenvalues.

(3) $A_3 = -\frac{d^2}{dx^2}$, D_{A_3} is defined as follows. We have

$$\langle -f'', g \rangle - \langle f, -g'' \rangle = -f'(x) g(x) + f(x) g'(x).$$

We choose:

$$D_{A_3} = \{f \in C^\infty[a,b] : f(a) = f(b) = 0\}.$$

Then A_3 is symmetric, and

$$\sigma(A_3) = \left\{ \frac{n^2\pi^2}{(b-a)^2} : n = 1, 2, ... \right\}.$$

This operator is essentially self-adjoint, which means that we may close the operator. Consider

$$\Gamma = \{(x, Ax) \in D_A \times \mathcal{H}\},$$

and the closure $\overline{\Gamma}$ yields a self-adjoint operator. The true self-adjoint operator is

$$\widetilde{D_{A_3}} = \left\{ f \in L^2 : f', f'' \text{ exist and are in } L^2, f(a) = f(b) = 0 \right\}.$$

Other possibilities are:

$$\begin{aligned} D_{A_4} &: f'(a) = f'(b) = 0 \\ D_{A_5} &: f'(a) + kf(a) = 0, f'(b) + kf(b) = 0 \\ D_{A_6} &: f(a) = f(b), f'(a) = f'(b). \end{aligned}$$

The latter is called periodic boundary conditions.

Example: $-\frac{d^2}{dx^2}$ on $L^2(\mathbb{R})$, $\sigma\left(-\frac{d^2}{dx^2}\right) = \mathbb{R}$.

9. Projective Representations

Recall Classical-to-Quantum terminology:

- The Hamiltonian space M becomes the quantum state space $\mathbb{P}\mathcal{H}$
- The true-false observables $\{M \to \{0,1\}\} = 2^M$ becomes the set of closed subspaces of $\mathcal{H}$
- The full observable space becomes $Gr(\mathcal{H})$ the space of (possibly unbounded) self-adjoint operators on $\mathcal{H}$

For $V \in Gr(\mathcal{H})$, the question "is $u \in V$?" for $u \in \mathcal{H}$ is a projective question, so states (elements of $\mathbb{P}\mathcal{H}$) are in particular, observables (the projection to the closed subspace containing the state $P_u v = \frac{(u,v)}{(u,u)} u$).

Symmetries of our quantum system correspond to automorphisms of $\mathbb{P}\mathcal{H}$. This means that angle-preserving bijections of $\mathbb{P}\mathcal{H}$ to itself, ie $f : \mathbb{P}\mathcal{H} \to \mathbb{P}\mathcal{H}$ so that

$$\frac{(fu, fv)}{\sqrt{(fu, fu)(fv, fv)}} = \frac{(u, v)}{\sqrt{(u, u)(v, v)}}.$$

Wigner showed that any such map lifts to a bijection$\mathcal{H} \to \mathcal{H}$ that is unitary or conjugate unitary ($(fu, fv) = (v, u)$). We want to study groups of symmetries, ie subgroups of $Aut(\mathbb{P}\mathcal{H})$ = space of automorphisms of $\mathbb{P}\mathcal{H}$. Since $Aut(\mathbb{P}\mathcal{H}) = \mathbb{P}U(\mathcal{H}) \sqcup \overline{\mathbb{P}U(\mathcal{H})}$, which is the union of connected components in the strong operator topology, so a connected group of symmetries would be a subgroup of $\mathbb{P}U(\mathcal{H})$. Each of those symmetries can lift, but only a pointwise lift. Instead of thinking of 'abstract' subgroups, we'll think of homomorphisms of $G \to Aut(\mathbb{P}\mathcal{H})$, where G is a topological group. If G is connected, we can factor

$$G \to \mathbb{P}U(\mathcal{H}) \to Aut(\mathbb{P}\mathcal{H}).$$

Natural question: Does this lift to a map $G \to U(\mathcal{H})$? Obviously, there is a pointwise lift, but it might not be a group homomorphism. Weaker: is there a continuous lift? Maybe yes, maybe no, but if G is simply connected, then the answer is definitely yes. Can we choose it to be a group homomorphism? Take any lift $\widehat{\rho}$ and test if it is a homomorphism, ie if

$$\begin{aligned} \widehat{\rho}(x)\,\widehat{\rho}(y) &= \widehat{\rho}(xy)? \text{ or} \\ 1 &= [\widehat{\rho}(x)\,\widehat{\rho}(y)]^{-1}\,\widehat{\rho}(xy)? \end{aligned}$$

Maybe or maybe not. The good news: the right hand side is a lift to $U(\mathcal{H})$ of

$$[\rho(x)\,\rho(y)]^{-1}\,\rho(xy) = 1.$$

Thus,

$$\omega_{\widehat{\rho}}(x, y) = [\widehat{\rho}(x)\,\widehat{\rho}(y)]^{-1}\,\widehat{\rho}(xy) \in S^1$$

For $x, y, z \in G$, we have

$$\begin{aligned} \partial\omega_{\widehat{\rho}}(x, y, z) &:= \omega_{\widehat{\rho}}(y, z)\,\omega_{\widehat{\rho}}(xy, z)^{-1}\,\omega_{\widehat{\rho}}(x, yz)\,\omega_{\widehat{\rho}}(x, y)^{-1} \\ &= [\widehat{\rho}(x)\,\widehat{\rho}(y)\,\widehat{\rho}(z)]^{-1}\,\widehat{\rho}(xyz)\,\omega_{\widehat{\rho}}(x, yz)\,\omega_{\widehat{\rho}}(x, y)^{-1} = 1. \end{aligned}$$

This is a cocycle condition, so

$$\partial\omega_{\widehat{\rho}} = 0 \Longrightarrow$$

$\omega_{\widehat{\rho}}$ represents an element of $H^2(G, S^1)$, and this element does not depend on the choice of lift:

$$\omega_\rho \in H^2\left(G, S^1\right).$$

Our point of view: ω_ρ represents the obstruction to lifting ρ to a group homomorphism. Why? ρ does lift to

$$G_{\omega_\rho} := G \times S^1$$

with group law

$$(g, \lambda)(h, \mu) = (gh, \omega_{\widehat{\rho}}(g, h)\lambda\mu).$$

This only depends on ω_ρ, up to isomorphism. The associator is exactly the coboundary above. The lift is

$$\rho(g, \lambda) := \lambda_{\widehat{\rho}}(g).$$

Note that ρ already lifts to G iff the exact sequence

$$1 \to S^1 \to G_{\omega_\rho} \to G \to 1$$

splits. In fact, ω_ρ may be recovered from the abstract group G_{ω_ρ}: $[(g,1),(h,1)] = (1, \omega_{\widehat{\rho}}(g,h))$.

(Some physics stuff ... want one-parameter groups of symmetries to correspond to observables. Recall that an observable is a self-adjoint operator A on $\mathcal{H}$, which corresponds to a one-parameter group of symmetries e^{itA}. Do all one-parameter subgroups arise this way? What is such a subgroup? $\mathbb{R} \to \mathbb{P}U(\mathcal{H})$, ie a projective representation of the Lie group $\mathbb{R}$. Bargmann: For simply connected Lie groups, we can "take logarithms": The group lifting obstruction : $H^2(G, S^1) \to H^2(\mathfrak{g}, \mathbb{R})$ (the Lie-algebra lifting obstruction). Great news: $H^2(\mathbb{R}, \mathbb{R}) = 0$ implies all 1-parameters groups of symmetries lift to unitary groups.)

10. Quanti"s"ation

Idea: Replace classical observables

$$f : M \to \mathbb{R}$$

(M is the symplectic manifold) by quantum observables $A \in SA(\mathcal{H})$ — self-adjoint operators. Here, $\mathcal{H}$ is a separable Hilbert space. The operators correspond to projection-valued measures on $\mathbb{R}$.

"Quanti's'ation" is like a map $f \mapsto A_f$ that is linear and preserves the Borel $\mathrm{Bor}(M, M)$ module structure (ie $A_{\phi f} = \phi(A_f)$) and preserve the Poisson bracket. The Poisson bracket is an antisymmetric pairing that satisfies the Jacobi identity. That is,

$$A_{[f,g]} = (i\hbar)^{-1}[A_f, A_g].$$

This $\hbar$ measures the quantum-ness, so as $\hbar$ goes to 0 one should recover the classical system.

In particular, corresponding to classical observables position x_i and momentum p_j are the quantum observables $X_i = A_{x_i}$ and $P_j = A_{p_j}$. These should satisfy

$$[X_i, X_j] = 0 = [P_i, P_j]$$

because the lower case guys commute. Since

$$\{x_i, p_j\} = \delta_{ij}\ ,$$

we have

$$[X_i, P_j] = i\hbar\delta_{ij}\ .$$

Problem: if X, P are self adjoint and satisfy $[X,P]=i\hbar$, then we use the identity

$$[X,AB]=[X,A]\,B+A\,[X,B]$$

to prove inductively that

$$[X,P^n]=ni\hbar P^{n-1},$$

which implies

$$\begin{aligned} 2\,\|X\|\,\|P\|^n &\geq \|[X,P^n]\| = n\hbar\left\|P^{n-1}\right\| \\ &= n\hbar\,\|P\|^{n-1}, \end{aligned}$$

so that $\|X\|$ and/or $\|P\|$ is infinite. Thus we must use unbounded operators. But then

$$[X,P]=i\hbar$$

can hold on the domain (cause the domain is too small) for stupid reasons. The "solution" is to view the three families of equations above as a Lie algebra. We define a Lie algebra by its structure constants in such a way that the desired relations are satisfied. (ie the quotient of the free $2n$-dim real Lie algebra modulo the relations). For example, the analogous construction for the relations

$$[X,P]=H,[H,X]=2X,\ [H,P]=2P$$

is $\mathfrak{sl}_2$.

What is this Lie algebra? Answer: the Heisenberg Lie algebra. Let V be a symplectic vector space over $\mathbb{R}$ and define $\mathfrak{h}(V):=V\oplus\mathbb{R}$ as a vector space with Lie bracket

$$[v\oplus t,v'\oplus t']=0\oplus(v,v'),$$

where (v,v') is the symplectic pairing. This is the Lie algebra of $H(V):=V\times\mathbb{R}$ as a set with multiplication

$$(v,t)\cdot(v',t')=\left(v+v',t+t'+\frac{1}{2}(v,v')\right).$$

This is just the twist of V by the 2-cocycle given by $(\cdot,\cdot)$. $H(V)$ is a 2-step nilpotent Lie group. Since the group commutator satisfies $[(v,t),(v',t')]=(0,(v,v'))$, we have $[H(V),H(V)]=\mathbb{R}=Z(H(V))$. If $\Lambda\subseteq V$ is a Lagrangian (i.e. a maximal self-annihilating subspace), then Λ imbeds in $H(V)$, and Λ then imbeds in $\mathfrak{h}(V)$. The subspaces $\operatorname{Span}(X_i)$ and $\operatorname{Span}(P_j)$ arise in this way.

In our case, we take $V=\mathbb{R}^n\oplus\mathbb{R}^n$ with symplectic pairing

$$(x\oplus y,x'\oplus y')=x\cdot y'-x'\cdot y.$$

In a natural way, regard $\operatorname{Span}(X_i)$ as $\mathbb{R}^n\oplus 0$ and $\operatorname{Span}(P_j)$ as $0\oplus\mathbb{R}^n$. According to Folland, a "good" way to choose the operators X_i and P_j on $\mathcal{H}$ is to find a unitary representation ρ of $H_n:=H(\mathbb{R}^n\oplus\mathbb{R}^n)$ and identify X_i with $d\rho(X_i)$ and P_j with $d\rho(P_j)$.

By quantization of the classical picture, we saw that we want self-adjoint operators X_i,P_j such that

$$\begin{aligned} [X_i,X_j] &= 0,[X_i,P_j]=0,i\neq j \\ [P_i,P_j] &= 0,[X_j,P_j]=i\hbar \end{aligned}$$

(Here, we are studying the thingy of n particles moving freely in 3-space; we put $n=3k$ and i,j range from 1 to n.) As Igor said: these operators cannot all be bounded, and commutators of unbounded operators have small domains. Magically, the appropriate domain condition is encoded by requiring that the representation of the Heisenberg algebra exponentiates to the Heisenberg group.

Specifically, a family of such operators gives a representation of

$$\mathfrak{h}_n = \mathbb{R}^n_x \oplus \mathbb{R}^n_p \oplus \mathbb{R}$$

(as a set) with the bracket

$$\left[(x \oplus p, t), (x' \oplus p', t')\right] = \left[0 \oplus 0, x \cdot p' - p \cdot x'\right],$$

where $\cdot$ is the usual Euclidean inner product. This is called the Heisenberg algebra, which has a matricial realization:

$$\mathfrak{h}_n = \left\{ \begin{pmatrix} 0 & x & t \\ & 0 & p \\ & & 0 \end{pmatrix} : x, p \in \mathbb{R}^n, t \in \mathbb{R} \right\}.$$

This is the Lie algebra of the Heisenberg group:

$$H_n = \mathbb{R}^n_x \oplus \mathbb{R}^n_p \oplus \mathbb{R}$$

with operation

$$\begin{aligned} & (x \oplus p, t)(x' \oplus p', t') \\ = & \left((x + x') \oplus (p + p'), t + t' + \frac{1}{2}(x \cdot p' - p \cdot x') \right) \end{aligned}$$

So we want our operators X_i, P_j to arise as $d\rho$ (basis vectors) for some unitary $\rho : H_n \to U(\mathcal{H})$. If this happens, then we must have that the action of $Z(H_n) = \mathbb{R}$ exponentiates the action of $\mathfrak{z}(\mathfrak{h}_n) = \mathbb{R}$. Since the commutation relations force $t \in \mathfrak{z}(\mathfrak{h}_n)$ to act by $i\hbar t$, we must have $t \in Z(H_n)$ acting by multiplication by $e^{i\hbar t}$.

Incidentally, if

$$\begin{aligned} A_j &= \frac{1}{\sqrt{2\hbar}}(X_j + iP_j), \\ A_j' &= \frac{1}{\sqrt{2\hbar}}(X_j - iP_j) \end{aligned}$$

are called the creation and annihilation operators, which are adjoint to each other.

So we want a representation ρ of H_n such that $Z(H_n)$ acts by the nontrivial character $\chi_\hbar : t \mapsto e^{i\hbar t}$. Stone-von Neumann: There's only one (irreducible, up to isomorphism). What does it look like? :-)

By Frobenius reciprocity,

$$0 \neq \mathrm{Hom}_{Z_n}(\rho, \chi_\hbar) \cong \mathrm{Hom}_{H_n}\left(\rho, Ind^{H_n}_{Z_n}\chi_\hbar\right).$$

For us, the induced representation $Ind^{H_n}_{Z_n}\chi_\hbar = L^2\left(\mathbb{R}^n_x \oplus \mathbb{R}^n_p\right)$, with H_n-action

$$\begin{aligned} & \left[(x_0 + p_0, t_0) f\right](x \oplus p) \\ = & \chi_{\hbar/2}(x \cdot p_0 - x_0 \cdot p)\chi_\hbar(t_0) f(x + x_0 \oplus p + p_0). \end{aligned}$$

The real picture:

$$Ind^{H_n}_{Z_n}\chi_\hbar = \{f : H_n \to \mathbb{C} : f(zh) = \chi_\hbar(z) f(h)\}$$

with H_n acting by right translations.

Problem: This representation $Ind_{Z_n}^{H_n}\chi_\hbar$ is reducible. We take a quotient:

$$\overline{f}(x) = \int_{\mathbb{R}_p^n} \chi_{-\hbar/2}(x \cdot p)\, f(x \oplus p)\, dp.$$

Then, $\overline{f} \in L^2(\mathbb{R}_x^n)$, and

$$\overline{[(x_0 \oplus p_0, t_0)\, f]}(x) = \chi_\hbar(x \cdot p_0)\, \chi_{\hbar/2}(x_0 \cdot p_0)\, \chi_\hbar(t_0)\, \overline{f}(x + x_0).$$

Specifically,

$$\begin{aligned} \overline{[(x_0 \oplus 0, 0)\, f]}(x) &= \overline{f}(x + x_0) \\ \overline{[(0 \oplus p_0, 0)\, f]}(x) &= \chi_\hbar(x \cdot p_0)\, \overline{f}(x). \end{aligned}$$

Once we are in $L^2(\mathbb{R}_x^n)$, we can take Fourier transforms: If $\phi \in L^2(\mathbb{R}_x^n)$,

$$\widehat{\phi}(p) := \int_{\mathbb{R}_x^n} \chi_\hbar(x \cdot p)\, \phi(x)\ dx,$$

and

$$\begin{aligned} (x_0 \widehat{\oplus 0, 0)\, \phi}(p) &= \chi_\hbar(-x_0 \cdot p)\, \widehat{\phi}(p) \\ &= \left[(0 \oplus -x_0, 0)\, \widehat{\phi}\right](p). \end{aligned}$$

Similarly,

$$\begin{aligned} (0 \widehat{\oplus p_0, 0)\, \phi}(p) &= \widehat{\phi}(p + p_0) \\ &= \left[(p_0 \oplus 0, 0)\, \widehat{\phi}\right](p). \end{aligned}$$

In other words, if w is the symplectomorphism of $\mathbb{R}_x^n \oplus \mathbb{R}_p^n$ given by $x_0 \oplus p_0 \mapsto p_0 \oplus -x_0$, then the Fourier transform intertwines ρ and $\rho \circ w$.

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