Quantum Mechanics for Mathematician

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Contents

Notation

1. Local coordinate $q = (q_1 ..., q_n)$ on a smooth n-dimensional manifold M are the Cartesian coordinates on $\varphi(U) \subset \mathbb{R}^n$, where (U, φ) is the coordinate chart on M. For $f : U \to \mathbb{R}^n$, we denote $f \circ \varphi^{-1}(q_1, ..., q_n)$ by $f(q)$
2. Denote by $\mathcal{A}^*(M) = \oplus_{k=0}^{n} \mathcal{A}^k(M)$ the graded algebra of smooth differential forms on M with respect to wedge product and by $d_k : \mathcal{A}^k(M) \to \mathcal{A}^{k+1}(M)$ the de Rham differential (a graded derivation of $\mathcal{A}^*(M)$ of degree 1)

Chapter 1

A review of Classical Mechanics

Week 1

1.1 Lagrangian formalism

1.2 Hamiltonian formalism

Definition 1. Algebra of Classical Mechanics.

Generally, for all mechanical system, all of the observable are smooth function of $p = (p_1, ..., p_n)$, $q = (q_1, ..., q_n)$. We have commutative algebra $\mathcal{A} = \mathcal{A}_{cl} = C^\infty\left(\mathbb{R}^{2n}\right)$, $f \in \mathcal{A}_{cl} : (q,p) \to \mathbb{R}$

Definition 2. Hamilton Equation of Motion.

$$\dot{q} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial q} \tag{1.2.1}$$

where $H = H(q,p) : \mathbb{R}^{2n} \to \mathbb{R}$. Cauchy problem of coupled PEDs with initial condition $q|_{t=0} = q_0,\ p|_{t=0} = p_0$ with(q_0, p_0) in $\mathbb{R}^{2n}$ space.

By assumption : There is unique global solution defined for all $t \in \mathbb{R}$: $\begin{cases} p = q(q_0, p_0, t) \\ p = q(q_0, p_0, t) \end{cases}$

In short, $\mu = (q,p) \in \mathcal{M} = \mathbb{R}^{2n}$ is an orbit in $\mathcal{M}$ (a Hamiltonian phase flow generated by Hamiltonian vector field V in phase space $\mathcal{M} = T^*N$ or cotangent bundle of configuration space) such that $\dot{\mu} = V(\mu) = (\dot{q}, \dot{p})(\mu) = \left(\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q}\right)$

Time reversible: $t \to -t$, $p \to -p$ and $q \to -q$ such that the form of the equation doesn't change (Loschmidt's paradox)
No: heat equation $\partial_t u = \Delta u$ limited by 2nd Law of Thermodynamics
Yes: $\partial_t u = -i(\Delta + V)u$

Definition 3. The Hamiltonian generate one parameter Abelian group of diffeomorphisms (index by time $t \in \mathbb{R}$) of transformation

$$G_t : \mathcal{M} \to \mathcal{M}\ (\forall t \in \mathbb{R})$$

of phase space in to itself .

$$G_{t_1} \circ G_{t_1} = G_{t_1+t_2} \tag{1.2.2}$$
$$G_{t_0} = id_{\mathcal{M}} \tag{1.2.3}$$
$$G_t^{-1} = G_{-t} \tag{1.2.4}$$

By definition, $\mu(t) = G_t\mu$ is the solution with initial condition $\mu(0) = G_0\mu$. By construction, uniqueness of solution to Cauchy problem for Hamiltonian equation. In return, G_t generates a family of transformation U_t of Algebra $\mathcal{A} = \mathcal{A}_{cl}$ of classical observation of solution such that for $\forall f \in \mathcal{A}_{cl} = C^\infty_{\mathbb{R}}(\mathcal{M}),\ \forall \mu \in \mathcal{M},\ \forall t \in \mathbb{R}$

$$\left(U_t f\right)(\mu) = f_t\left(\mu\right) = f\left(G_t\mu\right) \tag{1.2.5}$$

Note that $f_t \in \mathcal{A}_{cl}$, $f_t\left(q_0,p_0\right) = f_t\left(\mu_0\right) = f\left(q(q_0,p_0,t),p(q_0,p_0,t)\right)$

$$f_{t+s}\left(\mu\right) = f_t\left(G_s\mu\right)$$

Thus

$$\frac{\partial}{\partial s}\, f_t\left(G_s\mu\right)\big|_{s=0} = \nabla f_t(\mu)V(\mu) = \left(\frac{\partial f_t}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial f_t}{\partial p}\frac{\partial H}{\partial q}\right)(\mu) = X_H(f_t)(\mu)$$

Therefore, the evolution of any function of μ satisfies

$$\frac{df_t}{dt} = \{H,f\} = \frac{\partial H}{\partial p}\frac{\partial f_t}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial f_t}{\partial p} = X_H(f_t) \tag{1.2.6}$$

with initial condition $f_t(q,p)|_{t=0} = f(q.p)$, where $\{\ ,\ \}$ denotes the Poisson Bracket and $X_H = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}$ is a vector field generated by Hamiltonian. This means that the Cauchy problem for the time evolution of observable f (given by U_t) has a unique solution

$$f_t(q_0,p_0) = f\left(q(q_0,p_0,t),p(q_0,p_0,t)\right)\ \ i.e.\ f_t(\mu) = f(\mu(t)) = f\left(G_t\mu\right)$$

and not only the generalized coordinate(q,p) but also the observable $f(q,p)$ evolve with time.

Summary: The states of classical system is determined by a representative point in phase space $\mu = (q,p) \in \mathcal{M} = \mathbb{R}^{2n}$, which is an orbit in $\mathcal{M}$ (a flow generated by Hamiltonian vector field V in phase space $\mathcal{M}$) such that $\dot{\mu} = V(\mu) = (\dot{q},\dot{p})(\mu) = \left(\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q}\right)$ .The evolution of any observable $f : \mathbb{R} \to \mathcal{A}_{cl}$ is governed by the solution of Hamiltonian equation

$$\frac{df_t}{dt} = \{H,f\} \quad subjected\ to\ f_t|_{t=0} = f_0$$

Dictionary:	CM	QM	
Observable	f	A	self-adjoint operator in Hilbert space[1]
States	ω	Ψ	
Time envolve	f_t with $\frac{df_t}{dt} = \{H,f\}$	$A(t)$ with $\frac{dA(t)}{dt} = [H,A(t)]_\hbar$	$\{A,B\} \overset{\hbar\to 0}{\longleftarrow} \frac{i}{\hbar}[A,B]_\hbar$

Table 1.1: Dictionary of CM and QM

Mathematical Structure: Symplectic manifold

- A symplectic manifold is a $C^\infty(M)$ equipped with a differential 2-form Ω that is closed($d\Omega = 0$) and point-wise non-degenerate, i.e. for each $p \in M$ and $V \in T_pM$, $\Omega(V,W) = 0$ for all $W \in T_pM$ only when $W = 0$.
- Non-degeneracy forces the dimension of M to be even $dim(M) = 2n$
- The symplectic form Ω gives an identification of 1-forms with a vector fields (ensured by non-degeneracy). Namely, if ϕ is a1-form, the corresponding Vector field is defined by

  $$\Omega\left(X,Y_\phi\right) = \phi\left(X\right)$$

  for all vector fields. In particular, when $f \in C^\infty(M)$, $X_{df} = X_f$ is called Hamiltonian vector field of f s.t. $\Omega\left(X,Y_f\right) = df\left(X\right) = X\left(f\right)$
- The poisson bracket of two smooth function f,g is

  $$\{f,g\} = \Omega\left(X_f,X_g\right) = X_f\left(g\right) = -X_g\left(f\right)$$

  which makes $C^\infty(M)$ into a Lie algebra.
- Jacobi identity is a consequence of $d\Omega = 0$, and the correspondence $\pi : f \mapsto X_f$ is a Lie algebra homomorphism: $\pi\left\{f,g\right\} = \left\{\pi(f),\pi(g)\right\}$

  $$X_{\{f,g\}}h = \left\{\left\{f,g\right\},h\right\} = -\left\{\left\{g,h\right\},f\right\} - \left\{\left\{h,f\right\},g\right\} = X_fX_gh - X_gX_fh = \left[X_f,X_g\right]h$$

[1] $\mathcal{L}^2 = \left\{\psi : \mathbb{R}^N \to \mathbb{C} \middle| \int_{\mathbb{R}^N} |\psi(x)|^2 < \infty\right\}$

Mathematical Structure: Symplectic manifold

- Darboux theorem: for any point in a symplectic manifold M, $\exists(U_x,\varphi)$ where $\varphi(x)=(q^1...,q^n,p_1...,p_\mu)$ s.t. $\Omega = dp_\mu\wedge dq^\mu$. The coordinate system with this property is called canonical.
- Canonical transformation (symplectomorphism): a diffeomorphism $G_t : M\to M$ that preserves the symplectic structure. Then its infinitesimal generator, the vector field defined by $X(f_t)=\frac{d}{ds}f_t\circ G_s|_{s=0}$ satisfies $L_X\Omega=0$. (In fact $X=X_H$ which can be seen from equation (1.2.6))
- $L_{X_H}\Omega = L_{X_H}dp_\mu\wedge dq^\mu + dp_\mu\wedge L_{X_H}dq^\mu = d\left(L_{X_H}p_\mu\right)\wedge dq^\mu + dp_\mu\wedge d\left(L_{X_H}q^\mu\right) = -d\left(\frac{\partial H}{\partial q^\mu}\right)\wedge dq^\mu + dp_\mu\wedge d\left(\frac{\partial H}{\partial p_\mu}\right) = -d^2H=0$. In reverse, if $L_X\Omega=0$, then $L_X\Omega=(i_Xd+di_X)\Omega=di_X\Omega=0\Longrightarrow i_X\Omega=df$ which means there exists H s.t. $L_{X_H}\Omega=0$
- Hamiltonian vector field are precisely the infinitesimal generators for canonical transformations.

Week 2

Preview: In QM, the evolution equation is

$$\frac{dA_t}{dt}=[H,A_t]$$

where $t\to A_t,\mathbb{R}\to\mathcal{A}_{qm}$ ={unbounded self-adjonint operator in Hilbert space} , H is the Hamiltonian operator and $[A,B]=i/\hbar\,(AB-BA)$ is the commutator of A,$B\in\mathcal{A}_{qm}$

Definition 4. Self-adjoint: $A^*=A$ which satisfies $(AB)^*=B^*A^*=BA$, but $[A,B]^*=-i/\hbar\,(BA-AB)=[A,B]$ which preserves the algebra.

Properties of PB$\{\cdot,\cdot\}$: $\mathcal{A}_{cl}\times\mathcal{A}_{cl}\to\mathcal{A}_{cl}$, $(f,g)\mapsto\{f,g\}$

1. Bilinear
2. Skew-symmetry
3. Jacobian Identity
4. Leibniz rule: $\{f,gh\}=\{f,g\}\,h+g\,\{f,h\}$, i.e. $\{,\}$ is the derivation of the algebra $\mathcal{A}_{cl}$ in each variable.

Proof. (4) Define $\{f,g\}=X_fg$,where X_f is the first order differential operator (vector field), i.e. $X_f=\frac{\partial f}{\partial p}\frac{\partial}{\partial q}-\frac{\partial f}{\partial q}\frac{\partial}{\partial p}$. Now its clear that X_f is a derivation on $\mathcal{A}_{cl}$ such that $X_f\,(gh)=(X_fg)\,h+g\,(X_fh)$ ☐

Exercise 5. Show that $[X_f,X_g]=X_fX_g-X_gX_f$, $[X_f,X_g]\,h=X_{\{f,g\}}h=\{\{f,g\},h\}$. Then derive Jacobian Identity.

Claim 6. Algebra property of $\mathcal{A}_{cl}=C^\infty(M)$ which is equipped with $\{\}_{PB}$

- $\mathcal{A}_{cl}$ is a real vector space.
- $\mathcal{A}_{cl}$ is Lie algebra with the operation $\{\}_{PB}$ i.e. the properties of Lie bracket holds
- The last two operation, i.e. the product in $\mathcal{A}_{cl}$ and the Lie product $\{f,g\}$ are connected via the Leibniz rule 4. which states that $\{\}_{PB}$ is a deviation in each variable

Claim 7. Classical dynamics:

The algebra $\mathcal{A}_{cl}$ of classical observables exists a distinguished element $H=H\,(p,q)\in C^\infty(M)$, the rule of which is to describe the time evolution $t\to A_t,\mathbb{R}\to\mathcal{A}_{qm}$ of any classical observable. The evolution is governed by $\frac{df_t}{dt}=\{H,f\}$ with initial condition $f_t(q,p)|_{t=0}=f(q.p)$.

Finally, recall the definition of $U_t:\mathcal{A}_{cl}\to\mathcal{A}_{cl}$, $(U_tf)\,(\mu)=f_t\,(\mu)$ for $\forall f\in\mathcal{A}_{cl}=C^\infty(M)$. Then, its easy to check that U_t is an automorphism of the algebra $\mathcal{A}_{cl}$, i.e.

- U_t is linear
- $U_t\,(fg)=U_t\,(f)\,U_t\,(g)$
- U_t is invertible (i.e. U_t is bijective) and $U_t^{-1}=U_{-t}$

1.3 States

1.4 Liouville's theorem