MATH4104: Quantum nonlinear dynamics. Lecture Five. Review of quantum theory: operators and the Heisenberg picture, periodic potential.

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Classical dynamics.

Classical dynamics:

Definition.
A classical state, $P(q_1, q_2, \ldots, q_n, p_1, p_2, \ldots, p_n)$ is positive, real valued, integrable function (with norm one in L^1) on an even dimensional sympletic manifold, the phase space.

The normalisation is

$$\int_{-\infty}^{\infty} dq^n dp^n P(q_i, p_i) = 1$$

States, physical quantities, instruments and operationss.

A more general class of functions to represent states,

Definition.
A completely specified state is a pure *state and is given by*

$$P(q, p|q_0, p_0) = \delta^{(2n)}(q - q_0, p - p_0)$$

A pure state corresponds to a single point in phase space. A completely specified state means that we know everything there is to know about the state.

States, physical quantities, instruments and operationss.

Physical quantities.

Definition.
A physical quantity *is a real valued function $A(q, p)$ on the symplectic manifold (ie one with a Poisson bracket).*

Examples:

- kinetic energy $T = p^2/(2m)$
- potential energy $V(q)$
- total energy (Hamiltonian) $H = T + V$
- angular momentum $\vec{L} = \vec{q} \times \vec{p}$

States, physical quantities, instruments and operationss.

Definition.

The moments *of a physical quantity A in the state P is given by*

$$\langle A \rangle_P = \int_{-\infty}^{\infty} dq dp A(q,p) P(q,p)$$

Technical note: the moment defined by a state P is a bounded positive linear functional on the space L^{∞} of physical quantities.

Classical dynamics.

Two pictures for dynamics.

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Physical quantities change in time, with states independent of time. This is the Hamilton picture.

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States change in time, with physical quantities independent of time. This is the Liouville picture. Both pictures give the same results for moments of physical quantities.

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States change in time, with physical quantities independent of time. This is the Liouville picture. Both pictures give the same results for moments of physical quantities.

In the *Hamilton picture*, the evolution of physical quantities is given by Hamilton's equations,

$$\frac{dA}{dt} = -\{H, A\} + \frac{\partial A}{\partial t}$$

The $\{\ ,\ \}$ is the usual Poisson bracket.

Classical dynamics.

In the *Liouville picture*, evolution equation for $P(q,p,t)$. The total time derivative of a phase space function of the form $F(q,p,t)$is,

$$\begin{aligned}
\frac{dF}{dt} &= \frac{dq}{dt}\frac{\partial F}{\partial q} + \frac{dp}{dt}\frac{\partial F}{\partial p} + \frac{\partial F}{\partial t} \\
&= \{F, H\} + \frac{\partial F}{\partial t}
\end{aligned}$$

dynamics of the density $P(q,p,t)$ is like the flow of an incompressible fluid, so $\frac{dP}{dt} = 0$.

$$\frac{\partial P}{\partial t} = \{H, P\}$$

This is *Liouville's equation*.
Show that the evolution of moments of physical quantities are the same in both pictures.

Quantum dynamics.

Like classical mechanics, there are two ways to think of the dynamics:

- States change in time *Schrödinger* picture.
- physical quantities change in time *Heisenberg picture*

Both pictures give the same result for averages, $\langle \hat{A}(t) \rangle$.

Schrödinger picture.

$$\begin{aligned}\langle \hat{q}(t) \rangle &= \langle \psi(t) \hat{q} | \psi(t) \rangle & (1)\\ &= \int dx \; \psi^*(x,t) x \psi(x,t) & (2)\end{aligned}$$

where

$$|\psi(t)\rangle = \sum_n c_n |E_n\rangle e^{-iE_n t/\hbar}$$

where

$$\hat{H}|E_n\rangle = E_n|E_n\rangle$$

We can also write

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} \sum_n c_n |E_n\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle$$

Schrödinger picture.

Then the time dependent average is

$$\langle\psi(t)|\hat{q}|\psi(t)\rangle = \langle\psi(0)|e^{i\hat{H}t/\hbar}\hat{q}e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$$

Define the *unitary operator* ($UU^\dagger = 1$)

$$U(t) = e^{-i\hat{H}t/\hbar}$$

$$\langle\psi(t)|\hat{q}|\psi(t)\rangle = \langle\psi(0)|U^\dagger(t)\hat{q}U(t)|\psi(0)\rangle$$

$\hat{H}$ is a *hermitian operator*, $\hat{H}^\dagger = \hat{H}$, which implies it has real eigenvalues.

Heisenberg picture.

Define the new operators

$$\begin{aligned}\hat{q}(t) &= U^{\dagger}(t)\hat{q}U(t)\\ \hat{p}(t) &= U^{\dagger}(t)\hat{p}U(t)\end{aligned}$$

prove that this does not change the commutation relations:

$$[\hat{q}(t), \hat{p}(t)] = i\hbar$$

We then say that transformation is *canonical*.

Heisenberg picture.

The we can write,

$$\langle\psi(t)|\hat{q}|\psi(t)\rangle = \langle\psi(0)|\hat{q}(t)|\psi(0)\rangle$$

where

$$\begin{aligned}
\frac{d\hat{q}}{dt} &= \left(\frac{d}{dt}U^\dagger(t)\right)\hat{q}U(t) + U(t)^\dagger\hat{q}\left(\frac{d}{dt}U(t)\right) \\
&= \frac{i}{\hbar}\hat{H}\hat{q} - \frac{i}{\hbar}\hat{H}\hat{q} \\
&= -\frac{i}{\hbar}[\hat{q},\hat{H}]
\end{aligned}$$

using the definition of the commutator $[\cdot\ ,\ \cdot]$.

cf classical $\dot{q} = \{q, H(q,p)\}$, in terms of Poisson bracket

Heisenberg picture.

Example: SHO

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2$$

$$\frac{d\hat{q}}{dt} = -\frac{-i}{2m\hbar}[\hat{q}, \hat{p}^2] = \frac{\hat{p}}{m}$$

where we use the identity $[A, BC] = [A, B]C + B[A, C]$ and $[\hat{q}, \hat{p}] = i\hbar$.

Likewise

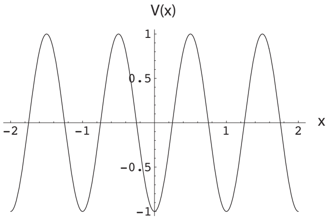
$$\frac{d\hat{p}}{dt} = -m\omega^2\hat{q}$$

Show that the solutions are the same form as the classical solutions

Particle in a periodic potential.

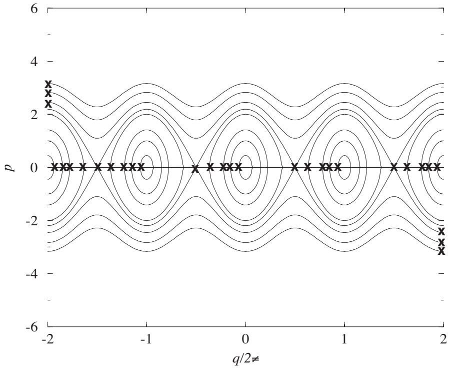
$$V(x) = -V_0 \cos(2\pi x/\lambda)$$

$$H = \frac{p_x^2}{2m} - V_0 \cos(2\pi x/\lambda)$$



Particle in a periodic potential.

Phase space orbits.



Particle in a periodic potential.

Dimensionles variables:

$$
\begin{aligned}
q &= 2\pi x/\lambda \\
p &= p_x^2/\mu
\end{aligned}
$$

The commutation relations are

$$[\hat{q}, \hat{p}] = i\bar{k}$$

where dimensionless Planck

$$\bar{k} = \frac{2\pi\hbar}{\lambda\mu}$$

Scale energy $H \rightarrow mH/\mu^2$, define dimensionless Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2} - \kappa \cos \hat{q}$$

where $\kappa = mV_0/\mu^2$

Particle in a periodic potential.

Quantisation (for bounded motion), with energy E

Only allowed orbits that enclose an area$= n \times 2\pi \times \hbar$ (with $n = 1, 2, \ldots$).

The classical action variable is

$$J(E) = area/2\pi$$

so

$$J(E_n) = n\hbar$$

Particle in a periodic potential.

Classical action

$$J = \sqrt{\kappa}\frac{8}{\pi}\begin{cases} \mathcal{E}(N) - (1-N^2)\mathcal{K}(N), & N < 1 \quad \text{bounded motion} \\ \frac{1}{2N}\mathcal{E}(N^{-1}), & N > 1 \quad \text{un-bounded motion,} \end{cases}$$

Here $2N^2 = 1 + E/\kappa$,

$\mathcal{E}$ and $\mathcal{K}$ are the complete elliptic integrals of the first and second kind and $\mathcal{F}$ is the incomplete integral of the first kind.

Particle in a periodic potential.

for allowed energies,

$$J(E_n) - J(E_{n-1}) = \hbar$$

and

$$J(E_n) - J(E_{n-1}) =\approx \left.\frac{dJ(E)}{dE}\right|_{E_n} .\Delta E_n$$

where $\Delta E_n = E_n - E_{n-1}$.

Now use

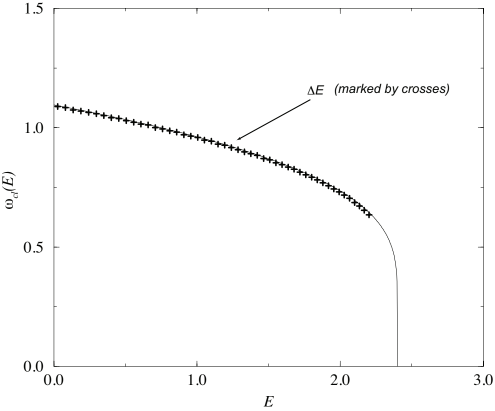
$$\frac{dJ(E)}{dE} = \omega_{cl}(E)$$

thus

$$\Delta E_n = \hbar\omega_{cl}(E)$$

Particle in a periodic potential.

Phase space orbits.



Particle in a periodic potential.

Dynamics of a *classical* distribution $Q(q,p)$:

$$\frac{\partial Q}{\partial t} = -\{H, Q\}_{q,p} = -p\frac{\partial Q}{\partial q} + \kappa \sin q \frac{\partial Q}{\partial p} \ ,$$

solved by the method of characteristics*.

$$Q_0(q,p) = \frac{1}{2\pi\sqrt{\sigma_q \sigma_p}} \exp\left[\frac{(p-p_0)^2}{2\sigma_p}\right] \exp\left[\frac{(q-q_0)^2}{2\sigma_q}\right]$$

$(q_0, p_0) = (-1.5, 0)$, $\sigma_q = 0.18$, $\sigma_p = 0.33$

$$Q(q,p,t) = Q_0\left[\bar{q}(q,p,-t), \bar{p}(q,p,-t)\right],$$

$\big(\bar{q}(q,p,t), \bar{p}(q,p,t)\big)$ is the solution to Hamilton's equations.

* *R. Courant and D. Hilbert, Methods of Mathematical Physics, vol II*

Particle in a periodic potential.

Dynamics of a *classical* distribution $Q(q,p)$: Plot contours of Q

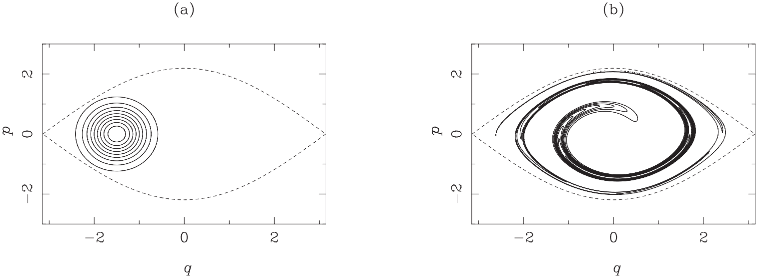


Figure: $\kappa = 1.2$, (a) initially the atom is localized in the region of bounded motion; (b) After just ten classical periods the distribution of the atom is sheered over the trajectories on which it has support.

Particle in a periodic potential.

Classical dynamics of moments of momentum:

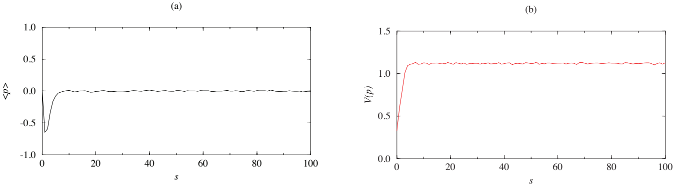


Figure: (a) the mean momentum, $\langle p \rangle$, rapidly collapses to zero due to the sheering action of the nonlinear motion;(b) the momentum variance, $V(p)$

Particle in a periodic potential.

Quantum dynamics of moments of momentum: