1.2 Foundations of Quantisation: Hamilton formalism

classical particle

$$H = H(x,p) \; ; \quad \dot{x} = \frac{\partial H}{\partial p} \, , \; \dot{p} = -\frac{\partial H}{\partial x} \qquad \text{e.o.m.}$$

Energy conservation (no explicit dep. on t: $\frac{\partial H}{\partial t} = 0$)

$$\frac{dH}{dt} \overset{!}{=} \frac{\partial H}{\partial x}\dot{x} + \frac{\partial H}{\partial p}\dot{p} = \frac{\partial H}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial H}{\partial x} = 0$$

Let x, p without argument be at equal time (e.g. $t=0$). Express the above with the Poisson-bracket $\{F, G\}_p \equiv \frac{\partial F}{\partial x}\frac{\partial G}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial G}{\partial x} = -\{G,F\}_p$

$$\Rightarrow \{x,x\}_p = \{p,p\}_p = 0 \, , \quad \boxed{\{x,p\}_p = 1} \qquad x, p \text{ conjugate var.}$$

$$\boxed{\dot{x}(t) = \{x, H\}_p \, , \quad \dot{p}(t) = \{p, H\}_p}$$

line 1: normalisation only (of phase space)

line 2: determine dynamics, time evolution; here we need H and V(x) pot.

Quantisation: (use units $\hbar = h/2\pi = 1$)

recipe: replace $x \to \hat{x}$, $p \to \hat{p}$ by operators $\Rightarrow H \to \hat{H}$ (non-com. objects!)

replace $\{\, , \,\}_p \to [\, , \,]\frac{1}{i}$ Poisson bracket by commutator $[A,B] = AB - BA$

$$\Rightarrow [\hat{x}, \hat{x}] = [\hat{p}, \hat{p}] = 0 \quad \boxed{[\hat{x}, \hat{p}] = i \, (\hbar)} \quad \text{equal time comm. rel.}$$

$$\boxed{i\frac{d}{dt}\hat{x}(t) = [\hat{x}, \hat{H}] \, , \quad i\frac{d}{dt}\hat{p}(t) = [\hat{p}, \hat{H}]} \quad \text{dynamics in \underline{Heisenberg picture}}$$

recall: equal time commutators are always the same, but the time dependence can be put into the operator (Heisenberg picture), states (Schrödinger ~) or both (Dirac ~, for interacting particles).

- Schrödinger picture: operator: t-indep, states: t-dep:

$$\boxed{i\frac{d}{dt}|t;s\rangle = \hat{H}|t;s\rangle} \quad \text{Schrödinger eq.} \qquad \left(\frac{d}{dt}\hat{H}=0\right)$$

$$\Rightarrow \quad \underline{|t;s\rangle = e^{-i\hat{H}t}|0;s\rangle}$$

Expectation values: $\langle t;s|\hat{O}_s|t;s\rangle = \langle 0;s|\underbrace{e^{i\hat{H}t}\hat{O}_s e^{-i\hat{H}t}}_{\hat{O}_H(t)}\overbrace{\underbrace{|0;s\rangle}_{|H\rangle}}^{|t;s\rangle}$

- Heisenberg picture: operators: t-dep, states: t-indep

$$|H\rangle \equiv |0;s\rangle \qquad \left(\frac{d}{dt}|H\rangle = 0\right)$$

$$\boxed{i\frac{d}{dt}\hat{O}_H(t) = [\hat{O}_H(t),\hat{H}]} \quad \text{Heisenberg e.o.m.}$$

$$\Rightarrow \quad \underline{\hat{O}_H(t) = e^{i\hat{H}t}\hat{O}_s e^{-i\hat{H}t}} \quad , \text{ exp. val. invariant!}$$

Dirac Ket Bra

- Standard example: Quantisation of the Harmonic Oscillator (HO)

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 \qquad m,\omega \text{ parameters} \quad (\omega=0 \text{ free particle})$$

Notation:

creation op

annihilation op

$$\hat{a} \equiv \sqrt{\frac{m\omega}{2}}\,\hat{x} + \frac{i}{\sqrt{2m\omega}}\,\hat{p}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2}}\,\hat{x} - \frac{i}{\sqrt{2m\omega}}\,\hat{p}$$

(as $\hat{x}=\hat{x}^\dagger$, $\hat{p}=\hat{p}^\dagger$ Hermitian $\Rightarrow \hat{H}=\hat{H}^\dagger$ too)

$$\Leftrightarrow \quad \hat{x} = \frac{1}{\sqrt{2m\omega}}(\hat{a}^\dagger + \hat{a})$$

$$\hat{p} = i\sqrt{\frac{m\omega}{2}}(\hat{a}^\dagger - \hat{a})$$

exercise 2.1 $\Rightarrow$ $[\hat{a},\hat{a}] = 0 = [\hat{a}^\dagger,\hat{a}^\dagger]$

$$\underline{[\hat{a},\hat{a}^\dagger] = 1}$$

classical solution

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

$$\frac{\partial H}{\partial p} = \{x, H\}_P \qquad -\frac{\partial H}{\partial x} = \{p, H\}_P$$

e.o.m.: $\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \Leftrightarrow p = m\dot{x}$

$$\dot{p} = m\ddot{x} = -\frac{\partial H}{\partial x} = -m\omega^2 x \Leftrightarrow \ddot{x} = -\omega^2 x$$

$\Rightarrow \quad x(t) = A\cos\omega t + B\sin\omega t \;, \quad p(t) = -\omega m A \sin\omega t + m\omega B\cos\omega t$

$\Rightarrow \quad x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t \;, \quad p(t) = -m\omega x(0)\sin(\omega t) + p(0)\cos\omega t$

in terms of boundary conditions at $t=0$ $\quad x(t=0), p(t=0)$

average over period $T = \frac{2\pi}{\omega}$: $\boxed{\langle x(t)^2\rangle \equiv \frac{1}{T}\int_0^T dt\, x(t)^2 = \frac{1}{2}x(0)^2 + \frac{1}{2}\left(\frac{p(0)}{m\omega}\right)^2} \in \mathbb{R}_+$

(and $\langle x(t)\rangle = 0$)

Poisson brackets $\{x(0), x(0)\}_P = 0$ equal time $\left(\frac{\partial}{\partial x} = \frac{\partial}{\partial x(0)}, \frac{\partial}{\partial p} = \frac{\partial}{\partial p(0)}\right)$

BUT: $\boxed{\{x(t), x(0)\}_P = \{x(0)\cos\omega t, x(0)\} + \frac{1}{m\omega}\{p(0)\sin\omega t, x(0)\}_P = -\frac{1}{m\omega}\sin\omega t \neq 0}$

QM solution: (Heisenberg pic.) $\quad \hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\hat{x}^2$

$$i\frac{d}{dt}\hat{x}_H(t) = [\hat{x}_H(t), \hat{H}(t)] = \frac{1}{2m}[\hat{x}_H, \hat{p}_H^2] = \frac{1}{2m}\left(\hat{p}_H[\hat{x}_H, \hat{p}_H] + [\hat{x}_H, \hat{p}_H]\hat{p}_H\right)$$

$$= \frac{i}{m}\hat{p}_H \qquad \text{as } [A, BC] = [A,B]C + B[A,C]$$

$$i\frac{d}{dt}\hat{p}_H(t) = [\hat{p}_H(t), \hat{H}(t)] = \frac{m\omega^2}{2}[\hat{p}_H, \hat{x}_H^2] = \frac{m\omega^2}{2}\left(\hat{x}_H[\hat{p}_H, \hat{x}_H] + [\hat{p}_H, \hat{x}_H]\hat{x}_H\right)$$

$$= -im\omega^2\hat{x}_H$$

$\Rightarrow \boxed{\frac{d^2}{dt^2}\hat{x}_H(t) = -\omega^2\hat{x}_H(t)}$ same as class. e.o.m.

solution $\hat{x}_H(t) = \hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t$

$\hat{p}_H(t) = -m\omega\hat{x}\sin\omega t + \hat{p}\cos\omega t$

in terms of b.c. $\hat{x} \equiv \hat{x}_H(0) = \hat{x}_S \;, \; \hat{p} \equiv \hat{p}_H(0) = \hat{p}_S$

reexpress with $\hat{a}, \hat{a}^\dagger$:

$$\hat{x}_H(t) = \frac{1}{\sqrt{2m\omega}}\left\{(\hat{a}+\hat{a}^\dagger)\cos\omega t + i(\hat{a}^\dagger - \hat{a})\sin\omega t\right\}$$

$$= \frac{1}{\sqrt{2m\omega}}\left\{\hat{a}\, e^{-i\omega t} + \hat{a}^\dagger e^{i\omega t}\right\}$$

as $\hat{x}_H(0) = \hat{x} = \frac{1}{\sqrt{2m\omega}}(\hat{a}+\hat{a}^\dagger)$, $\hat{p}_H(0) = \hat{p} = i\sqrt{\frac{m\omega}{2}}(\hat{a}^\dagger - \hat{a})$

(ditto $\hat{p}_H(t) = \sqrt{\frac{m\omega}{2}}\left(-(\hat{a}+\hat{a}^\dagger)\sin\omega t + i(\hat{a}^\dagger-\hat{a})\cos\omega t\right) = \sqrt{\frac{m\omega}{2}}\, i\left\{-\hat{a}\, e^{-i\omega t} + \hat{a}^\dagger e^{i\omega t}\right\}$

<u>different time commutator:</u> $\left([\hat{x}_H(0), \hat{x}_H(0)] = 0 \right)$

$$[\hat{x}_H(t), \hat{x}_H(0)] = \frac{1}{2m\omega}\left\{[\hat{a},\hat{a}^\dagger]e^{-i\omega t} + [\hat{a}^\dagger,\hat{a}]e^{i\omega t}\right\} = \frac{1}{2m\omega}\left\{e^{-i\omega t} - e^{i\omega t}\right\}$$

$$= \frac{-i}{m\omega}\sin\omega t$$, consistent with rule $\{\,,\,\}_P \to [\,,\,]\frac{1}{i}$

<u>average:</u> define n-oscillator state $|n\rangle$, $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$ (→ ex. 2.)

$$\Rightarrow \langle n|\hat{x}_H(t)^2|n\rangle = \frac{1}{2m\omega}\langle n|\left\{\hat{a}\hat{a}\, e^{-2i\omega t} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger e^{2i\omega t}\right\}|n\rangle$$

$$\overset{\text{ex. 2.}}{=} \frac{1}{2m\omega}(2n+1) > 0$$

$\langle n|\hat{x}|n\rangle = 0$

<u>QM vs. class.:</u>

- time dependence identical
- expectation value ("fluctuations"):
  - class is arbitrary, continuous function of $x(0)$, $p(0)$
  - QM is quantised, dictated by commutation relations