Quantum Mechanics: Introduction

Particle of mass m:

Schrödinger wave equation

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V(\vec{x})\psi$$

same as in classical mech

$$\psi(\vec{x},t) = \psi(\vec{x})e^{-\frac{iEt}{\hbar}}$$ - separation of variables

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V\psi = E\psi$$ energy

time indep. Schrödinger eq

Wave function ψ = probability amplitude

Meaning: $|\psi(\vec{x},t)|^2 dV$ - probability of finding particle in dV at $\vec{x}$, time t

ψ has to belong to $\mathcal{L}^2(\mathbb{R}^3)$ in order for total prob $= 1 = \int |\psi|^2 dV$

Hamiltonian formulation of QM:

Classical mech: time evolution gen. by Hamilt.

Similar here, but:

$\mathcal{H}$ - Hilbert space (usually inf. dim.)

$\mathcal{L}^2(M)$ - usually, M - conf. space.

Unbounded self-adjoint operators

eigenfunctions vs no eigenf.

$x, -i\frac{d}{dx}$ on $\mathcal{L}^2(\mathbb{R})$

"eigenfunctions": $-i\frac{d}{dx}e^{ipx} = p\,e^{ipx}$

$x\,\delta(x-a) = a\,\delta(x-a)$

"Rigged" Hilbert space:

Nested sequence: $\Omega \subset \mathcal{H} \cong \mathcal{H}^* \subset \Omega^*$

Ω - nuclear subspace - dense in $\mathcal{H}$ functions decreasing faster than any power of $|x|$ at infinity.

"eigenfunctions" - distributions from Ω^*

$f(x) \to \int dx\, f(x)e^{ipx} = \hat{f}(p)$

Inverse transform: $f(x) = \int \frac{dp}{2\pi}\hat{f}(p)e^{-ipx}$

decomp. in terms of eigenf.

State of QM system: normalized unit vector in $\mathcal{H}$.

classical mech: States - points in phase space coords + momenta

observables: positions of momenta, energies angular momenta - functions on phase space

QM: observables → Self-adj operators in $\mathcal{H}$

Notation: $|\psi\rangle$ - vectors in $\mathcal{H}$
(Dirac) mnemonic label, e.g.

$|a\rangle$ $A|a\rangle = a|a\rangle$
eigenv.

$(\phi, A\psi) \rightsquigarrow \langle\phi|A|\psi\rangle$
bra ket

Assume system is in state $|\psi\rangle$
Measure observable repr. by self-adj. A

$A|a\rangle = a|a\rangle$ $\langle a'|a\rangle = \delta_{aa'}$ $\langle a'|a\rangle = \delta(a-a')$
(assume spectrum is simple) discrete continuous

"Rigged" space framework: $|\psi\rangle = \int da' f(a')|a'\rangle$
for any $\phi, \psi \in \Omega$ $|\phi\rangle = \int da\, g(a)|a\rangle$
$\langle\psi|\phi\rangle = \int da\, f^*(a) g(a)$

For discrete spectrum:
result of measurement will be a
with probability $|\langle a|\psi\rangle|^2$ for discr.

and with prob. $|\langle a|\psi\rangle|^2 \Delta a$
between a and $a+\Delta a$ for continuous

Total prob. is 1 since $|\psi\rangle$ normalized.

Useful identity: $\sum_a |a\rangle\langle a| = 1$
$\int da$

e.g. $\sum_a |a\rangle\langle a|\psi\rangle = |\psi\rangle$ exp. in orth. basis

Average value obtained over many measurements of A in $|\psi\rangle$:

$$\sum_a a|\langle a|\psi\rangle|^2 = \sum_a a\langle\psi|a\rangle\langle a|\psi\rangle = \langle\psi|A|\psi\rangle$$

Observables q_i, p_i on phase space:
$[q_i, q_j] = [p_i, p_j] = 0$ $[q_j, p_k] = i\delta_{jk}$
$\hbar = 1$
$[\,,\,]$ - just a commutator.

$f(q,p) \longrightarrow f(\hat{q}, \hat{p})$ ambiguous
can be fixed in simple examples

$pq^2 = q^2 p = qpq$ - not true in quantum case

Deformation quantization
(M, π) - Poisson manifold
$Q: f \to$ operator
$Q^{-1}(Q_f Q_g) = f \underset{\hbar}{*} g = f\cdot g - \frac{i\hbar}{2}\{f,g\}_\pi + O(\hbar^2)$
star product

1) associative
2) unit function is a unit for $*$-product

Geometric quantiz. $Q(1) = Id$

$[Q(f), Q(g)] = i\hbar Q(\{f,g\})$

1) preq. → all smooth functions

polarization → cutting down variables $\int \frac{\omega}{2\pi\hbar} \in \mathbb{Z}$

$Q(f) = -i\hbar \nabla_{X_f} + f$ line bundle

Time evolution of QM.

$$|\psi(t)\rangle = e^{-i\frac{t}{\hbar}H}|\psi(0)\rangle$$

unitary operator

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

$$H|E\rangle = E|E\rangle \qquad |E(t)\rangle = e^{-iEt}|E(0)\rangle$$

Diag. H solves time evolution for any $|\psi\rangle$

$|\langle\psi|E(t)\rangle|^2$ - const. in time

$|E\rangle$ - stationary states

Schrödinger eq. in this framework

$\vec{x} = (x_1, x_2, x_3) \quad \vec{p} = (p_1, p_2, p_3)$

$x_i \longrightarrow x_i \cdot \qquad p_j \longrightarrow -i\hbar\frac{d}{dx_j}$

v. Neumann - only realiz. up to unitary equivalence

$$H = \frac{\vec{P}^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x})$$

Schrödinger eq ⟺ eigenvalue problem for H

Notice: $|\vec{y}\rangle = \delta^{(3)}(\vec{x}-\vec{y})$ eigenf. for position op $|x\rangle$ with eig. $\vec{y}$

$$\langle\vec{y}|\psi\rangle = \int d^3x\, \delta^3(x-y)\psi(x) = \psi(\vec{y})$$

↪ general postulates give interpr. of $\psi(\vec{y})$ as the prob. amplitude for finding part. near $\mathbb{R}^3 \ni \vec{y}$

Case $V=0$ - free particle $H = \frac{\vec{P}^2}{2m}$, $e^{i\vec{p}\cdot\vec{x}}$ - eig.

H has cont. spectrum ⇒ eigenfunct $\in S^*$

$\langle\vec{p}|\vec{p}'\rangle = \delta^{(3)}(\vec{p}-\vec{p}')$ - normaliz. $|p\rangle = (2\pi)^{-3/2}e^{i\vec{p}\cdot\vec{x}}$

Symmetries in QM.

G - Lie group → Unitary repr. of G in $\mathcal{H}$ commuting with $e^{-iHt} = U(t)$

$U(\theta) = e^{-i\theta A}$ - Stone's theorem

1-param. subgroup

A - Herm. generator

$\Rightarrow [A, H] = 0 \Rightarrow$

$\langle\phi(t)|A|\psi(t)\rangle = \langle\phi(0)|e^{iHt}Ae^{-iHt}|\psi(0)\rangle = \langle\phi(0)|A|\psi(0)\rangle$

thus A is conserved

Symmetries great for diagonalization:

$H|E\rangle = E|E\rangle \Rightarrow Hg|E\rangle = Eg|E\rangle$

Heisenberg picture

$|\psi\rangle \to U(t)|\psi\rangle = e^{-\frac{iHt}{\hbar}}|\psi\rangle$

$A \to U^\dagger(t)\, A\, U(t)$

$$\frac{d}{dt}A(t) = \frac{d}{dt}\, e^{\frac{i}{\hbar}Ht} A\, e^{-\frac{i}{\hbar}Ht} =$$

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

$\langle \varphi(t)| A |\psi(t)\rangle = \langle\varphi| A(t)|\psi\rangle$

making observables depend on time.

Remark

Remember the classical eq. of motion?

$$\frac{df}{dt} = \{H, f\}$$

Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{kx^2}{2} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

ω – frequency

Classical: $m\ddot{x} + kx = 0 \qquad x(t) = A\sin(\omega t + \phi)$

$$a = x\sqrt{\frac{m\omega}{2}} + ip\sqrt{\frac{1}{2m\omega}}$$

$$a^\dagger = x\sqrt{\frac{m\omega}{2}} - ip\sqrt{\frac{1}{2m\omega}}$$

$[a, a^\dagger] = 1$ since $[x,p] = i$

$$H = \frac{1}{2}\omega(aa^\dagger + a^\dagger a) = \omega(a^\dagger a + \tfrac{1}{2}) = \omega(N + \tfrac{1}{2})$$

$[N, a^\dagger] = a^\dagger \qquad [N, a] = -a$

Representation: $Na^\dagger|n\rangle = (n+1)a^\dagger|n\rangle$

$N a|n\rangle = (n-1)a|n\rangle$

H – sum of squares of self-adj. op $\Rightarrow$

$\Rightarrow$ no negative eigenv. $\Rightarrow \exists\, |0\rangle$

$a|0\rangle = 0$. Solving diff eq.

$\langle x|0\rangle = Ce^{-\frac{m\omega x^2}{2}}$

$N|0\rangle = 0 \Rightarrow H|0\rangle = \frac{\omega}{2}|0\rangle$

$|0\rangle$ – unique since first order diff. op.

$\langle n | a a^\dagger | n \rangle = \langle n | a^\dagger a + 1 | n \rangle = n+1$

normalized

$\| a^\dagger |n\rangle \|^2 \Rightarrow |n\rangle = (n!)^{-1/2} (a^\dagger)^n |0\rangle$

normalized eigenvalue

$a^\dagger |n\rangle = \sqrt{n+1}\, |n+1\rangle \qquad a|n\rangle = \sqrt{n}\, |n-1\rangle$

$\{|n\rangle\}$ - complete in $\mathcal{H}$!

$H\, |n\rangle = (n + \tfrac{1}{2})\, \omega$

Now can compute any $\langle m | A | n \rangle$ for any $A(x,p)$

S-matrix:

free states

$H = H_0 + V \qquad H_0 |\Phi_\alpha\rangle = E_\alpha |\Phi_\alpha\rangle$

$H |\Psi_\alpha^\pm\rangle = E_\alpha |\Psi_\alpha^\pm\rangle$ in / out — "in" and "out" states

$$\int d\alpha\, e^{-iE_\alpha \tau} g(\alpha) |\Psi_\alpha^\pm\rangle \xrightarrow[\tau \to \pm\infty]{} \int d\alpha\, e^{-iE_\alpha \tau} g(\alpha) |\Phi_\alpha\rangle$$

"wave packets"

In other words:

$$e^{-iH\tau} \int d\alpha\, g(\alpha) |\Psi_\alpha^\pm\rangle \to e^{-iH_0\tau} \int d\alpha\, g(\alpha) |\Phi_\alpha\rangle$$

$S_{\beta\alpha} = \langle \Psi_\beta^- | \Psi_\alpha^+ \rangle$

S-matrix — transition amplitude between in/out states

$S = \Omega(\infty)^\dagger\, \Omega(-\infty) = U(+\infty, -\infty)$

where $\Omega(\tau) = e^{iH\tau} e^{-iH_0\tau}$

$$U(\tau, \tau_0) = \Omega(\tau)^\dagger \Omega(\tau_0) = e^{iH_0\tau} e^{-iH(\tau-\tau_0)} e^{-iH_0\tau_0}$$

$$S_{\beta\alpha} = \langle \Phi_\beta | e^{iH_0\tau} e^{-iH(\tau-\tau_0)} e^{-iH_0\tau_0} | \Phi_\alpha \rangle \Big|_{\substack{\tau \to +\infty \\ \tau \to -\infty}}$$

$$i \frac{d}{d\tau} U(\tau, \tau_0) = V(\tau)\, U(\tau, \tau_0)$$

$$V(t) = e^{iH_0 t}\, V\, e^{-iH_0 t}$$

"interaction picture"

Solution $U(\tau, \tau_0) =$

$$= T \exp \int_{\tau_0}^{\tau} -i V(t)\, dt =$$

$$= 1 + \sum \frac{(-i)^n}{n!} \int_{\tau_0}^{\tau} \dots \int_{\tau_0}^{\tau} T(V(s_1) \dots V(s_n))\, ds_1 \dots ds_n$$

Thus,

$$S_{\beta\alpha} = \langle \Phi_\beta | T \exp \int_{-\infty}^{\infty} -iV(t)\,dt \,|\, \Phi_\alpha \rangle$$

$$V(t) = e^{iH_0 t} V e^{-iH_0 t}$$

Perturbation series

Let us realize it using path integral

$$[Q_a, P_b] = i\delta_{ab} \quad [Q_a, Q_b] = [P_a, P_b] = 0$$

$$Q_a|q\rangle = q_a|q\rangle \qquad \langle q'|q\rangle = \delta(q'-q) = \prod_a (q'_a - q_a)$$

$$1 = \int \prod_a dq_a |q\rangle\langle q|$$

$$P_a|p\rangle = p_a|p\rangle \quad \langle p'|p\rangle = \prod_a \delta(p_a - p'_a) = \delta(p'-p)$$

$$\langle q|p\rangle = \prod_a \frac{1}{\sqrt{2\pi}} e^{iq_a p_a}$$

Heisenberg picture: $\quad$ " $e^{iHt}|q\rangle$

$$Q_a(t)|q;t\rangle = q_a|q;t\rangle$$
$$P_a(t)|p;t\rangle = p_a|p;t\rangle$$

$$\langle q';\tau+\Delta\tau|q;\tau\rangle = \langle q';\tau|e^{-iH\Delta\tau}|q;\tau\rangle$$

$H(Q,P)$ - order s.t. Q on the left, P on the right

$$\int \prod_a dp_a \langle q';\tau| e^{-iH(Q(\tau),P(\tau))\Delta\tau}|p;\tau\rangle \times \langle p;\tau|q;\tau\rangle$$

$$= \int_{-\infty}^{\infty} \prod_a \frac{dp_a}{2\pi} e^{-iH(q',p)\Delta\tau + i\sum_a (q'_a - q_a)p_a}$$

$$\tau_{k+1} - \tau_k = \Delta\tau = \frac{(t'-t)}{N+1}$$

$$t, \tau_1 \ldots, \tau_N, t'$$

$$\langle q';t'|q;t\rangle = \int dq_1 \ldots dq_N \langle q';t'|q_N;\tau_N\rangle \ldots \langle q_1;\tau_1|q;t\rangle$$

$$\parallel$$

$$\int \left[\prod_{k=1}^{N} \prod_a dq_a\right] \left[\prod_{k=0}^{N} \prod_a dp_a/2\pi\right]$$

$$\exp\left(i\sum_{k=1}^{N+1}\left\{\sum_a (q_{k,a} - q_{k-1,a})p_{k-1,a} - H(q_k, p_{k-1})\Delta\tau\right\}\right)$$

$$q_0 = q \qquad q_{N+1} = q' \qquad q_a(\tau_k) = q_{k,a}$$
$$p_a(\tau_k) = p_{k,a}$$

$$\langle q', t' | q, t\rangle = \int \prod_{\tau, a} dq^a(\tau) \prod_{\tau, b} \frac{dp_b(\tau)}{2\pi}$$

$q_a(t) = q_a$
$q_a(t') = q'_a$

$$\exp\left(i \int_t^{t'} d\tau \left(\sum_a \dot{q}^a(\tau) p_a(\tau) - H(p(\tau), q(\tau))\right)\right)$$

<u>Generalization:</u> correlation function

$$\langle q', t' | O_A(p(t_A), Q(t_A)) O_B(p(t_B), Q(t_B)) \ldots | q, t\rangle$$

$$= \int [dq][dp] \; O_A(p(t_A), q(t_A)) O_B(p(t_B), q(t_B)) \ldots \exp(\ldots)$$

$t_A > t_B > \ldots$

$$\langle q', t' | \; e^{\int dt \sum_A J_A(t) O_A(t)} | q, t\rangle =$$

$$= \int [dq][dp] \exp i\left(\int_t^{t'} d\tau (\dot{q}^a p_a - H + \sum_A J_A O_A\right)$$

Let's put support of J_a in $t \in (a, b]$

$$\langle q', t' | q, t\rangle^J = \langle q' | U^J(t, t') | q\rangle =$$

$$= \langle q' | e^{-iH(t'-b)} U^J(a, b) e^{-iH(a-t)} | q\rangle$$

$$\langle q', t' | q, t\rangle^J =$$

$$= \sum_{m,n} \langle q' | e^{-iH(t'-b)} | m\rangle \langle m | U^J(a, b) | n\rangle \langle n | e^{-iH(a-t)} | q\rangle =$$

$$= \sum_{m,n} \langle q' | m\rangle \langle n | q\rangle e^{-iE_m(t'-b)} e^{-iE_n(a-t)} \langle m | U^J(a, b) | n\rangle$$

$t \to -\infty \quad t' \to +\infty$

$t = i\tau \quad \tau \to -\infty \quad \tau \to +\infty$

Wick rotation

Thus all m, n vanish except $|0\rangle$ $\quad E_0 = 0$

$$\langle q', t' | q, t\rangle^J \Big|_{\substack{t' \to +\infty \\ t \to -\infty}} = \langle q' | 0\rangle \langle 0 | q\rangle Z(J)$$

$$Z(J) = \langle 0 | U^J(a, b) | 0\rangle = \langle 0 | U^J(-\infty, +\infty) | 0\rangle$$

$Z(0) = 1$ - normalization

$$Z(J) = \frac{\langle q', t' | q, t\rangle^J \Big|_{\substack{t' \to +\infty \\ t \to -\infty}}}{\langle q' | 0\rangle \langle 0, q\rangle}$$

$$\to Z(J) = N \int [dq][dp] \, e^{iS^J}$$

$$\langle 0 | T(O_{A_1}(t_1) \ldots O_{A_n}(t_n)) | 0\rangle =$$

$$= (-i)^n \frac{\delta^n}{\delta J_{A_1}(t_1) \ldots \delta J_{A_n}(t_n)} Z(J) \Big|_{J=0}$$

Lagrangian version of path integral

$$H(Q,P) = \frac{1}{2}\sum_{n,m} A_{n,m}(Q) P_n P_m + \sum_n B_n(Q) P_n + C(Q)$$

$$\int d\tau \left[\sum_n p_n(\tau)\dot{q}^n(\tau) - H(q(\tau),p(\tau))\right] =$$

$$= -\frac{1}{2}\sum_{nm}\int d\tau \int d\tau' \tilde{A}_{n,m}(\tau,\tau')\, p_n(\tau) p_m(\tau')$$

$$- \int d\tau\, \tilde{B}_{\tau,n}[q(\tau)]\, p_n(\tau) - \tilde{C}(q)$$

$$\tilde{A}_{n,m}(\tau,\tau') = A_{nm}(q(\tau))\,\delta(\tau-\tau')$$

$$\tilde{B}_{\tau n}(q(\tau)) = B_n(q(\tau)) - \dot{q}_n(\tau)$$

$$\tilde{C}(q) = \int d\tau\, C[q(\tau)]$$

Formula $\int_{-\infty}^{\infty}\prod_s d\xi_s \exp\left(-\frac{i}{2}\sum_{sr}\hat{A}_{sr}\xi_s\xi_r - i\sum \hat{B}_s\xi_s - i\hat{C}\right)$

$$= \left(\mathrm{Det}\left(\frac{i\hat{A}}{2\pi}\right)\right)^{-1/2} \exp\left(-\frac{i}{2}\sum \hat{A}_{sr}\bar{\xi}_s\bar{\xi}_r - i\sum \hat{B}_s\bar{\xi}_s - i\hat{C}\right)$$

$$\bar{\xi}_s = -\sum_r (\hat{A}^{-1})_{sr}\hat{B}_r$$

$\bar{\xi}$ - stationary point!

$$\frac{\delta}{\delta p_n(\tau)}\int_{-\infty}^{\infty} d\tau\left[\dot{q}^n(\tau)p_n(\tau) - H(q(\tau),p(\tau))\right]$$

$$= \dot{q}_n(\tau) - \frac{\delta}{\delta p_n(\tau)} H(q(\tau),p(\tau))$$

$$L(q(\tau),\dot{q}(\tau)) = \dot{q}^n(\tau)\bar{p}_n(\tau) - H(q(\tau),\bar{p}(\tau))$$

$$N\int [dq][dp]\, e^{i\int\left[\dot{q}^n(\tau)p_n(\tau) - H(q(\tau),p(\tau))\right]d\tau}$$

$$= \tilde{N}\int [dq]\, e^{i\int L(q(\tau),\dot{q}(\tau))}$$

Now let's look at the example.

Harmonic oscillator via Path Integrals

Integrating over $\{p\}$ variables

$$\int d^n x\, e^{-x^T A x + J^T x} \;=$$

$$-x^T A x + J^T x = -(x - \tfrac{1}{2}A^{-1}J)^T A (x - \tfrac{1}{2}A^{-1}J) + \tfrac{1}{4} J^T A^{-1} J$$

$$y = x - \tfrac{1}{2} A^{-1} J$$

$$= e^{J^T A^{-1} J/4} \underbrace{\int d^n y\, e^{-y^T A y}}_{\text{normalization factor}}$$

$$Z(J) = N \int [Dq]\, e^{i\int dt (L + qJ)}$$

$$L = -\tfrac{1}{2} m q \underbrace{\left(\frac{d^2}{dt^2} + \omega^2\right)}_{A} q \qquad A^{-1}?$$

$$\left(\frac{d^2}{dt^2} + \omega^2\right) f(t) = g(t)$$

$$f(t) = \int ds\, G(t,s)\, g(s)$$

$$\left(\frac{d^2}{dt^2} + \omega^2\right) G(t,s) = \delta(t-s)$$

Assume $G(t,s) = G(t-s)$

$$\tilde{G}(k) = \int dt\, G(t)\, e^{-ikt}$$

$$G(t) = \int \frac{dk}{2\pi}\, \tilde{G}(k)\, e^{ikt}$$

$$(-k^2 + \omega^2)\, \tilde{G}(k) = 1$$

$$\tilde{G}(k) = P\frac{-1}{k^2 - \omega^2} + h(k)\, \delta(k^2 - \omega^2)$$

General solution in terms of distributions $\rightarrow e^{\pm i\omega t}$

(A has kernel - we have to specify boundary conditions)

$$G(t) = \int \frac{dk}{2\pi} \frac{-1}{k^2 - \omega^2} e^{ikt}$$

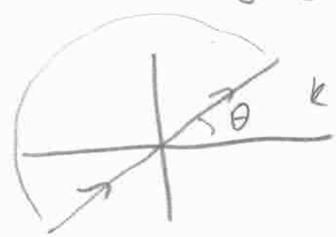
poles $k = \pm\omega$

solution:

$$G_E(k) = \frac{1}{k^2 + \omega^2} \qquad -\frac{d^2}{d\tau^2} + \omega^2$$

$$G(t) = \int \frac{dk}{2\pi} \frac{-1}{k^2 - \omega^2 + i\epsilon} e^{ikt}$$

$$k = \pm\sqrt{\omega^2 - i\epsilon}$$



contour passes below $k=-\omega$ and above $+\omega$

$$G(t) = \frac{i}{2\omega}\left[\theta(t)e^{-i\omega t} + \theta(-t)e^{i\omega t}\right]$$

$\theta(t)=0 \quad t<0 \quad \theta(t)=1 \quad \Rightarrow$

$$\Rightarrow Z(J) = e^{\frac{i}{2m}\int dt\,ds\,J(t)G(t-s)J(s)}$$

Thus:

$$\langle 0|T(q(t)q(t'))|0\rangle =$$

$$= (-i)^2 \frac{\delta^2}{\delta J(t)\delta J(t')} Z[J]\Big|_{J=0} =$$

$$= -\frac{i}{2m} G(t-t')$$

n-point correlation function:

n-odd $\Rightarrow$ result vanishes

$$\langle 0|T(x(t_1)x(t_2)x(t_3)x(t_4))|0\rangle =$$

$$= -\frac{1}{m^2}\Big[G(t_1-t_2)G(t_3-t_4) + $$
$$+ G(t_1-t_3)G(t_2-t_4) +$$
$$+ G(t_1-t_4)G(t_2-t_3)\Big]$$