$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

$$H\psi = -\sum \frac{\hbar^2}{2m_i} \nabla_i^2 \psi + V\psi$$

~~Claim~~ $\cancel{\|\psi_t\| = \|\psi_0\|}$

Claim
$$\frac{\partial |\psi_t(q)|^2}{\partial t} = -\sum_{i=1}^{N} \nabla_i \cdot \underline{j}_i(t,q).$$

$$\rho(t,q) = |\psi_t(q)|^2, \quad j_i(t,q) = \frac{\hbar}{m_i} \operatorname{Im}\left[\psi^*(t,q)\nabla_i\psi(t,q)\right]$$

$$q = (\underline{x}_1, \dots, \underline{x}_N) \in \mathbb{R}^{3N}$$

Pf of cont. eq. from Schr. eq.

$$\frac{\partial |\psi_t(q)|^2}{\partial t} = \frac{\partial}{\partial t}(\psi^*\psi) = \frac{\partial \psi^*}{\partial t}\psi + \psi^*\frac{\partial \psi}{\partial t} = 2\,\mathrm{Re}\left[\psi^*\frac{\partial\psi}{\partial t}\right]$$

$$= 2\,\mathrm{Re}\left[\psi^* \frac{\cancel{1}^{\,-i}}{\cancel{i}\hbar} H\psi\right] = 2\,\mathrm{Im}\left[\psi^*\frac{1}{\hbar}H\psi\right]$$

$$= \frac{2}{\hbar}\,\mathrm{Im}\left[-\sum_{i=1}^{N}\frac{\hbar^2}{2m_i}\psi^*\nabla_i^2\psi + \underbrace{\cancel{V\psi^*\psi}}_{\text{real}}\right]$$

$$= -\frac{\hbar}{m_i}\sum_i \mathrm{Im}\left(\psi^*\nabla_i^2\psi + \underbrace{(\nabla_i\psi^*)\cdot(\nabla_i\psi)}_{\text{real}}\right)$$

$$= -\sum_{i=1}^{N} \nabla_i \cdot j_i \,, \quad \text{QED.}$$

$\Rightarrow$ $|\psi|^2$ loc. conserved $\Rightarrow$ $\|\psi_t\|^2 = \|\psi_0\|^2$.

$\Rightarrow$ Born's rule is consistent with Schr. eq.

$$L^2(\mathbb{R}^{3N}, \mathbb{C}) = \{ \psi : \mathbb{R}^{3N} \to \mathbb{C} : \|\psi\| < \infty \}.$$

Thm (Ex. and uniqueness of sol.s of Schr. eq.)

For a large class of potentials V (including Coulomb, Newton's gravity, every bounded measurable fct. and linear combinations thereof) and for every $\psi_0 \in L^2(\mathbb{R}^{3N}, \mathbb{C})$, there is a unique weak solution (L^2 solution) $\psi(t,q)$ of the Schr. eq. with V and initial datum ψ_0. Moreover, $\psi_t \in L^2(\mathbb{R}^{3N}, \mathbb{C})$ $\forall t \in \mathbb{R}$.

Pf: Stone's thm, Kato's thm
[Reed & Simon].

Time Evolution Operators

$$U_t \psi_0 = \psi_t, \qquad U_t : L^2 \to L^2$$

propagator

- linear, i.e. $U_t(\psi + \phi) = U_t \psi + U_t \phi$
  $U_t(\lambda \psi) = \lambda U_t \psi \quad \forall \lambda \in \mathbb{C}$
  $\forall \psi, \phi \in L^2(\mathbb{R}^{3N}, \mathbb{C})$

- preserves norms : $\|U_t\psi\| = \|\psi\|$

  isometric

- composition law : $U_s U_t = U_{t+s}$, $U_0 = I$ $\forall s,t \in \mathbb{R}$

  I = identity, $I\psi = \psi$

  conseq : $U_{-t} U_t = I$, so $U_{-t} = U_t^{-1}$

  (U_t is a bijection)

A bijective isometry is called a unitary operator.

$\Rightarrow U_t$ is unitary.

Ex: $(\psi_1, \psi_2, \psi_3, \dots) \longmapsto (0, \psi_1, \psi_2, \psi_3, \dots)$

$L^2(\mathbb{N}, \mathbb{C}) = \ell^2$ square-summable sequences

$\sum_{n=1}^{\infty} |\psi_n|^2 < \infty$

isometric but not unitary
not surjective.

comp law: $U_s U_t = U_{t+s}$, $U_0 = I$

1-parameter group

Rem if not time translation invariant? $V(t, q)$

Then $U_{t_1}^{t_2}$, $U_{t_2}^{t_3} U_{t_1}^{t_2} = U_{t_1}^{t_3}$, $U_{t_1}^{t_1} = I$

$$U_t = e^{-iHt/\hbar}$$

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$ for bounded A.

converges in norm

$\|A\|$ = operator norm

H is unbounded, $H : \mathcal{D} \to L^2(\mathbb{R}^{3N}, \mathbb{C})$

domain

dense subspace

$e^{-iHt/\hbar}$

$$\phi_t := e^{-iHt/\hbar}\,\psi_0$$

U_t is bounded

valid for $\psi_0 \in \mathcal{D}$

~~Naive~~ computation:

$$i\hbar \frac{d\phi_t}{dt} = i\hbar \frac{d}{dt}\left(e^{-iHt/\hbar}\right)\psi_0$$

$$= i\hbar\left(-\frac{i}{\hbar}H\right)e^{-iHt/\hbar}\,\psi_0$$

$$= H\,\phi_t\,.$$

in finite dim: $\psi : \{1, \dots, n\} \to \mathbb{C}$

$$\|\psi\| = \left(\sum_{i=1}^{n} |\psi(i)|^2 \right)^{1/2} \quad \text{and}$$

$\psi = (\psi(1), \dots, \psi(n)) \in \mathbb{C}^n$,

unitary $U : \mathbb{C}^n \to \mathbb{C}^n$ $n \times n$ matrix

unitary iff $U^+ = U^{-1}$, $U^+ =$ adjoint matrix

$(U^+)_{ij} = U^*_{ji}$ conjugate transpose

Inner product

$\underline{u} \cdot \underline{v} = \sum_{i=1}^{3} u_i v_i$

$$\langle \psi | \phi \rangle = \int_{\mathbb{R}^d} \psi^*(q)\, \phi(q)\, dq.$$

$\forall \psi, \phi \in L^2(\mathbb{R}^{d}, \mathbb{C})$. Properties:

1. anti-linear in ψ

$$\langle \psi + \chi | \phi \rangle = \langle \psi | \phi \rangle + \langle \chi | \phi \rangle, \quad \langle \lambda \psi | \phi \rangle = \lambda^* \langle \psi | \phi \rangle$$

2. linear in ϕ, $\langle \psi | \phi + \chi \rangle = \ldots$, $\langle \psi | \lambda \phi \rangle = \lambda \langle \psi | \phi \rangle$

sesqui-linear   sesqui $= \frac{3}{2}$

3. conjugate-symm. = Hermitian

$$\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^*$$

4. positive definite:

$$\langle \psi | \psi \rangle > 0 \quad \text{for } \psi \neq 0$$

Analog in $\mathbb{C}^n$: $\langle \psi | \phi \rangle = \sum_{i=1}^{n} \psi^*(i)\, \phi(i).$

$$\|\psi\| = \sqrt{\langle \psi | \psi \rangle}$$

<u>Rem</u> $\langle \psi | \phi \rangle = \frac{1}{4}\left(\|\psi+\phi\|^2 - \|\psi-\phi\|^2 - i\|\psi+i\phi\|^2 + i\|\psi-i\phi\|^2 \right).$

polarization identity

Conseq U unitary $\Rightarrow$ $\langle U\psi | U\phi\rangle = \langle \psi | \phi\rangle$.

Def Hilbert space $\mathcal{H}$ is a complex vector space with inner product such that $\underbrace{\text{every Cauchy sequence converges.}}_{\text{complete}}$

Thm $L^2(\mathbb{R}^d, \mathbb{C}^n)$ is a Hilbert space.

1.4 Classical Mechanics

Def Newtonian mechanics

World consists of: 3-dim Euclidean space,
1-dim time (Euclidean),

N particles (material points), $\underline{Q}_i : \mathbb{R}_t \to \mathbb{R}^3_q$

eq. of motion:

$$m_i \frac{d^2 \underline{Q}_i(t)}{dt^2} = -\nabla_i V\left(\underline{Q}_1(t), \dots, \underline{Q}_N(t)\right)$$

with $V = -\sum_{i<j} \frac{e_i e_j / 4\pi\varepsilon_0}{|\underline{Q}_i - \underline{Q}_j|} + \sum_{i<j} \frac{m_i m_j G}{|\underline{Q}_i - \underline{Q}_j|}$.

ordinary diff. eq. (ODE)

initial data: $\underline{Q}_i(0)$ $\forall i$

$\mathbb{R}^{6N}$ = phase space $\dfrac{d\underline{Q}_i}{dt}(0)$ $\forall i$