Session 12
March 11, 2020

last time: • density $\rho_\psi = |\psi|^2$ and current (density) $j_\psi = \mathrm{Im}\, \overline{\psi} \nabla \psi$

satisfy continuity equation $\boxed{\partial_t \rho_\psi + \nabla j_\psi = 0}$

Note: this means $\underbrace{\partial_t \int_\Lambda \rho_\psi dx}_{\text{change of mass/probability/... in } \Lambda} = - \int_\Lambda \nabla j_\psi dx \overset{\text{Gauss (Stokes)}}{=} \underbrace{- \int_{\partial\Lambda} j_\psi d\sigma}_{\text{flow through boundary of } \Lambda}$

change of mass/probability/... in Λ = flow through boundary of Λ

now: current = density · velocity, i.e., $j_\psi = \rho_\psi \cdot v_\psi$

$$\Rightarrow \text{velocity vector field } v_\psi(t,x) = \frac{j_\psi(t,x)}{\rho_\psi(t,x)} = \frac{\mathrm{Im}\, \overline{\psi(t,x)} \nabla \psi(t,x)}{\overline{\psi(t,x)}\, \psi(t,x)} = \mathrm{Im}\, \underbrace{\frac{\nabla \psi(t,x)}{\psi(t,x)}}$$

looks dangerous at zeros of ψ, but this can be dealt with

Let us approximate v_ψ for large t, or v_{ψ_ε} for $\varepsilon \to 0$

↳ recall: macro scale $\frac{t}{\varepsilon}, \frac{x}{\varepsilon}$, $\psi_\varepsilon(t,x) = \varepsilon^{-\frac{d}{2}} \psi(\frac{t}{\varepsilon}, \frac{x}{\varepsilon})$,

$$\text{then } \psi_\varepsilon(t,x) = \frac{e^{i\frac{x^2}{2\varepsilon t}}}{(it)^{d/2}} \hat{\psi}_0\left(\frac{x}{t}\right) + \underbrace{\varepsilon^{-\frac{d}{2}} r\left(\frac{t}{\varepsilon}, \frac{x}{\varepsilon}\right)}_{\to 0 \text{ in } L^2 \text{ as } \varepsilon \to 0}$$

$$\Rightarrow v_{\psi_\varepsilon}(t,x) = \mathrm{Im} \frac{\nabla \psi_\varepsilon(t,x)}{\psi_\varepsilon(t,x)} = \mathrm{Im} \frac{(\nabla \psi)(\frac{t}{\varepsilon}, \frac{x}{\varepsilon})}{\psi(\frac{t}{\varepsilon}, \frac{x}{\varepsilon})} = v_\psi\left(\frac{t}{\varepsilon}, \frac{x}{\varepsilon}\right)$$

$$= \varepsilon\, \mathrm{Im} \frac{\nabla_x \psi(\frac{t}{\varepsilon}, \frac{x}{\varepsilon})}{\psi(\frac{t}{\varepsilon}, \frac{x}{\varepsilon})} = \varepsilon\, \mathrm{Im} \frac{\nabla_x \psi_\varepsilon(t,x)}{\psi_\varepsilon(t,x)}$$

$$\approx \varepsilon\, \mathrm{Im} \frac{\nabla_x \left(e^{i\frac{x^2}{2\varepsilon t}} \hat{\psi}_0(\frac{x}{t})\right)}{e^{i\frac{x^2}{2\varepsilon t}} \hat{\psi}_0(\frac{x}{t})}$$

$$= \varepsilon \operatorname{Im} i \frac{x}{\varepsilon t} + \mathcal{O}(\varepsilon)$$

$$= \frac{x}{t} + \mathcal{O}(\varepsilon)$$

$\Rightarrow v_{\psi_\varepsilon}(t,x) \approx \frac{x}{t}$ for small ε (or $v_\psi(t,x) \approx \frac{x}{t}$ for large t)

↳ in this sense classical trajectories appear in QM

Note: Regarding $v_\psi(t,x)$ as an actual velocity vector field for particles (i.e., integral curves give us the trajectories) gives Bohmian Mechanics (which explains the measurement formalism of QM – usually taken as additional axiom – in terms of particle trajectories)

3. The Schrödinger Equation with Potential

$i\partial_t \psi(t,x) = -\frac{\Delta}{2}\psi(t,x) + V(x)\psi(t,x) = H\psi(t,x)$ (here: V time-independent)

Fourier transformation turns V into convolution $\to$ not easy to find solution

Idea: regard $\psi : \mathbb{R}_t \to F$ for some function space F and solve ODE $i\frac{d}{dt}\psi(t) = H\psi(t)$ on F

$\Rightarrow$ formally $\psi(t) = e^{-iHt}\psi(0)$

Note: $\underbrace{\text{from physics}}_{|\psi(t,x)|^2 \text{ probability density}}$ and since $\|\psi(t,\cdot)\|_{L^2} = \|\psi_0\|_{L^2}$ for free SE we need to study $F = L^2(\mathbb{R}^d)$

3.1 Hilbert and Banach Spaces

Recall:
- Banach space = $\overbrace{\text{complete}}^{\text{every Cauchy sequence converges}}$ normed vector space
- Hilbert space = Banach space with scalar product $\langle\cdot,\cdot\rangle : \mathcal{H}\times\mathcal{H} \to \overbrace{\mathbb{C}}^{\text{or any other field}}$ s.t. $\|\psi\| = \sqrt{\langle\psi,\psi\rangle}$.

  Convention: $\langle\lambda\psi,\varphi\rangle = \bar{\lambda}\langle\psi,\varphi\rangle$

Ex.:
- $\mathbb{C}^n$ with $\langle x,y\rangle_{\mathbb{C}^n} = \sum_{j=1}^{n} \overline{x_j} y_j$
- ℓ^2 with $\langle x,y\rangle_{\ell^2} = \sum_{j=1}^{\infty} \overline{x_j} y_j$
- $L^2(M,\mu)$ for some measure space (M,μ), with $\langle\psi,\varphi\rangle_{L^2} = \int_M \overline{\psi(x)}\varphi(x)\,d\mu$

In the following, let $\mathcal{H}$ be a Hilbert space.

$\boxed{\text{Definition 3.3: A sequence } (\varphi_j)_j \text{ in } \mathcal{H} \text{ is called orthonormal sequence (ONS) if } \langle \varphi_i, \varphi_j \rangle = \delta_{ij} \quad \forall i,j}$

Properties of ONS $(\varphi_j)_j$:

- orthonormal decomposition: $\forall \psi \in \mathcal{H}$: $\psi = \underbrace{\sum_{j=1}^{n} \langle \varphi_j, \psi \rangle \varphi_j}_{=: \psi_n} + \underbrace{\left(\psi - \sum_{j=1}^{n} \langle \varphi_j, \psi \rangle \varphi_j \right)}_{=: \psi_n^\perp}$

  with $\langle \psi_n, \psi_n^\perp \rangle = \langle \psi_n, \psi - \psi_n \rangle = \langle \psi_n, \psi \rangle - \langle \psi_n, \psi_n \rangle = \sum_{j=1}^{n} \overline{\langle \varphi_j, \psi \rangle} \langle \varphi_j, \psi \rangle - \sum_{i,j=1}^{n} \overline{\langle \varphi_j, \psi \rangle} \underbrace{\langle \varphi_j, \varphi_i \rangle}_{=\delta_{ij}} \langle \varphi_i, \psi \rangle$

  $= 0$

  $\Rightarrow \langle \psi, \psi \rangle = \langle \psi_n + \psi_n^\perp, \psi_n + \psi_n^\perp \rangle = \langle \psi_n, \psi_n \rangle + \langle \psi_n^\perp, \psi_n^\perp \rangle$

- $\boxed{\text{Bessel inequality: } \|\psi\|^2 \geq \sum_{j=1}^{n} |\langle \varphi_j, \psi \rangle|^2}$ $\forall \psi \in \mathcal{H}, n \in \mathbb{N}$, follows directly from orthonormal decomposition

- $\boxed{\text{Cauchy-Schwarz: } |\langle \varphi, \psi \rangle| \leq \|\varphi\| \cdot \|\psi\|}$ $\forall \varphi, \psi \in \mathcal{H}$, follows from Bessel for $n = 1$, $\varphi_1 = \frac{\varphi}{\|\varphi\|}$

- $\boxed{\text{Polarisation identity}}$ for complex $\mathcal{H}$:

  $$\boxed{\langle \varphi, \psi \rangle = \frac{1}{4} \left(\|\varphi + \psi\|^2 - \|\varphi - \psi\|^2 - i \|\varphi + i\psi\|^2 + i \|\varphi - i\psi\|^2 \right)} \quad \forall \varphi, \psi \in \mathcal{H}$$

  (check by direct calculation)