

Next, we establish a more direct connection to velocity:

Consider the probability density  $\rho_\psi(t, x) = |\psi(t, x)|^2$  and  $i\partial_t \psi(t, x) = \left(-\frac{\Delta}{2} + V\right)\psi(t, x)$ ,  $V: \mathbb{R}^d \rightarrow \mathbb{R}$

$$\Rightarrow \partial_t \rho_\psi(t, x) = \partial_t |\psi(t, x)|^2 = \overline{\partial_t \psi(t, x)} \psi(t, x) + \psi(t, x) \overline{\partial_t \psi(t, x)}$$

$$= \frac{i}{2} \overline{(-\Delta \psi(t, x) + V(x)\psi(t, x))} \psi(t, x) - \frac{i}{2} \overline{\psi(t, x)} (-\Delta \psi(t, x) + V(x)\psi(t, x))$$

$$\frac{i}{2}z - \frac{i}{2}\overline{z} = \operatorname{Im} z$$

$$= \operatorname{Im} \overline{\psi(t, x)} (-\Delta \psi(t, x))$$

$$= -\nabla \underbrace{\operatorname{Im} \overline{\psi(t, x)} \nabla \psi(t, x)}_{=: j_\psi(t, x) = \text{current}} \quad (\text{since } \overline{\nabla \psi} \nabla \psi \in \mathbb{R})$$

$$\Rightarrow \partial_t \rho_\psi + \nabla \cdot j_\psi = 0, \text{ continuity equation}$$

Note: The continuity eq. implies:  $\partial_t \int \rho_\psi dx = - \int \nabla \cdot j_\psi dx \stackrel{\text{Gauss (Stokes)}}{=} - \int_{\partial \Lambda} j_\psi d\sigma$

change of mass/probability/... in  $\Lambda \subset \mathbb{R}^d$  (compact) = flow through boundary of  $\Lambda$

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

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

looks dangerous at zeros of  $\psi$ , but since  $\rho_\psi = 0$  at zeros of  $\psi$ , the velocity field never needs to be evaluated at the zeros.

Let us approximate  $v_\psi$  for large  $t$ .

$$v_\psi(t, x) = \lim \frac{\nabla \psi(t, x)}{\psi(t, x)}$$

We skip the rigorous estimate  $\approx$

$$\approx \lim \frac{\nabla_x \left( (it)^{-\frac{d}{2}} e^{i\frac{x^2}{2t}} \hat{\psi}_0\left(\frac{x}{t}\right) \right)}{(it)^{-\frac{d}{2}} e^{i\frac{x^2}{2t}} \hat{\psi}_0\left(\frac{x}{t}\right)}$$

$$= \lim \frac{i\frac{x}{t} e^{i\frac{x^2}{2t}} \hat{\psi}_0\left(\frac{x}{t}\right) + e^{i\frac{x^2}{2t}} \nabla_x \hat{\psi}_0\left(\frac{x}{t}\right)}{e^{i\frac{x^2}{2t}} \hat{\psi}_0\left(\frac{x}{t}\right)}$$

$$\approx \frac{x}{t} + O\left(\frac{1}{t}\right)$$

↳ So for example, in this sense classical trajectories appear in QM

### 3. The Schrödinger Equation with Potential

Next, we want to understand the Schrödinger equation

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

Note: • Fourier transformation turns  $V$  into convolution  $\Rightarrow$  not easy to find solutions for  $V \neq 0$ .

• Since  $|\psi(t, x)|^2$  is a probability density, we want to understand the SE on  $L^2$ .

(For the free SE we had  $\|\psi(t)\|_{L^2} = \|\psi(0)\|_{L^2}$  if  $\psi(0) \in L^2$ , and that should also hold for  $V \neq 0$ .)

Ideas that we will develop in this chapter:

• As we have done for the free SE, we try to make sense of  $e^{-iHt}$  for a large class of  $V$ , s.t. we can define  $\psi(t) = e^{-iHt} \psi(0)$ .

• We regard  $L^2$  as a subspace of  $S'$ , s.t. the SE holds in the sense of distributions; but hopefully it also holds on  $L^2$ , at least for some initial data.

First, we want to embed the free SE in the  $L^2$  framework, so we discuss Hilbert spaces (and operators on them) in general, and then how to define  $\mathcal{F}: L^2 \rightarrow L^2$ .

### 3.1 Hilbert and Banach Spaces

- Recall: • **Banach space** = <sup>every Cauchy sequence converges</sup> complete normed vector space
- **Hilbert space** = Banach space with scalar product  $\langle \cdot, \cdot \rangle: \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$  s.t.  $\|\psi\| = \sqrt{\langle \psi, \psi \rangle}$ . <sup>or any other field</sup>
- Convention:  $\langle \lambda \psi, \varphi \rangle = \overline{\lambda} \langle \psi, \varphi \rangle$ . "antilinearity in the first argument"

Examples: •  $\mathbb{C}^n$  with  $\langle x, y \rangle_{\mathbb{C}^n} = \sum_{j=1}^n \overline{x_j} y_j$

•  $\ell^2$  with  $\langle x, y \rangle_{\ell^2} = \sum_{j=1}^{\infty} \overline{x_j} y_j$

•  $L^2(M, \mu)$  for some measure space  $(M, \mu)$ , with  $\langle \psi, \varphi \rangle_{L^2} = \int_M \overline{\psi(x)} \varphi(x) d\mu$

Let us first prove some standard properties.

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

**Definition 3.3:** A sequence  $(e_j)_j$  in  $\mathcal{H}$  is called orthonormal sequence (ONS) if  $\langle e_i, e_j \rangle = \delta_{ij} \quad \forall i, j$ .

The following properties hold:

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

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

$= 0$

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