Definition 2.1 A *classical solution* to the Schrödinger equation is a function $\psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$ that satisfies the following regularity conditions:

- $\psi(x,\cdot) \in C^1([0,\infty))$ for every $x \in \mathbb{R}^d$. There exists $\tau > 0$ and $g \in L^1$ such that $\left| \frac{\partial}{\partial t} |\psi(x,t)|^2 \right| \leq g(x)$ $\forall t \in [s-\tau, s+\tau]$, $\forall s$.
- $\psi(\cdot,t) \in C^2(\mathbb{R}^d)$ for every t, and $\Delta\psi(\cdot,t) \in L^2(\mathbb{R}^d)$.
- $V(\cdot)\,\psi(\cdot,t) \in L^2(\mathbb{R}^d)$ for every t.

In addition, $\psi(x,t)$ satisfies the Schrödinger equation.

We shall see later that classical solutions exist. Now we discuss important properties.

Lemma 2.1 If ψ is a classical solution, then $\int |\psi(x,t)|^2 dx$ is constant in t.

Proof: Here we set $\hbar = 2m = 1$.

$$\frac{d}{dt} \int |\psi(x,t)|^2 dx = \int \frac{d}{dt} |\psi(x,t)|^2 dx$$

e.g. by Thm 2.27 in Folland

$$= \int \left[\overline{\frac{\partial}{\partial t}\psi(x,t)}\, \psi(x,t) + \overline{\psi(x,t)}\, \frac{\partial}{\partial t}\psi(x,t) \right] dx$$

$$\overset{\text{Schr. eq.}}{=} \int \left[-i\Delta\overline{\psi(x,t)}\, \psi(x,t) + i\,\overline{\psi(x,t)}\,\Delta\psi(x,t) + i\,V(x)\,|\psi(x,t)|^2 - i V |\psi|^2 \right] dx$$

$$\overset{\text{by parts}}{=} i \int \left[\nabla\overline{\psi(x,t)} \cdot \nabla\psi(x,t) - \nabla\overline{\psi(x,t)} \cdot \nabla\psi(x,t) \right] dx$$

$$= 0. \qquad \square$$

Corollary 2.2 If ϕ, ψ are two classical solutions such that $\psi(x,0) = \phi(x,0)$, then $\psi(x,t) = \phi(x,t)$ $\forall t$.

Proof: $\phi - \psi$ is also a classical solution, and $\int |\phi(x,0) - \psi(x,0)|^2 dx = 0$. By Lemma 2.1, $\int |\psi(x,t) - \phi(x,t)|^2 dx = 0$ for all t, so that $\psi = \phi$. $\square$

These are important properties: the Schrödinger equation conserves the L^2 norm, hence the probability density. And Corollary 2.2 implies *causality*, or *determinism*: the state of the system at time t is determined by the state at time 0.

2.2. Evolution of a free particle

This is the simplest case, there is no external potential (i.e. $V \equiv 0$). At time $t=0$ the particle is in the state $\psi(x,0)$. Its evolution can be found using Fourier theory. Let us first perform the computations formally, we shall make them rigorous after we

have obtained an expression for the solution.
Let $\mathcal{F} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ denote the Fourier transform (this is a Hilbert homomorphism, or unitary linear map). It is well-known that

$$\mathcal{F} \Delta \mathcal{F}^{-1} \hat{f}(k) = -\|k\|^2 \hat{f}(k),$$

that is, the Laplacian is a multiplication operator in the Fourier space. The Schrödinger equation becomes:

$$i \frac{\partial}{\partial t} \hat{\psi}(k,t) = \frac{\hbar}{2m} \|k\|^2 \hat{\psi}(k)$$

with $\hat{\psi}(k,0)$ given. The solution is $\hat{\psi}(k,t) = e^{-i \frac{\hbar}{2m} \|k\|^2 t}$, hence

$$\psi(x,t) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{ikx - i\frac{\hbar}{2m}\|k\|^2 t} \hat{\psi}(k,0)\, dk.$$

If we make some assumptions on $\psi(x,0)$, one can guarantee that $\psi(x,t)$ is well-defined and is a classical solution. Exercise: check the properties of Definition 2.1 in the case where $\psi(x,0)$ is a Schwartz function.
Observe that this solution has constant momentum (i.e. velocity) since $|\hat{\psi}(k,t)|^2 = |\hat{\psi}(k,0)|^2 \quad \forall t$.

<u>Exercise 1</u>. Show that, under some assumptions on $\psi(x,0)$ (e.g. Schwartz), we have

$$\psi(x,t) = \frac{1}{(2\pi i \frac{\hbar}{2m} t)^{d/2}} \int e^{i\frac{2m}{\hbar t}(x-y)^2} \psi(y,0)\, dy.$$

Hint: Replace $\int_{\mathbb{R}^d}$ by $\lim_{R\to\infty} \int_{B_R}$ and use Fubini. Gaussian integral with complex parameters.

<u>Exercise 2</u>. Consider a "wave packet" with initial position x_0 and velocity v_0. That is,

$$\psi(x,0) = \frac{1}{(2\pi\sigma^2)^{d/2}} e^{i\frac{2m}{\hbar} v_0 (x-x_0)} e^{-\frac{(x-x_0)^2}{\sigma^2}}.$$

Show that its free evolution is given by

$$\psi(x,t) = \frac{1}{(2\pi(\sigma^2 + i\frac{\hbar}{2m}t))^{d/2}} \exp\left\{ \frac{\left(\frac{2m}{\hbar}\sigma^2 v_0 + \frac{i}{2}(x-x_0)\right)^2}{\sigma^2 + i\frac{\hbar}{2m}t} - \left(\frac{2m}{\hbar}\right)^2 \sigma_0^2 v_0^2 \right\}.$$

Check that the mean position is $\int x |\psi(x,t)|^2 dx = x_0 + v_0 t$, and the variance is

$$\int \|x\|^2 |\psi(x,t)|^2 dx - \left\| \int x |\psi(x,t)|^2 dx \right\|^2 = \sigma^2 + \left(\frac{\hbar}{2m}\right)^2 \frac{t^2}{\sigma^2}.$$

We observe that
- The mean position has ballistic motion (i.e. constant velocity).
- Uncertainty increases over time.
- Velocity is related to oscillations. Indeed,

$$\operatorname{Re} \psi(x,0) = \frac{1}{(2\pi\sigma^2)^{d/2}} \cos\left(\frac{2m}{\hbar} v_0 (x-x_0)\right) e^{-\frac{(x-x_0)^2}{\sigma^2}}.$$

The faster the oscillations, the faster the velocity.