Chapter 7. Schrödinger equation

$$\begin{cases} -i\partial_t u - \Delta_x u = 0 & \text{in } \mathbb{R}^d \times (0,\infty) \\ u(x,0) = g(x) & \text{in } x \in \mathbb{R}^d. \end{cases} \qquad (i^2 = -1)$$

Heuristically, by using Fourier transform $x \mapsto k$ we have

$$\begin{cases} i\partial_t \hat{u}(k,t) = |2\pi k|^2 \hat{u}(k,t) \\ \hat{u}(k,0) = \hat{g}(k) \end{cases} \Rightarrow \hat{u}(k,t) = e^{-it|2\pi k|^2} \hat{g}(k)$$

This is similar to the heat equation

$$\hat{\tilde{u}}(k,t) = e^{-t|2\pi k|^2} \hat{g}(k)$$

$$\Rightarrow \tilde{u}(x,t) = (e^{t\Delta} g) = \frac{1}{(4\pi t)^{d/2}} \int_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} g(y)\, dy$$

If now we formally replace t by it (imaginary time), then the solution of the Schrödinger equation is

$$u(x,t) = (e^{it\Delta} g)(x) = \frac{1}{(4\pi i t)^{d/2}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{4t}} g(y)\, dy$$

Theorem: For $g \in L^1(\mathbb{R}^d)$ define

$$(e^{it\Delta} g)(x) = \frac{1}{(4\pi i t)^{d/2}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{4t}} g(y)\,dy.$$

Then:

a) $$\|e^{it\Delta} g\|_{L^2} = \|g\|_{L^2}, \quad \forall g \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d).$$

b) Consequently, we can define $e^{it\Delta} g$ for all $g \in L^2(\mathbb{R}^d)$ by the density argument. In this way $e^{it\Delta}$ is a unitary transformation in $L^2(\mathbb{R}^d)$:

$$\|e^{it\Delta} g\|_{L^2} = \|g\|_{L^2}, \quad \forall g \in L^2(\mathbb{R}^d).$$

c) $$\widehat{e^{it\Delta} g}(k) = e^{it|2\pi k|^2} \hat{g}(k), \quad \forall g \in L^2(\mathbb{R}^d).$$

Proof: a) Consider for $\varepsilon > 0$

$$\hat{G}_\varepsilon(k) = e^{-(it+\varepsilon)|2\pi k|^2} \Rightarrow G_\varepsilon(x) = \frac{1}{(4\pi(it+\varepsilon))^{d/2}} e^{-\frac{|x|^2}{4(it+\varepsilon)}}$$

(exercise, c.f. Fourier transform of Gaussians)
Here $\varepsilon > 0 \rightsquigarrow$ exp. decay)

Then we have for $g \in L^1$

$$(G_\varepsilon * g)(x) = \frac{1}{(4\pi(it+\varepsilon))^{d/2}} \int_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4(it+\varepsilon)}} g(y)\,dy$$

$$\begin{pmatrix}\text{Dominated} \\ \text{c.v.}\end{pmatrix} \xrightarrow{\varepsilon \to 0^+} (G_0 * g)(x), \quad \text{for all } x \in \mathbb{R}^d$$

On the other hand, for $g \in L^2$:

$$\widehat{G_\varepsilon * g}(k) = \widehat{G_\varepsilon}(k)\,\hat{g}(k) = e^{-(it+\varepsilon)|2\pi k|^2} \hat{g}(k)$$

$$\xrightarrow{\varepsilon \to 0} e^{-it|2\pi k|^2} \hat{g}(k) \quad \text{in } L^2(\mathbb{R}^d, dk)$$

by Dominated c.v. Thus:

$$G_\varepsilon * g \xrightarrow{\varepsilon \to 0^+} \left(e^{-it|2\pi k|^2} \hat{g}(k)\right)^\vee \quad \text{in } L^2(\mathbb{R}^d, dx)$$

$\rightarrow$ up to a subsequence $\varepsilon \to 0^+$ we get the pointwise convergence $\rightarrow$ the limit is the same to $(G_0 * g)$.

Thus

$$(G_0 * g) = \left(e^{-it|2\pi k|^2} \hat{g}(k)\right)^\vee \quad \text{in } L^2(\mathbb{R}^d)$$

Consequently for $g \in L^1 \cap L^2$:

$$\|\underbrace{G_0 * g}_{(= e^{it\Delta} g \text{ by def})}\|_{L^2} = \|e^{-it|2\pi k|^2} \hat{g}(k)\|_{L^2} = \|g\|_{L^2}.$$

b) For $g \in L^2(\mathbb{R}^d)$, take $\{g_n\} \subset L^1 \cap L^2$ s.t. $g_n \to g$ in L^2. Then:

$$\| e^{it\Delta} g_m - e^{it\Delta} g_n \|_{L^2} = \| g_m - g_n \|_{L^2} \to 0 \text{ as } m,n \to \infty$$

$\Rightarrow \{e^{it\Delta} g_n\}$ is a Cauchy sequence in L^2

$\Rightarrow$ we can define $e^{it\Delta} g = \lim_{n\to\infty} e^{it\Delta} g_n$.

This def is independent of the choice of $\{g_n\}$:

If $g_n \to g$ & $\tilde{g}_n \to g$, then

$$\| e^{it\Delta} g_n - e^{it\Delta} \tilde{g}_n \|_{L^2} = \| g_n - \tilde{g}_n \| \xrightarrow{n\to\infty} 0.$$

Thus $\forall g \in L^2$, $e^{it\Delta} g$ is well-defined. And:

$$\| e^{it\Delta} g \|_{L^2} = \lim_{n\to\infty} \| e^{it\Delta} g_n \|_{L^2} = \lim_{n\to\infty} \| g_n \|_{L^2} = \| g \|_{L^2}.$$

Note that we can define $e^{-it\Delta}$ by the same way, and hence $e^{it\Delta}$ is a unitary

$$(e^{it\Delta})^* = e^{-it\Delta}.$$

c) Also from $g_n \in L^1 \cap L^2$, $g_n \to g$ in L^2

$$\widehat{e^{it\Delta} g_n}(k) = e^{-it|2\pi k|^2} \hat{g}_n(k)$$

$$(n \to \infty) \quad \downarrow L^2 \qquad\qquad \downarrow L^2$$

$$\widehat{e^{it\Delta} g}(k) = e^{-it|2\pi k|^2} \hat{g}(k) \qquad \square$$

<u>Remark:</u> If $g \in L^1(\mathbb{R}^d)$,

$$\left|\left(e^{it\Delta} g\right)(x)\right| = \left| \frac{1}{(4\pi i t)^{d/2}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{4t}} g(y)\, dy \right|$$

$$\Rightarrow \|e^{it\Delta} g\|_{L^\infty} \leq \frac{\|g\|_{L^1}}{(4\pi t)^{d/2}} \to 0 \text{ as } t \to \infty$$

If $g \in L^2(\mathbb{R}^d)$:

$$\|e^{it\Delta} g\|_{L^2} = \|g\|_{L^2}.$$

Hence, if $g \in L^1 \cap L^2$:

$$\|e^{it\Delta} g\|_{L^q} \xrightarrow{(t\to\infty)} 0 \quad \text{for all } 2 < q \leq \infty$$

(exercise)

In fact, if $g \in L^p$ with $1<p<2$, then

$$\|e^{it\Delta} g\|_{L^{p'}} \xrightarrow[t\to\infty]{} 0 \quad \text{with} \quad \frac{1}{p}+\frac{1}{p'}=1.$$

(This is harder to prove. You can use the Riesz-Thorin interpolation inequality, similar to Young's ineq for Fourier transform)

<u>Theorem</u> (RAGE - Ruelle, Amrein-Georgescu, Enss)

If $g \in L^2(\mathbb{R}^d)$, then $\forall R>0$:

$$\int_{|x|<R} |e^{it\Delta} g(x)|^2 dx \longrightarrow 0 \quad \text{as} \quad t\to\infty.$$

<u>Proof:</u> We decompose $g = g_1 + g_2$ with

$$g_2 \in L^2, \ \|g_2\|_{L^2} \le \varepsilon, \quad g_1 \in L^1, \ \|g_1\|_{L^1} \le C_\varepsilon.$$

Then: $$\int_{|x|<R} |e^{it\Delta} g|^2 \le 2\int_{|x|<R} |e^{it\Delta} g_1|^2 + 2\int_{|x|<R} |e^{it\Delta} g_2|^2$$

$$\le C R^d \|e^{it\Delta} g_1\|_{L^\infty}^2 + 2\|e^{it\Delta} g_2\|_{L^2}^2$$

$$\le C R^d \frac{\|g_1\|_{L^1}^2}{t^d} + 2\|g_2\|_{L^2}^2 \le \frac{C_{R,\varepsilon}}{t^d} + C\varepsilon^2 \xrightarrow{t\to\infty} C\varepsilon^2 \xrightarrow{\varepsilon\to 0} 0.$$

<u>Theorem</u> (Classical solution) If $g \in C_c^\infty(\mathbb{R}^d)$, then

$$u = e^{it\Delta} g \in C^\infty\left(\mathbb{R}^d \times [0,\infty)\right)$$

and
$$\begin{cases} -i\partial_t u - \Delta_x u = 0 & \text{in } \mathbb{R}^d \times (0,\infty) \\ \lim_{t\to 0} u(x,t) = g(x) & \text{in } \mathbb{R}^d. \end{cases}$$

<u>Proof</u>:
$$\hat{u}(k,t) = e^{-it|2\pi k|^2} \hat{g}(k)$$

$\forall m \geq 1$:
$$\Rightarrow |k|^m \hat{u}(k,t) = e^{-it|2\pi k|^2} |k|^m \underbrace{\hat{g}(k)}_{\leq \frac{C_N}{(1+|k|)^N},\ \forall N \geq 1} \in L^2(\mathbb{R}^d, dk)$$

$$\Rightarrow \quad u(\cdot,t) \in \bigcap_{m\geq 1} H^m(\mathbb{R}^d) \subset C^\infty(\mathbb{R}^d).$$

Moreover, $\partial_t^m \hat{u}(k,t) = e^{-it|2\pi k|^2} \left(-i|2\pi k|^2\right)^m \hat{g}(k)$

$\rightsquigarrow \partial_t^m u(x,t) = (\quad)^\vee$ continuous in t, $\forall m \geq 1$

Thus $u \in C^\infty\left(\mathbb{R}^d \times (0,\infty)\right)$. Moreover,

$$-i\widehat{\partial_t u} = -i\, e^{-it|2\pi k|^2}\left(-i\,|2\pi k|^2\right)\hat{g}(k)$$
$$= e^{-it|2\pi k|^2}\left(-|2\pi k|^2\right)\hat{g}(k) = \widehat{\Delta_x u}$$

$$\Rightarrow -i\partial_t u - \Delta_x u = 0 \quad \text{in } \mathbb{R}^d \times (0,\infty).$$

Finally

$$\int_{\mathbb{R}^d} |\hat{u}(k,t) - \hat{g}(k)|\, dk = \int_{\mathbb{R}^d} |e^{-it|2\pi k|^2} - 1|\, \underbrace{|\hat{g}(k)|}_{\in L^1} dk \xrightarrow[t\to 0^+]{} 0$$

by Dominated C.V.

$\Rightarrow \quad u(x,t) \xrightarrow[t\to 0]{} g(x)$ uniformly $x \in \mathbb{R}^d$. $\square$

<u>Theorem</u> (Weak solution) a) If $g \in H^2(\mathbb{R}^d)$, then

$$u = e^{it\Delta} g \in C^1\big(L^2(\mathbb{R}^d), (0,T)\big) \text{ and}$$

$$\begin{cases} -i\partial_t u - \Delta_x u = 0 & \text{for a.e. } x \in \mathbb{R}^d, \forall t > 0 \\ \lim\limits_{t\to 0} u(\cdot, t) = g & \text{in } L^2(\mathbb{R}^d) \end{cases}$$

Here $\partial_t u(\cdot, t) = \lim\limits_{h\to 0} \dfrac{u(\cdot, t+h) - u(\cdot, t)}{h}$ in $L^2(\mathbb{R}^d)$.

b) If $g \in L^2(\mathbb{R}^d)$, then $u = e^{it\Delta} g$ satisfies

$$\begin{cases} -i\partial_t \langle \varphi, u \rangle - \langle \Delta\varphi, u \rangle = 0, \ \forall \varphi \in C_c^\infty(\mathbb{R}^d) \\ \lim\limits_{t\to 0} u(\cdot, t) = g \quad \text{in } L^2(\mathbb{R}^d). \end{cases}$$

Proof: a) If $g \in H^2(\mathbb{R}^d)$, then we prove that

$$-i\,\frac{u(\cdot,t+h)-u(\cdot,t)}{h} \xrightarrow[h\to 0]{} e^{it\Delta}(\underbrace{\Delta g}_{\in L^2}) \quad \text{in } L^2(\mathbb{R}^d).$$

Indeed,

$$\| \dots - e^{it\Delta}(\Delta g)\|_{L^2}^2 = \| \widehat{\dots} - \widehat{e^{it\Delta}(\Delta g)}\|_{L^2}^2$$

$$= \int_{\mathbb{R}^d} \left| -i\,\frac{e^{-i(t+h)|2\pi k|^2} - e^{-it|2\pi k|^2}}{h}\hat{g}(k) + e^{-it|2\pi k|^2}|2\pi k|^2\hat{g}(k)\right|^2 dk$$

$$= \int_{\mathbb{R}^d} \Bigg|\underbrace{-i\,\frac{e^{-ih|2\pi k|^2}-1}{h|2\pi k|^2}+1}_{\to\, 0 \text{ as } h\to 0}\Bigg|^2 \underbrace{|2\pi k|^4|\hat{g}(k)|^2}_{\in L^1} dk \longrightarrow 0$$

Dominated C.V.

and bounded uniformly

$$\left(|e^{i\theta}-1|^2 = |\cos\theta - 1|^2 + |\sin\theta|^2 \leq C\theta^2 \right)$$

Thus $u \in C^1(L^2(\mathbb{R}^d), (0,\infty))$ and

$$-i\,\partial_t u = e^{it\Delta}(\Delta g) \underset{\substack{\downarrow \\ \text{check by Fourier transform}}}{=} \Delta(e^{it\Delta}g) = \Delta u.$$

Moreover:

$$\| u(\cdot,t) - g \|_{L^2}^2 = \| \hat{u}(\cdot,t) - \hat{g} \|_{L^2}^2$$

$$= \int_{\mathbb{R}^d} |\underbrace{e^{-it|2\pi k|^2} - 1}_{\to 0 \text{ as } t\to 0}|^2 \, \underbrace{|\hat{g}(k)|^2}_{\in L^1} dk$$

and uniformly bounded

$$\xrightarrow[t\to 0]{} 0 \quad \text{by Dominated c.v.}$$

b) If $g \in L^2(\mathbb{R}^d)$, then: $\forall \varphi \in C_c^\infty(\mathbb{R}^d)$

$$-i\partial_t \langle \varphi, u \rangle = -i\partial_t \langle \hat{\varphi}, \hat{u} \rangle$$

$$= -i\partial_t \int_{\mathbb{R}^d} \underbrace{\overline{\hat{\varphi}(k)}}_{\leq \frac{C_N}{(1+|k|)^N},\ \forall N \geq 1} e^{-it|2\pi k|^2} \hat{g}(k)\, dk$$

(Dominated c.v.)

$$= \int_{\mathbb{R}^d} \underbrace{\overline{\hat{\varphi}(k)}} e^{-it|2\pi k|^2} \Big(\underbrace{(-i)^2 |2\pi k|^2}_{-|2\pi k|^2} \Big) \hat{g}(k)\, dk$$

$$= \int_{\mathbb{R}^d} \overline{\widehat{\Delta\varphi}}\, \hat{u} = \langle \Delta \varphi, u \rangle \qquad \square$$

General Spectral approach:

Let $\mathcal{H}$ be a separable Hilbert space (i.e. $\mathcal{H}$ has an orthonormal basis which is at most countable). Let $A: D(A) \to \mathcal{H}$ be a self-adjoint operator.

By Spectral theorem, $\exists$ unitary $U: \mathcal{H} \to L^2(\Omega)$ s.t.

$$U A U^* = \underset{\substack{\Downarrow \\ \text{multiplication operator}}}{M_f} \quad \text{on } L^2(\Omega)$$

where $f: \Omega \to \mathbb{R}$ a real-valued function and

$$(M_f \varphi)(x) = f(x)\varphi(x), \quad \forall \varphi \in L^2(\Omega).$$

This allows to define $e^{-itA}: \mathcal{H} \to \mathcal{H}$ by

$$U e^{-itA} U^* = e^{-itM_f} \quad \text{on } L^2(\Omega)$$

where

$$\left(e^{-itM_f}\varphi\right)(x) = e^{-itf(x)}\varphi(x), \quad \forall \varphi \in L^2(\Omega).$$

<u>Theorem:</u> (Stone) If A is self-adjoint, then:

a) $\forall g \in D(A)$, $u = e^{-itA} g$ satisfies

$$\begin{cases} i\partial_t u = Au, & \forall t \\ u \xrightarrow[t \to 0]{} g & \text{in } \mathcal{H} \end{cases}$$

where $$\partial_t u = \lim_{h \to 0} \frac{u(t+h) - u(t)}{h} \quad \text{in } \mathcal{H}$$

b) $\forall g \in \mathcal{H}$, $u = e^{-itA} g$ satisfies

$$\begin{cases} i\partial_t \langle \varphi, u \rangle = \langle A\varphi, u \rangle, & \forall t, \ \forall \varphi \in D(A) \\ u \xrightarrow[t \to 0]{} g & \text{in } \mathcal{H}. \end{cases}$$

<u>Example:</u> If $A = -\Delta$, $\mathcal{H} = L^2(\mathbb{R}^d)$,

then $U = \mathcal{F}$ (Fourier transform) and

$\mathcal{F}(-\Delta)\mathcal{F}^* = |2\pi k|^2$ multiplication operator

$$\rightsquigarrow \mathcal{F}(e^{-itA} g) = e^{-it|2\pi k|^2} \hat{g}(k)$$

The proof of the abstract theorem is similar to the case of $-\Delta$.

This abstract theory can be used also for the Schrödinger operator

$$A = -\Delta + V(x) \quad \text{on } \mathcal{H} = L^2(\mathbb{R}^d)$$

when $V: \mathbb{R}^d \to \mathbb{R}$ a nice function s.t. A is self-adjoint.

Then $\forall g \in L^2(\mathbb{R}^d)$, we can define the dynamics

$$u = e^{-it(-\Delta+V)} g$$

which solves $\begin{cases} i\partial_t u = (-\Delta+V)u \\ u(t=0) = g \end{cases}$ in appropriate sense

<u>RAGE:</u> If $-\Delta+V$ has no eigenfunction, then $\forall g \in L^2(\mathbb{R}^d)$,

$$\frac{1}{T}\int_0^T \int_{|x|\leq R} \left| e^{-it(-\Delta+V)} g(x)\right|^2 dx \longrightarrow 0 \text{ as } T\to\infty$$

<u>Asymptotic completeness:</u> If $0 \leq V \in C_c^\infty(\mathbb{R}^d)$ and small, then $\exists$ a unitary operator $R: L^2 \to L^2$,

$$\forall g \in L^2(\mathbb{R}^d), \quad \Big\| e^{-it(-\Delta+V)} g - \underbrace{e^{it\Delta}}_{\text{free dynamics}} Rg \Big\|_{L^2} \xrightarrow{t\to\infty} 0.$$