The one-dimensional periodic Schrödinger equation

Jordan Bell
jordan.bell@gmail.com
Department of Mathematics, University of Toronto

April 23, 2016

1 Translations and convolution

For $y \in \mathbb{R}$, let

$$\tau_y f(x) = f(x-y).$$

To say that $f : \mathbb{R} \to \mathbb{C}$ is uniformly continuous means that $\|\tau_h f - f\|_b \to 0$ as $h \to 0$, where

$$\|g\|_b = \sup_{x\in\mathbb{R}} |g(x)|.$$

Let $1 \le p < \infty$ and let $\mathscr{L}(L^p(\mathbb{R}))$ be the Banach algebra of bounded linear operators $L^p(\mathbb{R}) \to L^p(\mathbb{R})$, with the strong operator topology: a net T_i converges to T in the strong operator topology if and only if for each $f \in L^p(\mathbb{R})$, $\|T_i f - Tf\|_{L^p} \to 0$.

Lemma 1. *$y \mapsto \tau_y$ is continuous $\mathbb{R} \to \mathscr{L}(L^p(\mathbb{R}))$, using the strong operator topology.*

Proof. For $y \in \mathbb{R}$ and $f \in L^p(\mathbb{R})$, $\|\tau_{y+h} f - \tau_y f\|_{L^p} = \|\tau_h f - f\|_{L^p}$. Take $\epsilon > 0$ and let $\phi \in C_c(\mathbb{R})$ with $\|f-\phi\|_{L^p} < \infty$. Say $\operatorname{supp}\phi \subset [a,b]$. Let $K = [a-1, b+1]$. For $|h| \le 1$, if $x \notin K$ then $x-h, x \notin \operatorname{supp}\phi$, and hence

$$\begin{aligned}
\|\tau_h\phi - \phi\|_{L^p}^p &= \int_{\mathbb{R}} |\phi(x-h) - \phi(x)|^p dx \\
&= \int_K |\phi(x-h) - \phi(x)|^p dx \\
&\le (b-a+2)\, \|\tau_h\phi - \phi\|_b^p \\
&= (b-a+2)\, \|\tau_\phi - \tau_y\phi\|_b^p .
\end{aligned}$$

Because $\phi \in C_c(\mathbb{R})$, ϕ is uniformly continuous on $\mathbb{R}$, whence $\|\tau_h\phi - \phi\|_{L^p} \to 0$ as $h \to 0$, say $\|\tau_h\phi - \phi\|_{L^p} < \epsilon$ for $|h| \leq h_\epsilon$. Hence

$$\begin{aligned}\|\tau_{y+h}f - \tau_y f\|_{L^p} &= \|\tau_h f - f\|_{L^p} \\ &\leq \|\tau_h f - \tau_h\phi\|_{L^p} + \|\tau_h\phi - \phi\|_{L^p} + \|\phi - f\|_{L^p} \\ &= 2\|f - \phi\|_{L^p} + \|\tau_h - \phi\|_{L^p} \\ &< 3\epsilon.\end{aligned}$$

□

Define $A : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ by

$$A(x_1, x_2) = x_1 + x_2.$$

If μ_1, μ_2 are finite Borel measures on $\mathbb{R}$, let $\mu_1 \otimes \mu_2$ be the product measure on $\mathbb{R}^2$, and let

$$\mu_1 * \mu_2 = A_*(\mu_1 \otimes \mu_2)$$

be the pushforward of $\mu_1 \otimes \mu_2$ by A, called the **convolution** of μ_1 and μ_2. If $f : \mathbb{R} \to [0, \infty]$ is measurable then applying the change of variables formula and then Tonelli's theorem we obtain

$$\begin{aligned}\int f d(\mu_1 * \mu_2) &= \int f \circ A d(\mu_1 \otimes \mu_2) \\ &= \int \left(\int f \circ A(x_1, x_2) d\mu_1(x_1) \right) d\mu_2(x_2) \\ &= \int \left(\int f(x_1 + x_2) d\mu_1(x_1) \right) d\mu_2(x_2).\end{aligned}$$

If B is a Borel set in $\mathbb{R}$ then applying the above with $f = 1_B$,

$$\begin{aligned}(\mu_1 * \mu_2)(B) &= \int 1_B d(\mu_1 * \mu_2) \\ &= \int \left(\int 1_B(x_1 + x_2) d\mu_1(x_1) \right) d\mu_2(x_2) \\ &= \int \mu_1(B - x_2) d\mu_2(x_2).\end{aligned}$$

2 Periodic functions

Let $\mathbb{T} = \mathbb{R}/\mathbb{Z}$, and let $\mathscr{S}(\mathbb{T})$ be the collection of C^∞ functions $\phi : \mathbb{R} \to \mathbb{C}$ satisfying $\phi(x+1) = \phi(x)$ for all $x \in \mathbb{T}$. For $\phi, \psi \in \mathscr{S}(\mathbb{T})$, for $n \geq 1$ let

$$d_n(\phi, \psi) = \sup_{x \in [0,1]} |\phi^{(n)}(x) - \psi^{(n)}(x)|$$

and

$$d(\phi, \psi) = \sum_{n=0}^{\infty} 2^{-n} \frac{d_n(\phi, \psi)}{1 + d_n(\phi, \psi)}.$$

With this metric, $\mathscr{S}(\mathbb{T})$ is a Fréchet space.

For $n \in \mathbb{Z}$, define

$$e_n(x) = e^{2\pi i n x}, \qquad x \in \mathbb{R}.$$

For $f \in L^1(\mathbb{T})$, define $\widehat{f} : \mathbb{Z} \to \mathbb{C}$, for $n \in \mathbb{Z}$, by

$$\widehat{\phi}(n) = \int_0^1 \phi(x) e_{-n}(x) dx = \int_0^1 \phi(x) e^{-2\pi i n x} dx.$$

Denote by $\mathscr{S}'(\mathbb{T})$ the dual space of $\mathscr{S}(\mathbb{T})$, the collection of continuous linear maps $\mathscr{S}(\mathbb{T}) \to \mathbb{C}$. For $L \in \mathscr{S}'(\mathbb{T})$, define $\widehat{L} : \mathbb{Z} \to \mathbb{C}$ by

$$\widehat{L}(n) = L e_{-n}.$$

For $x \in \mathbb{R}$, define $\delta_x : \mathscr{S}(\mathbb{T}) \to \mathbb{C}$ by

$$\delta_x \phi = \phi(x).$$

δ_x belongs to $\mathscr{S}'(\mathbb{T})$, and

$$\widehat{\delta}_x(n) = \delta_x e_{-n} = e_{-n}(x) = e^{-2\pi i n x}.$$

For $f \in L^1(\mathbb{T})$, define $L_f \in \mathscr{S}'(\mathbb{T})$ by

$$L_f \phi = \int_0^1 f(x) \phi(x) dx, \qquad \phi \in \mathscr{S}(\mathbb{T}).$$

For $n \in \mathbb{Z}$,

$$\widehat{L_f}(n) = L_f e_{-n} = \int_0^1 f(x) e_{-n}(x) dx = \widehat{f}(n).$$

3 The Poisson summation formula

If $f \in \mathscr{L}^1(\mathbb{R})$,

$$\begin{aligned}
\int_0^1 \sum_{n \in \mathbb{Z}} |f(x+n)| dx &= \sum_{n \in \mathbb{Z}} \int_0^1 |f(x+n)| dx \\
&= \sum_{n \in \mathbb{Z}} \int_n^{n+1} |f(x)| dx \\
&= \int_{\mathbb{R}} |f(x)| dx.
\end{aligned}$$

This implies that there is a Borel set N_f in $\mathbb{R}$ with $\lambda(N_f) = 0$ such that for $x \in N_f^c$,

$$\sum_{n \in \mathbb{Z}} |f(x+n)| < \infty.$$

We define $Pf(x) = \sum_{n\in\mathbb{Z}} f(x+n)$ for $x \in N_f^c$ and $Pf(x) = 0$ for $x \in N_f$. Thus it makes sense to define $P : L^1(\mathbb{R}) \to L^1(\mathbb{R})$ by

$$Pf(x) = \sum_{n\in\mathbb{Z}} f(x+n),$$

in other words,

$$Pf = \sum_{n\in\mathbb{Z}} \tau_{-n} f.$$

Then

$$\begin{aligned}
\int_0^1 Pf(x) e^{-2\pi imx} dx &= \int_0^1 \left(\sum_{n\in\mathbb{Z}} f(x+n) \right) e^{-2\pi imx} dx \\
&= \sum_{n\in\mathbb{Z}} \int_0^1 f(x+n) e^{-2\pi imx} dx \\
&= \sum_{n\in\mathbb{Z}} \int_n^{n+1} f(x) e^{-2\pi imx} dx \\
&= \int_{\mathbb{R}} f(x) e^{-2\pi imx} dx \\
&= \widehat{f}(m).
\end{aligned}$$

That is,

$$\widehat{Pf}(m) = \widehat{f}(m).$$

Supposing that $Pf(x) = \sum_{n\in\mathbb{Z}} \widehat{Pf}(n) e^{2\pi inx}$,

$$Pf(x) = \sum_{n\in\mathbb{Z}} \widehat{f}(n) e^{2\pi inx}$$

and supposing $Pf(x) = \sum_{n\in\mathbb{Z}} f(x+n)$,

$$\sum_{n\in\mathbb{Z}} f(x+n) = \sum_{n\in\mathbb{Z}} \widehat{f}(n) e^{2\pi inx},$$

the **Poisson summation formula**.

For $N \geq 1$, let

$$L_N = \frac{1}{N} \sum_{j=0}^{N-1} \delta_{j/N}.$$

For $n \in \mathbb{Z}$,

$$\widehat{L}_N(n) = \frac{1}{N} \sum_{j=0}^{N-1} \delta_{j/N} e_{-n} = \frac{1}{N} \sum_{j=0}^{N-1} e_{-n}(j/N) = \frac{1}{N} \sum_{j=0}^{N-1} e^{-2\pi inj/N}.$$

If $n \in N\mathbb{Z}$ then $\widehat{L}_N(n) = 1$ and otherwise $\widehat{L}_N(n) = 0$. That is,

$$L_N = \frac{1}{N} \sum_{j=0}^{N-1} \delta_{j/N} \sim \sum_{k\in\mathbb{Z}} \widehat{L}_N(k) e_k = \sum_{k\in\mathbb{Z}} e_{Nk}.$$

4 The heat kernel

For $x \in \mathbb{R}$ and $t > 0$ define

$$H_t(x) = \int_{\mathbb{R}} e^{-4\pi^2 t\xi^2} e^{2\pi i\xi x} d\xi.$$

Using

$$\int_{\mathbb{R}} \exp\left(\frac{1}{2}iaw^2 + iJw\right) dw = \sqrt{\frac{2\pi i}{a}} \exp\left(-\frac{iJ^2}{2a}\right),$$

for $\frac{1}{2}ia = -4\pi^2 t$ we get $a = 8i\pi^2 t$ and $J = 2\pi x$, and we calculate

$$\begin{aligned} H_t(x) &= \sqrt{\frac{2\pi i}{8\pi^2 it}} \exp\left(-\frac{i}{16\pi^2 it} \cdot 4\pi^2 x^2\right) \\ &= \sqrt{\frac{1}{4\pi t}} \exp\left(-\frac{x^2}{4t}\right). \end{aligned}$$

By the Fourier inversion theorem,

$$\widehat{H_t}(\xi) = e^{-4\pi^2 t\xi^2}.$$

For $f \in L^1(\mathbb{R})$,

$$\widehat{\tau_y f}(\xi) = \int_{\mathbb{R}} f(x-y) e^{-2\pi i\xi x} dx = e^{-2\pi i\xi y} \widehat{f}(\xi) = e_{-n}(y)\widehat{f}(\xi).$$

5 The Schrödinger equation on $\mathbb{R}$

Let

$$\Gamma(t,x) = \sqrt{\frac{i}{t}} e^{-\pi i x^2/t},$$

which satisfies

$$\partial_x \Gamma(t,x) = -\frac{2\pi i x}{t}\Gamma(t,x), \quad \partial_x^2 \Gamma(t,x) = -\frac{4\pi^2 x^2}{t^2}\Gamma(t,x) - \frac{2\pi i}{t}\Gamma(t,x)$$

and

$$\partial_t \Gamma(t,x) = -\frac{1}{2}t^{-1}\Gamma(t,x) + \pi i x^2 t^{-2}\Gamma(t,x).$$

This satisfies

$$\begin{aligned} \partial_t \Gamma(t,x) &= \frac{1}{2}\left(-\frac{1}{t} + \frac{2\pi i x^2}{t^2}\right)\Gamma(t,x) \\ &= \frac{1}{4\pi i}\left(-\frac{2\pi i}{t} - \frac{4\pi^2 x^2}{t^2}\right)\Gamma(t,x) \\ &= \frac{1}{4\pi i}\partial_x^2 \Gamma(t,x). \end{aligned}$$

For $f : \mathbb{R} \to \mathbb{C}$, let

$$\psi(f)(t,x) = f * \Gamma(t,\cdot)(x) = \int_{\mathbb{R}} f(y)\Gamma(t,x-y)dy.$$

This satisfies

$$\begin{aligned}
\partial_t \psi(f)(t,x) &= \int_{\mathbb{R}} f(y) \cdot \partial_t \Gamma(t,x-y)dy \\
&= \int_{\mathbb{R}} f(y) \cdot \frac{1}{4\pi i} \partial_x^2 \Gamma(t,x-y)dy \\
&= \frac{1}{4\pi i} \partial_x^2 \psi(f)(t,x).
\end{aligned}$$

We also calculate

$$\begin{aligned}
\psi(f)(t,x) &= \int_{\mathbb{R}} f(y) \cdot \Gamma(t,x-y)dy \\
&= \int_{\mathbb{R}} f(y) \cdot \sqrt{\frac{i}{t}} e^{-\pi i(x-y)^2/t} dy \\
&= \int_{\mathbb{R}} f(y) \cdot \sqrt{\frac{i}{t}} \exp\left(-\frac{\pi i x^2}{t} + \frac{2\pi i x y}{t} - \frac{\pi i y^2}{t}\right) dy \\
&= \Gamma(t,x) \cdot \int_{\mathbb{R}} f(y) \exp\left(-\frac{\pi i}{t}(y^2 - 2xy)\right) dy.
\end{aligned}$$

Let

$$\widehat{f}(y) = \int_{\mathbb{R}} f(x) e^{-2\pi i x y} dx.$$

Using

$$\int_{\mathbb{R}} \exp\left(\frac{1}{2} i a w^2 + i J w\right) dw = \sqrt{\frac{2\pi i}{a}} \exp\left(-\frac{i J^2}{2a}\right),$$

we get, with $a = 2\pi t$ and $J = 2\pi u$,

$$\begin{aligned}
&\Gamma(t,x)\cdot\psi(\widehat{f})(-1/t,-x/t)\\
=&\Gamma(t,x)\cdot\int_{\mathbb{R}}\widehat{f}(y)\Gamma\left(-\frac{1}{t},-\frac{x}{t}-y\right)dy\\
=&\Gamma(t,x)\cdot\int_{\mathbb{R}}\widehat{f}\left(-\frac{x}{t}-y\right)\Gamma\left(-\frac{1}{t},y\right)dy\\
=&\sqrt{\frac{i}{t}}e^{-\pi ix^2/t}\cdot\int_{\mathbb{R}}\left(\int_{\mathbb{R}}f(u)e^{-2\pi iu\left(-\frac{x}{t}-y\right)}du\right)\cdot\sqrt{-it}e^{\pi ity^2}dy\\
=&e^{-\pi ix^2/t}\int_{\mathbb{R}}f(u)e^{2\pi iux/t}\left(\int_{\mathbb{R}}e^{2\pi iuy+\pi ity^2}dy\right)du\\
=&e^{-\pi ix^2/t}\int_{\mathbb{R}}f(u)e^{2\pi iux/t}\cdot\sqrt{\frac{2\pi i}{2\pi t}}\exp\left(-\frac{i}{4\pi t}(2\pi u)^2\right)du\\
=&e^{-\pi ix^2/t}\sqrt{\frac{i}{t}}\int_{\mathbb{R}}f(u)e^{2\pi iux/t}\exp\left(-\frac{\pi iu^2}{t}\right)du\\
=&\sqrt{\frac{i}{t}}\int_{\mathbb{R}}f(u)\exp\left(-\frac{\pi ix^2}{t}+\frac{2\pi iux}{t}-\frac{\pi iu^2}{t}\right)du\\
=&\sqrt{\frac{i}{t}}\int_{\mathbb{R}}f(u)e^{-\frac{\pi i(x-u)^2}{t}}du\\
=&\int_{\mathbb{R}}f(u)\Gamma(t,x-u)du\\
=&\psi(f)(t,x).
\end{aligned}$$

In other words,

$$\begin{aligned}
\psi(f)(t,x)&=\Gamma(t,x)\cdot\psi(\widehat{f})(-1/t,-x/t)\\
&=\sqrt{\frac{i}{t}}e^{-\pi ix^2/t}\cdot\int_{\mathbb{R}}\widehat{f}(\xi)\cdot\sqrt{-it}\exp\left(\pi it\left(-\frac{x}{t}-\xi\right)^2\right)d\xi\\
&=\int_{\mathbb{R}}\widehat{f}(\xi)\exp\left(-\frac{\pi ix^2}{t}+\frac{\pi ix^2}{t}+2\pi ix\xi+\pi it\xi^2\right)d\xi\\
&=\int_{\mathbb{R}}\widehat{f}(\xi)e^{2\pi ix\xi+\pi it\xi^2}d\xi.
\end{aligned}$$

6 The Schrödinger equation on $\mathbb{T}$

Given t and x, let $\gamma(y) = \Gamma(t, x-y)$. We calculate

$$\begin{aligned}
\widehat{\gamma}(\xi) &= \int_{\mathbb{R}} \gamma(y) e^{-2\pi i \xi y} dy \\
&= \int_{\mathbb{R}} \sqrt{\frac{i}{t}} e^{-\pi i (x-y)^2/t} e^{-2\pi i \xi y} dy \\
&= \int_{\mathbb{R}} \sqrt{\frac{i}{t}} \exp\left(-\frac{\pi i x^2}{t} + \frac{2\pi i x y}{t} - \frac{\pi i y^2}{t} - 2\pi i \xi y \right) dy.
\end{aligned}$$

Using

$$\int_{\mathbb{R}} \exp\left(\frac{1}{2} i a w^2 + i J w\right) dw = \sqrt{\frac{2\pi i}{a}} \exp\left(-\frac{i J^2}{2a}\right)$$

with $a = -\frac{2\pi}{t}$ and $J = \frac{2\pi x}{t} - 2\pi\xi$, for which $J^2 = \frac{4\pi^2 x^2}{t^2} - \frac{8\pi^2 x \xi}{t} + 4\pi^2 \xi^2$,

$$\begin{aligned}
\widehat{\gamma}(\xi) &= \sqrt{\frac{i}{t}} \exp\left(-\frac{\pi i x^2}{t}\right) \cdot \sqrt{-it} \exp\left(\frac{it}{4\pi} J^2\right) \\
&= \exp\left(-\frac{\pi i x^2}{t}\right) \exp\left(\frac{i\pi x^2}{t} - 2\pi i x \xi + \pi i \xi^2 t\right) \\
&= \exp\left(-2\pi i x \xi + \pi i \xi^2 t\right).
\end{aligned}$$

The Poisson summation formula tells us

$$\sum_{n\in\mathbb{Z}} \gamma(n) = \sum_{n\in\mathbb{Z}} \widehat{\gamma}(n),$$

i.e.

$$\sum_{n\in\mathbb{Z}} \Gamma(t, x-n) = \sum_{n\in\mathbb{Z}} e^{-2\pi i n x + \pi i t n^2} = \sum_{n\in\mathbb{Z}} e^{2\pi i n x + \pi i t n^2}.$$

Define

$$\Theta(t, x) = \sum_{n\in\mathbb{Z}} e^{\pi i (t n^2 + 2 x n)} = \sum_{n\in\mathbb{Z}} e^{\pi i t n^2} e^{2\pi i x n} = \sum_{n\in\mathbb{Z}} \Gamma(t, x-n).$$

For $\phi \in \mathscr{S}$, namely a Schwartz function, define

$$\Theta_t \phi(x) = \sum_{n\in\mathbb{Z}} \int_{\mathbb{R}} \phi(x) e^{\pi i t n^2} e^{2\pi i x n} dx,$$

which satisfies

$$\Theta_t \phi(x) = \sum_{n\in\mathbb{Z}} \widehat{\phi}(-n) e^{\pi i t n^2} = \sum_{n\in\mathbb{Z}} \widehat{\phi}(n) e^{\pi i t n^2}.$$

If f is 1-periodic, for $n \in \mathbb{Z}$ let

$$\widehat{f}(n) = \int_0^1 f(y) e^{-2\pi i n y} dy.$$

Define

$$\psi(f)(t,x) = \Theta_t * f(x) = \int_0^1 \Theta(t, x-y) f(y) dy,$$

which satisfies

$$\begin{aligned}
\psi(f)(t,x) &= \int_0^1 \sum_{n \in \mathbb{Z}} e^{\pi i t n^2} e^{2\pi i (x-y) n} f(y) dy \\
&= \sum_{n \in \mathbb{Z}} e^{\pi i t n^2} e^{2\pi i x n} \int_0^1 f(y) e^{-2\pi i n y} dy \\
&= \sum_{n \in \mathbb{Z}} e^{\pi i t n^2} e^{2\pi i x n} \widehat{f}(n).
\end{aligned}$$

We remind ourselves

$$\Theta(t,x) = \Theta_t(x) = \sum_{n \in \mathbb{Z}} e^{\pi i t n^2} e^{2\pi i x n}$$

and

$$\widehat{\Theta}_t(n) = e^{\pi i t n^2}.$$

Say $t = \frac{2M}{N}$. Then for $k \in \mathbb{Z}$,

$$\begin{aligned}
\widehat{\Theta}_t(k+N) &= \exp\left(\pi i \cdot \frac{2M}{N} \cdot (k+N)^2\right) \\
&= \exp\left(\pi i \cdot \frac{2M}{N} \cdot k^2\right).
\end{aligned}$$