The Schrödinger Equation and the Fresnel Integral

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Abstract

We treat the Schrödinger equation

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2}, \quad u(0,x) = f(x),$$

applying the Fourier transform to write

$$u(t,x) = S(t)f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-it\xi^2} \hat{f}(\xi) e^{ix\cdot\xi}\, d\xi,$$

which differs from the solution to the heat equation only in replacing $e^{-t\xi^2}$ by $e^{-it\xi^2}$. Analytic continuation of the heat kernel $H_t(y) = (4\pi t)^{-1/2} e^{-y^2/4t}$ produces

$$S(t)f(x) = \int_{-\infty}^{\infty} f(x-y) S_t(y)\, dy, \quad S_t(y) = (4\pi i t)^{-1/2} e^{-y^2/4it}.$$

Applying this formula to important special cases leads to the study of the Fresnel integral,

$$\mathrm{Fr}(x) = (\pi i)^{-1/2} \int_0^x e^{iy^2}\, dy,$$

which is seen to be a smooth, odd function, with lots of oscillation, but nevertheless satisfying

$$\lim_{x\to\pm\infty} \mathrm{Fr}(x) = \pm\frac{1}{2}.$$

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1 Introduction

We discuss the 1D Schrödinger equation

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2}, \tag{1.1}$$

for $t, x \in \mathbb{R}$, with initial condition

$$u(0, x) = f(x). \tag{1.2}$$

Note that the partial Fourier transform

$$\hat{u}(t, \xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(t, x)e^{-ix\xi}\, dx \tag{1.3}$$

satisfies

$$\partial_t \hat{u}(t, \xi) = -i\xi^2 \hat{u}(t, \xi), \quad \hat{u}(0, \xi) = \hat{f}(\xi), \tag{1.4}$$

so

$$\hat{u}(t, \xi) = e^{-it\xi^2} \hat{f}(\xi), \tag{1.5}$$

and we have

$$u(t, x) = \mathcal{F}^* e^{-it\xi^2} \mathcal{F} f(x). \tag{1.6}$$

Since, by the Plancherel theorem, the Fourier transform

$$\mathcal{F} : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}) \tag{1.7}$$

is bijective and norm preserving (i.e., unitary), with inverse $\mathcal{F}^*$, we see that (1.5)–(1.6) defines a solution

$$u(t, x) = S(t)f(x) \tag{1.8}$$

to (1.1)–(1.2), for $f \in L^2(\mathbb{R})$. Furthermore, for each $t \in \mathbb{R}$,

$$S(t) : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}) \tag{1.9}$$

is unitary, with inverse

$$S(t)^{-1} = S(t)^* = S(-t). \tag{1.10}$$

2 Relation to heat equation, and integral formula

We have defined the solution operator $S(t) : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ to the Schrödinger equation in §1. If $f \in L^2(\mathbb{R})$ and also $\hat{f} \in L^1(\mathbb{R})$, then $S(t)f$ is given by the absolutely convergent integral

$$S(t)f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-it\xi^2} \hat{f}(\xi) e^{ix\xi} \, d\xi. \tag{2.1}$$

We relate this to the solution operator

$$H(t)f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-t\xi^2} \hat{f}(\xi) e^{ix\xi} \, d\xi \tag{2.2}$$

for the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2}, \quad u(0, x) = f(x). \tag{2.3}$$

As seen in [1], §§3.3–3.5, we have, for $t > 0$,

$$H(t)f(x) = \int f(x - y) H_t(y) \, dy, \tag{2.4}$$

with

$$\begin{aligned} H_t(y) &= \frac{1}{2\pi} \int e^{-t\xi^2 + iy\xi} \, d\xi \\ &= (4\pi t)^{-1/2} e^{-y^2/4t}, \quad t > 0. \end{aligned} \tag{2.5}$$

Now, we can extend (2.2) and (2.4)–(2.5), from $t \in (0, \infty)$ to complex t with positive real part. Let us denote such a complex number by $s + it$, $s > 0$, $t \in \mathbb{R}$. We have

$$\begin{aligned} H(s + it)f(x) &= \frac{1}{\sqrt{2\pi}} \int e^{(s+it)\xi^2} \hat{f}(\xi) e^{ix\xi} \, d\xi \\ &= \frac{1}{\sqrt{2\pi}} \int f(x - y) H_{s+it}(y) \, dy, \end{aligned} \tag{2.6}$$

with

$$H_{s+it}(y) = \big[2\pi(s + it)\big]^{-1/2} e^{-y^2/4(s+it)}, \quad s > 0, \ t \in \mathbb{R}. \tag{2.7}$$

The Fourier integral represenation (2.6), with the Plancherel theorem, gives

$$H(s + it) : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}), \quad \|H(s + it)\|_{\mathcal{L}(L^2)} = 1, \quad s > 0, \ t \in \mathbb{R}, \tag{2.8}$$

and furthermore, for $f \in L^2(\mathbb{R})$,

$$S(t)f = \lim_{s \searrow 0} H(s+it)f, \quad \text{in } L^2\text{-norm}. \tag{2.9}$$

Comparison with (2.1) shows that, if $f \in L^2(\mathbb{R})$ and also $\hat{f} \in L^1(\mathbb{R})$ (so $f \in C(\mathbb{R})$), then, for each $t \in \mathbb{R}$,

$$H(s+it)f(x) \longrightarrow S(t)f(x), \quad \text{uniformly in } x, \text{ as } s \searrow 0. \tag{2.10}$$

If, in addition, $f \in L^1(\mathbb{R})$, i.e.,

$$f \in \mathcal{A}(\mathbb{R}), \tag{2.11}$$

then we can pass to the limit $s \searrow 0$ and write, for each $t \in \mathbb{R} \setminus 0$,

$$S(t)f(x) = \int f(x-y) S_t(y)\, dy, \tag{2.12}$$

with

$$S_t(y) = \frac{1}{\sqrt{4\pi}} (0+it)^{-1/2} e^{-y^2/4it}. \tag{2.13}$$

Here

$$(0+it)^{-1/2} = \lim_{s \searrow 0} (s+it)^{-1/2} = \begin{cases} e^{-\pi i/4} |t|^{-1/2}, & \text{if } t > 0, \\ e^{\pi i/4} |t|^{-1/2}, & \text{if } t < 0. \end{cases} \tag{2.14}$$

Note that

$$e^{\pi i/4} = \frac{1+i}{\sqrt{2}}. \tag{2.15}$$

Having this formula for $S_t(y)$, we can readily extend $S(t)$ to act on $f \in L^1(\mathbb{R})$, for $t \neq 0$, obtaining

$$S(t) : L^1(\mathbb{R}) \longrightarrow L^\infty(\mathbb{R}), \quad \|S(t)f\|_{L^\infty} \le \frac{1}{\sqrt{4\pi|t|}} \|f\|_{L^1}. \tag{2.16}$$

3 The Fresnel integral

We start this section off with a study of $S(t)\chi_{a,b}$, where, for $a, b \in \mathbb{R}$, $a < b$, we set

$$\chi_{a,b}(x) = \begin{array}{ll} 1, & \text{if } \ a < x < b, \\ 0, & \text{otherwise.} \end{array} \tag{3.1}$$

For simplicity, we take $t > 0$, though we note that, if $f \in L^1(\mathbb{R})$ or $L^2(\mathbb{R})$,

$$f \text{ real valued } \Longrightarrow S(-t)f = \overline{S(t)f}. \tag{3.2}$$

By (2.12)–(2.14), we have

$$S(t)\chi_{a,b}(x) = \frac{e^{-\pi i/4}}{\sqrt{4\pi t}} \int_{x-b}^{x-a} e^{-y^2/4it}\, dy. \tag{3.3}$$

We are hence motivated to look at

$$\begin{aligned} \frac{e^{-\pi i/4}}{\sqrt{4\pi t}} \int_0^x e^{-y^2/4it}\, dy &= (\pi i)^{-1/2} \int_0^{x/\sqrt{4t}} e^{iu^2}\, du \\ &= \operatorname{Fr}\Bigl(\frac{x}{\sqrt{4t}}\Bigr), \end{aligned} \tag{3.4}$$

where we bring in the Fresnel integral

$$\operatorname{Fr}(x) = \frac{e^{-\pi i/4}}{\sqrt{\pi}} \int_0^x e^{iy^2}\, dy. \tag{3.5}$$

Using this special function, we have, for $t > 0$,

$$S(t)\chi_{a,b}(x) = \operatorname{Fr}\Bigl(\frac{x-a}{\sqrt{4t}}\Bigr) - \operatorname{Fr}\Bigl(\frac{x-b}{\sqrt{4t}}\Bigr). \tag{3.6}$$

We are now motivated to study the special function $\operatorname{Fr}(x)$, defined by (3.5). Clearly

$$\operatorname{Fr} \in C^\infty(\mathbb{R}), \quad \operatorname{Fr}(-x) = -\operatorname{Fr}(x). \tag{3.7}$$

We will show below that

$$\lim_{x \to \pm\infty} \operatorname{Fr}(x) = \pm \frac{1}{2}. \tag{3.8}$$

In particular, Fr is bounded,

$$|\operatorname{Fr}(x)| \le A < \infty, \quad \forall\, x \in \mathbb{R}, \tag{3.9}$$

for some $A < \infty$. To get started, note the identity

$$\partial_y\Bigl(\frac{1}{y}e^{iy^2}\Bigr) = 2ie^{iy^2} - \frac{1}{y^2}e^{iy^2}, \tag{3.10}$$

or equivalently

$$e^{iy^2} = \frac{1}{2i}\partial_y\Bigl(\frac{1}{y}e^{iy^2}\Bigr) + \frac{1}{2iy^2}e^{iy^2}, \tag{3.11}$$

which gives, for $0 < x < R < \infty$,

$$\int_x^R e^{iy^2}\,dy = \frac{1}{2i}\Bigl(\frac{e^{iR^2}}{R} - \frac{e^{ix^2}}{x}\Bigr) + \frac{1}{2i}\int_x^R \frac{1}{y^2}e^{iy^2}\,dy. \tag{3.12}$$

Hence, for each $x > 0$,

$$\lim_{R\to\infty} \mathrm{Fr}(R) = \mathrm{Fr}(x) + \frac{1}{2i}(\pi i)^{-1/2}\Bigl\{-\frac{e^{ix^2}}{x} + \int_x^\infty \frac{1}{y^2}e^{iy^2}\,dy\Bigr\}. \tag{3.13}$$

This shows that the limits on the left side of (3.8) exist. It remains to identify them.

For this evaluation, we look at

$$I(a) = \int_0^\infty e^{-ay^2}\,dy = \frac{\sqrt{\pi}}{2}a^{-1/2}, \tag{3.14}$$

valid for $a > 0$ via the change of variable $t = a^{1/2}y$. Now both the integral defining $I(a)$ and $a^{-1/2}$ are holomorphic in $\{a \in \mathbb{C} : \operatorname{Re} a > 0\}$, so this identity holds in the right half plane; cf. [2], §2.6. Hence we have

$$\begin{aligned}\int_0^\infty e^{-\varepsilon y^2}e^{iy^2}\,dy = I(\varepsilon - i) &= \frac{\sqrt{\pi}}{2}(\varepsilon - i)^{-1/2} \\ &\to \frac{\sqrt{\pi}}{2}e^{\pi i/4}, \quad \text{as } \varepsilon \searrow 0.\end{aligned} \tag{3.15}$$

We also know that

$$\int_0^R e^{iy^2}\,dy \longrightarrow L, \quad \text{as } R \to \infty, \tag{3.16}$$

for some $L \in \mathbb{C}$. The result (3.8) follows from the fact that, if (3.16) holds,

$$\lim_{\varepsilon\searrow 0}\int_0^\infty e^{-\varepsilon y^2}e^{iy^2}\,dy = L. \tag{3.17}$$

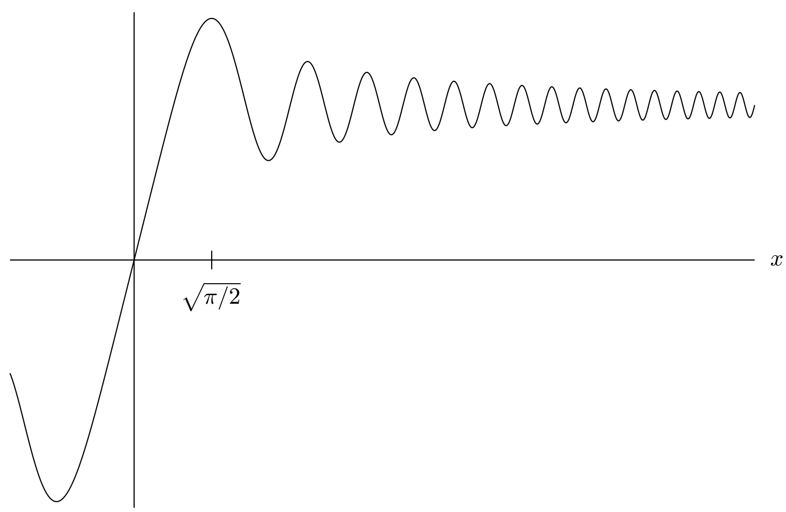

Figure 1: Graph of $\mathrm{Fr}_c(x)$

This implication is known as an *Abelian theorem*, and is discussed in Appendix A.

For graphical purposes, it is convenient to write

$$\begin{aligned} \mathrm{Fr}(x) &= e^{-\pi i/4} \frac{1}{\sqrt{\pi}} \int_0^x \Big[\cos y^2 + i \sin y^2\Big]\, dy \\ &= e^{-\pi i/4} \big[\mathrm{Fr}_c(x) + i\, \mathrm{Fr}_s(x)\big]. \end{aligned} \tag{3.18}$$

Figure 1 depicts the graph of $\mathrm{Fr}_c(x)$.

Here is a variant of (3.6), which applies to a general class of initial data.

Proposition 3.1 *If $f \in C_0^1(\mathbb{R})$, then, for $t > 0$,*

$$S(t)f(x) = \int_{-\infty}^{\infty} \mathrm{Fr}\Big(\frac{y}{\sqrt{4t}}\Big) f'(x-y)\, dy, \tag{3.19}$$

with a similar formula for $t < 0$.

Proof. Denote the right side of (3.19) by $v(t,x)$. Integration by parts gives

$$v(t,x) = \int_{-\infty}^{\infty} \partial_y \, \mathrm{Fr}\Big(\frac{y}{\sqrt{4t}}\Big)\, f(x-y)\, dy. \tag{3.20}$$

But

$$\begin{aligned} \partial_y \, \mathrm{Fr}\Big(\frac{y}{\sqrt{4t}}\Big) &= \frac{1}{\sqrt{4t}} \, \mathrm{Fr}'\Big(\frac{y}{\sqrt{4t}}\Big) \\ &= \frac{1}{\sqrt{4t}} \, \frac{e^{-\pi i/4}}{\sqrt{\pi}} e^{iy^2/4t} \\ &= S_t(y), \end{aligned} \tag{3.21}$$

the second identity by (3.5), and the third by (2.13). Then (2.12) yields

$$v(t,x) = S(t)f(x), \tag{3.22}$$

as asserted. □

We then have the following counterpart to (2.16).

Corollary 3.2 *Given $f \in C_0^1(\mathbb{R})$, A as in* (3.9),

$$\|S(t)f\|_{L^\infty} \le A \|f'\|_{L^1}. \tag{3.23}$$

We next give a second proof of (3.8), taking off from (3.13), which shows that

$$\lim_{x\to\pm\infty} \mathrm{Fr}(x) = \pm B, \tag{3.24}$$

for some $B \in \mathbb{C}$. We seek another proof that $B = 1/2$, not relying on the Abelian theorem used above. Our reasoning proceeds as follows. From (3.6) and (3.24), we know that

$$S(t)\chi_{a,b}(x) \longrightarrow 2B, \quad \text{uniformly in} \;\; x \in [a+\varepsilon, b-\varepsilon], \tag{3.25}$$

as $t \searrow 0$, for each $\varepsilon > 0$. On the other hand, we know that

$$S(t)\chi_{a,b} \longrightarrow \chi_{a,b}, \quad \text{in } L^2\text{-norm}, \tag{3.26}$$

as $t \to 0$. Comparison of (3.25) and (3.26) forces $B = 1/2$.

Remark. Given $B = 1/2$, we can rewrite (3.13) as

$$\mathrm{Fr}(x) - \frac{1}{2} = \frac{1}{2i}(\pi i)^{-1/2}\Big\{\frac{e^{ix^2}}{x} - \int_x^\infty \frac{1}{y^2} e^{iy^2}\, dy\Big\}, \tag{3.27}$$

for $x > 0$. Going further, we can write

$$\begin{aligned}\int_x^\infty \frac{1}{y^2} e^{iy^2}\, dy &= \frac{1}{2i}\int_x^\infty \frac{1}{y^3}\, d(e^{iy^2}) \\ &= \frac{1}{2i}\Big\{-\frac{e^{ix^2}}{x^3} + 3\int_x^\infty \frac{1}{y^4} e^{iy^2}\, dy\Big\},\end{aligned} \tag{3.28}$$

and proceed inductively to derive a complete asymptotic expansion, as $x \to \infty$, of $\mathrm{Fr}(x)$.

A An Abelian theorem

The following result justifies passing from (3.16) to (3.17), used to prove (3.8). For more general Abelian theorems, see Appendix A.5 of [2].

Proposition A.1 *Let* $f : \mathbb{R}^+ \to \mathbb{C}$ *be bounded and continuous. Assume*

$$\lim_{R\to\infty} \int_0^R f(t)\, dt = L. \tag{A.1}$$

Then

$$\lim_{\varepsilon\searrow 0} \int_0^\infty e^{-\varepsilon t} f(t)\, dt = L. \tag{A.2}$$

Proof. Set $g(s) = \int_0^s f(t)\, dt$, so $g(R) \to L$ as $R \to \infty$. Then, for $\varepsilon > 0$,

$$\begin{aligned}\int_0^\infty e^{-\varepsilon t} f(t)\, dt &= \int_0^\infty e^{-\varepsilon t} g'(t)\, dt \\ &= \varepsilon \int_0^\infty e^{-\varepsilon t} g(t)\, dt \\ &= L + \varepsilon \int_0^\infty e^{-\varepsilon t} [g(t) - L]\, dt.\end{aligned} \tag{A.3}$$

Pick $\delta > 0$ and then take $K < \infty$ such that

$$t \geq K \Longrightarrow |g(t) - L| \leq \delta. \tag{A.4}$$

Then

$$\begin{aligned}&\varepsilon \int_0^\infty e^{-\varepsilon t} |g(t) - L|\, dt \\ &\leq \varepsilon \int_0^K e^{-\varepsilon t} |g(t) - L|\, dt + \varepsilon\delta \int_K^\infty e^{-\varepsilon t}\, dt \\ &\leq \Big(\sup_{t\leq K} |g(t) - L|\Big) K\varepsilon + \delta.\end{aligned} \tag{A.5}$$

Hence

$$\limsup_{\varepsilon\searrow 0} \Big| \int_0^\infty e^{-\varepsilon t} f(t)\, dt - L \Big| \leq \delta, \quad \forall\, \delta > 0, \tag{A.6}$$

and we have (A.2). □

References

[1] M. Taylor, Partial Differential Equations, Vols. 1–3, Springer, NY 1996 (2nd ed. 2011).

[2] M. Taylor, Introduction to Complex Analysis, GSM #202, AMS, Providence RI, 2019.