The Schrödinger equation and Gauss sums

Michael E. Taylor

Consider the one-dimensional Schrödinger equation

$$(1) \qquad i\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2},$$

with solution operator $e^{-it\Delta}$. If $u(t,x)$ is defined on $\mathbb{R}\times S^1$, where $S^1=\mathbb{R}/2\pi\mathbb{Z}$ is the unit circle, then $e^{-it\Delta}$ has a very complicated behavior. It turns out that, if t is a rational multiple of 2π, then

$$(2) \qquad S(t,x) = e^{-it\Delta}\delta(x)$$

can be written as a finite linear combination of delta functions (as Jeffrey Rauch pointed out to me). The coefficients are Gauss sums. In this note we show how an analysis of the Schrödinger equation yields classical identities for Gauss sums.

We begin with a derivation of a basic reciprocity formula. To get this, we use the fact that $e^{-it\Delta}$ has a simple formula when acting on a (generalized) function $f(x)$ defined on the line. If one uses $f(x)=\sum_{\nu\in\mathbb{Z}}\delta(x-2\pi\nu)$ and compares the two representations for $S(t,x)$, at $t=2\pi m/n$, one gets a neat derivation of the reciprocity formula. We now show how that goes. Assume m and n are positive integers.

Working with Fourier series in S^1, we have

$$(3) \qquad S(2\pi m/n,x) = \frac{1}{2\pi}\sum_{k=-\infty}^{\infty} e^{2\pi i k^2 m/n}\, e^{ikx},$$

with convergence in $\mathcal{D}'(S^1)$. Setting $k=nj+\ell$, we obtain a double sum,

$$(4) \qquad S(2\pi m/n,x) = \sum_{\ell=0}^{n-1} e^{2\pi i\ell^2 m/n}\, e^{i\ell x}\sum_{j=-\infty}^{\infty} e^{injx}.$$

Now

$$(5) \qquad \sum_{j=-\infty}^{\infty} e^{injx} = \frac{2\pi}{n}\sum_{j=0}^{n-1}\delta_{2\pi j/n},$$

so we have

$$(6) \qquad S(2\pi m/n,x) = \frac{1}{n}\sum_{j=0}^{n-1}\Bigl(\sum_{\ell=0}^{n-1} e^{2\pi i\ell^2 m/n}\, e^{2\pi i\ell j/n}\Bigr)\delta_{2\pi j/n}(x).$$

Now let's go to the line. There, analytic continuation of the well known fundamental solution to the heat equation gives, for $t > 0$,

$$e^{-it\Delta}\delta(x) = \frac{1+i}{\sqrt{2}}\frac{1}{\sqrt{4\pi t}}\, e^{-ix^2/4t}. \tag{7}$$

Now, if $S(t,x)$ is regarded as defined for $x \in \mathbb{R}$, periodic of period 2π in x, we have $S(t,x) = \sum_{\nu\in\mathbb{Z}} e^{-it\Delta}\delta(x-2\pi\nu)$, with convergence in $\mathcal{S}'(\mathbb{R})$. Hence

$$\begin{aligned} S(2\pi m/n, x) &= \frac{1+i}{4\pi}\Big(\frac{n}{m}\Big)^{1/2} \sum_{\nu=-\infty}^{\infty} e^{-i(x-2\pi\nu)^2 n/8\pi m} \\ &= \frac{1+i}{4\pi}\Big(\frac{n}{m}\Big)^{1/2} e^{-ix^2 n/8\pi m} \sum_{\nu=-\infty}^{\infty} e^{-\pi i\nu^2 n/2m}\, e^{i\nu n x/2m}. \end{aligned} \tag{8}$$

Setting $\nu = 2mj + \ell$, we obtain a double sum

$$S(2\pi m/n, x) = \frac{1+i}{4\pi}\Big(\frac{n}{m}\Big)^{1/2} e^{-ix^2 n/8\pi m} \sum_{\ell=0}^{2m-1} e^{-\pi i\ell^2 n/2m} e^{i\ell n x/2m} \sum_{j=-\infty}^{\infty} e^{ijnx}. \tag{9}$$

The sum over j is evaluated as in (5), and (descending to S^1) we have

$$S(2\pi m/n, x) = \frac{1+i}{2n}\Big(\frac{n}{m}\Big)^{1/2} \sum_{j=0}^{n-1} e^{-\pi i j^2/2mn}\Big(\sum_{\ell=0}^{2m-1} e^{-\pi i\ell^2 n/2m}\, e^{\pi i j\ell/m}\Big)\delta_{2\pi j/n}(x). \tag{10}$$

Comparing (6) and (10), we have the identity

$$\sum_{\ell=0}^{n-1} e^{2\pi i\ell^2 m/n}\, e^{2\pi i\ell j/n} = \frac{1+i}{2}\Big(\frac{n}{m}\Big)^{1/2} e^{-\pi i j^2/2mn} \sum_{\ell=0}^{2m-1} e^{-\pi i\ell^2 n/2m}\, e^{\pi i j\ell/m}, \tag{11}$$

for each $j \in \{0, 1, \dots, n-1\}$. In particular, for $j = 0$, we have

$$\sum_{\ell=0}^{n-1} e^{2\pi i\ell^2 m/n} = \frac{1+i}{2}\Big(\frac{n}{m}\Big)^{1/2} \sum_{\ell=0}^{2m-1} e^{-\pi i\ell^2 n/2m}. \tag{12}$$

The case $m = 1$ of (12) is the most classical Gauss sum:

$$\sum_{\ell=0}^{n-1} e^{2\pi i\ell^2/n} = \frac{1+i}{2}\, n^{1/2}(1+i^{-n}). \tag{13}$$

Other analytical proofs of (11)–(13) can be found in a number of places; we mention particularly [A] and [Ld].

Let us denote the left side of (11) by $G(m,n,j)$, i.e.,

$$G(m,n,j) = \sum_{\ell=0}^{n-1} e^{2\pi i(\ell^2 m + \ell j)/n}. \tag{14}$$

Then the formula (6) reads

$$S(2\pi m/n, x) = \frac{1}{n}\sum_{j=0}^{n-1} G(m,n,j)\,\delta_{2\pi j/n}(x). \tag{15}$$

Clearly the expression (11) is even in j. Hence, on the right side one can replace $e^{\pi i j\ell/m}$ by $e^{-\pi i j\ell/m}$.

One still has a somewhat different looking sum on the right side of (11), and we are motivated to define

$$\Gamma(m,k,j) = \frac{1}{2k}\sum_{\ell=0}^{2k-1} e^{\pi i(\ell^2 m + \ell j)/k}. \tag{16}$$

The relation between (15) and (16) is simple:

$$\Gamma(m,k,j) = \frac{1}{2k} G(m,2k,j). \tag{17}$$

Note also that, for nonzero $a \in \mathbb{Z}$, $\Gamma(am,ak,aj) = \Gamma(m,k,j)$. If we set $n = 2k$ in (15), we have $G(m,2k,j) = 2k\,\Gamma(m,k,j)$, and hence

$$S(\pi m/k, x) = \sum_{j=0}^{2k-1} \Gamma(m,k,j)\,\delta_{\pi j/k}(x). \tag{18}$$

Meanwhile, the reciprocity formula (11) takes the form

$$\Gamma(m,k,j) = \left(\frac{m}{k}\right)^{1/2} e^{\pi i/4}\, e^{-\pi i j^2/4mk}\, \overline{\Gamma(k,m,j)}. \tag{19}$$

when $n = 2k$.

Let us set $m = 1$. By definition,

$$\Gamma(k,1,j) = \frac{1}{2}\left[1 + (-1)^{j+k}\right] = \varepsilon(j+k), \tag{20}$$

where $\varepsilon(j)$ is 1 for j even and 0 for j odd. Hence

$$\Gamma(1,k,j) = k^{-1/2} e^{\pi i/4}\, e^{-\pi i j^2/4k}\,\varepsilon(j+k). \tag{21}$$

Therefore

$$e^{-(\pi i/k)\Delta}\delta(x) = k^{-1/2} e^{\pi i/4} \sum_{j=0}^{2k-1} e^{-\pi i j^2/4k}\,\varepsilon(j+k)\,\delta_{\pi j/k}(x). \tag{22}$$

Let us denote by G_ℓ the multiplicative subgroup of S^1 generated by $e^{2\pi i/\ell}$, a cyclic group of order ℓ. Clearly (6) implies that $S(\pi/k,x)$ is supported on G_{2k}, but in fact (22) implies the more precise containment:

$$\begin{aligned} k \text{ even} &\Longrightarrow S(\pi/k,x) \ \text{ supported on } \ G_k \\ k \text{ odd} &\Longrightarrow S(\pi/k,x) \ \text{ supported on } \ G_{2k} \setminus G_k = e^{\pi i/k}\cdot G_k. \end{aligned} \tag{23}$$

Using the group property of $e^{-it\Delta}$, we see that

$$k \text{ even} \Longrightarrow S(m\pi/k, x) \ \text{ supported on } \ G_k, \tag{24}$$

and

$$\begin{aligned} k \text{ odd} \Longrightarrow S(2\mu\pi/k, x) \ &\text{ supported on } \ G_k, \\ S((2\mu+1)\pi/k, x) \ &\text{ supported on } \ e^{\pi i/k} \cdot G_k. \end{aligned} \tag{25}$$

In view of the formula (18), we deduce that

$$mk + j \text{ odd} \Longrightarrow \Gamma(m,k,j) = 0. \tag{26}$$

Let us set $\Gamma(m,k) = \Gamma(m,k,0)$. The following was established in [HB]:

Lemma 1. *Assume that m and k are relatively prime. Let μ solve $\mu m = 1$ mod k.*
(i) If mk and j are even, then

$$\Gamma(m,k,j) = e^{-\pi i(m/k)(j/2)^2\mu^2}\, \Gamma(m,k). \tag{27}$$

(ii) If mk and j are odd, then, with ν solving $4\nu m = 1$ mod k,

$$\Gamma(m,k,j) = e^{-4\pi i(m/k)\nu^2 j^2}\, \Gamma(4m,k). \tag{28}$$

Proof. We follow [HB]. To establish (27), expand the left side of

$$\sum_{\ell=0}^{2k-1} e^{\pi i m(\ell + j\mu/2)^2/k} = \sum_{\ell=0}^{2k-1} e^{\pi i m \ell^2/k},$$

valid whenever j is even. To establish (28), one can use the following observation. Suppose $\varphi : \mathbb{Z} \to \mathbb{C}$ is periodic of period k, which is odd, and set $\varphi_2(\ell) = \varphi(2\ell)$. Then φ and φ_2 have the same mean. Hence it follows that, if mk and j are odd, then

$$\Gamma(m,k,j) = \frac{1}{2k} \sum_{\ell=0}^{2k-1} e^{\pi i(4\ell^2 m + 2\ell j)/k},$$

and then an argument similar to the previous one yields (28).

We hence have the following:

Theorem 2. *Assume m and k are relatively prime. Let μ solve $\mu m = 1$ mod k.*
(i) If mk is even, then

$$e^{-(m/k)\pi i\Delta}\, \delta(x) = \Gamma(m,k) \sum_{\ell=0}^{k-1} e^{-\pi i(m/k)\ell^2\mu^2}\, \delta_{2\pi\ell/k}(x). \tag{29}$$

(ii) If mk is odd, then, with ν solving $4\nu m = 1$ mod k,

$$e^{-(m/k)\pi i\Delta}\, \delta(x) = \Gamma(4m,k) \sum_{\ell=0}^{k-1} e^{-4\pi i(m/k)\nu^2(2\ell+1)^2}\, \delta_{(2\ell+1)\pi/k}(x). \tag{30}$$

Using unitarity of $e^{-it\Delta}$ we have:

Corollary 3. *Assume m and n are relatively prime. then*

$$\begin{aligned} mk \ odd &\Longrightarrow \Gamma(m,k) = 0, \\ mk \ even &\Longrightarrow |\Gamma(m,k)| = k^{-1/2}. \end{aligned} \tag{31}$$

These identities specify $\Gamma(m,k)$ up to phase. Note that (13) with $n = 2k$ gives

$$\Gamma(1,k) = \varepsilon(k)\, e^{\pi i/4}\, k^{-1/2}. \tag{32}$$

Results on $\Gamma(m,k)$ are special cases of results on $G(m,n) = G(m,n,0)$, defined by the left side of (12), i.e.,

$$G(m,n) = \sum_{\ell=0}^{n-1} e^{2\pi i \ell^2 m/n}. \tag{33}$$

Note that

$$G(m,2k) = 2k\, \Gamma(m,k). \tag{34}$$

The identity (13) is a formula for $G(1,n)$. In addition, the following results hold; proofs can be found on pp. 85–88 of [Lg].
(i) If p is an odd prime and $j \geq 2$, then

$$G(m,p^j) = p\, G(m,p^{j-2}). \tag{35}$$

(ii) If $(n,k) = 1$ and $(m,nk) = 1$, then

$$G(m,nk) = G(mn,k) G(mk,n). \tag{36}$$

(iii) If $n \geq 1$ is odd and $(m,n) = 1$, then

$$G(m,n) = (m|n)\, G(1,n), \tag{37}$$

where $(m|n)$ is the Jacobi symbol, taking values ± 1.
(iv) If m is odd,

$$G(m,2^j) = (-2^j|m)\, \sigma(m)\, G(1,2^j), \tag{38}$$

where $\sigma(m) = 1$ if $m = 1 \bmod 4$, $\sigma(m) = i$ if $m = 3 \bmod 4$.

Of these four results, (i) and (ii) are straightforward. One first proves (iii) for $n = p$, prime, and then deduces it in general, using (i)–(ii). The proof of (iv) makes use of the computation of $G(1,n)$, for $n = 2^j$. It also uses the fact that, if $\zeta = e^{2\pi i/2^j}$, then $\zeta \mapsto \zeta^m$ yields an automorphism of the field $\mathbb{Q}(\zeta)$, which hence sends $G(1,2^j)$ to $G(m,2^j)$. See [Lg] for details. Evidently $G(m,n)$ can be evaluated in general via (ii)–(iv), and the formula (13). We mention that the proof of (13) given in [Lg] is the same as that in [Ld], and is due to Dirichlet.

We make a few more comments on the reciprocity formula (12). When $n = 2k$ is even, it takes the form

$$\Gamma(m,k) = \Big(\frac{m}{k}\Big)^{1/2} e^{\pi i/4}\, \overline{\Gamma(k,m)}, \tag{39}$$

specializing (19). When m is odd, the right side of (12) involves yet a different sort of Gauss sum. Let us set

$$\gamma(m,k) = \frac{1}{k}\sum_{\ell=0}^{k-1} e^{\pi i (m/k)\ell^2}. \tag{40}$$

Then (12) can be written

$$G(m,n) = (1+i)\,(mn)^{1/2}\,\overline{\gamma(n,2m)}. \tag{41}$$

Note that

$$G(m,n) = n\,\gamma(2m,n). \tag{42}$$

Also, if we decompose the sum for $\Gamma(m,k)$ into $0 \le \ell < k$ and $k \le \ell < 2k$, we obtain the identity

$$\Gamma(m,k) = \frac{1+e^{\pi i m k}}{2}\,\gamma(m,k). \tag{43}$$

From this we see that

$$mk \text{ odd} \Longrightarrow \Gamma(m,k) = 0, \tag{44}$$

which is a special case of (26), and that

$$mk \text{ even} \Longrightarrow \Gamma(m,k) = \gamma(m,k). \tag{45}$$

Hence we deduce from (42) that

$$G(m,n) = n\,\Gamma(2m,n). \tag{46}$$

Note also that substitution of the identities (45) and (46) into (41) yields

$$\Gamma(2m,n) = (1+i)\Big(\frac{m}{n}\Big)^{1/2}\,\overline{\Gamma(n,2m)},$$

which is merely a special case of (39).

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