Notes on the Harmonic Oscillator and the Fourier Transform

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In these notes we first derive two well-known results and relate them in an elegant way. We show that the Hermite functions, the eigenfunctions of the harmonic oscillator, are an orthonormal basis for L^2, the space of square-integrable functions. Secondly we establish the Fourier inversion theorem on L^2. We then infer some simple properties of the Schwartz space of well-behaved functions.

I The Fourier Transform

Define the Fourier transform operator $\mathfrak{F}$ as the linear transformation on integrable functions f,

$$\left(\mathfrak{F}f\right)(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(y) e^{-ipy}\, dy = \widehat{f}(p) \;. \tag{I.1}$$

One sometimes writes $\left(\mathfrak{F}f\right)(p) = \widehat{f}(p)$. The Fourier inversion theorem says $\mathfrak{F}^2 f$ exists, and

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\mathfrak{F}f\right)(p) e^{ipx}\, dp = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{f}(p) e^{ipx}\, dp \;. \tag{I.2}$$

The pair of identities (I.1) and (I.2) are the fundamental identities for Fourier transforms.

We show in these notes that these relations hold and have a meaning for arbitrary $f \in L^2$. The L^2-inner product is

$$\langle f, g \rangle_{L^2} = \int_{-\infty}^{\infty} \overline{f(x)} g(x) dx \;. \tag{I.3}$$

Square-integrable functions $f \in L^2$ are those of length $\|f\|_{L^2} = \langle f, f \rangle_{L^2}^{1/2} < \infty$. A subset $\mathcal{D} \subset L^2$ is said to be *dense*, if any $f \in L^2$ can be approximated by a sequence $f_n \in \mathcal{D}$. This means $\lim_n \|f - f_n\|_{L^2} = 0$. An orthonormal basis $\{\Omega_n\}$ is a set of orthonormal vectors whose finite linear combinations are dense. A linear transformation T is continuous on L^2 if $\|Tf\|_{L^2} \le M \|f\|_{L^2}$ for some constant $M < \infty$. A continuous transformation defined on a basis extends uniquely to all L^2.

II The Fourier Transform is Unitary

The transformation $\mathfrak{F}$ is *unitary* on L^2. What does this mean? Define the matrix elements of the adjoint $\mathfrak{F}^*$ of $\mathfrak{F}$ by $\langle f, \mathfrak{F}^* g \rangle_{L^2} = \langle \mathfrak{F} f, g \rangle_{L^2}$. For integrable functions f, g, one can compute $\mathfrak{F}^*$ as

$$\langle f, \mathfrak{F}^* g \rangle_{L^2} = \langle \mathfrak{F} f, g \rangle_{L^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ixy} \overline{f(y)} g(x)\, dx dy = \langle f, P\mathfrak{F} g \rangle_{L^2} \;. \tag{II.1}$$

Here we introduce the operator of reflection through the origin, namely

$$\left(Pf\right)(x) = f(-x) \;. \tag{II.2}$$

Note that $P\mathfrak{F} = \mathfrak{F}P$. The computation (II.1) shows that on integrable functions,

$$\mathfrak{F}^* = P\mathfrak{F} = \mathfrak{F}P \;. \tag{II.3}$$

From these relations it is not clear that $\mathfrak{F}$ has an inverse. We claim the striking fact that the inverse $\mathfrak{F}^{-1}$ does exist, and moreover that it equals $\mathfrak{F}^*$. In other words we claim that

$$I = \mathfrak{F}^* \mathfrak{F} = \mathfrak{F} \mathfrak{F}^* \;. \tag{II.4}$$

The relations (II.4) state that $\mathfrak{F}$ is unitary. We prove (II.4) in §VII using properties of the harmonic oscillator that we establish in §IV–§V.

III Some Consequences of Unitarity

The property that $\mathfrak{F}$ is unitary has numerous beautiful consequences. We now mention two. The relation $I = \mathfrak{F}^*\mathfrak{F}$ in (II.4) is known as Plancherel's theorem. Written in terms of expectations,

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} |\widehat{f}(p)|^2 \, dp \; . \tag{III.1}$$

A second consequence of the unitarity is the Fourier inversion formula. From (II.3–II.4) we infer

$$I = \mathfrak{F}P\mathfrak{F} \; , \qquad \text{or} \quad f = \mathfrak{F}P\mathfrak{F}f \; , \tag{III.2}$$

applied to any $f \in L^2$. Use the definitions to write out (III.2); it is just the desired inversion (I.2).

IV The Harmonic Oscillator

The operator

$$a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \; , \qquad \text{and its adjoint} \quad a^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right) \; , \tag{IV.1}$$

are the lowering and raising operators for the harmonic oscillator with unit mass and frequency equal, and units with $\hbar = 1$. They satisfy $[a, a^*] = I$, and $[a, a^{*n}] = n a^{*n-1}$. The operator

$$H = a^* a = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2 - 1\right) \tag{IV.2}$$

is the corresponding Hamiltonian. Note that

$$[H, a^{*n}] = a^{*n+1} a + a^*[a, a^{*n}] - a^{*n} H = n a^{*n} \; . \tag{IV.3}$$

The differential equation $\sqrt{2} a \Omega_0(x) = \Omega_0(x) + \Omega_0'(x) = 0$ has the normalized solution

$$\Omega_0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2} \; , \tag{IV.4}$$

and yields a zero-energy ground state of H satisfying $H\Omega_0 = a^* a \Omega_0 = 0$.

Introduce the Hermite functions $\Omega_n(x)$ and the Hermite polynomials $H_n(x)$ defined by

$$\Omega_n(x) = \frac{1}{\sqrt{n!}} a^{*n} \Omega_0(x) = \frac{1}{2^{n/2}\sqrt{n!}} H_n(x) \Omega_0(x) \; . \tag{IV.5}$$

From (IV.3), we infer that Ω_n is an eigenfunction of H with eigenvalue n. Furthermore

$$\langle \Omega_n, \Omega_n \rangle = \frac{1}{n} \langle \Omega_{n-1}, a a^* \Omega_{n-1} \rangle = \frac{1}{n} \langle \Omega_{n-1}, (H + I)\Omega_{n-1} \rangle = \langle \Omega_{n-1}, \Omega_{n-1} \rangle = \cdots = \langle \Omega_0, \Omega_0 \rangle = 1 \; , \tag{IV.6}$$

so using the fact that the eigenvalues of the Ω_n are different for different n, these functions satisfy

$$\langle \Omega_n, \Omega_m \rangle = \delta_{nm} \; . \tag{IV.7}$$

In other words, the Hermite functions are an orthonormal set of eigenfunctions of H, with the eigenvalues are $n = 0, 1, 2, \ldots$.

V The Oscillator Eigenfunctions are a Basis

If the $\{\Omega_n\}$ are not a basis, then there is a non-zero vector $\chi \in L^2$ perpendicular to all of the Ω_n. We assume that there exists a vector $\chi \in L^2$ satisfying $\chi \perp \Omega_n$ for all n. We then show that $\chi = 0$.

We use the generating function for Hermite polynomials, namely $G(z;x) = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x)$. We now compute $G(z;x)$, which also was a homework problem. Use the definition (IV.5) to write $G(z;x) = \Omega_0^{-1}\, e^{\sqrt{2}za^*}\Omega_0$. For any constant λ, the "translation identity" $e^{-\lambda a} a^* e^{\lambda a} = a^* - \lambda$ follows from expanding each side of this equality as a power series in λ. Now define $f(\lambda) = e^{\lambda a^*} e^{\lambda a} e^{-\lambda(a^*+a)} e^{\lambda^2/2}$. Using the translation identity, we infer $f'(\lambda) = 0$. Consequently $f(\lambda) = f(0) = I$, and we have proved the "rearrangement identity" $e^{\lambda a^*} e^{\lambda a} = e^{\lambda(a^*+a)} e^{-\lambda^2/2}$. Since also $e^{\sqrt{2}za}\,\Omega_0 = \Omega_0$, we apply the rearrangement identity with $\lambda = \sqrt{2}z$ to show $e^{\sqrt{2}za^*}\Omega_0 = e^{-z^2+2zx}\,\Omega_0$. Therefore dividing by Ω_0,

$$G(z;x) = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x) = e^{-z^2+2zx} \; . \tag{V.1}$$

Suppore we are given a vector χ orthogonal to all the Ω_n. Using (V.1), we have for any real p,

$$\sum_{n=0}^{\infty} \frac{(-ip/\sqrt{2})^n}{\sqrt{n!}} \langle \Omega_n, \chi\rangle_{L^2} = \int_{-\infty}^{\infty} G(-ip/2;x)\Omega_0(x)\chi(x)dx = \sqrt{2\pi}e^{p^2/4}\mathfrak{F}\left(\chi\Omega_0\right)(p) = 0 \; . \tag{V.2}$$

Hence $\mathfrak{F}\left(\chi\Omega_0\right) = 0$. Therefore, unless $\chi = 0$, the Fourier transform $\mathfrak{F}$ has no inverse!

In order to show that $\chi = 0$, multiply the (vanishing) Fourier transform of $\chi\Omega_0$ by e^{ipa}. Then

$$\int_{-\infty}^{\infty} \chi(x)\Omega_0(x)e^{-ip(x-a)}\, dx = 0 \; . \tag{V.3}$$

Take $\epsilon > 0$. Then multiply (V.3) by $e^{-\epsilon p^2}$, and integrate over p. By completing the square for the Gaussian p-integration, we obtain

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \chi(x)\Omega_0(x)e^{-\epsilon p^2 - ip(x-a)}\, dxdp = \sqrt{\frac{\pi}{\epsilon}}\int_{-\infty}^{\infty} \chi(x)\Omega_0(x)e^{-(x-a)^2/4\epsilon}\, dx = 0 \; . \tag{V.4}$$

Let $\epsilon \to 0$, and recall that $\sqrt{\frac{1}{\epsilon\pi}}e^{-(x-a)^2/\epsilon} \to \delta(x-a)$. Thus $\chi(a)\Omega_0(a) = 0$, for all a. But $\Omega_0(a) > 0$, so divide by this function to conclude $\chi(a) = 0$. This is a contradiction to the assumption that $\chi \neq 0$. Therefore we conclude that the $\{\Omega_n\}$ form a basis.

VI Oscillator Eigenfunctions are Fourier Eigenfunctions

Recall that the operators in (IV.1) denote the lowering and raising operators for the simple harmonic oscillator. Note $Pa^* = -a^*P$. Thus using (I.1), (II.3), and $P^2 = I$, we obtain the commutation relations

$$\mathfrak{F}\, a = -ia\,\mathfrak{F} \; , \qquad \text{and} \quad \mathfrak{F}\, a^* = ia^*\,\mathfrak{F} \; . \tag{VI.1}$$

As a consequence, the oscillator Hamiltonian $H = a^*a = \frac{1}{2}\left(-d^2/dx^2 + x^2 - 1\right)$ commutes with $\mathfrak{F}$, and $\mathfrak{F}$ and H can be simultaneously diagonalized. In other words, the oscillator eigenfunctions Ω_n of H are also eigenfunctions of $\mathfrak{F}$. The corresponding eigenvalues are $\pm 1, \pm i$, as follows from the representation of the n^{th}-eigenfunction $\Omega_n = \frac{1}{\sqrt{n!}}a^{*n}\Omega_0$. Using (VI.1) and $\mathfrak{F}\Omega_0 = \Omega_0$, we infer that

$$\mathfrak{F}\,\Omega_n = \frac{1}{\sqrt{n!}}\mathfrak{F}\, a^{*n}\Omega_0 = i^n\frac{1}{\sqrt{n!}}a^{*n}\mathfrak{F}\,\Omega_0 = i^n\Omega_n \; . \tag{VI.2}$$

VII The Fourier Inversion Theorem

From (VI.2) and $P\Omega_n = (-1)^n \Omega_n$, we conclude that $\mathfrak{F} P \mathfrak{F}\, \Omega_n = \Omega_n$. Thus

$$\mathfrak{F} P \mathfrak{F} = I \ , \qquad \text{on the span of the functions } \Omega_n \ . \tag{VII.1}$$

Using the discussion in §I and the continuity of the identity I, we infer that the equality (VII.1) extends to all L^2 if and only if the collection of harmonic oscillator eigenfunctions $\{\Omega_n\}$ are a basis for L^2. In that case, (VII.1) shows that $\mathfrak{F}$ has a left and right inverse $\mathfrak{F}P = P\mathfrak{F} = \mathfrak{F}^*$. But in §V we established that the $\{\Omega_n\}$ are a basis. So we conclude that (VII.1) extends of L^2 and $\mathfrak{F}^{-1} = \mathfrak{F}^*$.

VIII Schwartz Space of Well-Behaved Functions

The Schwartz space $\mathcal{S}$ of well-behaved functions is defined as those functions $f(x) \in L^2$ for which $H^n f \in L^2$ for all $n = 0, 1, 2, 3, \ldots$, where H is the oscillator Hamiltonian. Since we showed in §VI that $[H, \mathfrak{F}] = 0$, we conclude that $\mathfrak{F}\mathcal{S} \subset \mathcal{S}$. But as $\mathfrak{F}^{-1} = \mathfrak{F}P$, and $P\mathcal{S} \subset \mathcal{S}$, it follows that

$$\mathfrak{F}\mathcal{S} = \mathcal{S} \ . \tag{VIII.1}$$

Note that $\Omega_n \in \mathcal{S}$, for every n. Furthermore any $f \in L^2$ has an expansion in the $\{\Omega_n\}$-basis,

$$f(x) = \sum_{j=0}^{\infty} f_j \, \Omega_j(x) \ . \tag{VIII.2}$$

We write the condition that $f \in L^2$ actually is an element of $\mathcal{S}$ as

$$\| H^n f \|_{L^2}^2 = \sum_{j=0}^{\infty} j^{2n} \, |f_j|^2 < \infty \ , \tag{VIII.3}$$

for all $n = 0, 1, 2, 3, \ldots$. In other words, the Schwartz space has “rapidly decreasing” coefficients in the oscillator/Fourier basis $\{\Omega_n\}$.

Any $f \in L^2$ has a sequence of approximating functions $f_R \in \mathcal{S}$. In fact for f of the form (VIII.2), define

$$f_R(x) = \sum_{j=0}^{\infty} f_j \, e^{-j^2/R} \, \Omega_j(x) \ . \tag{VIII.4}$$

Clearly $f_R \in \mathcal{S}$. Furthermore, as $e^{-j^2/R}$ is monotonically decreasing in j,

$$\| f_R - f \|_{L^2}^2 = \sum_{j=1}^{\infty} |f_j|^2 \left(1 - e^{-j^2/R} \right)^2 \leq \| f \|_{L^2}^2 \left(1 - e^{-1/R} \right)^2 \to 0 \ , \qquad \text{as } R \to \infty \ . \tag{VIII.5}$$

Exercise. Show that the Schwartz functions are exactly those for which

$$\sup_{x \in \mathbb{R}} \left| x^r \frac{d^s}{dx^s} f(x) \right| < \infty \ , \tag{VIII.6}$$

for all $r, s = 0, 1, 2, 3, \ldots$.