Hermite Function and Its Application to 1D Quantum Harmonic Oscillator Model

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Abstract

Quantum Harmonic Oscillator (QHO) is the quantum mechanical analog of the classical harmonic oscillator, which is one of the few quantum mechanic systems whose analytical solution are known [1]. In this paper, the author gives an insight into the solution of a QHO system via the tool of **Fourier Transform** and **Hermite Function**.

Keywords: QHO, Fourier Analysis, Hermite Functions, Hermite Polynomials, Hermite Operator, Annihilation and Creation Operators.

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1 Hermite Functions & Hermite Polynomials

Definition 1.1 (Hermite Function [3])**:** The Hermite functions $h_k(x)$ are defined by the generating identity

$$\sum_{k=0}^{\infty} h_k(x)\frac{t^k}{k!} = e^{-(x^2/2-2tx+t^2)}.$$

Since we can write $e^{-(x^2/2-2tx+t^2)}$ as $e^{x^2/2}e^{-(x-t)^2}$, using Taylor's formula

$$e^{x^2/2}e^{-(x-t)^2} = e^{x^2/2}\sum_{k=0}^{\infty}(-1)^k\frac{t^k}{k!}\left(\frac{d}{dx}\right)^k e^{-x^2},$$

we then have another identity for Hermite functions

$$h_k(x) = (-1)^k e^{x^2/2}\left(\frac{d}{dx}\right)^k e^{-x^2}. \tag{1}$$

Equation (1) reveals that the Hermite function $h_k(x)$ is a product of a polynomial $H_k(x)$ and $e^{-x^2/2}$, where $H_k(x)$ is the **Hermite polynomial**[1]. Thus $h_k(x)$ belongs to the **Schwartz space** $\mathcal{S}(\mathbb{R})$, which consists of **Schwartz functions**, i.e. functions satisfy

$$\sup_{x\in\mathbb{R}} |x|^k|f^{(l)}(x)| < \infty \qquad \forall k,l \geq 0.$$

And we will prove that

Theorem 1.1. *Hermite functions form an orthogonal basis in* $\mathcal{S}(\mathbb{R})$.

[1] Precisely, $H_k(x)$ defined here are called **physicists' Hermite polynomials**

1.1 Completeness

To prove the completeness of the family $\{h_k\}_{k=0}^{\infty}$, we need

Lemma 1.2. *If the Fourier transform $\hat{f}(\xi)$ of a function $f(x) \in \mathcal{S}(\mathbb{R})$ is 0, then $f(x)$ is identically 0.*

It's nearly obvious since we have the **Fourier Inversion formula** for functions in $\mathcal{S}(\mathbb{R})$

Theorem 1.3 (Fourier Inversion)**.** *If $f(x)$ is a function in $\mathcal{S}(\mathbb{R})$ and $\hat{f}(\xi)$ is the Fourier transform of $f(x)$*

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)e^{-2\pi ix\xi}dx,$$

then we have

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi)e^{2\pi ix\xi}d\xi.$$

Fourier transforms are useful when we are dealing with convolutions. Because we have the

Theorem 1.4 (Convolution Theorem)**.** *Let $\hat{f}$ and $\hat{g}$ denote the Fourier transforms of f and g, and the convolution $f * g$ defined by*

$$(f * g)(x) = \int_{-\infty}^{\infty} f(x-t)g(t)dt.$$

We have the Fourier transform $\widehat{f * g}$ of $f * g$ equals the product of $\hat{f}$ and $\hat{g}$

$$\widehat{(f * g)}(\xi) = \hat{f}(\xi)\hat{g}(\xi).$$

Suppose that we have a function f in Schwartz space and is orthogonal to every h_k, in the sense that (where the bar means complex conjugation)

$$(f, h_k) = \int_{-\infty}^{\infty} f(x)\overline{h_k(x)}dx = 0 \qquad \forall k \geq 0,$$

Multiply each expression by $e^{t^2}\frac{t^k}{k!}$ and sum together, we have

$$\begin{aligned}
\sum_{k=0}^{\infty}\int_{-\infty}^{\infty} f(x)h_k(x)e^{t^2}\frac{t^k}{k!}dx &= \int_{-\infty}^{\infty} f(x)e^{t^2}\sum_{k=0}^{\infty} h_k(x)\frac{t^k}{k!}dx \\
&= \int_{-\infty}^{\infty} f(x)e^{-\frac{1}{2}(2t-x)^2}dx \\
&= (f * g)(2t),
\end{aligned}$$

where $g(x) = e^{-x^2/2}$, thus via convolution theorem and lemma 1.2, we conclude that $f = 0$ and the family $\{h_k\}_{k=0}^{\infty}$ is a complete basis.

I will postpone the proof for the orthogonality later until we figure out some more properties of h_k.

1.2 Hermite operator, Annihilation and Creation operator

Definition 1.2 (Hermite operator [3])**:** The Hermite operator which acts on Schwartz functions is defined by this formula

$$L(f) = -\frac{d^2}{dx^2}f + x^2 f,$$

or simply

$$L = -\frac{d^2}{dx^2} + x^2.$$

We can quickly verify some properties of this operator.

Proposition 1: L is a **symmetric operator**

$$(f, Lg) = (Lf, g).$$

Proof.

$$\begin{aligned}(f, Lg) &= \int_{-\infty}^{\infty} f(x)\overline{\left(-\frac{d^2}{dx^2} + x^2\right) g(x)}dx \\ &= \int_{-\infty}^{\infty} x^2 f(x)\overline{g(x)}dx - \int_{-\infty}^{\infty} f(x)\overline{g''(x)}dx \\ &= \int_{-\infty}^{\infty} x^2 f(x)\overline{g(x)}dx - \int_{-\infty}^{\infty} f''(x)\overline{g(x)}dx \\ &= (Lf, g),\end{aligned}$$

where we have used integration by parts twice. □

Hermite operator and Hermite functions are connected through this theorem

Theorem 1.5. *Hermite functions are eigenfunctions of Hermite operator, in fact*

$$Lh_k = (2k+1)h_k.$$

Once the theorem is proved, we will have the orthogonality of h_k as a corrollary, we talk about this latter. To prove this theorem, the definitions of **annihilation** and **creation** operators are useful.

Definition 1.3 (Annihilation & Creation operator)**:** The annihilation operator is defined as

$$A(f) = \frac{d}{dx}f + xf,$$

while the creation operator is defined as

$$A^*(f) = -\frac{d}{dx}f + xf.$$

Proposition 2:

$$A^*A = L - I.$$

Proof.

$$\begin{aligned}A^*A &= \left(-\frac{d}{dx} + x\right)\left(\frac{d}{dx} + x\right) \\ &= -\frac{d^2}{dx^2} + x\frac{d}{dx} - \frac{d}{dx}x + x^2 \\ &= -\frac{d^2}{dx^2} + x\frac{d}{dx} - I - x\frac{d}{dx} + x^2 \\ &= L - I.\end{aligned}$$

□

We can derive this lemma from the definition of Hermite funcitons

Lemma 1.6.

$$Ah_k = 2kh_{k-1} \qquad A^*h_k = h_{k+1}.$$

Proof. Take differentiation on both sides of the identity

$$\sum_{k=0}^{\infty} h_k(x)\frac{t^k}{k!} = e^{-(x^2/2-2tx+t^2)},$$

we have

$$\sum_{k=0}^{\infty} h_k'(x)\frac{t^k}{k!} = (-x+2t)e^{-(x^2/2-2tx+t^2)}.$$

Using the identity on the right-hand side and compare the coefficients of t we find

$$h_k'(x) = -xh_k(x) + 2kh_{k-1}(x), \tag{2}$$

this yields $Ah_k = 2kh_{k-1}$. However when we differentiate equation (1) on both sides

$$\begin{aligned} h_k'(x) &= (-1)^k \frac{d}{dx} e^{x^2/2} \left(\frac{d}{dx}\right)^k e^{-x^2} \\ &= x(-1)^k e^{x^2/2} \left(\frac{d}{dx}\right)^k e^{-x^2} - (-1)^{k+1} e^{x^2/2} \left(\frac{d}{dx}\right)^{k+1} e^{-x^2} \\ &= xh_k(x) - h_{k+1}(x), \end{aligned}$$

this yields $A^* h_k = h_{k+1}(x)$. $\square$

Thus we are led to

$$A^* A h_k = 2kA^* h_{k-1} = 2kh_k.$$

Apply $A^* A = L - I$ and we conclude theorem 1.5.

1.3 Orthogonality and L^2-norm

Hermite functions are orthogonal, since

$$(2k+1)(h_k, h_l) = (Lh_k, h_l) = (h_k, Lh_l) = (2l+1)(h_k, h_l).$$

So we have concluded theorem 1.1. The significance of this theorem will be seen in the next section where we will apply this to the system of quantum harmonic oscillator. But before that, we need to calculate the L^2-norm of $h_k(x)$. From the definition of Hermite functions, we have

$$\int_{-\infty}^{\infty} |g(x)|^2 dx = \sum_{k=0}^{\infty} \frac{t^{2k}}{(k!)^2} \int_{-\infty}^{\infty} |h_k(x)|^2 dx \qquad \text{where } g(x) = e^{t^2} e^{-\frac{1}{2}(x-2t)^2}$$

since $\{h_k\}_{k=0}^{\infty}$ is an orthogonal basis in $\mathcal{S}(\mathbb{R})$. Evaluate the left-hand side integral

$$\begin{aligned} \int_{-\infty}^{\infty} |g(x)|^2 dx &= e^{2t^2} \int_{-\infty}^{\infty} e^{-(x-2t)^2} dx \\ &= \sum_{k=0}^{\infty} \sqrt{\pi} \frac{2^k t^{2k}}{k!}. \end{aligned}$$

Comparing the coefficients we have

$$||h_k||_2 = \sqrt{\int_{-\infty}^{\infty} |h_k(x)|^2 dx} = \sqrt{2^k k! \sqrt{\pi}}.$$

2 One-dimensional Quantum Harmonic Oscillator

The quantum harmonic oscillator is the quantum analog of classical harmonic oscillator where the **Hamiltonian** $\hat{H}$ of the particle is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2,$$

where m is the particle's mass, ω is the angular frequency of the oscillator, $\hat{x}$ is the position operator and $\hat{p}$ is the momentum operator, given by $\hat{p} = -i\hbar \dfrac{\partial}{\partial x}$. [2]

2.1 Time-independent Schrödinger Equation

If the state of the system is $|\psi\rangle$, then the so-called wave function $\psi(x)$ is defined to be

$$\psi(x) = \langle x|\psi\rangle,$$

where the bra vector $\langle x|$ is the state where the system has exactly the position x, i.e. an eigenstate of position operator which satisfies $\hat{x}|x\rangle = x|x\rangle$.

Then solving the time-independent Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle,$$

where E is the eigenvalue of Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$, is equivalent to solving this one

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x) = E\psi(x).$$

A change of variable $x = \lambda y$ where $\lambda = \sqrt{\frac{\hbar}{m\omega}}$, reduces this equation to

$$\left(-\frac{\partial^2}{\partial y^2} + y^2\right)\psi(\lambda y) = \frac{2}{\omega\hbar}E\psi(\lambda y).$$

Using the knowledge of Hermite functions, if we assume ψ is a Schwartz function[2], the solution to this equation is

$$\psi_k(\lambda y) = \frac{1}{c_k}h_k(y) \qquad E_k = \frac{\omega\hbar}{2}(2k+1) \quad c_k = ||h_k||_2 = \sqrt{2^k k!\sqrt{\pi}},\ k \geq 0,$$

which forms an orthogonal basis.

2.2 Time-dependent Schrödinger Equation

Since we've totally solved the time-independent Schrödinger equation, it becomes easy to solve the time-dependent one

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{i\hbar}\hat{H}\psi(x,t).$$

Because $\psi_k(y)$ forms an orthogonal basis and is independent of time, we have

$$\psi(x,t) = \sum_{k=0}^{\infty}\psi_k(x)a_k(t) \qquad a_k(t) = \int_{-\infty}^{\infty}\psi(z,t)\overline{\psi_k(z)}dz.$$

Substitute this into the time-dependent Schrödinger equation, we get

$$a_k'(t) = \frac{1}{i\hbar}E_k a_k(t).$$

Hence $a_k(t) = e^{-i\frac{E_k}{\hbar}t}a_k(0)$, and the wave function of our particle can be written explicitly

$$\psi(x,t) = \sum_{k=0}^{\infty} a_k(0)\frac{1}{\sqrt{2^k k!\sqrt{\pi}}}h_k\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-i\omega(k+1/2)},$$

where $a_k(0)$ is our initial data.

References

[1] David Jeffery Griffiths. *Introduction to quantum mechanics.* Pearson Education India, 2005.

[2] *Quantum Harmonic Ocsillator.* URL: `https://en.wikipedia.org/wiki/Quantum_harmonic_oscillator`.

[3] Elias M Stein and Rami Shakarchi. *Fourier analysis: an introduction.* 2003.

[2]Actually ψ satisfies $\int_{-\infty}^{\infty}|\psi(x)|^2dx = 1$