Hilbert transformation, Gaussian & Dawson Function and the Harmonic Quantum Oscillator Model

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The one-dimensional model of the quantum oscillator is considered. The corresponding function space is the periodic function on the unit circle. The spectrum of the energy levels of the harmonic quantum oscillator is given by the set of eigen-pairs of the Schrödinger (energy=Hamiltonian) operator equation

$$H_E := -\frac{1}{2m}P^2 + V^2$$

with potential V^2 and the Schrödinger momentum operator

$$P := -i\hbar\frac{d}{dx} \quad \text{i.e.} \quad P^2 := \hbar^2\frac{d^2}{dx^2} = (-i\hbar\frac{d}{dx})^2 \ .$$

The corresponding energy norm is defined by

$$\|\psi\|_E^2 := (H_E\psi, \psi) \ .$$

The spectrum of the energy level is given by the eigenvalues and its corresponding excited state (wave functions) functions ψ_n defined by

$$H_E\psi_n = E_n\psi_n \ .$$

The wave function of the ground state is given by the Gaussian function in the form

$$\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4} e^{-m\omega x^2/(2\hbar)} \ .$$

For the eigen-function the following recursion formula is valid

$$\psi_n(x) = \sqrt{\frac{m\omega}{2\hbar n}}(x - \frac{\hbar}{m\omega}\frac{d}{dx})\psi_{n-1}(x) \ .$$

The challenge is about the "eigen-functions" of the momentum operator: Those are plane wave

$$\rho_n(x) = e^{ikx}$$

with eigenvalues

$$p = \hbar k \qquad \text{(de-Broglie condition).}$$

The eigen-functions of the momentum operator cannot be normed, as for the absolute value of the Gaussian function it holds

$$|\rho_n(x)|^2 = |e^{ikx}|^2 = 1 \ .$$

In essence a minimal momentum and a minimal location expansion (ground state energy) needs to be given, which is not equal zero, caused by the uncertainty relation. The root cause is given by the ground state wave function, which fulfills

$$\psi_0(0) = (\frac{m\omega}{\pi\hbar})^{1/4} \neq 0 \ .$$

The eigen-functions of the Hamiltonian operator are built by the product of the Hermite polynomials and the ground state wave function. As the Gaussian function is even, the generation and annihilation operators do not "converge" symmetrically from "both sides" (upstairs, downstairs) to the ground state zero energy. The Hermite polynomials are built on the Gaussian function and span the $L_2(-\infty,\infty)-$Hilbert space. From the properties below the same capabilities can be provided by the odd Dawson function.

What will happen, if there is an alternative ground state wave function with $\psi_0^*(0)=0$?

We propose the Hilbert transform of the Gaussian function

$$f(x) = e^{-x^2} ,$$

which is the Dawson function

$$F(x) := e^{-x^2}\int_0^x e^{t^2}dt = \frac{\sqrt{\pi}}{2}\frac{1}{\pi} p.v.\int_{-\infty}^{\infty}\frac{e^{-y^2}}{x-y}dy = H[f](x)$$

as alternative model for the ground state wave function. We further propose the normal derivative operator T *of the double layer potential (which is self-adjoint) as alternative to the Schrödinger momentum operator.*

The Hilbert transforms of $x^{2n}f(x)$ are also related to the Dawson function. From the properties of the Hilbert transform below it follows, that both functions are orthogonal with respect to the $L_2(-\infty,\infty)-$ Hilbert space, i.e.

$$(f,F)_{L_2(-\infty,\infty)} = 0 \ .$$

This property in combination with the below commutator properties indicate the usefulness of the theory of complementary variational principles ([ArA]), e.g. the method of Trefftz, the hyper circle method of Prager/Synge, the method of orthogonal projection ([VeW] 4) for an alternative (complementary) harmonic quantum oscillator energy spectrum model.

Lemma 1: The Hilbert transform of the Gauss-Weierstrass density function $f(x)$ is given by

$$[H(f)](x) = 4\pi\int_0^\infty f(\xi)\sin(2\pi\xi x)d\xi \ .$$

The proof is given in the appendix.

Some key properties of the Hilbert transform

$$(Hu)(x) := \lim_{\varepsilon \to 0} \frac{1}{\pi} \oint_{|x-y|>\varepsilon} \frac{u(y)}{x-y} dy = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{u(y)}{x-y} dy$$

are given in

Lemma: i) The constant Fourier term vanishes, i.e. $(Hu)_0 = 0$

ii) $$H(xu(x)) = xH(u(x)) - \frac{1}{\pi} \int_{-\infty}^{\infty} u(y) dy$$

iii) For odd functions it hold

$$H(xu(x)) = x(Hu)(x)$$

iv) If $u, Hu \in L_2$ then u and Hu are orthogonal, i.e.

$$\int_{-\infty}^{\infty} u(y)(Hu)(y) dy = 0$$

v) $\|H\| = 1$, $H^* = -H$, $H^2 = -I$, $H^{-1} = H^3$,

vi) $H(f * g) = f * Hg = Hf * g \qquad f * g = -Hf * Hg$

vii) If $(\varphi_n)_{n \in N}$ is an orthogonal system, so it is for the system $(H(\varphi_n))_{n \in N}$,

i.e. $(H\varphi_n, H\varphi_n) = -(\varphi_n, H^2 \varphi_n) = (\varphi_n, \varphi_n)$.

viii) $\|Hu\|^2 = \|u\|^2$, i.e. if $u \in L_2$, then $Hu \in L_2$.

Proof:

i) , v)-viii) see [PeB], 2.9

ii) Consider the Hilbert transform of $xu(x)$

$$H(xu(x)) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{yu(y)}{x-y} dy \ .$$

The insertion of a new variable $z = x - y$ yields

$$H(xu(x)) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{(x-z)u(x-z)}{z} dz = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{(xu(x-z)}{z} dz - \frac{1}{\pi} \int_{-\infty}^{\infty} u(x-z) dz = xH(u(x)) - \frac{1}{\pi} \int_{-\infty}^{\infty} u(y) dy$$

iii) It follows from i) and ii)

iv) $$\int_{-\infty}^{\infty} u(y)(Hu)(y) dy = \frac{i}{2\pi} \int_{-\infty}^{\infty} sign((\omega)|\hat{u}(\omega)|^2 d\omega$$ whereby $|\hat{u}(\omega)|^2$ is even •

The proposed operator of concern is the normal derivative operator

$$T : H_{1/2} \to H_{-1/2}$$

of the double layer potential

$$K : H_{1/2} \to H_{1/2} .$$

In case of the unit circle this is the Calderon-Zygmund given by **(**[LiI] (1.2.31)-(1.2.33), [LiI1]):

$$Tu(x) := \oint \frac{1}{4\sin^2 \frac{x-y}{2}} u(y)dy \; .$$

This enables an alternative energy operator in the form

$$H_E^* := -\frac{1}{2m} T^2 + V^2 \; ,$$

whereby the operator T is self-adjoint (in opposite to the Schrödinger momentum operator P), i.e. it holds

$$(Tu, v)_0 = (u, Tv)_0 \qquad \forall u, v \in H_{1/2} \; .$$

Remark: The single layer potential

$$Au(x) := -\oint \log 2\sin \frac{x-y}{2} u(y)dy$$

is related to the operators H, T by

$$A[u_x](x) = -H[u](x)$$

resp.

$$(HA)[u_x](x) = u(x) \; .$$

The corresponding commutator are defined by

$$\overline{H} := xH - Hx$$

$$\overline{P} := xP - Px$$

$$\overline{T} := xT - Tx$$

.

Corollary:

i) $\overline{H}u = 0$ if u is odd

ii) $\overline{P}u = u$

iii) $\overline{T}u = Hu$

and therefore

iv) $(\overline{P}u, \overline{T}u) = 0$

APPENDIX

Proof of lemma 1: The Fourier transform of

$$\varphi_0(t) := \pi^{-1/4} e^{-t^2/2}$$

is given by

$$\hat{\varphi}_0(t) := \sqrt{2}\pi^{1/4} e^{-\omega^2/2} \ .$$

With

$$(Hu)_\nu = -i\,\mathrm{sgn}(\nu) u_\nu$$

one gets

$$\left[H(\varphi_0)\right]^\wedge(\omega) = -i\,\mathrm{sgn}(\omega)\hat{\varphi}_0(\omega) \ .$$

Applying the inverse Fourier transform then gives

$$\left[H(\varphi_0)\right](t) = \sqrt{2}\pi^{1/4}\int_{-\infty}^{\infty}(-i\,\mathrm{sgn}(\omega))e^{-\omega^2/2}e^{-i\omega t}d\omega \ .$$

Since $\mathrm{sgn}(\omega)e^{-\omega^2/2}$ is odd we have

$$\left[H(\varphi_0)\right](t) = 2\sqrt{2}\pi^{1/4}\int_0^{\infty} e^{-\omega^2/2}\sin(\omega t)d\omega \ .$$

With

$$f(x) = \pi^{1/4}\varphi_0(\sqrt{2\pi}x)$$

it follows

$$\pi^{1/4}\left[H(\varphi_0)\right](\sqrt{2\pi}x) = 2\sqrt{2\pi}\int_0^{\infty} e^{-\omega^2/2}\sin(\sqrt{2\pi}\omega x)d\omega \ .$$

Substituting the variables $\omega = \sqrt{2\pi}\xi$ then leads to

$$\left[H(f)\right](x) = 4\pi\int_0^{\infty} e^{-\pi\xi^2}\sin(2\pi\xi x)d\xi \qquad \bullet$$

Hermite Polynomials

The weighted Hermite polynomials

$$\varphi_n(x) := \frac{e^{-\frac{x^2}{2}} H_n(x)}{\sqrt{2^n n! \sqrt{\pi}}} \quad \text{with} \quad H_n(x) := (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \ , \quad H_0(x) = 1 \, , \quad H_1(x) = x \, ,$$

form a set of orthonormal functions in $L_2(-\infty, \infty)$, i.e. the Hermite polynomials have only real zeros. The relation to the Gaussian function is given by

$$f(x) = \pi^{1/4} \varphi_0(\sqrt{2\pi} x) \ .$$

The Hermite polynomials $H_n(x)$ fulfill the recursion formula

(2.9) $$H_n(\sqrt{2\pi} x) = 2x H_{n-1}(\sqrt{2\pi} x) - (n-1) b_n \varphi_{n-2}(x) - 2(n-1) H_{n-2}(\sqrt{2\pi} x) \ .$$

Using the abbreviation

$$a_n := \sqrt{\frac{2(n-1)!}{n!}} \qquad b_n := \sqrt{\frac{(n-2)!}{n!}}$$

this gives the recursion formula

(2.10) $$\varphi_n(x) := a_n x \varphi_{n-1}(x) - (n-1) b_n \varphi_{n-2}(x) \, , \quad \varphi_0(x) := \pi^{-1/4} e^{-\frac{x^2}{2}} \, , \quad \varphi_1(x) := 2^{-1/2} \pi^{-1/4} x e^{-\frac{x^2}{2}} \quad ,$$

from which the recursion formula for the corresponding Hilbert transforms can be calculated

(2.11) $$\hat{\varphi}_n(x) := a_n \left[x \hat{\varphi}_{n-1}(x) - \frac{1}{\pi} \int_{-\infty}^{\infty} \varphi_{n-1}(y) dy \right] - (n-1) b_n \hat{\varphi}_{n-2}(x)$$

$$\hat{\varphi}_0(x) = \pi^{1/4} \int_{-\infty}^{\infty} e^{-\frac{\omega^2}{2}} \sin(\omega x) d\omega \ .$$

As $\varphi_n, H\varphi_n \in L_2$ is follows by lemma xxx

$$L_2 := H := span[\varphi_n(x)] = span[H(\varphi_n(x))] \ .$$

The Dawson Function

For the Gauss error function and the Dawson integral

$$erf(z) = 2\int_0^z e^{-\pi t^2} dt \quad , \quad F(z) := e^{-z^2}\int_0^z e^{-u^2} du$$

we recall from [LeN]:

Lemma $F(z)$ is an entire function with the following properties

i) $F(z) = \sum_0^\infty (-1)^k \frac{2^k z^{2k+1}}{1\cdot 3..\cdot(2k+1)} = z\cdot {}_1F_1(1,\frac{3}{2},-z^2) = \frac{1}{4\sqrt{\pi}} f_H(\frac{z}{\sqrt{\pi}})$

ii) $F(0) = 0$, $F'(x) + 2xF(x) = 1$, $\lim_{z\to\infty} 2xF(x) = 1$, i.e. $F(x) \approx \frac{1}{2x}$ for $z \to \infty$

iii) for the single maximum and inflection points it holds

$F(0.924...) = 0.541.. > 1/2$ and $F(1.50...) = 0.42...$ ([AbM] 7.1.17)

iv) $\frac{d}{dx}(xF(x)) = x + F(x)(1-2x) \geq F(x) > 0$

v) $erf(x) = \frac{2x}{\sqrt{\pi}}\,{}_1F_1(\frac{1}{2};\frac{3}{2},-x^2) = \frac{2}{\sqrt{\pi}}\sum_0^\infty \frac{(-1)^k x^{2k+1}}{k!(2k+1)}$.

Remark: From [AbM] 13, ([GaW], [GrI] we recall the formulas

i) ${}_1F_1(\frac{1}{2};\frac{3}{2},-\pi x^2) = \frac{1}{x}\int_0^x e^{-\pi t^2} dt = \frac{1}{x}\int_0^x f(t)dt$

ii) ${}_1F_1(1;\frac{3}{2},\pi x^2) = \frac{f(x)}{x}\int_0^x f(t)dt$

iii) $\sqrt{\frac{x}{\pi}} f_H(\sqrt{\frac{x}{\pi}}) = 4xe^{-x}\,{}_1F_1(\frac{1}{2};\frac{3}{2},x) = 4e^{\frac{x}{2}} M_{\frac{1}{4},\frac{1}{4}}(x)$, $f_H(x)$ denotes the Hilbert transformation of $f(x)$

iv) $e^{-x^2}\,{}_1F_1(\frac{1}{2};\frac{3}{2},x^2) = \sum_{n=0}^\infty \frac{2^n}{1\cdot 3\cdots(2n+1)}(ix)^{2n}$

v) $(xH - Hx)[f_H] = 0$

vi) $H[f_H] = -4\pi\int_0^\infty e^{-\pi y^2}\cos(2\pi xy)dy$

vii) $H\left[\frac{e^{-x}}{x}\right] = c\frac{F(\sqrt{x})}{\sqrt{x}}$ ([GaW] 7.1.17).

Ball symmetric potential of linear oscillator

For the energy

$$E = \frac{1}{2}\hbar\omega$$

the radial function $f(r)$ of the corresponding eigen-function of the Schrödinger equation is given by

$$f(r) = e^{\lambda\frac{r^2}{2}}\left[c_1 \cdot {}_1F_1(\frac{1}{2};\frac{3}{2},\lambda r^2) + c_2\frac{1}{r}{}_1F_1(\frac{1}{2};\frac{3}{2},\lambda r^2)\right] .$$

Remark (Yukawa potential): The $Ei(-x)-$function is also related to the Yukawa potential of a point charge in the form

$$e^{-\mu r}/r \quad , \quad \mu > 0$$

in order to define a nuclear force potential which decays rapidly at infinity. Yukawa assumed that μ^{-1} was of the order of magnitude of a nuclear radius. It results that the potential u of a charge distribution satisfies the Yukawa equation

$$\Delta u = \mu^2 u$$

at points of free space. Thus the Yukawa potentials are invariant under the group of rotations and translations of space, like those of Newton potentials. As μ approaches zero the Yukawa potentials approach those of Newton. The function $e^{-\mu r}/r$ is a member of the Bessel family of functions. Bessel functions have certain advantages over Newtonian potentials in functional analysis.

Analog to the above we propose a modified Yukawa potential dY^* by the substitution

$$e^{-\mu r}/r \to \mu F'(\mu r) .$$

The Dawson function $F(x)$ shows similar behavior as the Yukawa potential with the additional properties that $F(0) = 0$ and the long distance behavior

$$F(x) \approx x^{-1} .$$

We recall the alternative option for the exponential integral function density (and the eigenfunction of the ground state energy of the harmonic quantum oscillator)

$$\frac{e^{-x}}{x}dx \to -2\,{}_1F_1'(\frac{1}{2};\frac{3}{2},-x)dx$$

leading to an alternative "Yukawa" potential with same long range behavior as both, the gravitation (Newton) and the electromagnetic (Coulomb) potential (whereby the Coulomb potential is aligned with weak interaction potential by the Higgs mechanism) in the form

$$-g^2\frac{e^{-\frac{mc}{\hbar}x}}{x} \to -2ag^2\,{}_1F_1'(\frac{1}{2};\frac{3}{2},-ax) = -2g^2\frac{mc}{\hbar}\,{}_1F_1'(\frac{1}{2};\frac{3}{2},-\frac{mc}{\hbar}x) .$$

With the standard notation and corresponding abbreviation

$$n\cdot\sigma_n := \frac{Zme^2}{\hbar^2} \quad , \quad \sigma := \sigma_1 \quad V^*(r) := \frac{2\sigma}{r} \quad , \quad E^* := \frac{2mE}{\hbar^2}$$

the Coulomb eigenvalue problem, based on the corresponding Schrödinger equation,

$$u''(r) + \left[E^* + V^*(r)\right]u(r) = 0$$

has the eigen-pair solutions

$$\psi^*(r) := \frac{1}{\sqrt{\pi}}\sigma_n^{3/2} e^{-\sigma_n r}\, {}_1F_1'(1-n;2,\sigma_n r)$$

$$E_n := -\frac{1}{2}\sigma_n^2\hbar^2 \qquad \text{Rydberg formula.}$$

The Yang-Mills theory seeks to describe the behavior of elementary particles and is the core of the unification of electromagnetic and weak forces, as well as quantum chromodynamics, the theory of strong forces. It is the basis of the Standard Model. It is a special example of gauge theory with non-abelian symmetry group.

According to the above we propose a modified potential $V^{**}(r)$ of the Schrödinger equation, which delivers (not symmetric) eigen-functions in the form

$$\psi^{**}(r) \approx \sqrt{\frac{\sigma_n}{\pi}}\frac{\sigma_n r\cdot e^{-\sigma_n r}}{r}\, {}_1F_1(\frac{1}{2}-n;\frac{3}{2},\sigma_n r) \quad .$$

Applying the Dawson function to define the total energy in a one-dimensional Schrödinger equation by

$$E(x) := E_{kin}(x) + E_{pot}(x) := \alpha x F(\gamma x) + \frac{\beta}{x}F(\gamma x) = \frac{1}{2\gamma}(\alpha x + \frac{\beta}{x})\cdot\frac{d}{dx}\left[erf^2(\gamma x)\right]$$

with some constants α,β,γ provides a model with finite zero and infinity energy according to

$$E(x) \to \begin{cases} \beta & for \quad x\to 0 \\ \frac{\alpha}{2\gamma} & for \quad x\to\infty \end{cases}$$

Calderon-Zygmund and Riesz Operators

The Calderon-Zygmund operator with symbol $|v|$ ([EsG] (3.17), (3.35)) is defined by

$$(\Lambda u)(x)=(\sum_{k=1}^{n}R_kD_ku)(x)=\frac{\Gamma(\frac{n+1}{2})}{\pi^{\frac{n+1}{2}}}\sum_{k=1}^{n}p.v.\int_{-\infty}^{\infty}\sum_{k=1}^{n}\frac{x_k-y_k}{|x-y|^{n+1}}\frac{\partial u(y)}{\partial y_k}dy=-\frac{\Gamma(\frac{n-1}{2})}{2\pi^{\frac{n+1}{2}}}p.v.\int_{-\infty}^{\infty}\frac{\Delta_y u(y)}{|x-y|^{n-1}}dy=-(\Delta\Lambda^{-1})u(x)$$

whereby R_k denotes the Riesz operators ([AbH] p. 19, 106, [PeB] example 9.9)

$$R_ku=-i\pi^{-(n+1)/2}\Gamma(\frac{n+1}{2})p.v.\int_{-\infty}^{\infty}\frac{x_k-y_k}{|x-y|^{n+1}}u(y)dy\,.$$

For $n\geq 2$ it holds ([EsG] (3.15))

$$\Lambda^{-1}u=\frac{1}{2}\pi^{-(n+1)/2}\Gamma(\frac{n-1}{2})\int_{-\infty}^{\infty}\frac{u(y)dy}{|x-y|^{n-1}}\quad .$$

The Riesz operators fulfill certain properties with respect to commutation with translations homothesis and rotation ([PeB], [StE]). Let $SO(n)$ denote the rotation group. If $j\neq j$ then R_jR_k is a singular convolution operator. On the other hand it holds $R_j^2=-(1/n)I+A_j$ where A_j is a convolution operator. The following identities are valid

$$\|R_j\|=1\quad,\quad R_j^*=-R_j\quad,\quad\sum R_j^2=-I\quad,\quad\sum\|R_ju\|^2=\|u\|^2\quad,u\in L_2\ .$$

Let

$$m:=m(x):=(m_1(x),...m_n(x))$$

be the vector of the Mikhlin multipliers of the Riesz operators and $\rho=\rho_{ik}\in SO(n)$, then

$$m(\rho(x))=\rho(m(x))\,,$$

whereby

$$m_j(\rho(x))=\sum\rho_{jk}m_k(x)$$

and

$$m(\rho(x))=c_n\int_{S^{n-1}}(\frac{\pi i}{2}sign(x\rho^{-1}(y))+\log\left|\frac{1}{x\rho^{-1}(y)}\right|)\frac{y}{|y|}d\sigma(y)$$

$$=c_n\int_{S^{n-1}}(\frac{\pi i}{2}sign(xy)+\log\left|\frac{1}{xy}\right|)\frac{y}{|y|}d\sigma(y)\ .$$

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