Tsirelson's Constant

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All infinite-dimensional, separable, complex Hilbert spaces are isometrically isomorphic [1]. Fix such a space X for consideration. Let P, Q be self-adjoint linear operators on X that satisfy the canonical commutation relations

$$P\,Q - Q\,P = -i\,I$$

where i is the imaginary unit and I is the identity operator. Such unbounded operators P, Q are each defined only on a dense linear subspace of X, and the intersection of two dense linear subspaces generally need not be dense. The commutation relations ensure, however, that

$$R = -(P + Q)$$

is well-defined and is a self-adjoint linear operator. Hence we have three operators P, Q, R such that $P + Q + R = 0$ and

$$P\,Q - Q\,P = Q\,R - R\,Q = R\,P - P\,R = -i\,I.$$

Let us define a **sign function** for operators [2]. First, the scalar sign function is given by

$$\operatorname{sgn}(z) = \begin{cases} 1 & \text{if } \operatorname{Re}(z) > 0, \\ -1 & \text{if } \operatorname{Re}(z) < 0 \end{cases}$$

for $z \in \mathbb{C}$ lying off the imaginary axis. Next, the matrix sign function is given by

$$\operatorname{sgn}(M) = U\,\operatorname{sgn}(\Lambda)\,U^{-1}$$

where $M \in \mathbb{C}^{n\times n}$ is a Hermitian matrix with no eigenvalues on the imaginary axis. The unitary $n \times n$ matrix U has column vectors equal to the orthonormal eigenvector basis of $\mathbb{C}^n$ determined by M, and the diagonal $n \times n$ matrix Λ has components equal to the (real) eigenvalues of M:

$$M = U\,\Lambda\,U^{-1}.$$

By $\operatorname{sgn}(\Lambda)$ is meant the diagonal $n \times n$ matrix with sgn applied component-wise to Λ. Finally, the operator sign function can be defined similarly by use of the spectral theorem for unbounded operators (upon which we do not elaborate).

It is remarkable that the operator norm [3]

$$c = \|\mathrm{sgn}(P) + \mathrm{sgn}(Q) + \mathrm{sgn}(R)\| \approx 1.2$$

is independent of the choice of P, Q, R . It is a nontrivial constant and a more precise estimate would be good to see. We will provide a limiting expression for c shortly.

0.1. Schrödinger Representation. Let $X = L_2(\mathbb{R})$ and, for wave functions $\psi \in L_2(\mathbb{R})$,

$$(P\psi)(x) = -i\frac{d}{dx}\psi(x), \qquad (Q\psi)(x) = x\,\psi(x).$$

These are the momentum and position (or coordinate) operators that arise in quantum mechanics. Further, the time-independent Schrödinger ODE for the quantum harmonic oscillator [4, 5, 6, 7]:

$$\frac{d^2\psi}{dx^2} + \left(\lambda - x^2\right)\psi = 0$$

(in natural units) can be written as

$$(P^2 + Q^2)\psi = \lambda\,\psi$$

with eigenvalues $\lambda_n = 2n + 1$ for $n = 0, 1, 2, \ldots$ and orthonormal eigenfunctions

$$\psi_n(x) = \left(\sqrt{\pi}n!2^n\right)^{-1/2} e^{-x^2/2} H_n(x).$$

The Hermite polynomials $H_n(x)$ satisfy Rodrigues' formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

as well as the recurrence

$$H_{n+1}(x) = 2x\,H_n(x) - 2n\,H_{n-1}(x), \qquad H_0(x) = 1, \qquad H_1(x) = 2x.$$

It is well-known that

$$\int_{-\infty}^{\infty} \psi_n(x)^2 dx = 1$$

and $\psi_n(x)^2$ is the probability density for location of a particle in the n^{th} energy state of a harmonic oscillator. Corresponding to any observable physical quantity, there is a self-adjoint linear operator T, and its expected value for the same particle is

$$\mathrm{E}_n(T) = \int_{-\infty}^{\infty} \psi_n(x)(T\psi_n)(x)dx.$$

[0]The addendum clarifies the meaning of $P\,Q - Q\,P = -i\,I$ and the well-definition of c.

For example,

$$\sqrt{\mathrm{Var}_n(P)}\sqrt{\mathrm{Var}_n(Q)} = n + \frac{1}{2} \geq \frac{1}{2}$$

which constitutes the Heisenberg uncertainty principle for a quantum harmonic oscillator (in dimensionless variables). The fact that the product of uncertainties is bounded away from zero can be proved under much more general circumstances.

In the following section, the Laguerre polynomials

$$L_n(x) = \frac{1}{n!} e^x \frac{d^n}{dx^n} \left(x^n e^{-x} \right)$$

are essential. These obey the recurrence

$$(n+1)L_{n+1}(x) = (2n+1-x)\, L_n(x) - n\, L_{n-1}(x), \qquad L_0(x) = 1, \qquad L_1(x) = 1 - x$$

and are orthogonal with respect to the exponential distribution Exp(1), just as the Hermite polynomials are orthogonal with respect to the normal distribution $\mathrm{N}(0, 1/2)$.

0.2. Wigner Function. One might believe that, to estimate c, all we must do is to find $n \times n$ matrices P, Q satisfying the commutation relations for arbitrarily large n. Unfortunately no such matrices exist since otherwise we would have

$$0 = \mathrm{tr}(P\,Q) - \mathrm{tr}(Q\,P) = \mathrm{tr}(P\,Q - Q\,P) = \mathrm{tr}(-i\,I) = -i\,n,$$

a contradiction. A different approach must be found.

The **Wigner function** (or **quasi-distribution**) offers a way to compute c. All we require are its values on the Hermite eigenfunction basis of $L_2(\mathbb{R}) \times L_2(\mathbb{R})$:

$$\begin{aligned} w_{m,n}(x,y) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi_m\left(x + \frac{\xi}{2}\right) e^{i\,\xi\,y} \psi_n\left(x - \frac{\xi}{2}\right) d\xi \\ &= \begin{cases} \dfrac{(-1)^m}{\pi} \sqrt{\dfrac{m!}{n!}} (2\bar{z})^{n-m} e^{-2|z|^2} L_m^{(n-m)}\left(4|z|^2\right) & \text{if } m \leq n, \\ w_{n,m}(x,y) & \text{if } m > n \end{cases} \end{aligned}$$

where $z = (x + i\,y)/\sqrt{2}$ and $\bar{z} = (x - i\,y)/\sqrt{2}$. See [8, 9, 10, 11] for details. The generalized Laguerre polynomials are related to the (ordinary) Laguerre polynomials via

$$L_m^{(k)}(x) = (-1)^k \frac{d^k}{dx^k} L_{m+k}(x).$$

The n^{th} expected value of any physical quantity $f(Q, P)$ can alternatively be calculated via

$$\mathrm{E}_n(f(Q,P)) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) w_{n,n}(x,y)\, dy\, dx.$$

For example,

$$\mathrm{Var}_n(P) = \frac{(-1)^n}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} y^2 e^{-(x^2+y^2)} L_n(2(x^2+y^2)) dy\, dx = n + \frac{1}{2}$$

and $\mathrm{Var}_n(Q)$ likewise, confirming Heisenberg's principle. Note that $w_{1,1}(0,0) = -1/\pi$, for instance, and thus the Wigner function is not a probability density in the usual sense (because it may take negative values).

0.3. Operator Norm. The $(m,n)^{\text{th}}$ element in the matrix representation of the operator $T = \mathrm{sgn}(P)$ relative to the Hermite eigenfunction basis of $L_2(\mathbb{R})$ is

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_m(x)(T\psi_n)(x) dx &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{sgn}(y) w_{m,n}(x,y)\, dy\, dx \\ &= \int_{-\infty}^{\infty} \int_{0}^{\infty} w_{m,n}(x,y)\, dy\, dx - \int_{-\infty}^{\infty} \int_{-\infty}^{0} w_{m,n}(x,y)\, dy\, dx \end{aligned}$$

for integers $m \geq 0$, $n \geq 0$. Changing to polar coordinates

$$x = r\cos(\theta), \qquad y = r\sin(\theta)$$

in the upper half plane, we obtain

$$\begin{aligned} \int_{-\infty}^{\infty} \int_{0}^{\infty} w_{m,n}(x,y)\, dy\, dx &= \int_{0}^{\pi} \int_{0}^{\infty} w_{m,n}(r\cos(\theta), r\sin(\theta))\, r\, dr\, d\theta \\ &= \int_{0}^{\pi} e^{i(m-n)\theta} d\theta \int_{0}^{\infty} w_{m,n}(r,0)\, r\, dr, \end{aligned}$$

$$\begin{aligned} \int_{-\infty}^{\infty} \int_{-\infty}^{0} w_{m,n}(x,y)\, dy\, dx &= \int_{\pi}^{2\pi} \int_{0}^{\infty} w_{m,n}(r\cos(\theta), r\sin(\theta))\, r\, dr\, d\theta \\ &= \int_{\pi}^{2\pi} e^{i(m-n)\theta} d\theta \int_{0}^{\infty} w_{m,n}(r,0)\, r\, dr. \end{aligned}$$

When $m \le n$,

$$\int_0^\infty w_{m,n}(r,0)\, r\, dr = \frac{(-1)^m}{\pi}\sqrt{\frac{m!}{n!}}\int_0^\infty \left(\sqrt{2}r\right)^{n-m} e^{-r^2} L_m^{(n-m)}\left(2r^2\right) r\, dr$$

and thus the $(m,n)^{\text{th}}$ matrix element simplifies to [12]

$$\gamma_{m-n}\frac{(-1)^{m+n}}{\pi}\sqrt{m!\,n!}\sum_{k=\max\{m,n\}}^{m+n}(-1)^k 2^{k-(m+n)/2-1}\frac{\Gamma(k-(m+n)/2+1)}{(m+n-k)!\,(k-m)!\,(k-n)!}$$

where

$$\gamma_j = \int_0^\pi e^{i\,j\,\theta} d\theta - \int_\pi^{2\pi} e^{i\,j\,\theta} d\theta = \begin{cases} 0 & \text{if } j \equiv 0 \bmod 2, \\ 4i/j & \text{if } j \equiv 1 \bmod 2. \end{cases}$$

The norm $\|\operatorname{sgn}(P)\|$ of the infinite matrix is found by numerically evaluating the largest eigenvalue of the upper left $N \times N$ submatrix of $\operatorname{sgn}(P)$ and letting $N \to \infty$.

The matrices $\operatorname{sgn}(Q)$ and $\operatorname{sgn}(R)$ are obtained similarly, with γ_{m-n} replaced by δ_{m-n} and ε_{m-n} respectively, where

$$\delta_j = \int_{-\pi/2}^{\pi/2} e^{i\,j\,\theta} d\theta - \int_{\pi/2}^{3\pi/2} e^{i\,j\,\theta} d\theta = \begin{cases} 0 & \text{if } j \equiv 0 \bmod 2, \\ 4/j & \text{if } j \equiv 1 \bmod 4, \\ -4/j & \text{if } j \equiv 3 \bmod 4 \end{cases}$$

and

$$\varepsilon_j = \int_{-5\pi/4}^{-\pi/4} e^{i\,j\,\theta} d\theta - \int_{-\pi/4}^{3\pi/4} e^{i\,j\,\theta} d\theta = \begin{cases} 0 & \text{if } j \equiv 0 \bmod 2, \\ 2\sqrt{2}(-1-i)/j & \text{if } j \equiv 1 \bmod 8, \\ 2\sqrt{2}(-1+i)/j & \text{if } j \equiv 3 \bmod 8, \\ 2\sqrt{2}(1+i)/j & \text{if } j \equiv 5 \bmod 8, \\ 2\sqrt{2}(1-i)/j & \text{if } j \equiv 7 \bmod 8. \end{cases}$$

Adding the three matrices and taking the largest eigenvalue, we obtain a limiting value ≈ 1.2 for the operator norm.

0.4. Quantum Probability. For convenience, define the **indicator function**

$$\operatorname{ind}(\xi) = \begin{cases} 1 & \text{if } \xi > 0, \\ 0 & \text{if } \xi < 0 \end{cases} = \frac{1}{2} + \frac{1}{2}\operatorname{sgn}(\xi).$$

Let $q\cos(t) + p\sin(t)$ denote the coordinate of a classical harmonic oscillator at time t, where q, p are the initial coordinate and momentum, and the period is 2π. Choose

$\tau \in \{0, 2\pi/3, 4\pi/3\}$ at random. What is the probability that $q\cos(\tau) + p\sin(\tau) > 0$? Clearly this depends on the initial state and is given by

$$
\begin{aligned}
&\sum_{k=0}^{2} \mathrm{P}\left(q\cos(\tau) + p\sin(\tau) > 0 \mid \tau = \tfrac{2\pi k}{3}\right) \mathrm{P}\left(\tau = \tfrac{2\pi k}{3}\right) \\
=\ & \tfrac{1}{3}\left(\mathrm{ind}\,(q) + \mathrm{ind}\left(-\tfrac{1}{2}q + \tfrac{\sqrt{3}}{2}p\right) + \mathrm{ind}\left(-\tfrac{1}{2}q - \tfrac{\sqrt{3}}{2}p\right)\right) \\
=\ & \begin{cases} \tfrac{2}{3} & \text{if } \tfrac{\pi}{6} < \theta < \tfrac{\pi}{2} \text{ or } \tfrac{5\pi}{6} < \theta < \tfrac{7\pi}{6} \text{ or } -\tfrac{\pi}{2} < \theta < -\tfrac{\pi}{6}, \\ \tfrac{1}{3} & \text{if } -\tfrac{\pi}{6} < \theta < \tfrac{\pi}{6} \text{ or } \tfrac{\pi}{2} < \theta < \tfrac{5\pi}{6} \text{ or } -\tfrac{5\pi}{6} < \theta < -\tfrac{\pi}{2} \end{cases}
\end{aligned}
$$

where θ is the polar angle of (q, p) in the plane. Thus the solution is $\frac{1}{2} \pm \frac{1}{6}$.

Consider now the quantum harmonic oscillator $Q\cos(t) + P\sin(t)$ [13]. Answering the same question reduces to evaluating the spectral bounds of the operator

$$\tfrac{1}{2}I + \tfrac{1}{6}\left(\mathrm{sgn}\,(Q) + \mathrm{sgn}\left(-\tfrac{1}{2}Q + \tfrac{\sqrt{3}}{2}P\right) + \mathrm{sgn}\left(-\tfrac{1}{2}Q - \tfrac{\sqrt{3}}{2}P\right)\right)$$

which turn out to be

$$\tfrac{1}{2} \pm \tfrac{1}{6}c \approx \tfrac{1}{2} \pm 0.21.$$

The maximum probability ≈ 0.71 is calculated in [12] and is rigorously proved to be < 1. We wonder if there are other such fascinating numbers in the intersection between functional analysis and quantum mechanics.

0.5. Generalized Oscillator. The Schrödinger ODE for the anharmonic oscillator:

$$\frac{d^2\psi}{dx^2} + \left(\lambda - x^4\right)\psi = 0$$

with quartic potential cannot be solved in closed-form (unlike the harmonic oscillator). It is worthy to mention that the smallest eigenvalue is

$$\lambda_0 = 1.0603620904...$$

and this constant is now known to over 1000 digits [14, 15, 16, 17]. The corresponding eigenvalues for the sextic and octic potentials are 1.1448024537... and 1.2258201138... [18, 19]. See [20] for mention of the linear potential case.

0.6. Addendum. Tsirelson [3] warns readers that he uses $PQ - QP = -iI$ merely as shorthand for the Weyl relations

$$\exp(i\alpha P)\exp(i\beta Q) = \exp(i\alpha\beta)\exp(i\beta Q)\exp(i\alpha P) \qquad \text{for all } \alpha, \beta \in \mathbb{R}.$$

The consequential independence of $\|\mathrm{sgn}(P) + \mathrm{sgn}(Q) + \mathrm{sgn}(R)\|$ of the choice of P, Q, R follows from von Neumann's theorem [1].

He also offers the following explanation for [0.2]: "The operator norm is the supremum of the corresponding quadratic form over the unit sphere. We may choose an increasing sequence of finite-dimensional subspaces whose union is dense, and consider the corresponding finite-dimensional suprema; they increase to the infinite-dimensional supremum. Thus the operator norm is the limit of an increasing sequence of matrix norms. A good choice of a basis (in the Hilbert space) simplifies the calculation of the matrices. We use the basis of eigenvectors of the Hamiltonian (of the oscillator). The calculation of the matrices may be made via the Wigner function."

REFERENCES

[1] M. Reed and B. Simon, *Methods of Modern Mathematical Physics. I. Functional Analysis*, 2^{nd} ed., Academic Press, 1980, pp. 47, 71, 249–250, 270–275, 302–305; MR0751959 (85e:46002).

[2] N. J. Higham, *Functions of Matrices: Theory and Computation*, SIAM, 2008, pp. 39–43, 107–132; MR2396439.

[3] B. Tsirelson, Automorphisms of the type II_1 Arveson system of Warren's noise, arXiv:math.OA/0612303.

[4] G. F. Simmons, *Differential Equations with Applications and Historical Notes*, McGraw-Hill, 1972, pp. 194–196; MR0499365 (58 #17258).

[5] C. A. Tracy, Lectures on Ordinary Differential Equations (2007), https://www.math.ucdavis.edu/~tracy/courses/math22B/.

[6] S. A. Ponomarenko, Quantum harmonic oscillator revisited: A Fourier transform approach, *Amer. J. Phys.* 72 (2004) 1259–1260.

[7] A. Engel, Comment on 'Quantum harmonic oscillator revisited: A Fourier transform approach', *Amer. J. Phys.* 74 (2006) 837.

[8] H. J. Groenewold, On the principles of elementary quantum mechanics, *Physica* 12 (1946) 405–460; MR0018562 (8,301a).

[9] M. S. Bartlett and J. E. Moyal, The exact transition probabilities of quantum-mechanical oscillators calculated by the phase-space method, *Proc. Cambridge Philos. Soc.* 45 (1949) 545–553; MR0034709 (11,631e).

[10] T. Takabayasi, The formulation of quantum mechanics in terms of ensemble in phase space, *Progress Theoret. Physics* 11 (1954) 341–373; MR0064670 (16,319b).

[11] T. Curtright, T. Uematsu and C. Zachos, Generating all Wigner functions, *J. Math. Phys.* 42 (2001) 2396–2415; MR1821868 (2002f:81060).

[12] B. Tsirelson, How often is the coordinate of a harmonic oscillator positive? arXiv:quant-ph/0611147.

[13] P. Nardone, Heisenberg picture in quantum mechanics and linear evolutionary systems, *Amer. J. Phys.* 61 (1993) 232–237.

[14] M. Trott, High-precision value for the quartic anharmonic oscillator ground state, arXiv:quant-ph/0012147.

[15] H. A. Alhendi and E. I. Lashin, Spectrum of one-dimensional anharmonic oscillators, *Canad. J. Phys.* 83 (2005) 541–550; arXiv:quant-ph/0305128.

[16] P. Kościk and A. Okopińska, Application of the Frobenius method to the Schrödinger equation for a spherically symmetric potential: an anharmonic oscillator, *J. Phys. A* 38 (2005) 7743–7755; MR2169486 (2006j:81051).

[17] A. J. Zakrzewski, Highly precise solutions of the one-dimensional Schrödinger equation with an arbitrary potential, *Comput. Phys. Comm.* 175 (2006) 397–403; MR2260324 (2007d:81056).

[18] F. Vinette and J. Čížek, Upper and lower bounds of the ground state energy of anharmonic oscillators using renormalized inner projection, *J. Math. Phys.* 32 (1991) 3392–3404; MR1137393 (93m:81024).

[19] E. J. Weniger, J. Čížek, and F. Vinette, The summation of the ordinary and renormalized perturbation series for the ground state energy of the quartic, sextic, and octic anharmonic oscillators using nonlinear sequence transformations, *J. Math. Phys.* 34 (1993) 571–609; MR1201021 (93j:81018).

[20] S. R. Finch, Airy function zeroes, unpublished note (2004).