Distributional Quantum Mechanics

Michael Maroun

Institute for Pure and Applied Mathematics
@ the University of California, Los Angeles

Entropy Inequalities, Quantum Information, and Quantum Physics

marounm@gmail.com
visit arXiv:2101.07876

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Introduction

The system of interest is the ill-posed expression

$$H\psi(x) = \left[-\frac{h^2}{2m}\nabla^2 - \alpha\,\delta(x)\right]\psi(x) = E\,\psi(x)$$

In one dimension, this system is trivial, and yields a single energy eigenvalue. For the trivial one dimensional system all of the following methods work and produce the same bound state energy

- Integrating the 1d equation over an epsilon ball centered at the point support (the origin)
- Calculating the average of the pseudo-operator H in the state ψ iff the distributional 2$^{\text{nd}}$ derivative is used
- Calculating the spatial Green Function for the resolvent operator via the Fourier Transform and finding its pole

This is possible in 1d since the fundamental solution to the Helmholtz equation is continuous on all of $\mathbb{R}$. Note that the odd solution is "invisible" to the potential.

Motivation $(\mathrm{H}\Psi) \in \mathcal{D}'(\mathbb{R}^{\mathrm{d}})$ I of II

Definition 1.1 (Locally Square Integrable Functions v1)

Let $T : \mathbb{R}^d \to \mathbb{C}$, then one says $T \in L^2_{\mathsf{loc}}(\mathbb{R}^d)$ if it is the case that

$$\int_{x \in K \subset \mathbb{R}^d} |T|^2 \, \mathsf{d}x < \infty \qquad \forall \, K \subset \mathbb{R}^d.$$

Definition 1.2 (Locally Square Integrable Functions v2)

$$L^2_{\mathsf{loc}}(\mathbb{R}^d) := \left\{ \, T \in \mathcal{D}'(\mathbb{R}^d) \; : \forall \, \varphi \in \mathcal{D}(\mathbb{R}^d), \text{ one has } \; (\varphi \, T) \in L^2(\mathbb{R}^d) \, \right\}$$

Lemma 1.3 (Bourbaki-Strichartz Equivalence)

Definition 1.1 $\iff$ *Definition 1.2*

Motivation $(\mathrm{H}\Psi) \in \mathcal{D}'(\mathbb{R}^{\mathrm{d}})$ II of II

Some key features to keep in mind.

1. There is no obvious way to extended the Max Born probability interpretation into the Gelfand triple. In fact, this search has led to, and uncovered powerful and beautiful mathematics of the theory of Bergman, Segal-Bargmann and Hardy spaces, which give rise to weights and reproducing kernels on such Hilbert spaces.
2. Nonetheless, no single version of these spaces is versatile enough to capture the full phenomena of the rich possibilities of multi-particle scattering and quantum field theory.
3. One specific trouble is trying to identify the proper weight to attach to the scattering solutions of the Schrodinger equation. For a fixed potential a suitable weight can be found but there is no known universal connection between all the possible physically interesting interactions, nor a notion of “correct” weight on a Hilbert space.
4. While the L^2_{loc} approach works well for scattering theory, it cannot accommodate highly singular potentials. See poster for two key types of singular potentials.

A Generalization of Quantum Theory

Definition 1.4 (The C-Spectrum)

When $\langle H\psi, \varphi\rangle = E\langle\psi, \varphi\rangle \ \forall\, \varphi \in \mathcal{D}(\mathbb{R}^d)$, with $(H\psi) \in \mathcal{D}'(\mathbb{R}^d)$ then E is said to be in the **C-Spectrum**. Note, it may not be valid for all φ, or it may require distributional identities be substituted.

Definition 1.5 (Proxy Test Functions)

If, $\langle H\psi, \psi\rangle = E$ for $L^2(\mathbb{R}^d) \ni \psi \notin \mathcal{D}(\mathbb{R}^d)$ then ψ is said to be a **proxy test function**. In addition, it may also be the case that $\psi \notin L^2(\mathbb{R}^d)$ but that it is a distribution itself. While $(V\psi) \in \mathcal{D}'(\mathbb{R}^d)$, the definitions hold.

Lemma 1.6 (Test Sequence Convergence)

Finally, every proxy test function $L^2(\mathbb{R}^d) \ni \psi \notin \mathcal{D}(\mathbb{R}^d)$ *is necessarily given by some sequence* $\varphi_n \in \mathcal{D}(\mathbb{R}^d) \ \forall\, n \in \mathbb{N}$ *such that* $\varphi_n \xrightarrow{n\to\infty} \psi$.

The Breaking of Unitarity I of II

Definition 1.7 (Regular Distribution)

A distribution $T \in \mathcal{D}'(\mathbb{R}^d)$ is said to be **regular** if $\exists\ f : \mathbb{R}^d \to \mathbb{R}$ s.t.

$$\int_{x \in \mathbb{R}^d} f(x)\varphi(x)\mathrm{d}\mu(x) \ \ \forall\ \varphi \in \mathcal{D}(\mathbb{R}^d)$$

where $\mathrm{d}\mu(x)$ is Lebesgue measure. Otherwise, the distribution is **singular**.

Definition 1.8 (Singular Function)

An $f : \mathbb{R}^d \to \mathbb{R}$ is said to be **singular** if $f \notin L^p(\mathbb{R}^d)$ for any $1 \leq p \leq \infty$.

Remark 1.1 (Non-Self-Adjoint Hamiltonians)

Inter-atomic/molecular potentials are known empirically to be described by inverse positive powers of the Euclidean norm. Such potentials are all singular functions in the above sense. E.g. VdW, Buck, L-J, B-L, LDF.

The Breaking of Unitarity II of II

Remark 1.2 (An Arrow of Time)

Unitary operators are **only** *generated from self-adjoint operators. With singular potentials, the Hamiltonian fails to be self-adjoint. There is often a family of self-adjoint extensions, which can be parametrized by an index whose index set has cardinality of the continuum.*

Proposition 1.1 (The Origin of Randomness)

Let $\theta \in \mathbb{R}$ be the index parametrizing the family of all possible self-adjoint extensions of a Hamiltonian with singular potential, $H(\theta)$. With no preference for a given extension over another, there then exists an a priori uniform distribution from which the random variable θ is sampled. Then, one has

$$U_t(\theta) = e^{-\frac{i}{\hbar} t\, H(\theta)}.$$

Note in general $\mathrm{E}[\mathbf{U_t}(\theta)] \neq \mathbf{U_t}(\mathrm{E}[\theta])$. Finally, $\mathrm{E}[\mathbf{U_t}(\theta)] = \bar{\mathbf{U}}(\mathbf{t})$ need not be invertible for $t \neq 0$.

Thank You for Your Attention!

For the C-spectrum in $\mathbb{R}^3$, see arXiv:2101.07876

Stay tuned for the solution to the delta prime pseudo-potential to appear on the arxiv soon.

marounm@gmail.com

References I of II

[AGHH] Albeverio, S., Gesztesy, F., Hoegh-Krohn, R. and Holden, H., *Solvable Models in Quantum Mechanics*, 2^{nd} ed. AMS Chelsea Publishing, Providence, 2005.

[AlKu] Albeverio, S., Kurasov, P., *Singular Perturbations of Differential Operators*, London Mathematical Society: Lecture Series, **271**, 2000.

[AlG] Al-Gwaiz, M. A., *Theory of Distributions*. Chapman & Hall/CRC Press/Marcel Dekker, New York, 1992.

[Boh] Bohm, A., *Quantum Mechanics: Foundations and Applications*. Springer, New York, 1993.

[ChSh] Cheon, T. and Shigehara, T., "Realizing discontinuous wave functions with renormalized short-range potentials", *Phys. Lett. A.* 243 (1998), 111-116.

[DyZw] Dyatlov, S. and Zworski, M., *Mathematical Theory of Scattering Resonances*. American Mathematical Society, Providence, 2010.

[FrJo] Friedlander, F. G. and Joshi, M., *Introduction to the Theory of Distributions*. Cambridge University Press, Cambridge, 1999.

[Fri] Friedman, C.N., "Perturbations of the Schrodinger equation by potentials with small support". *J. Funct. Anal.* 10(1972), 346-360.

References II of II

[KuBo] Kurasov, P. and Boman, J. (comm. Jorgensen, P.), "Finite rank singular perturbations and distributions with discontinuous test functions", *Proc. Am. Soc.* 126 (1998) 1673-1683.

[JoLa] Johnson, G. W. and Lapidus, M. L., *The Feynman Integral and Feynman's Operational Calculus*. Oxford U. Press, New York, 2000.

[Mar] Maroun, M., *Generalized Quantum Theory and Mathematical Foundations of Quantum Field Theory*. Ph.D. Dissertation, University of California, Riverside, Riverside, CA, 2013.

[Mau] Maurin, K., *General Eigenfunction Expansions and Unitary Representations of Topological Groups*. Polish Scientific Publishers, Warsaw, 1968.

[PeZe] Perelomov, A. M. and Zel'dovich, Y. B., *Quantum Mechanics: Selected Topics*. World Scientific, Singapore, 1998.

[ReSi] Reed, M. and Simon, B., *Methods of Modern Mathematical Physics*. Vol. I, *Functional Analysis*. Academic Press, New York, 1980.

[Rud] Rudin, W., *Functional Analysis*. McGraw-Hill, New York, 1991.

[Str] Strichartz, R., *A Guide to Distribution Theory and Fourier Transforms*, 2^{nd}ed. World Scientific, Singapore, 2003.