Distributional Quantum Mechanics

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Abstract

The mathematics of quantum theory is not always as straightforward as it seems. The Dirac delta "function" as a potential in the Schrodinger equation in one dimension is considered a very elementary problem and models the ground states of many real life quantum systems. But the Dirac delta function is not a function at all, and it turns out that trying to "solve" the Schrodinger equation for the same potential in two and three dimensions is extremely difficult. There is also the derivative of the Dirac delta potential in one dimension, which models infinitesimal dipoles extremely well in classical Maxwell theory. It too is an extremely challenging model to solve for a bound state energy.

This poster shows how to deal with such mathematical challenges by proposing a slight generalization in standard quantum theory that accounts for distributional potentials. As a bonus, the modified theory puts bound states and scattering states on equal footing. It can also make precise the mathematical foundations of quantum statistical mechanics, where the breaking of self-adjointness leads to the breaking of the unitary time evolution.

Remark: Scattering Theory

In the theory of scattering, the scattering states are not elements of $L^2(\mathbb{R}^d)$, and the S-matrix (scattering matrix) always contains a Dirac delta distribution as required by momentum conservation.

Definition 1.1 (*Singular Distribution*)

A distribution $T \in \mathcal{D}'(\mathbb{R}^d)$ is said to be **singular** if it is not regular.

Definition 1.2 (*Regular Distribution*)

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

$$\int\limits_{x\in\mathbb{R}^d} f(x)\varphi(x)\mathrm{d}\mu(x) \quad \forall\, \varphi \in \mathcal{D}(\mathbb{R}^d)$$

where $\mathrm{d}\mu(x)$ is Lebesgue measure.

Definition 1.3 (*Singular Function*)

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

Definition 1.4 (Locally Square Integrable Functions v1)

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

$$\int\limits_{x\in K\subset\mathbb{R}^d} |T|^2\,\mathrm{d}x < \infty \quad \forall\, K \subset \mathbb{R}^d. \tag{1}$$

Definition 1.5 (Locally Square Integrable Functions v2)

$$L^2_{\text{loc}}(\mathbb{R}^d) := \left\{ T \in \mathcal{D}'(\mathbb{R}^d) \ : \ (T\varphi) \in L^2(\mathbb{R}^d) \right\} \tag{2}$$

Lemma 1.6 (Bourbaki-Strichartz Equivalence)

Definition 1.4 $\Longleftrightarrow$ **Definition 1.5**

Proof of Lemma 1.6 (Bourbaki-Strichartz Equivalence)

Clearly,

$$\|\varphi\|_\infty \int\limits_{x\in K} |T|^2\,\mathrm{d}x \geq \int\limits_{x\in K} |\varphi|^2|T|^2\,\mathrm{d}x = \int\limits_{x\in U} |\varphi T|^2\,\mathrm{d}x$$

Let $d := d(K, \partial U) > 0$, where the notation $t := d(\mathbb{A}, \partial\mathbb{B})$ stands for the family of metric distances between points in the set $\mathbb{A}$ and points on the boundary of the set $\mathbb{B}$, denoted $\partial\mathbb{B}$. Also, let ε be such that $d > 2\varepsilon > 0$. Now consider the compact sets K_ε and $K_{2\varepsilon}$ as closed $(\varepsilon, 2\varepsilon)$-neighborhoods of K. One has the set inclusion $K \subset K_\varepsilon \subset K_{2\varepsilon} \subset U$ with $d_{K_\varepsilon} - \varepsilon > \varepsilon > 0$. Define a mollifier, φ_ε, and take χ_{K_ε} as the characteristic function supported on the compact set K_ε. The convolution $\chi_{K_\varepsilon^*}\varphi_\varepsilon =: \varphi_K$ together with its inequalities lead to $|\varphi_K|^2 \geq |\chi_K|^2$. Hence, one sees

$$\infty > \int\limits_{x\in U} |T|^2|\varphi_K|^2\,\mathrm{d}x \geq \int\limits_{x\in U} |T|^2|\chi_K|^2\,\mathrm{d}x = \int\limits_{x\in K} |T|^2\,\mathrm{d}x.$$

Remark: Master Equations and the Origin of Randomness

Given the definitions of singular potentials, both for distributions and singular functions, there is an overarching trend. The trend is that such Hamiltonian expressions, even once well defined, do not give rise to self-adjoint operators. When the operators exist, there is a continuum of possible self-adjoint extensions. Such a circumstance arises for example when there is a real valued but singular potential that can define a symmetric operator but the would-be domain fails to be a single closed dense subset of the Hilbert space.

One can then promote the continuous parameter indexing all the possible self-adjoint extensions to a random variable with an a priori uniform distribution reflecting that no one extension is preferred over another. There is then a family of Hamiltonians parametrized by a random variable. Invoking the usual measure theoretic principles gives rise to a family of time-evolution operators also parametrized by a random variable. This is a natural method of inducing the random phase condition required to justify the Pauli Master equation.

Remark: The Ill-posed Hamiltonian

Consider the bound state problem for a Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\Delta - \alpha\delta(x)$$

with $\alpha \in \mathbb{R}\backslash\{0\}, x \in \mathbb{R}^d$, and where the notation $\delta(x)$ stands for the linear functional $\delta(\varphi) = \varphi(0) \ \ \forall\, \varphi \in \mathcal{D}(\mathbb{R}^d)$.

The Hamiltonian Juxtaposed with the $L^2(\mathbb{R}^d)$ Fundamental Solution of the Helmholtz Equation

The summed expression above makes no sense! Instead one can consider $(H\psi) \in \mathcal{D}'(\mathbb{R}^d)$ in the following way.

$$\langle H\psi,\, \varphi\rangle = E\langle\psi,\, \varphi\rangle$$

Proposition 1.7 ($(H\psi) \in \mathcal{D}'(\mathbb{R}^d)$

Thus one must verify that$(H\psi) \in \mathcal{D}'(\mathbb{R}^d)$, where H is given below with $x \in \mathbb{R}^d$, $\hbar$, $m > 0$, and $\alpha \in \mathbb{R}\backslash\{0\}$.

$$H = -\frac{\hbar^2}{2m}\Delta - \alpha\delta(x)$$

Proof of Proposition 1.7

Let $-\Delta$ be the distributional Laplace operator, then $\Delta\psi \in \mathcal{D}'(\mathbb{R}^d)$. Since ψ is the fundamental solution to the Helmholtz equation, one has that $-\Delta\psi + b^2\psi = \delta$, where δ is again the Dirac distribution in $\mathcal{D}'(\mathbb{R}^d)$, and $b \in \mathbb{R}$. Thus, it implies that

$$-\Delta\psi = \delta - b^2\psi.$$

Now both, δ, and ψ (trivially so) are in $\mathcal{D}'(\mathbb{R}^d)$, it follows that so is the sum. The only remaining piece (and the most dubious) is to check that $V\psi \in \mathcal{D}'(\mathbb{R}^d)$. In this case, $V = \delta$,and so $\psi(x)\delta(x) \doteq \psi(0)\delta(x)$, which of course $\psi(0)\delta(x) \in \mathcal{D}'(\mathbb{R}^d)$. This means that whenever $\psi(0)$ is defined as a finite value $\psi \in \mathbb{C}$, then the distributional inclusion is justified. This condition is sufficient but it turns out it is not necessary. In the case $d = 3$, $\psi(0)$ is divergent but the theory is well-defined. See arXiv:2101.07876.

Definition 1.8 (C-Spectrum)

Let $\langle\cdot,\,\cdot\rangle$ denote the Schwartz bracket linear functional that pairs a test function $\varphi \in \mathcal{D}(\mathbb{R}^d)$ with a distribution $T \in \mathcal{D}'(\mathbb{R}^d)$ as,

$$\langle T,\, \varphi\rangle = T(\varphi) \in \mathbb{R} \subseteq \mathbb{C}.$$

Then whenever $\langle H\psi,\, \varphi\rangle = E\langle\psi,\, \varphi\rangle$, E is said to be in the distributionally generalized spectrum called the **C-spectrum**.

Definition 1.9 (Proxy Test Functions)

Proxy test functions are exactly all the elements of the operator domain (when it exists) being the closed dense subset $D(H) \subset L^2(\mathbb{R}^d)$ that make the usual notion of eigenvalue (elements of the pure point spectrum) correct with the Hilbert inner product replacing the Schwartz bracket in Definition 1.8 above. In addition, they include the set of generalized eigenvalues which are not elements of the Hilbert space, $L^2(\mathbb{R}^d)$. Therefore also, the *C-spectrum* can contain more than just the pure point spectrum.

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