Rigged Hilbert Spaces

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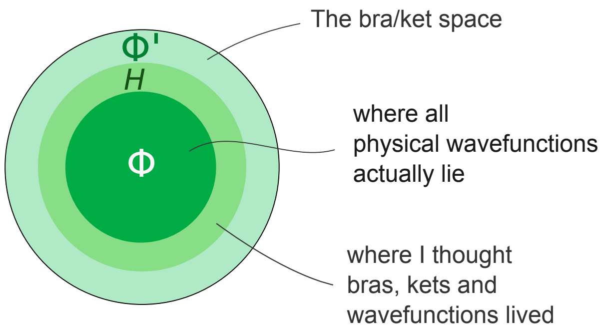

This report accompanies the seminar given by me on 25th November 2009 on the topic of Rigged Hilbert spaces and is based on [7]. Standard quantum mechanics involves Hilbert spaces which are not sufficient to describe operators which are unbounded and have continuous spectra. It is shown in this report that we need to augment the Hilbert space structure with a pair of spaces to give a rigorous description of the Dirac bra-ket formalism.

Introduction

Two of the most important required mathematical structures in quantum mechanics are linearity and scalar product. Linearity is needed to superpose two wavefunctions or eigenkets as may be the case. Since wavefunctions or eigenkets are not physically observable, we define a scalar product which is actually the physically observable probability amplitude.

This naturally gives rise to the structure of linear vector spaces and thus to the Hilbert space which is just a vector space completed with respect to the norm topology. A Hilbert space is an extension of the vector space structure; in addition to linear combinations of finitely many basis vectors, it also contains the limit points (it is closed) in the way that if a vector is expressible in the form $v = \sum c_n|\phi_n\rangle$ then v belongs to the Hilbert space iff $\sum |c_n|^2 < \infty$.

While Hilbert spaces are perfectly fine for describing quantum mechanics in finite dimensions, they fail to do so for operators with continuous spectra. The absence of a rigorous mathematical foundation to the bra-ket formalism was recognised by both Dirac and von Neumann. Dirac's delta function, which was later put on a firm mathematical footing by Schwartz [5] kicked off a new branch of functional analysis: the theory of distributions. Later, Israel Gelfand introduced the rigged Hilbert space formalism by combining the Hilbert space with the theory of distributions [3]. Essentially the "rigged" Hilbert space is the Hilbert space equipped with the theory of distributions; a triad of spaces $\Phi \subset \mathcal{H} \subset \Phi^\times$, with the smaller subspace Φ denoting the space of physical states (on the following page) and the larger space $\Phi^\times$ denoting the space of eigenkets.

There has been a slow acceptance of RHS as the proper mathematical foundation for quantum mechanics and it has started appearing in some textbooks recently [6]. It is important to note that "rigged" in this context means fully equipped (like a rigged ship) and not to any unscientific deed like fixing a result.

Finite dimensions

Life is simpler in finite dimensions. Suppose that the physical states of the system are denoted by vectors (known as kets and represented as $|a\rangle$). These belong to the Hilbert space V. Bras (which look like $\langle b|$) are defined as **linear functionals** over kets. A functional here is a map from a linear vector space V to the set of complex numbers $\mathbb{C}$ formally defined as $F : V \to \mathbb{C}$. For $\varphi, \psi \in V$, a linear functional is one for which $F(a\varphi + b\psi) = aF(\varphi) + bF(\psi)$ and an antilinear functional is one where $F(a\varphi + b\psi) = a^*F(\varphi) + b^*F(\psi)$.

There is a one-to-one correspondence between linear functionals F in V' and vectors f in V when V is finite dimensional, such that all linear functionals have the form $F(\phi) = (f, \phi)$ where f is a fixed vector and ϕ an arbitrary vector (Riesz theorem, proof in appendix). Thus every ket has a corresponding bra and vice-versa. To simplify notation, the same character is used to signify a ket and its corresponding bra. If the ket is denoted by $|a\rangle$ then the corresponding bra is $\langle a|$.

Consider a finite (N) dimensional problem. We consider the eigenkets of a particular operator which span the corresponding the Hilbert space. Then an arbitrary eigenket $|\psi\rangle$ can be expanded in terms of the basis kets:

$$|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + \cdots + c_N|\phi_N\rangle$$

In the finite dimensional case, we can represent any operator A as an $N \times N$ matrix acting on the N-dimensional Hilbert space, where the matrix representation of the operator is $A_{ij} = \langle e_i|A|e_j\rangle$ where $|e_i\rangle$ are the eigenkets of the observable A. The operators corresponding to physical operators are self-adjoint ($A = A^\dagger$) and the spectral theorem for the finite dimensional case guarantees the existence of an orthonormal basis of the Hilbert space containing the eigenvectors (eigenkets) of A. As there are finitely many discrete states, an operator's action on an arbitrary vector (which can be represented as a column vector) remains within the space.

However, the Hilbert space formulation is insufficient for describing wavefunctions and bra-kets of unbounded operators with continuous spectra. We call an operator A **bounded** if there is some finite K such that $\|Af\| < K\|f\|$ for all $f \in \mathcal{H}$, where $\|\ \|$ denotes the norm defined for the Hilbert space $\mathcal{H}$. For one-dimensional problems, the Hilbert space norm is usually defined using the scalar product

$$(f, g) \equiv \int_{-\infty}^{\infty} f^*(x)g(x)dx \qquad \text{(in 1D)}$$

$$||f|| \equiv \sqrt{(f, f)} = \sqrt{\int_{-\infty}^{\infty} |f(x)|^2 dx}$$

Rigged Hilbert Space

Why we need it

In this section, I shall consider some examples in one dimension which shall simplify calculations. The main reason why we need the rigged Hilbert space formalism is because of the unstable action of operators on the Hilbert space. In 1D the Hilbert space is the space of all square-integrable functions L^2

$$L^2 = \left\{ f(x) : \int_{-\infty}^{\infty} |f(x)|^2 dx < \infty \right\}$$

Now consider the position operator which in the x-representation can be written as

$$Q|x\rangle = x|x\rangle$$

$\mathcal{D}(Q)$ is the domain of Q. Thus $\mathcal{D}(Q)$ contains all the functions

$$\mathcal{D}(Q) = \left\{ f(x) \in L^2 : \int_{-\infty}^{\infty} |xf(x)|^2 dx < \infty \right\}$$

We can easily see that the function $f(x) = 1/(x+i)$ belongs to L^2 but is not in $\mathcal{D}(Q)$. Another problem is the non-invariance of domains of unbounded operators as $Q\mathcal{D}(Q) \nsubseteq \mathcal{D}(Q)$ which we can see by taking the function $h(x) = \frac{1}{x^2+1}$. This causes much trouble in the Hilbert space framework, for example in calculating $(\phi, Q\phi)$ (expectation values) or $\sqrt{(\phi, Q^2\phi) - (\phi, Q\phi)^2}$ (uncertainties).

If we now consider the momentum operator in x-representation given by $Pf(x) = -i\hbar\frac{d}{dx}f(x)$, then PQ defined for the functions in L^2 for which

$$PQf(x) = -i\hbar\frac{d}{dx}xf(x) = -i\hbar(f(x) + xf'(x))$$

is defined and in L^2. Thus we have to take functions f where f is differentiable and f, f' and xf' are in L^2. Even then we run into the same problems as above, viz. the non-invariance of domain of the operator PQ.

The space of physical states

Thus we seek a subspace Φ of $\mathcal{H}$ on which physical quantities like expection values and uncertainties are well-defined. The domains of the relevant operators (say Q, P, H) must be *invariant* under the action of these operators. A natural choice is to take the intersection of all domains of arbitrary powers of the operators

$$\Phi = \bigcap_{n,m,l=0}^{\infty} \mathcal{D}(P^n Q^m H^l)$$

This is the maximal invariant subspace of the Hilbert space under the actions of the operators P, Q and H. Thus $A\Phi \subset \Phi \quad (A = Q, P, H)$. Then we can construct the dual space $\Phi^\times$ (space of antilinear functionals over a vector space) of Φ. There is also an antidual space corresponding to Φ, the linear functionals correspond to bras in the Dirac bra-ket notation and the antilinear functionals correspond to kets.

In general, *smaller a space the larger is the dual space*. For example, for the free particle Hamiltonian (the factor of 1 is present to ensure that the condition goes to the L^2 condition as $|x| \to 0$)

$$\Phi = \{\phi : \int_{-\infty}^{\infty} dx|\phi(x)|^2(1+|x|)^m < \infty\}$$

Φ contains all the functions which decay faster than any arbitrary power of x. Therefore the dual space $\Phi^\times$ can contain functions which have divergent norm as long as they do not diverge faster than any arbitrary power of x. Thus $\mathcal{H}^\times \subset \Phi^\times$. Riesz representation theorem for infinite dimensional Hilbert spaces states that $\mathcal{H} = \mathcal{H}^\times$ (proof in appendix). Thus we get the Gelfand triple

$$\Phi \subset \mathcal{H} \subset \Phi^\times$$

We can now think of $\langle\varphi|f\rangle$ in two ways [2]: f as a functional (corresponding function in $\Phi^\times$) acting on the function $\varphi \in \Phi$. $\langle\varphi|f\rangle = f(\varphi)$, or φ as a functional belonging to the dual space of $\Phi^\times$ ($\Phi^{\times\times}$) which acts on the functional f belonging to $\Phi^\times$ to give the same answer $f(\varphi)$ using the bijective relation between Φ and $\Phi^{\times\times}$ which is given by

$$G(f) = f(g) \quad \text{where we identify } g \leftrightarrow G$$

Technicalities

Operators act on the smaller space (Φ). When we write an eigenket equation like $A|\varphi\rangle = a|\varphi\rangle$, then we *can not* use the same definition. Therefore, we must extend A to $A^\times$ to be defined over the larger space $\Phi^\times$ in which the eigenfunctions live.

$$A : \Phi \to \Phi$$

$$A^\times : \Phi^\times \to \Phi^\times$$

$$\langle\phi|A^\times|F\rangle = \langle A\phi|F\rangle$$

The functional F over Φ is called the *generalised eigenvector* of A on Φ with eigenvalue ω iff

$$\langle A\phi|F\rangle = \omega\langle\phi|F\rangle \quad \forall\, \phi \in \Phi$$

The generalised eigenvector with eigenvalue ω is denoted by $|\omega\rangle$

If $F \leftrightarrow f \in \mathcal{H}$ then $\langle A\phi|F\rangle = \omega\langle\phi|F\rangle$ becomes

$$(A\phi, f) = (\phi, A^\dagger) = \omega(\phi, f) \quad \forall\, \phi \in \Phi$$

when A is self-adjoint, then this just becomes the standard eigenvector equation $Af = \omega f$. The existence of the generalised eigenvector corresponding to an element in the continuous spectrum of A is guaranteed by the nuclear spectral theorem.

A practical use

Up till now we have been considering the RHS as an abstract, though necessary formulation required to put the Dirac bra-ket formalism on a firmer mathematical ground. However as we shall see now we can get some non-trivial insights out of a simple problem [6], which we wouldn't have got in the Hilbert space formalism. We consider the 1D free particle Hamiltonian

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi$$

The eigenfunctions are e^{ikx}, eigenvalues $\frac{\hbar^2 k^2}{2m}$.

The Φ subspace is defined as

$$\Phi = \{\phi : \int |\phi(x)|^2(1+|x|)^n dx < \infty\} \quad n = 0, 1, 2, \ldots$$

Here $|x|$ comes from the position operator. The extra term of 1 comes to make the integral approach the condition for $\phi \in \mathcal{H}$, i.e. the square integrability condition in the limit of large n.

A complex value of k is allowed by mathematics but ruled out by physics (as we must have $E > 0$). In the RHS only real k is allowed. The reasoning is thus: The conjugate space $\Phi^\times$ has functions which can be divergent but not faster than any arbitrary power of x. When k is complex then there is an exponential divergence at $\pm\infty$ which means e^{ikx} won't be in $\Phi^\times$. Thus in the RHS formalism there is no need to impose the extra physical condition of $E > 0$; the energy eigenfunctions having real, positive eigenvalues are automatically selected by the RHS formalism.

Conclusion

The RHS assigns a proper place for eigenfunctions and physical states. It also provides a stricter description of quantum mechanics, disallowing states which earlier had to be ruled out on physical grounds. A disadvantage is that it introduces spaces Φ and $\Phi^\times$ which are problem dependent. Earlier for example, for any one dimensional problem we could use L^2 as the Hilbert space.

It can be used to formulate *microscopic* irreversibility (not arising due to environmental interactions) and also gives a more rigorous description of scattering theory which cannot be done under the Hilbert space formulation [1][8]

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Appendix

Theorem 1. *[Riesz] [6]There is a one-to-one correspondence between linear functionals F in V' and vectors f in V when dim V is finite, such that all linear functionals have the form*

$$F(\phi) = (f, \phi)$$

where f is a fixed vector and ϕ an arbitrary vector.

Proof. It is obvious that any $f \in V$ defines a linear functional. We need to show that for an arbitrary linear functional F we can construct a fixed f. Let $\{\phi_n\}$ be a system of orthonormal basis vectors in V. $\Psi = \sum_n x_n \phi_n$ is an arbitrary vector in V.

Then the action of F on ψ is given as

$$F(\psi) = \sum_n x_n F(\phi_n)$$

We can then construct the vector f as $f = \sum_n [F(\phi_n)]^* \phi_n$. Taking the scalar product with ψ, we get $F(\psi)$.

$$(f, \psi) = \sum_n F(\psi_n) x_n$$

□

Theorem 2. *[Riesz representation theorem][4] If $f \in \mathcal{H}^\times$, then there is an unique $y \in \mathcal{H}$ where $\mathcal{H}$ is a Hilbert space such that $f(x) = (x, y) \quad \forall x \in \mathcal{H}$ with $\|f\| = \|y\|$.*

Proof. Case (i) Let Ker$(f) = \mathcal{H}$. Then $f = 0$. Take $y = 0$. We have trivially $\|f\| = \|y\|$.

Case (ii) Let Ker$(f) \neq \mathcal{H}$. Then by the Projection Theorem there exists a nonzero element $z \in \mathcal{H}$ such that $z \perp$ Ker(f). Consider

$$M = \{zf(x) - xf(z) : x \in \mathcal{H}\}$$

Since $f(z)f(x) - f(x)f(z) = 0$ it follows that $M \subset$ Ker(f). Also $z \perp M$ gives $(zf(x) - xf(z), z) = 0 \quad \forall x \in \mathcal{H}$ .This implies $f(x)\|z\|^2 = (x, z)f(z)$ whence

$$f(x) = (x, y) \, \forall \, x \in \mathcal{H}, \text{ where } y = \frac{z\bar{f}(z)}{\|z\|^2}$$

y is unique. If not, suppose $(x, y) = (x, y') \, \forall \, x \in \mathcal{H}$, then $(x, y - y') = 0$ and so $(y - y', y - y') = 0$. So $y - y' = 0$, that is $y = y'$.

Finally, note that $f(y) = \|y\|^2$ and so $\|y\|^2 \leq |f(y)| \leq \|f\|\|y\|$ whence $\|y\| \leq \|f\|$. On the other hand $|f(x)| = |(x, y)| \leq \|x\|\|y\|$ and so

$$\|f\| = \sup_{\|x\| \leq 1} |f(x)| \leq \|y\|$$

Hence $\|f\| = \|y\|$. □