Dirac's bra-ket formalism and the rigged Hilbert space

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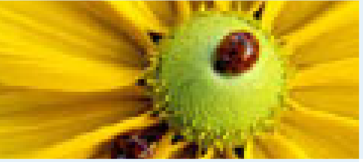


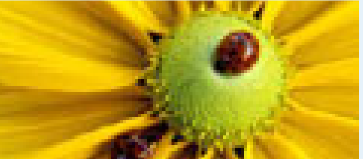
Overview

Little History

Example

Conclusions

A brief History of the rigged Hilbert space



Dirac's bra-ket formalism

- Left and a right eigenvectors:

$$A|a_n\rangle = a_n|a_n\rangle\,; \qquad A|a\rangle = a|a\rangle \tag{1}$$

$$\langle a_n|A = a_n\langle a_n|\,; \qquad \langle a|A = a\langle a| \tag{2}$$

- Completeness relations:

$$I = \sum_n |a_n\rangle\langle a_n| + \int da\,|a\rangle\langle a| \tag{3}$$

$$\varphi = \sum_n |a_n\rangle\langle a_n|\varphi\rangle + \int da\,|a\rangle\langle a|\varphi\rangle \tag{4}$$

- Normalization

$$\langle a_n|a_m\rangle = \delta_{nm}\,; \qquad \langle a|a'\rangle = \delta(a-a') \tag{5}$$

- Algebraic operations, e.g., commutation relations,

$$[A,B] = AB - BA \tag{6}$$

Hilbert space implementation

- **Von Neumann**

  1. “*Dirac has given a representation of quantum mechanics which is scarcely to be surpassed in brevity and elegance,* [...].”
  2. “*The method of Dirac, mentioned above, (and this is overlooked today in a great part of quantum mechanical literature, because of the clarity and elegance of the theory) in no way satisfies the requirements of mathematical rigor – not even if these are reduced in a natural and proper fashion to the extent common elsewhere in theoretical physics.*”
  3. “[...],*this requires the introduction of ‘improper’ functions with self-contradictory properties. The insertion of such mathematical ‘fiction’ is frequently necessary in Dirac’s approach,*[...].”

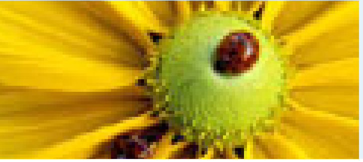
  [J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton (1955)]

- **Dirac**: “*the bra and ket vectors that we now use form a more general space than a Hilbert space.*”

  [P.A.M. Dirac, *The principles of Quantum Mechanics*, 3rd ed., Clarendon Press, Oxford (1947)]

Implementation in the rigged Hilbert space

- Schwartz
- Gelfand and his school 1950s
- Maurin
- Roberts, Bohm, Antoine 1960s
- Shortcomings: No systematic procedure to construct RHSs



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- A.Z. Capri, *Nonrelativistic Quantum Mechanics*, Benjamin (1985).
- D.A. Dubin, M.A. Hennings, *Quantum Mechanics, Algebras and Distributions*, Longman (1990).
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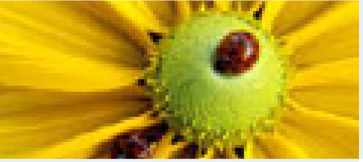
- "*...rigged Hilbert space seems to be a more natural mathematical setting for quantum mechanics than Hilbert space*"

[L.E. Ballentine, *Quantum Mechanics* (1990), page 19]

Construction of the rigged Hilbert space



Steps to construct the rigged Hilbert space

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$$\Phi \subset \mathcal{H} \subset \Phi' \tag{7}$$

and

$$\Phi \subset \mathcal{H} \subset \Phi^{\times} \tag{8}$$

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Steps

Step 1

Steps 2 and 3

Step 3

Step 4

Step 5

Kets

Bras

Eigenequations

Further

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- Illustrative example: 1D rectangular barrier potential

Step 1: Identify the observables

- Position, momentum and energy

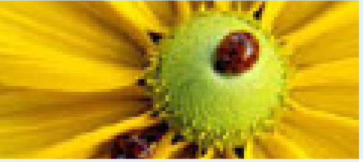
$$Qf(x) = xf(x) \tag{9}$$

$$Pf(x) = -i\hbar \frac{d}{dx} f(x) \tag{10}$$

$$Hf(x) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) f(x) \tag{11}$$

where

$$V(x) = \begin{cases} 0 & -\infty < x < a \\ V_0 & a < x < b \\ 0 & b < x < \infty \end{cases} \tag{12}$$



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- The observables satisfy

$$[Q,P] = i\hbar I\,; \quad [H,Q] = -i\frac{\hbar}{m}P\,; \quad [H,P] = i\hbar\frac{\partial V}{\partial x} \tag{13}$$

Steps 2 and 3: Hilbert space and domains

- The Hilbert space is

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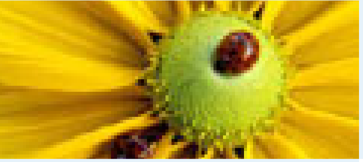

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- The domains of the observables are

$$\mathcal{D}(Q) = \left\{f \in L^2 \,|\, xf \in L^2\right\} \tag{16}$$

$$\mathcal{D}(P) = \left\{f \in L^2 \,|\, f \in AC,\ Pf \in L^2\right\} \tag{17}$$

$$\mathcal{D}(H) = \left\{f \in L^2 \,|\, f \in AC^2,\ Hf \in L^2\right\} \tag{18}$$

Step 3: spectra and eigenfunctions

- The spectra are continuous

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$$\mathrm{Sp}(Q) = \mathrm{Sp}(P) = (-\infty, \infty)\,; \quad \mathrm{Sp}(H) = [0, \infty) \tag{19}$$

- The eigenfunctions of Q are delta functions,

$$\langle x|x'\rangle = \delta(x - x') \tag{20}$$

- The eigenfunctions of P are plane waves,

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \tag{21}$$

Step 3

- The eigenfunctions of H are

$$\langle x|E^+\rangle_{\mathrm{r}} = \left(\frac{m}{2\pi k\hbar^2}\right)^{1/2} \times \begin{cases} T(k)e^{-ikx} & -\infty < x < a \\ A_{\mathrm{r}}(k)^{i\kappa x} + B_{\mathrm{r}}(k)e^{-i\kappa x} & a < x < b \\ R_{\mathrm{r}}(k)e^{ikx} + e^{-ikx} & b < x < \infty \end{cases} \tag{22}$$

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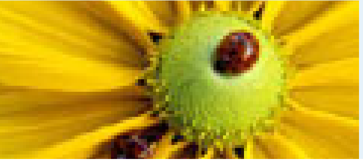
Step 4

- Expectation values must be well defined:

$$(\varphi, A\varphi)\,, \quad \varphi \in \mathcal{D}(A) \text{ only}, \quad A = P, Q, H \tag{24}$$



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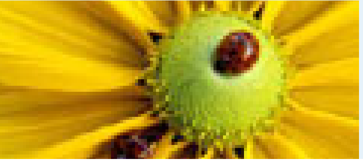
- Algebraic operations such as the commutator of two operators must be well defined:

$$[A, B]\varphi = AB\varphi - BA\varphi\,, \quad \varphi \in \mathcal{D}(AB), \mathcal{D}(BA) \text{ only}, \quad A, B = P, Q, H \tag{26}$$



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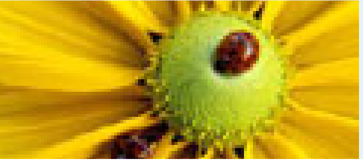
$$\Phi = \bigcap_{\substack{n,m=0 \\ A,B=Q,P,H}}^{\infty} \mathcal{D}(A^n B^m) \qquad (27)$$



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- Schwartz-like space

Step 5

- Dual (Φ') and antidual ($\Phi^\times$) spaces
- We have

$$\Phi \subset \mathcal{H} \subset \Phi^\times \tag{29}$$

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- Antilinear functional

$$F(\varphi) \equiv \int dx\, \overline{\varphi(x)} f(x) \tag{31}$$

$$\langle \varphi | F \rangle = \int dx\, \langle \varphi | x \rangle \langle x | f \rangle \tag{32}$$

- Linear functional

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Kets

- Momentum

$$\langle \varphi | p \rangle \equiv \int_{-\infty}^{\infty} dx\, \overline{\varphi(x)} \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \equiv \int_{-\infty}^{\infty} dx\, \langle \varphi | x \rangle \langle x | p \rangle \qquad (34)$$

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$$\langle \varphi | x \rangle \equiv \int_{-\infty}^{\infty} dx'\, \overline{\varphi(x')} \delta(x - x') \equiv \int_{-\infty}^{\infty} dx'\, \langle \varphi | x' \rangle \langle x' | x \rangle \qquad (35)$$

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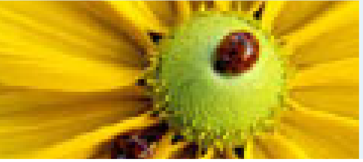
- Energy

$$\langle\varphi|E^+\rangle_{\mathrm{l,r}} \equiv \int_{-\infty}^{\infty} dx\, \overline{\varphi(x)}\langle x|E^+\rangle_{\mathrm{l,r}} \equiv \int_{-\infty}^{\infty} dx\, \langle\varphi|x\rangle\langle x|E^+\rangle_{\mathrm{l,r}} \tag{36}$$



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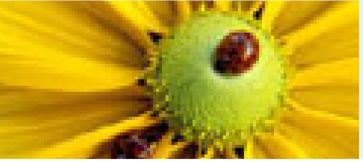
- $|p\rangle$, $|x\rangle$ and $|E^+\rangle_{\mathrm{l,r}}$ belong to $\Phi^\times$



Bras

- Momentum

$$\langle p|\varphi\rangle \equiv \int_{-\infty}^{\infty} dx\, \varphi(x) \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \equiv \int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|\varphi\rangle \tag{37}$$

- Position

$$\langle x|\varphi\rangle \equiv \int_{-\infty}^{\infty} dx'\, \varphi(x')\delta(x-x') \equiv \int_{-\infty}^{\infty} dx'\, \langle x|x'\rangle\langle x'|\varphi\rangle \tag{38}$$

- Energy

$$_{\mathrm{l,r}}\langle {}^{+}E|\varphi\rangle \equiv \int_{-\infty}^{\infty} dx\ \varphi(x)\ {}_{\mathrm{l,r}}\langle {}^{+}E|x\rangle \equiv \int_{-\infty}^{\infty} dx\ {}_{\mathrm{l,r}}\langle {}^{+}E|x\rangle\langle x|\varphi\rangle \tag{39}$$

- $\langle p|$, $\langle x|$ and $_{\mathrm{l,r}}\langle {}^{+}E|$ belong to Φ'

Right and left eigenvectors

- Ket eigenequations

$$P|p\rangle = p|p\rangle \, , \quad p \in \mathbb{R} \tag{40}$$

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$$H|E^+\rangle_{\mathrm{l,r}} = E|E^+\rangle_{\mathrm{l,r}} \, , \quad E \in [0, \infty) \tag{42}$$

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$$\langle x|Q = x\langle x|\,, \quad x \in \mathbb{R} \tag{44}$$

$${}_{\mathrm{l,r}}\langle^+ E|H = E\;{}_{\mathrm{l,r}}\langle^+ E|\,, \quad E \in [0,\infty) \tag{45}$$

Further results

- The bras and kets of an observable give a completeness relation

$$\int_{-\infty}^{\infty} dp \, |p\rangle \langle p| = I \tag{46}$$

$$\int_{-\infty}^{\infty} dx' \, |x'\rangle \langle x'| = I \tag{47}$$

$$\int_{0}^{\infty} dE \, |E^+\rangle_{\mathrm{l}\,\mathrm{l}}\langle^+E| + \int_{0}^{\infty} dE \, |E^+\rangle_{\mathrm{r}\,\mathrm{r}}\langle^+E| = I \tag{48}$$

- Also

$$P = \int_{-\infty}^{\infty} dp \, p|p\rangle \langle p| \tag{49}$$

$$Q = \int_{-\infty}^{\infty} dx \, x|x\rangle \langle x| \tag{50}$$

$$H = \int_{0}^{\infty} dE \, E|E^+\rangle_{\mathrm{l}\,\mathrm{l}}\langle^+E| + \int_{0}^{\infty} dE \, E|E^+\rangle_{\mathrm{r}\,\mathrm{r}}\langle^+E| \tag{51}$$

Further results

- Also

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\, e^{i(p-p')x/\hbar} = \delta(p-p') \tag{52}$$

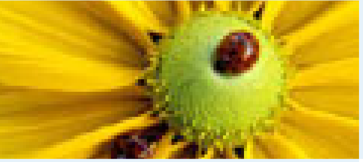
$$\int_{-\infty}^{\infty} dx\ {}_{\alpha}\langle^{\pm}E'|x\rangle\langle x|E^{\pm}\rangle_{\beta} = \delta(E-E')\,\delta_{\alpha\beta} \tag{53}$$

- All these relation hold in the distributional sense, i.e.,

$$P|p\rangle = p|p\rangle \tag{54}$$

means

$$\langle\varphi|P|p\rangle = p\langle\varphi|p\rangle\,, \quad \varphi\in\Phi \tag{55}$$



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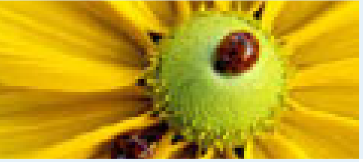

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- The RHS expresses the physical principles of quantum mechanics better than the Hilbert space