HILBERT SPACES

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Abstract. This handout gives a brief introduction to the theory of Hilbert spaces with applications to quantum mechanics.

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Introduction

In the theory of quantum mechanics, the configuration space of a system has the structure of a vector space, which means that linear combinations of states are again allowed states for the system (a fact that is known as the superposition principle). More precisely, the state space is a so-called *Hilbert space*.

1. Fundamental Definitions and Theorems

Definition 1. A *Banach space*[1] V is a complete normed vector space. That is, every Cauchy sequence in V tends to a limit in V (in the metric induced by the norm: $d(x, y) := \|x - y\|$).

In a Banach space, there is a well defined notion of distance between elements in the space. But in order to have a notion of geometry, one needs the additional inner product structure:

Definition 2. Let V be a vector space over the field $\mathbb{F}$, which, in this context, is either $\mathbb{R}$ or $\mathbb{C}$. An *inner product* on V is a map $\langle \cdot, \cdot \rangle : V \times V \mapsto \mathbb{F}$ that satisfies the following axioms for all $x, y, z \in V$ and for all scalars $\lambda \in \mathbb{F}$:

[1] Named after Stefan Banach (1892-1945), a Polish mathematician.

- $\langle x, y\rangle = \overline{\langle y, x\rangle}$
- $\langle \lambda x, y\rangle = \overline{\lambda}\langle x, y\rangle$ and $\langle x, \lambda y\rangle = \lambda\langle x, y\rangle$, as well as $\langle x+y, z\rangle = \langle x, z\rangle + \langle y, z\rangle$
- $\langle x, x\rangle > 0$ for all $x \neq 0$

Two vectors $x, y \in V$ are said to be *orthogonal* if $\langle x, y\rangle = 0$.

Remark 1. In short: an inner product is a positive definite hermitian sesquilinear form on V.

Definition 3. A *Hilbert space*[2] $(\mathcal{H}, \langle\cdot,\cdot\rangle)$[3] is a complete inner product space. The completeness is with respect to the metric induced by the inner product:

$$d(x, y) = \|x - y\| = \sqrt{\langle x - y, x - y\rangle}$$

An inner product space that is not complete is called a *Pre-Hilbert space*. Here we will only consider complete spaces, since one can always replace $\mathcal{H}$ by its completion.

An important theorem is the *Cauchy-Schwarz* inequality:

Theorem 1 (Cauchy-Schwarz)**.** *Let $\mathcal{H}$ be a Hilbert space. Then for every $f, g \in \mathcal{H}$ we have*

$$|\langle f, g\rangle| \leq \|f\|\|g\|$$

with equality if and only if f and g are parallel.

Definition 4. A set $\{\psi_k\}$ of vectors in $\mathcal{H}$ is called *orthogonal* if $\langle \psi_i, \psi_j\rangle = 0$ for $i \neq j$. It is called *orthonormal* if furthermore $\langle \psi_i, \psi_i\rangle = \|\psi\|^2 = 1$ for all i.

Lemma 1. *Suppose $\{\psi_j\}_{j=1}^n$ is an orthonormal set. Then every $\varphi \in \mathcal{H}$ can be decomposed as*

$$\varphi = \varphi_\| + \varphi_\perp, \quad \text{with} \quad \varphi_\| = \sum_{j=1}^{n} \langle \psi_j, \varphi\rangle \psi_j,$$

where $\langle \varphi_\|, \varphi_\perp\rangle = 0$. Moreover, $\langle \psi_j, \varphi_\perp\rangle = 0$ for all $1 \leq j \leq n$. In particular,

$$\|\varphi\|^2 = \sum_{j=1}^{n} |\langle \psi_j, \varphi\rangle|^2 + \|\varphi_\perp\|^2. \tag{1.1}$$

From equation (1.1), we obtain *Bessel's inequality*

$$\sum_{j=1}^{n} |\langle \psi_j, \varphi\rangle|^2 \leq \|\varphi\|^2$$

with equality holding if and only if φ lies in the span of $\{\psi_j\}_{j=1}^n$.

An orthonormal set $\{\psi_j\}_{j=1}^N$ is called an *orthonormal basis* if

$$\|\varphi\|^2 = \sum_{j=1}^{N} |\langle \psi_j, \varphi\rangle|^2$$

for all $\varphi \in \mathcal{H}$. This is equivalent to

$$\varphi = \sum_{j=1}^{N} \langle \psi_j, \varphi\rangle \psi_j$$

[2]Named after David Hilbert (1862-1943), a German mathematician.

[3]From now on we will just write $\mathcal{H}$ instead of $(\mathcal{H}, \langle\cdot,\cdot\rangle)$.

for all $\varphi \in \mathcal{H}$.

In quantum mechanics one deals with so called *separable* Hilbert spaces:

Definition 5. A Hilbert space[4] is called *separable* if it contains a countable dense subset.

In particular, this means that there is a countable orthonormal basis.

Theorem 2. *Any two separable infinite-dimensional Hilbert spaces are isomorphic.*

Another important concept in the theory of Hilbert spaces is that of a *dual space*:

Definition 6. A *linear functional* over V is a map $f : V \to \mathbb{F}$ that is linear. The set of all linear functionals over V is called the (algebraic) *dual space* of V and is denoted by V'. The set of all *continuous* linear functionals over V is denoted by V^*, the set of all *continuous antilinear* (that is conjugate linear) functionals over V is called the *antidual space* and is denoted by $V^\times$.

2. Examples

2.1. **Trivial examples.** Of course, the spaces $\mathbb{R}^n$ and $\mathbb{C}^n$ with $n \geq 1$ are Hilbert spaces if they are equipped with the usual Euclidean inner product:

$$\langle x, y\rangle := \sum_{i=1}^{n} \overline{x}_i \, y_i$$

The space $\mathbb{C}^2$ has a common use in quantum mechanics: It is used to describe the spin of a particle.

2.2. **The ℓ^2 space of square-summable sequences.** The sequence spaces ℓ^p are a natural generalization of the p-Norm for "vectors" with an infinite number of components.

For example, on $\mathbb{R}^n$ the p-Norm is defined as

$$\|x\|_p := \left(\sum_{i=1}^{n} |x|^p\right)^{1/p}, \qquad (x \in \mathbb{R}^n)$$

whereas on ℓ^p, the norm of a sequence $(x_n)_{n\in\mathbb{N}}$ takes the form of a series:

$$\|x\|_{\ell^p} := \left(\sum_{n\in\mathbb{N}} |x_n|^p\right)^{1/p}.$$

Of the ℓ^p spaces, only ℓ^2 is a Hilbert space with inner product

$$\langle x, y\rangle := \sum_{n\in\mathbb{N}} \overline{x_n} y_n.$$

Elements of ℓ^2 are called "square-summable sequences".

[4]More generally: a topological space.

2.3. **The L^2 space of square-integrable functions.** The L^p spaces, named after Henri Lebesgue[5], are function spaces using generalizations of p-Norms that are used on finite-dimensional vector spaces. The norm of L^p is defined as

$$\|f\|_{L^p(\Omega)} := \left(\int_\Omega |f(x)|^p \; dx \right)^{1/p} . \tag{2.1}$$

Remark 2. Note that the set of functions for which (2.1) holds is just a seminormed vector space (that is, $\|x\|$ may be zero even for some $x \neq 0$) and is denoted by $\mathcal{L}^p(\Omega)$. To make $\mathcal{L}^p(\Omega)$ a normed space, one considers the quotient space $L^p(\Omega) := \mathcal{L}^p(\Omega)/_\sim$ with $f \sim g \iff \|f - g\| = 0$, that is, if $f = g$ almost everywhere (up to a set of measure zero). Therefore, elements of L^p are equivalence classes of functions.

Of the L^p spaces, only the L^2 space is a Hilbert space with its inner product given by

$$\langle f, g \rangle := \int_\Omega \overline{f(x)} g(x) \, dx.$$

2.4. **The Sobolev spaces H^k.** The space

$$H^k(\Omega) := W^{k,2}(\Omega) = \left\{ u \in L^2(\Omega) : \; D^\alpha u \in L^2(\Omega) \, \forall \, |\alpha| \leq k \right\},$$

where α is a multi-index[6] and D^α are the weak partial derivatives, is a Hilbert space with norm

$$\|u\|_{H^k(\Omega)} := \left(\sum_{|\alpha| \leq k} \|D^\alpha u\|^2_{L^p(\Omega)} \right)^{1/2} .$$

Normed spaces in which the norm is a combination of L^P-norms of the function itself as well as its derivatives are called *Sobolev spaces.*

3. Operators on Hilbert spaces

In quantum mechanics, observables correspond to linear operators on a Hilbert space.

A *linear operator* A is a linear mapping

$$A : \mathrm{dom}(A) \mapsto \mathcal{H},$$

where $\mathrm{dom}(A)$ is a linear subspace of $\mathcal{H}$, called the *domain* of A. A linear operator A is called

- *bounded* if
$$\|A\| := \sup_{\|\psi\|=1} \|A\psi\|$$
is finite. If this is the case, $\|A\|$ is called the (operator) norm of A.
- *symmetric* if
$$\langle f, Ag \rangle = \langle Af, g \rangle \quad f, g \in \mathrm{dom}(A)$$
and $\mathrm{dom}(A)$ is dense in $\mathcal{H}$[7].

[5] French mathematician, 1875-1941.

[6] A multi-index α is a k-tupel $(\alpha_1, \alpha_2, ..., \alpha_k)$, $\alpha_{1,2,...,k} \in \mathbb{N}$, $|\alpha| := \sum_{i=1}^k \alpha_i$ Multi-indices are used as a convenient notation to denote for instance partial derivatives of higher order: $D^\alpha u := \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \ldots \partial x_k^{\alpha_k}}$.

[7] In some texts, however, the second condition is dropped from the definition.

– *hermitian* if A is symmetric and bounded[8].
– *compact* if every sequence $(A\,f_n)_{n\in\mathbb{N}}$ has a convergent subsequence whenever (f_n) is bounded.

Proposition 1. *A linear operator A is bounded if and only if A is continuous.*

Proof. ($\Rightarrow$) For $f, g \in \mathrm{dom}(A)$, $h := f - g$, $\tilde{h} := \frac{h}{\|h\|}$ we have

$$\|A(f-g)\| = \left\|A(\|h\|\tilde{h})\right\| = \|h\|\,\|A\tilde{h}\| \leq \|f-g\|\,\|A\|,$$

thus A is Lipschitz continuous.

($\Leftarrow$) First note that since A is linear we have $A(0) = 0$. From continuity at the zero vector it follows that there exists a $\delta > 0$ such that $\|A(f)\| = \|A(f) - A(0)\| \leq 1\,\forall f \in \mathcal{H} : \|f\| \leq \delta$. Choose $g \in \mathcal{H} : \|g\| = 1$, then

$$\|Ag\| = \left\|\frac{1}{\delta} A\,(\delta\,g)\right\| \leq \frac{1}{\delta}.$$

Thus $\sup_{\|g\|=1} \|Ag\| \leq \frac{1}{\delta} < \infty$. □

Definition 7 (Adjoint operator)**.** Given a linear operator A on $\mathcal{H}$ with a dense domain[9] one defines its *adjoint* $A^\dagger : \mathrm{dom}(A^\dagger) \to \mathcal{H}$ as follows: its domain is specified by

$$\mathrm{dom}(A^\dagger) := \{x \in \mathcal{H} : y \mapsto \langle x, Ay\rangle \text{ is a continuous linear functional}\}.$$

Now the Riesz representation theorem (see Theorem 4) says that for $x \in \mathrm{dom}A^\dagger$ there exists a unique $z =: A^\dagger x \in \mathcal{H}$ such that

$$\langle x, Ay\rangle = \langle z, y\rangle\,\forall y \in \mathrm{dom}(A).$$

Remark 3. Note that if A is symmetric it follows that $\mathrm{dom}(A) \subseteq \mathrm{dom}(A^\dagger)$ (because for $x \in \mathrm{dom}(A)$: $y \mapsto \langle x, Ay\rangle \Leftrightarrow y \mapsto \langle Ax, y\rangle$ which clearly is continuous[10]) and therefore $A = A^\dagger|_{\mathrm{dom}(A)}$. If furthermore $\mathrm{dom}(A) = \mathrm{dom}(A^\dagger)$, A is called *self-adjoint*.

Definition 8 (Spectrum of a linear operator)**.** The *spectrum* $\sigma(A)$ of a densely defined (unbounded) linear operator A is defined by

$$\sigma(A) := \{\lambda \in \mathbb{C} :\ (A - \lambda\mathbb{I})^{-1} \text{ is unbounded}\}.$$

Remark 4. If A is a bounded operator, boundedness of $(A - \lambda\mathbb{I})^{-1}$ follows automatically if the inverse exists at all.

The spectrum is a generalization of the notion of eigenvalues: If λ is an eigenvalue, then $\lambda \in \sigma(A)$, the converse, however, does not hold in general. This generalization is needed in quantum mechanics, because unbounded operators might not have any eigenvalues at all, but the eigenvalues (or rather spectral values) of an observable have a physical meaning, namely the possible results of a measurment of that observable.

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[8]Again the second condition is dropped from the definition in some texts.

[9]This condition ensures that each continuous linear functional of the form $y \mapsto \langle x, Ay\rangle$ can be extended to a unique continuous linear functional on all of $\mathcal{H}$, which is required to apply the Riesz representation theorem.

[10]Using Cauchy-Schwarz one obtains $|\langle z, y_1\rangle - \langle z, y_2\rangle| \leq ||z||\,||y_1 - y_2||$, showing that for fixed $z \in \mathcal{H}$ the map $y \mapsto \langle z, y\rangle$ is even Lipschitz-continuous.

4. Theorems

4.1. **Spectral theorem.** There are a number of results called spectral theorem, ranging from statements about (diagonalizability of) finite dimensional hermitian matrices to (unbounded) self-adjoint operators. It's exact formulation in the more general cases, however, is way beyond the scope of this presentation.

Therefore we are only going to state a relatively easy version, namely the one for compact symmetric operators, although many operators encountered in quantum mechanics won't even be bounded let alone compact.

Theorem 3 (Spectral theorem for compact symmetric operators)**.** *Suppose $\mathcal{H}$ is a Hilbert space and $A : \mathcal{H} \to \mathcal{H}$ is a compact symmetric operator. Then there exists a sequence of real eigenvalues α_j converging to 0. The corresponding normalized eigenvectors u_j form an orthonormal set and every $f \in \mathrm{Ran}(A) = \{Ax : x \in \mathrm{dom}A\}$ can be written as*

$$f = \sum_{j=0}^{\infty} \langle u_j, f \rangle \, u_j$$

If $\mathrm{Ran}(A)$ is dense, then the eigenvectors form an orthonormal basis.

4.2. **Riesz representation theorem.** The Riesz representation theorem for Hilbert spaces is an important result in functional analysis which relates a Hilbert space $\mathcal{H}$ to its continuous dual space $\mathcal{H}^*$. It also justifies the use of Dirac's bracket-notation in quantum mechanics.

Theorem 4 (Riesz representation theorem)**.** *Let $\mathcal{H}$ be a Hilbert space and let $\mathcal{H}^*$ be its continuous dual space. Suppose ℓ is a bounded linear functional on $\mathcal{H}$, then there is a unique $\varphi \in \mathcal{H}$ such that $\ell(\psi) = \langle \varphi, \psi \rangle$ for all $\psi \in \mathcal{H}$.*

Proof. If $\ell \equiv 0$, choose $\varphi = 0$. Otherwise there exists a unit vector $\tilde{\varphi} \in \ker(\ell)^\perp = \{\psi : \ell(\psi) = 0\}^\perp$[11]. For $\psi \in \mathcal{H}$ we have $\ell(\ell(\psi)\tilde{\varphi} - \ell(\tilde{\varphi})\psi) = \ell(\psi)\ell(\tilde{\varphi}) - \ell(\tilde{\varphi})\ell(\psi) = 0$ by linearity and hence

$$0 = \langle \underbrace{\tilde{\varphi}}_{\in \ker(\ell)^\perp}, \underbrace{\ell(\psi)\tilde{\varphi} - \ell(\tilde{\varphi})\psi}_{\in \ker(\ell)} \rangle = \ell(\psi) - \ell(\tilde{\varphi}) \langle \tilde{\varphi}, \psi \rangle .$$

Choosing $\varphi = \overline{\ell(\tilde{\varphi})}\, \tilde{\varphi}$ yields $\ell(\psi) = \langle \varphi, \psi \rangle$.

To see uniqueness, let φ_1 and φ_2 be two vectors satisfying $\ell(\psi) = \langle \varphi_i, \psi \rangle \ \forall \psi \in \mathcal{H}$. Then $\langle \varphi_1 - \varphi_2, \psi \rangle = \langle \varphi_1, \psi \rangle - \langle \varphi_2, \psi \rangle = 0 \ \forall \psi$. Therefore $\varphi_1 - \varphi_2 \in \mathcal{H}^\perp = \{0\}$, implying $\varphi_1 = \varphi_2$. ☐

In quantum mechanics, Theorem 4 guarantees that every ket $|\psi\rangle$ has an unambiguously corresponding bra $\langle \psi|$.

5. Hilbert spaces in quantum mechanics

In this section, we present a few selected topics concerning the use of Hilbert spaces and their extensions in quantum mechanics.

[11] Here $A^\perp$ denotes the orthogonal complement of A in $\mathcal{H}$: $A^\perp := \{x \in \mathcal{H} : \langle x, y \rangle = 0$ for all y in $A\}$.

5.1. **Application of the spectral theorem: Heisenberg's matrix mechanics.** Given a (classical) Hamiltonian function $H(q_1, ..., q_k, p_1, ..., p_k)$, Heisenberg's matrix theory gives the following rules to derive the allowed energy: If one can find a system of $2k$ (infinite, symmetric) "matrices" $Q_1, ..., Q_k, P_1, ..., P_k$ satisfying

$$[Q_m, Q_n] = [P_m, P_n] = 0 \quad \text{and} \quad [P_m, Q_n] = \begin{cases} 0 & m \neq n \\ \frac{h}{2\pi i}\,\mathrm{I} & m = n \end{cases} \tag{5.1}$$

for all $m, n = 0, ..., k$ and for which the matrix

$$D := H(Q_1, ..., Q_k, P_1, ..., P_k)$$

becomes a diagonal matrix, the allowed energy levels are given by the diagonal elements of H.

This problem can be split into two parts: finding matrices $\tilde{Q}_j, \tilde{P}_j$ satisfying the commutation relations given in (5.1) and finding a transformation matrix S such that

$$D = H(S^{-1}\tilde{Q}_1 S, ..., S^{-1}\tilde{Q}_k S, S^{-1}\tilde{P}_1 S, ..., S^{-1}\tilde{P}_k S) = S^{-1}\tilde{H}S$$

becomes diagonal. The second part leads to an eigenvalue problem: $SD = \tilde{H}S \iff \sum_j s_{ij} d_j \delta_{jk} = \sum_j h_{ij} s_{jk} \forall i$ means that the columns $(s_{jk})_{j\in\mathbb{N}}$ of S and the diagonal elements of D are the solutions of

$$\tilde{H}x = \lambda x.$$

Allowing only $x \in \ell^2$ (which is equivalent to S being orthogonal [this condition also ensures that the Q_i, P_i are symmetric if $\tilde{Q}_i, \tilde{P}_i$ are], since for orthogonal S each column $(s_{jk})_{j\in\mathbb{N}}$ has to satisfy $1 = \sum_i s_{ik} s_{ki}^{-1} = \sum_i s_{ik}\overline{s_{ik}}$) we find ourselves in a Hilbert space, therefore the spectral theorem guarantees the existence of countably many solutions $(x_i)_{i\in\mathbb{N}}$ and λ_i (if $\tilde{H}$ is compact, which unfortunately won't be true in general).

5.2. **Projective Hilbert space.** In quantum theory the wave functions ψ and ϕ represent the same physical state, if there exists a $\lambda \in \mathbb{C}$ such that $\phi = \lambda\psi$. This implies that for a given state there exists a whole equivalence class of functions $\psi \in \mathcal{H}$, which motivates the following definition:

Definition 9. The *projective Hilbert space* $P(\mathcal{H})$ of a complex Hilbert space $\mathcal{H}$ is the set of equivalence classes of vectors $\psi \in \mathcal{H}$, $\psi \neq 0$ for the relation given by

$$\psi \sim \phi :\iff \exists \lambda \in \mathbb{C} : \phi = \lambda\psi,$$

in other words $P(\mathcal{H}) = \mathcal{H}/_\sim$.

Remark 5. The elements of $P(\mathcal{H})$ can be interpreted as equivalence classes of vectors $\psi \in \mathcal{H}$, $\psi \neq 0$, as equivalence classes of unit vectors, as the one-dimensional subspaces of $\mathcal{H}$, or as the one-dimensional orthogonal projections acting in $\mathcal{H}$. Elements of $P(\mathcal{H})$ are called *"rays"* of the space.

5.3. **Rigged Hilbert space.** Although the mathematical concept of a Hilbert space is sufficient when dealing with compact self adjoint operators (that is with a *countable* set of eigenvectors) one can not (mathematically) justify some aspects of the Dirac method in a Hilbert space alone, since the eigenbras and eigenkets of an Operator are (in general) no longer elements of a Hilbert space[12]. This leads to the (in a way more general) concept of a *rigged Hilbert space*.

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[12] Dirac himself writes in [Dir58, p.40] that "the bra and ket vectors that we now use form a more general space than a Hilbert space."

Definition 10. Loosely speaking, a *rigged Hilbert space* (or *Gelfand triple*[13]) is a triple $(\Phi, \mathcal{H}, \Phi^*)$, where Φ is a dense subspace of $\mathcal{H}$ and Φ^* its continuous dual space.

Proposition 2. *The Gelfand triple $(\Phi, \mathcal{H}, \Phi^*)$ satisfies the following inclusion relations:*

$$\Phi \subseteq \mathcal{H} \text{ and } \mathcal{H}^* \subseteq \Phi^*$$

Proof. Since Φ is a dense *subset* of $\mathcal{H}$ the first inclusion is trivial. To show the second inclusion, let $\psi \in \mathcal{H}$ be arbitrary, then $x \mapsto \langle \psi, x \rangle$ defines a continuous linear functional $f : \mathcal{H} \to \mathbb{C}$, $f \in \mathcal{H}^*$ (by the Riesz representation theorem every element of $\mathcal{H}^*$ can be represented in this way). Now consider $f|_\Phi : \Phi \to \mathbb{C}$: clearly $f|_\Phi \in \Phi^*$ and, because Φ is dense, $f|_\Phi$ can be extended to a unique continuous functional on $\mathcal{H}$, which is exactly the function f. □

Associated with each triple $(\Phi, \mathcal{H}, \Phi^*)$ of spaces is a fourth space, namely the space $\Phi^\times$, that is the antidual space of Φ. The basic reasons why those spaces are needed are:

- the *bras* associated with the elements in the continuous spectrum of an observable *belong to* Φ^*,
- whereas the *kets belong to* $\Phi^\times$.
- unbounded operators can not be defined on the whole of $\mathcal{H}$. The space Φ is the largest space on which the observables are defined and which is invariant under the action of the observables.

Example 1. Let $\mathcal{H} = L^2(\mathbb{R})$ and consider the position observable $\mathcal{O}$ given by

$$\mathcal{O}\psi(x) = x\psi(x).$$

Although the action of $\mathcal{O}$ is in principle well defined for all $\psi \in L^2$, there are functions which are in L^2, but for which $\mathcal{O}\psi$ is no longer an element of L^2 (consider for instance $\psi(x) := \frac{\sin x}{x}$). Therefore the domain of $\mathcal{O}$ is given by

$$\mathrm{dom}(\mathcal{O}) = \{\psi(x) \in L^2 : \int_{-\infty}^{\infty} |x\psi(x)|^2 dx < \infty\} \subset L^2.$$

Similarly $\mathrm{dom}(\mathcal{O}^2) = \{\psi(x) \in L^2 : \int_{-\infty}^{\infty} |x^2\psi(x)|^2 dx < \infty\} \subset \mathrm{dom}(\mathcal{O})$ and so forth. Therefore if we are only interested in the position observable we define

$$\Phi := \bigcap_{n=0}^{\infty} \mathrm{dom}(\mathcal{O}^n).$$

This ensures that for every $\psi \in \Phi$ expectation values, uncertainities,... are well defined.

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[13]Named after Israel Gelfand (1913-2009), a Soviet mathematician.