# Diachrony of Spectra

Ikhan Choi

Postech - Unist - Kaist Joint Seminar

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### Example

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### Question

Why is it defined like this?

### Contents

### Hydrogen atom

Spectral theory on Hilbert spaces

Gelfand theory

Algebraic geometry







### Question

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How can we explain and compute this phenomenon?

A: By the following formula!

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right), \quad \text{for} \quad n_1, n_2 \in \mathbb{N}.$$

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The constant h is called the Planck constant and  $\hbar:=\frac{h}{2\pi}.$ 

From the three relations

$$\label{eq:mur} \text{mvr} = \text{nh}, \quad \frac{\text{m} \nu^2}{r} = -k \frac{(+e)(-e)}{r^2}, \quad \text{E} = \text{K} + \text{V} = \frac{1}{2} \text{m} \nu^2 - k \frac{e^2}{r},$$

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$$\label{eq:mur} m\nu r = n\hbar, \quad \frac{m\nu^2}{r} = -k\frac{(+e)(-e)}{r^2}, \quad E = K + V = \frac{1}{2}m\nu^2 - k\frac{e^2}{r},$$

we deduce

$$E = -\frac{k^2 e^4 m}{2 \hbar^2} \frac{1}{n^2} \approx -13.6 \frac{1}{n^2} \ (eV).$$

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### Proposition (Rydberg formula)

The wavelengths  $\lambda$  of absorbed or emitted photons from a hydrogen atom is estimated by the following formula:

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right), \quad \textit{for} \quad n_1, n_2 \in \mathbb{N},$$

where  $R := \frac{k^2 e^4 m}{4\pi \hbar^3 c}$  is the Rydberg constant.

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In quantum mechanics, an electron around a hydrogen atom is described by the Schrödinger equation: for  $(t,x)\in\mathbb{R}^{1+3}$ 

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By solving it, we obtain the probability distribution  $|\Psi(t,x)|^2$  of the electron at time t, hence the assumption  $\forall t$ ,  $\int |\Psi(t,x)|^2 dx = 1 < \infty$ . Let's solve.

$$\label{eq:delta-psi} i\hbar\frac{\partial\Psi(t,x)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(t,x) + V(x)\Psi(t,x).$$

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for some constant E, which is interpreted as the energy of electron. ... We have two *eigenvalue problems* with *shared eigenvalue* E:

$$\label{eq:delta_t} i\frac{d}{dt}\varphi(t) = \mathsf{E}\varphi(t), \qquad (-\Delta + V(x))\psi(x) = \mathsf{E}\psi(x).$$

(Solutions may or may not exist according to E!)

Suppose we already have found the solutions  $\phi_E(t)$ ,  $\psi_E(x)$  of the eigenvalue problems for each complex number E. Here are some facts:

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- ▶ Since  $\phi_E(t) \propto e^{-iEt}$  is easily solved, the main difficulty is  $\psi_E$ .

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#### Remark

Simply,  $L^2(\mathbb{R}^3)$  is the space of  $f:\mathbb{R}^3\to\mathbb{R}$  such that  $\int |f|^2<\infty$ . In fact, there are many technical issues to formalize this problem, for example,  $L^2$  function is in general not differentiable.

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Don't be so pedantic in doing physics.

Anyway, with long long calculations and hard hard mathematics, experts have found the following result:

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- ► Eigenvalues embody the possible energies of an electron, so we can give the Rydberg formula a reasonable explanation.
- ► This result explains not only the discretized energy spectrum but also the number of orbitals in each electron shell!
- ▶ We call the set of eigenvalues by **spectrum** of  $\mathcal{H}$ .

The simultaneous equation is solved when  $E = -\frac{1}{n^2}$  for some  $n \in \mathbb{N}$ :

$$\label{eq:delta-def} \dot{t}\frac{d}{dt}\varphi(t) = \mathsf{E}\varphi(t), \qquad (-\Delta + V(x))\psi(x) = \mathsf{E}\psi(x).$$

The simultaneous equation is solved when  $E = -\frac{1}{n^2}$  for some  $n \in \mathbb{N}$ :

$$\label{eq:delta_t} i\frac{d}{dt}\varphi(t) = E\varphi(t), \qquad (-\Delta + V(x))\psi(x) = E\psi(x).$$

General solution of the Schrödinger equation is like

$$\begin{split} \Psi(t,x) &= \sum_{n=1}^{\infty} \varphi_n(t) \psi_n(x) \\ &= \sum_{n=1}^{\infty} e^{i\frac{1}{n^2}t} \left( \sum_{i=1}^{n^2} c_{n,i} \psi_{n,i}(x) \right) \\ &= \sum_{n=1}^{\infty} e^{i\frac{1}{n^2}t} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} c_{nlm} \ \psi_{nlm}(x). \end{split}$$

#### Conclusion of Section 1

#### Contents

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In this section, we

- review the spectral theory on finite dimensional vector spaces,
- introduce Hilbert spaces a typical example of infinite dimensional vector spaces — to state some results which extend the spectral theory to infinite dimensional spaces,
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From now, we basically assume the scalar field as  $\mathbb{C}$ .

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Vector space with inner product

Vector space without additional structure

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The most famous examples are for:

#### Definition

Let V be a finite dimensional complex inner product space and  $A:V\to V$  be linear. (i.e., let A be a complex square matrix.) Then, A is said to be normal if  $AA^*=A^*A$ , and Hermitian if  $A=A^*$ 

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Note that the conjugate transpose depends on the inner product structure:  $A^*$  is defined by

$$\langle x, Ay \rangle = \langle A^*x, y \rangle.$$



### Theorem (Spectral theorem for normal matrices)

A complex square matrix A is normal if unitarily diagonalizable.

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#### TFAE: a matrix is/has

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Remind what we did in the previous section. The purpose of separation of variables is to *construct an orthonormlal basis for the solution space*.

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- Conversly, Hilbert space usually means the L<sup>2</sup> space of wave functions, by physicists.
- ▶ The space  $\ell^2(\mathbb{C})$  of sqare summable sequeces is a Hilbert space with  $\langle (a_n), (b_n) \rangle := \sum_n a_n b_n$ .

#### Theorem (?)

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A linear operator  $T: H \to H$  on a Hilbert space is called *bounded* if there is a constant C>0 such that for all  $x\in H$ 

$$\|Ax\| \leqslant C\|x\|.$$

The set of bounded operators on H is denoted by B(H).

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#### **Theorem**

A linear operator on a Hilbert space is bounded iff continuous.



## Compact operators

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### Example

An operator  $T:\ell^2\to\ell^2$  defined by

$$T(\alpha_1,\alpha_2,\alpha_3,\cdots)=(\alpha_1,\frac{\alpha_2}{2},\frac{\alpha_3}{3},\cdots)$$

is compact, but the identity  $I \to \ell^2 \to \ell^2$ 

$$I(\alpha_1, \alpha_2, \alpha_3, \cdots) = (\alpha_1, \alpha_2, \alpha_3, \cdots),$$

which is clearly bounded, is not compact.



## Spectral theorem for compact normal operators

### Theorem (Spectral theorem for compact normal operators)

Let T be a compact normal operator on a separable Hilbert space. Then, there exists a countable orthonormal basis consisting of eigenvectors, with corresponding eigenvalues that converges to 0.

### Theorem (Spectral theorem for compact self-adjoint operators)

Let T be a compact self-adjoint operator on a separable Hilbert space. Then, there exists a countable orthonormal basis consisting of eigenvectors, with corresponding eigenvalues that are reals and converges to 0.

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#### Remark

There are some concepts we will skip:

- we did not define "separable" space,
- we did not define "countable (Schauder) basis".

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The eigenvalues are distributed like

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For a free particle  $\Rightarrow \mathcal{H} = -\Delta + V = -\Delta$ , we cannot; eigenvectors exist for E  $\geqslant$  0, and they are "linear combinations" of

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- ▶ Energy spectrum of free particle is not *quantized* = *discretized*.
- ▶ We want to say  $-\Delta$  has the spectrum  $[0, \infty)$ .

#### Definition

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In particular,

#### Definition

The *point spectrum* of T is defined by the set of eigenvalues:

$$\sigma_p(T) := \{\lambda \in \mathbb{C} : T - \lambda I \text{ is not injective } \}.$$

#### Definition

The continuous spectrum of T is defined by

$$\sigma_c(T) := \{\lambda \in \mathbb{C} : T - \lambda I \text{ is injective but has proper dense image } \}.$$

### Conclusion of Section 2

- ▶ In infinite dimensional spaces, the spectral theorems are generalized for compact operators.
- ▶ The spectrum of an operator T is defined by

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### Example (1)

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### Example (2)

Let X be a compact space. Then, the set of complex-valued continuous functions  $C(X,\mathbb{C})$  is a commutative  $C^*$ -algebra.

Assumption: unless mentioned otherwise, we will only discuss *commutative unital* C\*-algebras.

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What can be told for a continuous function on a compact X? For C(X),

- $ightharpoonup \sigma(f) = im(f),$
- every maximal ideal is of the form  $\{f: f(x) = 0\}$  for a single point  $x \in X$ .

The following is also an important exmple to formulate functional calculus:

#### Definition

Let A be a (possibly non-commutative) C\*-algebra. An element  $\alpha\in A$  is called *normal* if  $\alpha^*\alpha=\alpha\alpha^*.$  For a normal element, a C\*-subalgebra defined by

$$C^*(\alpha) := \overline{\{\, p(\alpha,\, \alpha^*) : p \in \mathbb{C}[x,y]\,\}} \subset A$$

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- ▶ the maps above are inverses of each other.

Therefore,



### Proposition

There is a 1-1 correspondence between

 $\textit{spectrum of } \alpha \quad \Longleftrightarrow \quad \textit{maximal ideal space of } C^*(\alpha).$ 

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#### Definition

Let us define the *spectrum* of general commutative unital  $C^*$ -algebra A as the **set of maximal ideals** and denote it by  $\sigma(A)$ .

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We set up the topology of pointwise convergence on  $\sigma(A)$ : for example, consider C(X). Since X is naturally corresponded to  $\sigma(C(X))$  as a set,

$$x \to y \in X \iff f(x) \to f(y) \text{ for all } f \in C(X).$$

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### Example

For the space  $\ell^1$  of summable sequences, the spectrum is the unit circle:  $\sigma(\ell^1)=\mathbb{T}.$ 

## Example

Let X be compact Hausdorff. Then,  $\sigma(C(X))$  is homeomorphic to X.



## Gelfand-Naimark theorem

Finally, we state the Gelfand-Naimark theorem.

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Theorem (Gelfand-Naimark, 1943)

Let A be a commutative unital  $C^*$ -algebra. Then, we have a  $C^*$ -algebra isomorphism

$$A \to C(\sigma(A)).$$

This map is called Gelfand representation.

## Conclusion of Section 3

#### Transitions of definition:

- ▶ Spectrum of  $a \in A \rightarrow$  generalized eigenvalues;
- ▶ Spectrum of  $a \in C(X) \rightarrow \text{image of function}$ ;
- ▶ Spectrum of  $a \in C^*(a) \to \text{maximal ideals};$   $\Downarrow$
- ▶ Spectrum of C(X) := maximal ideals = domain = image of inj,
- ▶ Spectrum of A := maximal ideals (≈ domain(?)).

```
\mathsf{Spectrum} \quad \Longleftrightarrow \quad \{\mathsf{Maximal ideals}\} \quad \Longleftrightarrow \quad \{\mathsf{Points}\}
```

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In this section, assume that a "ring" is a commutative and unital one.

#### Remark

We give basic definitions here. For simplicity, we will do everything in the three dimension  $\mathbb{C}^3$ . Every concept is directly generalized to arbitrary dimensions.

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Let  $T \subset \mathbb{C}[x, y, z]$  and define

$$\mathcal{Z}(T) := \{ p \in \mathbb{C}^3 : f(p) = 0 \text{ for all } f \in T \}.$$

An algebraic set is a subset V of  $\mathbb{C}^n$  satisfying V=Z(T) for some T.

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#### Definition

Let  $Y \subset \mathbb{C}^n$  and define

$$\label{eq:J} \mathfrak{I}(Y) := \{f \in \mathbb{C}[x,y,z] : f(p) = 0 \text{ for all } p \in Y\}.$$

This is always a radical(square-free) ideal.



## Proposition

- ▶ For an algebraic set  $V \subset \mathbb{C}^3$ , we have  $\mathcal{V}(\mathfrak{I}(V)) = V$ .
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If an algebraic set is not a union of two proper algebraic subsets, then it is called *algebraic variety*.

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algebraic sets \iff radical ideals, algebraic varieties \iff prime ideals.
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# Coordinate ring

Consider an algebraic variety  $S^2=\{x^2+y^2+z^2=1\}$ . The following two functions are same on  $S^2$ :

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A coordinate ring or structure ring of an algebraic set V is the ring  $\mathbb{C}[x,y,z]/\mathbb{I}(V)$ .

Every ring of the form  $\mathbb{C}[x,y,z]/I$ , where I is an ideal, we can interpret the ring as the set of functions on the algebraic set  $\mathcal{V}(I)$ . Why do we introduce this?

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#### Main Philosophy of AG:

analyze the function space to study geometric objects!



## Krull dimension

Let us see an example that shows the power of structure rings.

Equation	ldeal	Dimension
Ø	Ø	3
x = 1	(x-1)	2 (plane)
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Coordinate rings are

#### Definition

The Krull dimension of a ring R is the maximal length of chain of prime ideals.

.. The Krull dimension of coordinate ring is same with the "dimension" of the corresponding algebraic sets.



# Maximal ideal is a point

Second example.

#### Theorem

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This theorem implies that we have the following correspondence:

points  $\iff$  maximal ideals.



Alexander Grothendieck (1928 - 2014)

"Every ring should be recognized as the set of functions on a space."



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original major: functional analysis!!!

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## Problems of maximal ideals

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But it had two problems:

- 1. The codomain is not unified;
- 2. We want the spectrum to have a functoriality.

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For C\*-algebras, we could just use the maximal ideals because the field  $R/\mathfrak{m}$  is always isomorphic to  $\mathbb{C}$ :

Theorem (Gelfand-Mazur)

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- 2. Compromise the unifies codomain.(v)

We want Spec :  $\mathbf{CRing} \to \mathbf{Set}$  to be a (contravariant) functor: functoriality allows to define schemes and apply the powerful theory of sheaves to AG.

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## Example

Consider the ring homomorphism  $i:\mathbb{Z}\hookrightarrow\mathbb{Q}.$  The most reasonable choice of the naturally induced map is

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## Proposition

Inverse image of prime ideal under a ring homomorphism is prime.



### Conclusion

When Grothendieck transplanted the idea of spectrum from functional analysis to algebraic geometry, the following definition comes up:

#### Definition

Let R be a ring. The spectrum of R is the set of prime ideals.