Mathematical structure of quantum mechanics

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$$\mathbb{C}^N = \left\{ \mathbf{z} = \begin{pmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_N \end{pmatrix}, \ z_n \in \mathbb{C} \text{ for all } 1 \leq n \leq N \right\} \quad \text{(column vectors of size } N\text{)}$$

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$$\mathbb{C}^{M \times N} = \left\{ \mathbf{A} = \begin{pmatrix} z_{1,1} & \cdots & z_{1,N} \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ z_{M,1} & \cdots & z_{M,N} \end{pmatrix}, \ z_{m,n} \in \mathbb{C} \text{ for all } 1 \leq m \leq M, \ 1 \leq n \leq N \right\}$$

(complex matrices with M **rows and** N **columns)**

$\mathbb{C}^N$ is endowed with a natural complex vector space structure:

- **addition of two vectors of $\mathbb{C}^N$**

$$\mathbf{z} = \begin{pmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_N \end{pmatrix}, \quad \mathbf{z}' = \begin{pmatrix} z'_1 \\ \cdot \\ \cdot \\ \cdot \\ z'_N \end{pmatrix} \quad \Rightarrow \quad \mathbf{z} + \mathbf{z}' = \begin{pmatrix} z_1 + z'_1 \\ \cdot \\ \cdot \\ \cdot \\ z_N + z'_N \end{pmatrix}$$

- **multiplication of a vector of $\mathbb{C}^N$ by a scalar**

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Conjugate transpose of a column vector $\mathbf{z} \in \mathbb{C}^N$, a matrix $\mathbf{A} \in \mathbb{C}^{M\times N}$:

$$\mathbf{z}^* = (\overline{z_1}, \cdots, \overline{z_N}) \quad \textbf{(line vector)}, \qquad \mathbf{A}^* \in \mathbb{C}^{N\times M} \textbf{ s.t. } [A^*]_{ij} = \overline{A_{ji}}.$$

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The vectors $\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \end{pmatrix}, \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 0 \end{pmatrix}, \cdots \mathbf{e}_N = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 1 \end{pmatrix}$ **form an orthonormal basis of $\mathbb{C}^N$:**

any vector $\mathbf{z} \in \mathbb{C}^N$ is a unique linear combination of $\mathbf{e}_1$, $\mathbf{e}_2$, $\cdots \mathbf{e}_N$ and

$$\langle \mathbf{e}_j | \mathbf{e}_k \rangle = \mathbf{e}_j^* \mathbf{e}_k = \delta_{j,k}.$$

Definition. **Let** $\mathbf{A} \in \mathbb{C}^{N\times N}$**.**

- $\lambda \in \mathbb{C}$ **is called an eigenvalue of** $\mathbf{A}$**, and** $\mathbf{z} \in \mathbb{C}^N$ **an associated eigenvector if**

$$\mathbf{z} \neq 0 \quad \textbf{and} \quad \mathbf{A}\mathbf{z} = \lambda \mathbf{z};$$

- **the spectrum of** $\mathbf{A}$ **is the set of complex numbers**

$$\sigma(\mathbf{A}) = \{\lambda \in \mathbb{C} \mid \lambda \mathbf{I}_N - \mathbf{A} \textbf{ non-invertible}\}\,.$$

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Theorem. **Let** $\mathbf{A} \in \mathbb{C}^{N\times N}$**.**

$$\begin{aligned}\sigma(\mathbf{A}) &= \{\textbf{eigenvalues of } \mathbf{A}\} \\ &= \{\textbf{roots of the polynomial } p_{\mathbf{A}}(z) := \textbf{det}(z\mathbf{I}_N - \mathbf{A})\}\end{aligned}$$

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Example: **compute the eigenvalues (with their algebraic multiplicities) of**

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad A = \begin{pmatrix} 5 & 1 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & -3i \end{pmatrix}.$$

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2. **$\mathbf{A}$ is diagonalizable in an orthonormal basis, i.e. there exist $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ in $\sigma(A)$ and an orthonormal basis $(\mathbf{z}_1, \mathbf{z}_2, \cdots, \mathbf{z}_N)$ of $\mathbb{C}^N$ s.t.**

$$\forall 1 \leq j,k \leq N, \quad \mathbf{A}\mathbf{z}_j = \lambda_j \mathbf{z}_j, \quad \langle \mathbf{z}_j | \, \mathbf{z}_k \rangle = \delta_{j,k}.$$

Each eigenvalues λ of $\mathbf{A}$ appears in the list $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ as many times as its algebraic multiplicity;

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3. **for each polynomial function $q(t) = \alpha_d t^d + \alpha_{d-1} t^{d-1} + \cdots + \alpha_1 t + \alpha_0$, we have**

$$q(\mathbf{A}) := \alpha_d \mathbf{A}^d + \alpha_{d-1}\mathbf{A}^{d-1} + \cdots + \alpha_1 \mathbf{A} + \alpha_0 \mathbf{I}_N = \sum_{j=1}^{N} q(\lambda_j)\mathbf{z}_j\mathbf{z}_j^*.$$

   By extension, we can define the matrix $f(A)$, for any function $f : \mathbb{R} \to \mathbb{C}$, as

$$f(A) = \sum_{j=1}^{N} f(\lambda_j)\mathbf{z}_j\mathbf{z}_j^* \quad \textbf{(functional calculus)}.$$

Some fundamental principles of quantum mechanics

1. **the pure states of a given quantum system are normalized vectors (or in fact rays) of some complex separable Hilbert space $\mathcal{H}$;**
2. **observables are self-adjoint operators on $\mathcal{H}$;**
3. **the result of the measurement of some scalar physical quantity a (e.g. the energy) is always a point of the spectrum of the associated observable A;**
4. **if the system is in the pure state $\Psi \in \mathcal{H}$ (with $\|\Psi\| = 1$) just before the measurement of a, the probability that the result lays in the range $[\alpha, \beta] \subset \mathbb{R}$ is $\|\mathbb{1}_{[\alpha,\beta]}(A)\Psi\|^2$, where the operator $\mathbb{1}_{[\alpha,\beta]}(A)$ is defined by functional calculus.**

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Good news: if $\mathcal{H}$ is finite-dimensional,

- **$\mathcal{H}$ can be identified with $\mathbb{C}^N$ by means of an orthonormal basis of $\mathcal{H}$;**
- **using this identification, any self-adjoint operator A on $\mathcal{H}$ can be identified with a hermitian matrix $\mathbf{A}$;**
- **the spectrum of the operator A coincides with the spectrum of the matrix $\mathbf{A}$;**
- **$\mathbb{1}_{[\alpha,\beta]}(A)$ is identified with the hermitian matrix $\mathbb{1}_{[\alpha,\beta]}(\mathbf{A})$.**

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Bad news: most quantum systems encountered in physics and chemistry cannot be described by finite-dimensional Hilbert spaces.

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Outline of the lecture

1. Hilbert spaces
2. Self-adjoint operators
3. Spectra of self-adjoint operators
4. Functional calculus

1 - Hilbert spaces

Definition (complex Hilbert space). **A complex Hilbert space is**

- **a complex vector space $\mathcal{H}$,**

i.e. a set $\mathcal{H}$, whose elements are sometimes denoted by "kets", endowed with addition and scalar multiplication laws s.t. $\forall \alpha, \beta \in \mathbb{C},\ \forall |\phi\rangle, |\chi\rangle, |\psi\rangle \in \mathcal{H}$**,**

$|\phi\rangle + (|\chi\rangle + |\psi\rangle) = (|\phi\rangle + |\chi\rangle) + |\psi\rangle$ **(associativity of the addition)**
$|\phi\rangle + |\psi\rangle = |\psi\rangle + |\phi\rangle$ **(commutativity of the addition)**
$|\psi\rangle + |0\rangle = |\psi\rangle$ **(existence of a neutral element for the addition)**
$|\psi\rangle + |-\psi\rangle = |0\rangle$ **(existence of an inverse for the addition)**
$\alpha(|\phi\rangle + |\psi\rangle) = \alpha|\phi\rangle + \alpha|\psi\rangle, \qquad (\alpha + \beta)|\psi\rangle = \alpha|\psi\rangle + \beta|\psi\rangle,$
$0|\psi\rangle = |0\rangle, \qquad 1|\psi\rangle = |\psi\rangle, \qquad \alpha(\beta|\psi\rangle) = (\alpha\beta)|\psi\rangle$

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- **a complex vector space $\mathcal{H}$,**
- **endowed with an inner product denoted by $\langle\cdot|\cdot\rangle$,**

i.e. a mapping $\langle\cdot|\cdot\rangle : \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ such that $\forall\alpha,\beta\in\mathbb{C},\ \forall|\phi\rangle,|\chi\rangle,|\psi\rangle\in\mathcal{H}$,

$$\langle\phi|\alpha\chi+\beta\psi\rangle=\alpha\langle\phi|\chi\rangle+\beta\langle\phi|\psi\rangle \qquad \textbf{(right-linearity)}$$

$$\langle\alpha\chi+\beta\psi|\,\phi\rangle=\overline{\alpha}\langle\chi|\phi\rangle+\overline{\beta}\langle\psi|\phi\rangle \qquad \textbf{(left-antilinearity)}$$

$$\overline{\langle\phi|\psi\rangle}=\langle\psi|\phi\rangle \qquad \textbf{(hermiticity)}$$

$$\langle\psi|\psi\rangle\geq 0 \quad \textbf{and} \quad (\langle\psi|\psi\rangle=0 \ \Leftrightarrow\ |\psi\rangle=|0\rangle) \qquad \textbf{(positive-definiteness)}.$$

Cauchy-Schwarz inequality

$$\forall|\phi\rangle,|\psi\rangle\in\mathcal{H},\quad |\langle\psi|\phi\rangle|\leq\|\psi\|\,\|\phi\|.$$

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- **complete for the norm $\|\cdot\|$ associated with this inner product.**

$$\|\psi\| := \langle\psi|\psi\rangle^{1/2} \geq 0, \quad \|\alpha\psi\| = |\alpha|\,\|\psi\|, \quad \|\phi+\psi\| \leq \|\phi\| + \|\chi\|, \quad (\|\psi\| = 0 \Leftrightarrow \psi = 0)$$

A sequence $(\psi_n)_{n\in\mathbb{N}}$ of elements of the normed vector space $\mathcal{H}$ is called Cauchy if

$$\forall \varepsilon > 0, \quad \exists N \in \mathbb{N} \quad \textbf{s.t.} \quad \forall q \geq p \geq N, \quad \|\psi_p - \psi_q\|_V \leq \varepsilon.$$

$\mathcal{H}$ is called complete if any Cauchy sequence of elements of $\mathcal{H}$ converges in $\mathcal{H}$, i.e. $\exists \psi \in \mathcal{H}$ s.t. $\|\psi_n - \psi\| \underset{n\to\infty}{\to} 0$.

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Physical consequence of completeness: **Dirac's bra-ket duality (Riesz representation theorem)**

- **for each $\psi \in \mathcal{H}$, $\mathcal{H} \ni \phi \mapsto \langle \psi | \phi \rangle \in \mathbb{C}$ is linear and continuous;**
- **conversely, any continuous linear map $\mathcal{H} \ni \phi \mapsto l(\phi) \in \mathbb{C}$ can be represented in a unique way by a "bra" $\langle \psi |$:**

$$\exists ! \psi \in \mathcal{H} \text{ s.t. } \forall \phi \in \mathcal{H},\ l(\phi) = \langle \psi | \phi \rangle.$$

Fundamental example 1: $\mathbb{C}^N$ endowed with its canonical inner product

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_N \end{pmatrix} \in \mathbb{C}^N, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_N \end{pmatrix} \in \mathbb{C}^N, \quad \langle \mathbf{x} | \mathbf{y} \rangle = \sum_{n=1}^{N} \overline{x_n} y_n, \quad \|\mathbf{x}\| = \left(\sum_{n=1}^{N} |x_n|^2 \right)^{1/2}.$$

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Fundamental example 2: $l^2(\mathbb{N}, \mathbb{C})$

$$l^2(\mathbb{N}, \mathbb{C}) = \left\{ |\psi\rangle = (\psi_n)_{n \in \mathbb{N}} \in \mathbb{C}^{\mathbb{N}} \mid \sum_{n=0}^{+\infty} |\psi_n|^2 < \infty \right\}$$

$$\forall |\psi\rangle, |\phi\rangle \in l^2(\mathbb{N}, \mathbb{C}), \quad \langle \psi | \phi \rangle = \sum_{n=0}^{+\infty} \overline{\psi_n} \phi_n, \quad \|\psi\| = \left(\sum_{n=0}^{+\infty} |\psi_n|^2 \right)^{1/2}$$

Fundamental example 3: $L^2(\mathbb{R}^d, \mathbb{C})$**.**

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- **The mapping**

$$(u, v) \mapsto (u, v)_{L^2} := \int_{\mathbb{R}^d} \overline{u} v := \int_{\mathbb{R}^d} \overline{u(\mathbf{r})}\, v(\mathbf{r})\, d\mathbf{r}$$

defines an inner product on the complex vector space

$$C_c^\infty(\mathbb{R}^d, \mathbb{C}) := \left\{ v \in C^\infty(\mathbb{R}^d, \mathbb{C}) \mid \ v = 0 \text{ outside some bounded set} \right\},$$

but $C_c^\infty(\mathbb{R}^d, \mathbb{C})$**, endowed with the inner product** $(\cdot, \cdot)_{L^2}$**, is not a Hilbert space.**

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- **To obtain a Hilbert space, we have to "complete" it with "all the limits of the Cauchy sequences of elements of $C_c^\infty(\mathbb{R}^d)$". We thus obtain the set**

$$L^2(\mathbb{R}^d, \mathbb{C}) := \left\{ u : \mathbb{R}^d \to \mathbb{C} \mid \int_{\mathbb{R}^d} |u|^2 < \infty \right\},$$

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- **Technical details:**
  - **one must use the Lebesgue integral (doesn't work with Riemann integral);**
  - **the elements of $L^2(\mathbb{R}^d, \mathbb{C})$ are in fact equivalence classes of measurable functions (for the Lebesgue measure) for the equivalence relation $u \sim v$ iff $u = v$ everywhere except possibly on a set of Lebesgue measure equal to zero.**

Fundamental example 4: the Sobolev spaces $H^1(\mathbb{R}^d, \mathbb{C})$ and $H^2(\mathbb{R}^d, \mathbb{C})$.

- **The sets**

$$H^1(\mathbb{R}^d, \mathbb{C}) := \left\{ u \in L^2(\mathbb{R}^d, \mathbb{C}) \mid \nabla u \in (L^2(\mathbb{R}^d, \mathbb{C}))^d \right\},$$
$$H^2(\mathbb{R}^d, \mathbb{C}) := \left\{ u \in L^2(\mathbb{R}^d, \mathbb{C}) \mid \nabla u \in (L^2(\mathbb{R}^d, \mathbb{C}))^d \text{ and } D^2 u \in (L^2(\mathbb{R}^d, \mathbb{C}))^{d\times d} \right\}$$

are complex vector spaces. Respectively endowed with the inner products

$$(u, v)_{H^1} := \int_{\mathbb{R}^d} \overline{u} v + \int_{\mathbb{R}^d} \overline{\nabla u} \cdot \nabla v,$$
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- **Technical detail: the gradient and the second derivatives are defined by means of distribution theory.**

Fundamental example 4: the Sobolev spaces $H^1(\mathbb{R}^d, \mathbb{C})$ and $H^2(\mathbb{R}^d, \mathbb{C})$.

- **The sets**

$$H^1(\mathbb{R}^d, \mathbb{C}) := \left\{ u \in L^2(\mathbb{R}^d, \mathbb{C}) \mid \nabla u \in (L^2(\mathbb{R}^d, \mathbb{C}))^d \right\},$$
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they are Hilbert spaces.

- **Technical detail: the gradient and the second derivatives are defined by means of distribution theory.**

Remark. Let $u \in H^1(\mathbb{R}^d)$. A function $\widetilde{u} \in H^1(\mathbb{R}^d)$ can be a very accurate approximation of u in $L^2(\mathbb{R}^d)$ and a terrible approximation of u in $H^1(\mathbb{R}^d)$.

For instance, let $u(x) = \frac{1}{1+x^2}$ and $u_n(x) = \left(1 + \frac{\sin(n^2 x^2)}{n}\right) u(x)$. The sequence $(u_n)_{n\in\mathbb{N}^*}$ converges to u in $L^2(\mathbb{R})$ and goes to infinity in $H^1(\mathbb{R})$.

Finite-dimensional complex Hilbert spaces

If there exists a finite family $(|\psi_1\rangle, \cdots, |\psi_N\rangle)$ **of vectors of** $\mathcal{H}$ **such that**

$$\forall |\psi\rangle \in \mathcal{H}, \quad \exists!(\alpha_1, \cdots, \alpha_N) \in \mathbb{C}^N \text{ such that } |\psi\rangle = \alpha_1|\psi_1\rangle + \cdots + \alpha_N|\psi_N\rangle,$$

then $\mathcal{H}$ **is called finite-dimensional and such a family is called a basis of** $\mathcal{H}$**.**

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Example: two bases of $\mathbb{C}^3$

$$\mathcal{B}_1 = \left(\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right) \quad \textbf{(canonical basis)}, \quad \mathcal{B}_2 = \left(\begin{pmatrix} 1/2 \\ 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 4 \\ 1 \end{pmatrix} \right).$$

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If $\mathcal{H}$ is finite-dimensional, then all the bases have the same number N of elements. This number is called the dimension of $\mathcal{H}$ and is denoted by $\dim(\mathcal{H})$.

In particular, $\boxed{\dim(\mathbb{C}^N) = N}$

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The basis $(|\psi_1\rangle, \cdots, |\psi_N\rangle)$ is called orthonormal if $\forall 1 \leq m, n \leq N,\ \langle\psi_m|\psi_n\rangle = \delta_{m,n}$.

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The basis $(|\psi_1\rangle, \cdots, |\psi_N\rangle)$ is called orthonormal if $\forall 1 \leq m, n \leq N,\ \langle\psi_m|\psi_n\rangle = \delta_{m,n}$.

Any non-orthonormal basis can be transformed into an orthonormal basis by the Gram-Schmidt orthonormalization process.

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If $\mathcal{H}$ is not finite-dimensional, it is called infinite-dimensional.

Example: $l^2(\mathbb{N}, \mathbb{C})$ is an infinite-dimensional Hilbert space.

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Example: $l^2(\mathbb{N},\mathbb{C})$ **is an infinite-dimensional Hilbert space.**

Nevertheless, $l^2(\mathbb{N},\mathbb{C})$ **possesses orthonormal bases in the following sense:**

- **let** $|0\rangle = (1,0,0,0,0,\cdots)$**,** $|1\rangle = (0,1,0,0,0,\cdots)$**,** $|2\rangle = (0,0,1,0,0,\cdots)$**, ...**
- **the family** $(|n\rangle)_{n\in\mathbb{N}}$ **of elements of** $l^2(\mathbb{N},\mathbb{C})$ **satisfies**

$$\langle m|n\rangle = \delta_{m,n} \qquad \textbf{(orthonormality)}$$

$$\forall |\psi\rangle \in l^2(\mathbb{N},\mathbb{C}), \qquad \|\psi\|^2 = \sum_{n\in\mathbb{N}} |\langle n|\psi\rangle|^2 \qquad \textbf{(Parseval relation)}$$

$$|\psi\rangle = \sum_{n\in\mathbb{N}} \langle n|\psi\rangle\, |n\rangle \qquad \textbf{(completeness)}$$

Separable Hilbert spaces

A Hilbert space $\mathcal{H}$ is called separable if it has a countable dense subset, that is if there exists a countable family $(\chi_n)_{n\in\mathbb{N}}$ of elements of $\mathcal{H}$ such that

$$\forall \psi \in \mathcal{H}, \quad \forall \varepsilon > 0, \quad \exists n \in \mathbb{N} \text{ s.t. } \|\psi - \chi_n\| \leq \varepsilon.$$

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Examples of separable Hilbert spaces:

- **all finite-dimensional Hilbert spaces are separable;**
- **$l^2(\mathbb{N}, \mathbb{C})$ is an infinite-dimensional separable Hilbert space;**
- **all the Hilbert spaces arising in QM (e.g. $L^2(\mathbb{R}^d, \mathbb{C})$, $H^1(\mathbb{R}^d, \mathbb{C})$) are separable.**

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- **all the Hilbert spaces arising in QM (e.g.** $L^2(\mathbb{R}^d, \mathbb{C})$**,** $H^1(\mathbb{R}^d, \mathbb{C})$**) are separable.**

Any infinite-dimensional separable Hilbert space $\mathcal{H}$ possesses orthonormal bases: there exists a countable family $(|e_n\rangle)_{n\in\mathbb{N}}$ of elements of $\mathcal{H}$ such that

$$\langle e_m | e_n \rangle = \delta_{m,n} \qquad \textbf{(orthonormality)}$$

$$\forall |\psi\rangle \in \mathcal{H}, \qquad \|\psi\|^2 = \sum_{n\in\mathbb{N}} |\langle e_n | \psi \rangle|^2 \qquad \textbf{(Parseval relation)}$$

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Unitary transforms

Let $\mathcal{H}$ and $\mathcal{K}$ be two Hilbert spaces. A mapping $U : \mathcal{H} \to \mathcal{K}$ is called a unitary operator if

- **U is a linear operator;**
- **U is invertible;**
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If a quantum system described by

- **the Hilbert space $\mathcal{H}$;**
- **observables A_1, A_2, ... (self-adjoint operators on $\mathcal{H}$),**

and if $U : \mathcal{H} \to \mathcal{K}$ is a unitary operator, then the physics of the system can be reformulated in a totally equivalent way using

- **the Hilbert space $\mathcal{K}$ (the ket $|\psi\rangle \in \mathcal{H}$ is transformed into $|\phi\rangle = U|\psi\rangle \in \mathcal{K}$);**
- **observables $B_1 = UA_1U^{-1}$, $B_2 = UA_2U^{-1}$, ... (self-adjoint operators on $\mathcal{K}$).**

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These two formulations correspond to two different representations of the same physical quantum system.

Fundamental example: one-dimensional quantum harmonic oscillator

	Position rep.	Momentum rep.	Energy rep.
Hilbert space	$\mathcal{H}_{\text{pos}} = L^2(\mathbb{R}, \mathbb{C})$		
Pure state	$\psi_{\text{pos}}(x)$		
Position op.	$x_{\text{pos}} = x$		
Momentum op.	$p_{\text{pos}} = -i\hbar\frac{d}{dx}$		
Kinetic energy op.	$T_{\text{pos}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$		
Potential energy op.	$V_{\text{pos}} = \frac{1}{2}\kappa x^2$		
Total energy op.	$H_{\text{pos}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\kappa x^2$		

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Pure state	$\psi_{\text{pos}}(x)$	$\psi_{\text{mom}}(p)$	
Position op.	$x_{\text{pos}} = x$	$x_{\text{mom}} = i\hbar \frac{d}{dp}$	
Momentum op.	$p_{\text{pos}} = -i\hbar \frac{d}{dx}$	$p_{\text{mom}} = p$	
Kinetic energy op.	$T_{\text{pos}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$	$T_{\text{mom}} = \frac{p^2}{2m}$	
Potential energy op.	$V_{\text{pos}} = \frac{1}{2}\kappa x^2$	$V_{\text{mom}} = -\frac{\hbar^2}{2}\kappa\frac{d^2}{dp^2}$	
Total energy op.	$H_{\text{pos}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\kappa x^2$	$H_{\text{mom}} = \frac{p^2}{2m} - \frac{\hbar^2}{2}\kappa\frac{d^2}{dp^2}$	

$$\psi_{\text{mom}}(p) = \left(U_{\text{pos}\to\text{mom}}\psi_{\text{pos}}\right)(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \psi_{\text{pos}}(x) e^{-i\,px/\hbar}\,dx \quad \textbf{(Fourier transform)}$$

Fundamental example: one-dimensional quantum harmonic oscillator

	Position rep.	Momentum rep.	Energy rep.
Hilbert space	$\mathcal{H}_{\rm pos} = L^2(\mathbb{R},\mathbb{C})$	$\mathcal{H}_{\rm mom} = L^2(\mathbb{R},\mathbb{C})$	$\mathcal{H}_{\rm e} = l^2(\mathbb{N},\mathbb{C})$
Pure state	$\psi_{\rm pos}(x)$	$\psi_{\rm mom}(p)$	$\lvert\psi_{\rm e}\rangle = \sum_{n\in\mathbb{N}} \psi_{{\rm e},n}\lvert n\rangle$
Position op.	$x_{\rm pos} = x$	$x_{\rm mom} = i\hbar\frac{d}{dp}$	$x_{\rm e} = \left(\frac{\hbar}{2}\frac{1}{m\omega}\right)^{1/2}(a^\dagger + a)$
Momentum op.	$p_{\rm pos} = -i\hbar\frac{d}{dx}$	$p_{\rm mom} = p$	$p_{\rm e} = i\left(\frac{\hbar}{2}m\omega\right)^{1/2}(a^\dagger - a)$
Kinetic energy op.	$T_{\rm pos} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$	$T_{\rm mom} = \frac{p^2}{2m}$	$T_{\rm e} = -\frac{\hbar\omega}{4}(a^\dagger - a)^2$
Potential energy op.	$V_{\rm pos} = \frac{1}{2}\kappa x^2$	$V_{\rm mom} = -\frac{\hbar^2}{2}\kappa\frac{d^2}{dp^2}$	$V_{\rm e} = \frac{\hbar\omega}{4}(a^\dagger + a)^2$
Total energy op.	$H_{\rm pos} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\kappa x^2$	$H_{\rm mom} = \frac{p^2}{2m} - \frac{\hbar^2}{2}\kappa\frac{d^2}{dp^2}$	$H_{\rm e} = \sum(n+\frac{1}{2})\hbar\omega\lvert n\rangle\langle n\rvert$

$|0\rangle = (1,0,0,0,\cdots)$, $|1\rangle = (0,1,0,0,\cdots)$, $|2\rangle = (0,0,1,0,\cdots),\cdots$, $\omega = \sqrt{\frac{k}{m}}$, $a^\dagger|n\rangle = \sqrt{n+1}\,|\,n{+}1\rangle$, $a|n\rangle = \sqrt{n}\,|\,n{-}1\rangle$

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Position op.	$x_{\text{pos}} = x$	$x_{\text{mom}} = i\hbar \frac{d}{dp}$	$x_{\text{e}} = \left(\frac{\hbar}{2}\frac{1}{m\omega}\right)^{1/2} (a^\dagger + a)$
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$$U_{\text{pos}\to\text{e}} = \sum_{n\in\mathbb{N}} |n\rangle\langle\phi_{\text{pos},n}|, \qquad \phi_{\text{pos},n}(x) = \frac{1}{\sqrt{2^n\, n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega x^2}{2\hbar}}, \qquad H_n(z) = (-1)^n\, e^{z^2} \frac{d^n}{dz^n}\left(e^{-z^2}\right).$$

2 - Self-adjoint operators

Notation: in this section, $\mathcal{H}$ denotes a separable complex Hilbert space, $\langle \cdot | \cdot \rangle$ its inner product, and $\| \cdot \|$ the associated norm.

Bounded linear operators on Hilbert spaces

Definition-Theorem (bounded linear operator). A bounded operator on $\mathcal{H}$ is a linear map $A : \mathcal{H} \to \mathcal{H}$ such that

$$\|A\| := \sup_{u \in \mathcal{H} \setminus \{0\}} \frac{\|Au\|}{\|u\|} < \infty.$$

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Definition-Theorem (adjoint of a bounded linear operator). Let $A \in \mathcal{B}(\mathcal{H})$. The operator $A^* \in \mathcal{B}(\mathcal{H})$ defined by

$$\forall (u, v) \in \mathcal{H} \times \mathcal{H}, \quad \langle u|A^*v\rangle = \langle Au|v\rangle,$$

is called the adjoint of A.

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Endowed with its norm $\|\cdot\|$ and the $*$ operation, $\mathcal{B}(\mathcal{H})$ is a C*-algebra.

(Non necessarily bounded) linear operators on Hilbert spaces

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Definition (linear operator). A linear operator on $\mathcal{H}$ is a linear map $A : D(A) \to \mathcal{H}$, where $D(A)$ is a subspace of $\mathcal{H}$ called the domain of A.

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Definition (extensions of operators). Let A_1 and A_2 be operators on $\mathcal{H}$. A_2 is called an extension of A_1 if $D(A_1) \subset D(A_2)$ and if $\forall u \in D(A_1)$, $A_2 u = A_1 u$.

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Symmetric operators are not very interesting. Only self-adjoint operators represent physical observables and have nice mathematical properties:

- **real spectrum;**
- **spectral decomposition and functional calculus.**

Definition (adjoint of a linear operator with dense domain). Let A be a linear operator on $\mathcal{H}$ with dense domain $D(A)$, and $D(A^*)$ the vector space defined as

$$D(A^*) = \{v \in \mathcal{H} \mid \exists w_v \in \mathcal{H} \text{ s.t. } \forall u \in D(A),\ \langle Au|v\rangle = \langle u|w_v\rangle\}\,.$$

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Case of unbounded operators:

symmetric (easy to check) $\begin{matrix}\Rightarrow\\ \Leftarrow\end{matrix}$ **self-adjoint (sometimes difficult to check)**

Some unbounded self-adjoint operators arising in quantum mechanics

- **position operator along the j axis:**
  - $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C})$,
  - $D(\widehat{r}_j) = \left\{u \in L^2(\mathbb{R}^d, \mathbb{C}) \mid r_j u \in L^2(\mathbb{R}^d, \mathbb{C})\right\}$, $(\widehat{r}_j \phi)(\mathbf{r}) = r_j \phi(\mathbf{r})$;
- **momentum operator along the j axis:**
  - $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C})$,
  - $D(\widehat{p}_j) = \left\{u \in L^2(\mathbb{R}^d, \mathbb{C}) \mid \partial_{r_j} u \in L^2(\mathbb{R}^d, \mathbb{C})\right\}$, $(\widehat{p}_j \phi)(\mathbf{r}) = -i\partial_{r_j} \phi(\mathbf{r})$;
- **kinetic energy operator:**
  - $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C})$,
  - $D(T) = H^2(\mathbb{R}^d, \mathbb{C}) = \left\{u \in L^2(\mathbb{R}^d, \mathbb{C}) \mid \Delta u \in L^2(\mathbb{R}^d, \mathbb{C})\right\}$, $T = -\frac{1}{2}\Delta$;
- **Schrödinger operators in 3D: let $V \in L^2_{\text{unif}}(\mathbb{R}^3, \mathbb{R})$ ($V(\mathbf{r}) = -\frac{Z}{|\mathbf{r}|}$ OK)**
  - $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C})$,
  - $D(H) = H^2(\mathbb{R}^3, \mathbb{C})$, $H = -\frac{1}{2}\Delta + V$.

3 - Spectra of self-adjoint operators

Notation: **in this section, $\mathcal{H}$ denotes a separable complex Hilbert space, $\langle \cdot | \cdot \rangle$ its inner product, and $\| \cdot \|$ the associated norm.**

Definition-Theorem (spectrum of a linear operator). Let A be a closed[1] linear operator on $\mathcal{H}$.

- **The open set $\rho(A) = \{z \in \mathbb{C} \mid (z - A) : D(A) \to \mathcal{H}$ invertible$\}$ is called the resolvent set of A.**

[1] **The operator A is called closed if its graph $\Gamma(A) := \{(u, Au),\ u \in D(A)\}$ is a closed subspace of $\mathcal{H} \times \mathcal{H}$.**

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- **The closed set $\sigma(A) = \mathbb{C} \setminus \rho(A)$ is called the spectrum of A.**

- **If A is self-adjoint, then $\sigma(A) \subset \mathbb{R}$ and it holds $\sigma(A) = \sigma_{\rm p}(A) \cup \sigma_{\rm c}(A)$, where $\sigma_{\rm p}(A)$ and $\sigma_{\rm c}(A)$ are respectively the point spectrum and the continuous spectrum of A defined as**

$$\sigma_{\rm p}(A) = \{z \in \mathbb{C} \mid (z - A) : D(A) \to \mathcal{H} \text{ non-injective}\} = \{\text{eigenvalues of } A\}$$

$$\sigma_{\rm c}(A) = \overline{\{z \in \mathbb{C} \mid (z - A) : D(A) \to \mathcal{H} \text{ injective but non surjective}\}}.$$

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$\mathcal{H}_{\mathrm{p}}$: **set of bound states,** $\mathcal{H}_{\mathrm{c}}$: **set of scattering states**

Diagonalizable self-adjoint operators and Dirac's bra-ket notation

Let A be a self-adjoint operator that can be diagonalized in an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ (this is not the case for many useful self-adjoint operators!).

Dirac's bra-ket notation: $$A = \sum_{n\in\mathbb{N}} \lambda_n |e_n\rangle\langle e_n|, \quad \lambda_n \in \mathbb{R}, \quad \langle e_m|e_n\rangle = \delta_{mn}.$$

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- **functional calculus for diagonalizable self-adjoint operators: for all $f : \mathbb{R} \to \mathbb{C}$, the operator $f(A)$ defined by**

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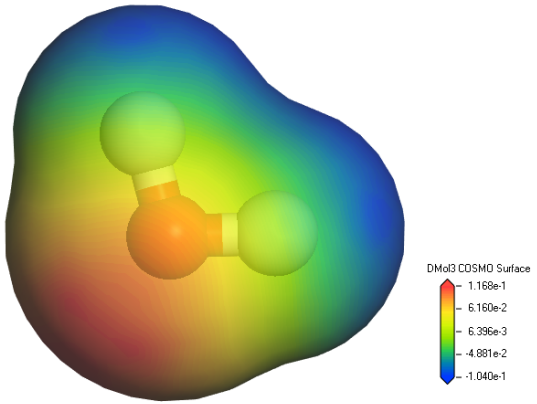
is independent of the choice of the spectral decomposition of A.

Electronic problem for a given nuclear configuration $\{\mathrm{R}_k\}_{1\leq k\leq M}$



Ex: water molecule $\mathrm{H_2O}$

$M = 3$, $N = 10$, $z_1 = 8$, $z_2 = 1$, $z_3 = 1$

$$v_{\mathrm{ext}}(\mathbf{r}) = -\sum_{k=1}^{M} \frac{z_k}{|\mathbf{r} - \mathbf{R}_k|}$$

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$$\forall p \in \mathfrak{S}_N, \quad \Psi(\mathbf{r}_{p(1)}, \cdots, \mathbf{r}_{p(N)}) = \varepsilon(p)\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N), \qquad \textbf{(Pauli principle)}$$

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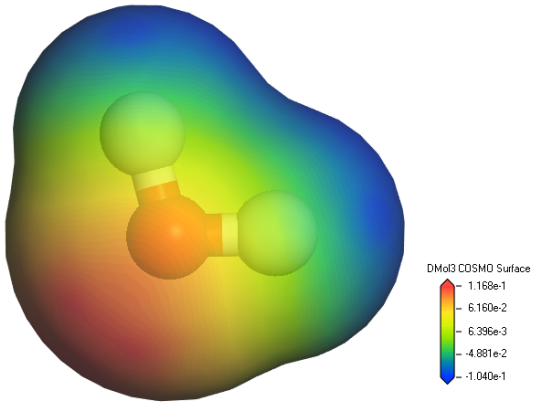

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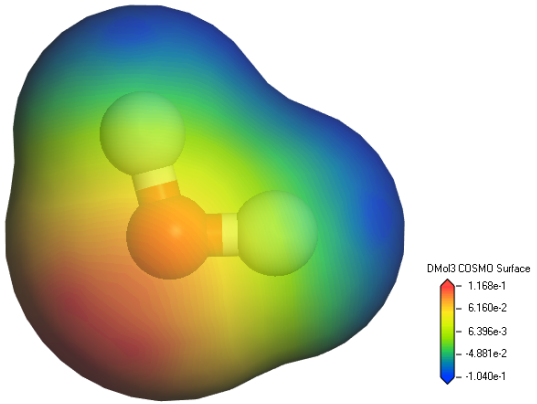

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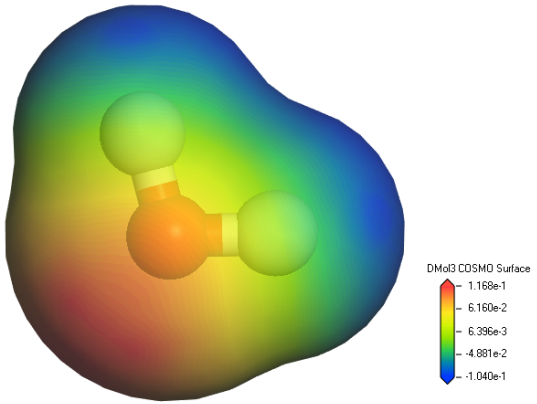
$$\Psi \in \mathcal{H}_N = \bigwedge^N \mathcal{H}_1, \qquad \mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C}^2) \quad \textbf{with spin}$$

Electronic problem for a given nuclear configuration $\{\mathbf{R}_k\}_{1\le k\le M}$



Ex: water molecule H_2O

$M = 3$, $N = 10$, $z_1 = 8$, $z_2 = 1$, $z_3 = 1$

$$v_{\text{ext}}(\mathbf{r}) = -\sum_{k=1}^{M} \frac{z_k}{|\mathbf{r} - \mathbf{R}_k|}$$

$$\left(-\frac{1}{2}\sum_{i=1}^{N} \Delta_{\mathbf{r}_i} + \sum_{i=1}^{N} v_{\text{ext}}(\mathbf{r}_i) + \sum_{1\le i<j\le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \right) \Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N) = E\, \Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)$$

$|\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)|^2$ **probability density of observing electron 1 at $\mathbf{r}_1$, electron 2 at $\mathbf{r}_2$, ...**

$$\Psi \in \mathcal{H}_N = \bigwedge^N \mathcal{H}_1, \qquad \mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C})$$

Theorem (Kato '51). The operator $H_N := -\frac{1}{2}\sum_{i=1}^{N} \Delta_{\mathbf{r}_i} + \sum_{i=1}^{N} v_{\text{ext}}(\mathbf{r}_i) + \sum_{1\le i<j\le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$

with domain $D(H_N) := \mathcal{H}_N \cap H^2(\mathbb{R}^{3N}, \mathbb{C})$ **is self-adjoint on** $\mathcal{H}_N$**.**

Theorem (spectrum of H_N).

1. HVZ theorem (Hunziger '66, van Winten '60, Zhislin '60)

$\sigma_{\rm c}(H_N) = [\Sigma_N, +\infty)$ **with** $\Sigma_N = \min \sigma(H_{N-1}) \leq 0$ **and** $\Sigma_N < 0$ **iff** $N \geq 2$.

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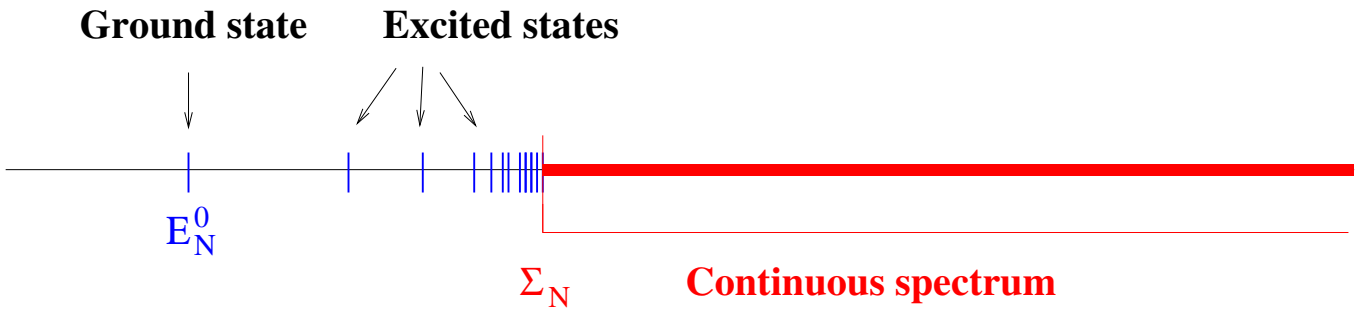
2. Bound states of neutral molecules and positive ions (Zhislin '61)

If $N \leq Z := \sum_{k=1}^{M} z_k$**, then** H_N **has an infinite number of bound states**.



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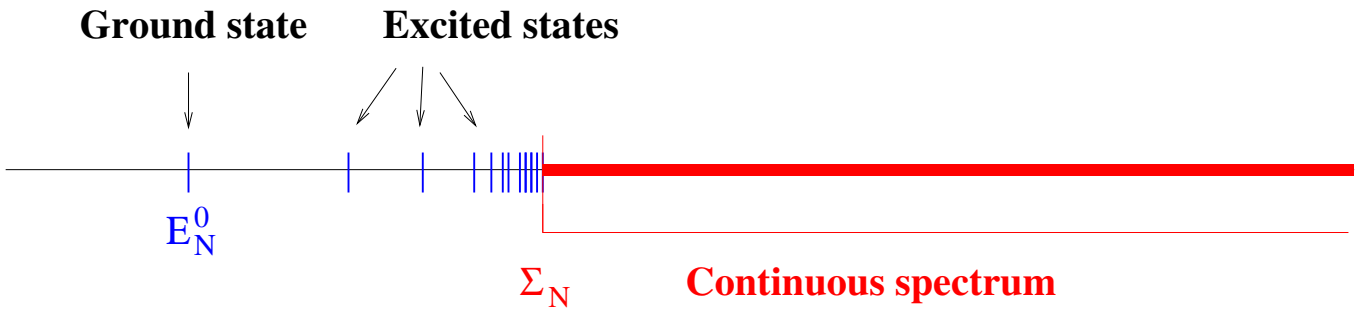

3. Bound states of negative ions (Yafaev '72)

If $N \geq Z + 1$**, then** H_N **has at most a finite number of bound states.**

Spectra of Schrödinger operators with confining potentials

$$\mathcal{H} = L^2(\mathbb{R}^d), \qquad V \in C^0(\mathbb{R}^d, \mathbb{R}), \qquad \lim_{|\mathbf{r}|\to+\infty} V(\mathbf{r}) = +\infty \textbf{ (confining potential)}$$

$$D(H) = \left\{ u \in L^2(\mathbb{R}^d) \mid -\frac{1}{2}\Delta u + Vu \in L^2(\mathbb{R}^d) \right\}, \quad \forall u \in D(H),\ Hu = -\frac{1}{2}\Delta u + Vu.$$

H is bounded below and its spectrum is purely discrete ($\sigma_{\rm d}(H) = \sigma(H)$, $\sigma_{\rm c}(H) = \emptyset$).

As a consequence, H is diagonalizable in a orthonormal basis: there exist

- **a non-decreasing sequence $(E_n)_{n\in\mathbb{N}}$ of real numbers going to $+\infty$;**
- **an orthonormal basis $(\psi_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$ composed of vectors of $D(H)$,**

such that

$$\forall n \in \mathbb{N}, \quad H\psi_n = E_n\psi_n.$$

In addition, the ground state eigenvalue E_0 is non-degenerate and the corresponding eigenvector can be chosen positive on $\mathbb{R}^d$.

Spectra of 3D Schrödinger operators with potentials decaying at infinity

V **such that** $\forall \varepsilon > 0,\ \exists (V_2, V_\infty) \in L^2(\mathbb{R}^3, \mathbb{R}) \times L^\infty(\mathbb{R}^3, \mathbb{R})$ **s.t.** $V = V_2 + V_\infty$ **and** $\|V_\infty\|_{L^\infty} \leq \varepsilon$,

$$\mathcal{H} = L^2(\mathbb{R}^3), \qquad D(H) = H^2(\mathbb{R}^3), \qquad \forall u \in D(H),\ Hu = -\frac{1}{2}\Delta u + Vu.$$

The operator H **is self-adjoint, bounded below, and** $\sigma_{\mathrm{c}}(H) = [0, +\infty)$**.**

Depending on V**, the discrete spectrum of** H **may be**

- **the empty set;**
- **a finite number of negative eigenvalues;**
- **a countable infinite number of negative eigenvalues accumulating at** 0 **(ex: Ridberg states).**

If H **has a ground state, then its energy is a non-degenerate eigenvalue and the corresponding eigenvector can be chosen positive on** $\mathbb{R}^d$**.**

The special case of Kohn-Sham LDA Hamiltonians

$$H_\rho = -\frac{1}{2}\Delta + V_\rho^{\mathrm{KS}} \quad \textbf{with} \quad V_\rho^{\mathrm{KS}}(\mathbf{r}) = -\sum_{k=1}^{M} \frac{z_k}{|\mathbf{r}-\mathbf{R}_k|} + \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}' + \frac{de_{\mathrm{xc}}^{\mathrm{LDA}}}{d\rho}(\rho(\mathbf{r}))$$

For any $\rho \in L^1(\mathbb{R}^3,\mathbb{R}) \cap L^3(\mathbb{R}^3,\mathbb{R})$, the KS potential V_ρ^{KS} satisfies the assumptions in the previous slide. In particular H_ρ is bounded below and $\sigma_{\mathrm{c}}(H_\rho) = [0,+\infty)$.

Let $Z = \sum_{k=1}^{M} z_k$ be the total nuclear charge of the molecular system and $N = \int_{\mathbb{R}^3} \rho$.

- **If $N < Z$ (positive ion), H_ρ has a countable infinite number of negative eigenvalues accumulating at 0.**
- **If $N = Z$ (neutral molecular system) and if ρ is a ground state density of the system, then H_ρ has at least N non-positive eigenvalues.**

Spectra of Hartree-Fock Hamiltonians

Let $\Phi = (\phi_1, \cdots, \phi_N) \in (H^1(\mathbb{R}^3))^N$ **be such that** $\displaystyle\int_{\mathbb{R}^3} \phi_i^* \phi_j = \delta_{ij}$**,**

$$\gamma(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^{N} \phi_i(\mathbf{r}) \phi_i(\mathbf{r}')^*, \qquad \rho_\gamma(\mathbf{r}) = \gamma(\mathbf{r}, \mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2.$$

$$\mathcal{H} = L^2(\mathbb{R}^3), \quad D(H) = H^2(\mathbb{R}^3),$$

$$(H\phi)(\mathbf{r}) = -\frac{1}{2}\Delta\phi(\mathbf{r}) - \sum_{k=1}^{M} \frac{z_k}{|\mathbf{r} - \mathbf{R}_k|}\phi(\mathbf{r}) + \left(\int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}' \right) \phi(\mathbf{r}) - \int_{\mathbb{R}^3} \frac{\gamma(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\, \phi(\mathbf{r}')\, d\mathbf{r}'$$

Let $Z := \sum_{k=1}^{M} z_k$**. The operator** H **is self-adjoint, bounded below, and we have:**

- $\sigma_{\text{ess}} = [0, +\infty)$**;**
- **if** $N < Z$ **(positive ion),** H **has a countable infinite number of negative eigenvalues accumulating at** 0**;**
- **if** $N = Z$ **(neutral molecular system) and if** Φ **is a HF minimizer of the system, then** H **has at least** N **negative eigenvalues (counting multiplicities).**

Spectra of Dirac Hamiltonians

$$\mathcal{H} = L^2(\mathbb{R}^3;\mathbb{C}^4), \qquad D(D_0) = H^1(\mathbb{R}^3;\mathbb{C}^4), \qquad D_0 = c\vec{p}\cdot\vec{\alpha} + mc^2\beta$$

$$p_j = -\mathrm{i}\hbar\partial_j, \qquad \alpha_j = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \in \mathbb{C}^{4\times 4}, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix} \in \mathbb{C}^{4\times 4}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \textbf{(Pauli matrices)}$$

The free Dirac operator D_0 is self-adjoint and

$$\sigma(D_0) = \sigma_{\mathrm{ac}}(D_0) = (-\infty, -mc^2] \cup [mc^2, +\infty).$$

Theorem. **Let** $\alpha := \frac{e^2}{4\pi\varepsilon_0\hbar c} \simeq 1/137.036$ **be the fine structure constant. Let**

$$D_Z = D_0 - \frac{Z}{|\mathbf{r}|}, \qquad Z \in \mathbb{R} \quad \textbf{(physical cases: } Z = 1, 2, 3, \cdots\textbf{)}.$$

- **if** $|Z| < \frac{\sqrt{3}}{2\alpha} \simeq 118.677$**, the Dirac operator** D_Z **is essentially self-adjoint (meaning that there exists a unique domain** $D(D_Z)$ **containing** $C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)$ **for which** D_Z **is self-adjoint);**
- **if** $|Z| > \frac{\sqrt{3}}{2\alpha} \simeq 118.677$**,** D_Z **has many self-adjoint extensions;**
- **if** $|Z| < \frac{1}{\alpha} \simeq 137.036$**,** D_Z **has a special self-adjoint extension, considered as the physical one. The essential spectrum of this self-adjoint extension is** $(-\infty, -mc^2] \cup [mc^2, +\infty)$ **and its discrete spectrum consist of the eigenvalues**

$$E_{nj} = mc^2 \left[1 + \left(\frac{Z\alpha}{n - j - \frac{1}{2} + \sqrt{(j+\frac{1}{2})^2 - Z^2\alpha^2}} \right)^2 \right]^{-1/2}, \quad n \in \mathbb{N}^*, \ j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots \leq n - \frac{1}{2}.$$

Many-body Dirac-Coulomb Hamiltonian are not understood mathematically.

4 - Functional calculus

Notation: **in this section, $\mathcal{H}$ denotes a separable complex Hilbert space, $\langle \cdot | \cdot \rangle$ its inner product, and $\| \cdot \|$ the associated norm.**

Theorem (functional calculus for bounded functions). Let $\mathfrak{B}(\mathbb{R},\mathbb{C})$ be the $*$-algebra of bounded $\mathbb{C}$-valued Borel functions on $\mathbb{R}$ and let A be a self-adjoint operator on $\mathcal{H}$. Then there exists a unique map

$$\Phi_A : \mathfrak{B}(\mathbb{R},\mathbb{C}) \ni f \mapsto f(A) \in \mathcal{B}(\mathcal{H})$$

satisfies the following properties:

1. **Φ_A is a homomorphism of $*$-algebras:**

$$(\alpha f+\beta g)(A) = \alpha f(A)+\beta g(A), \quad (fg)(A) = f(A)g(A), \quad \overline{f}(A) = f(A)^*;$$

2. $\|f(A)\| \leq \sup_{x\in\mathbb{R}} |f(x)|$**;**

3. **if $f_n(x) \to x$ pointwise and $|f_n(x)| \leq |x|$ for all n and all $x \in \mathbb{R}$, then**

$$\forall u \in D(A), \quad f_n(A)u \to Au \text{ in } \mathcal{H};$$

4. **if $f_n(x) \to f(x)$ pointwise and $\sup_n \sup_{x\in\mathbb{R}} |f_n(x)| < \infty$, then**

$$\forall u \in \mathcal{H}, \quad f_n(A)u \to f(A)u \text{ in } \mathcal{H};$$

In addition, if $u \in \mathcal{H}$ is such that $Au = \lambda u$, then $f(A)u = f(\lambda)u$.

Theorem (spectral projections and functional calculus - general case -).

Let A be a self-adjoint operator on $\mathcal{H}$.

- **For all $\lambda \in \mathbb{R}$, the bounded operator $P_\lambda^A := \mathbb{1}_{]-\infty,\lambda]}(A)$, where $\mathbb{1}_{]-\infty,\lambda]}(\cdot)$ is the characteristic function of $]-\infty, \lambda]$, is an orthogonal projection.**

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- **Spectral decomposition of A: for all $u \in D(A)$ and $v \in \mathcal{H}$, it holds**

$$\langle v|Au\rangle = \int_{\mathbb{R}} \lambda \underbrace{d\langle v|P_\lambda^A u\rangle}_{\text{Bounded complex measure on } \mathbb{R}}, \quad \textbf{which we denote by} \quad A = \int_{\mathbb{R}} \lambda \, dP_\lambda^A.$$

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- **Functional calculus: let f be a (not necessarily bounded) $\mathbb{C}$-valued Borel function on $\mathbb{R}$. The operator $f(A)$ can be defined by**

$$D(f(A)) := \left\{ u \in \mathcal{H} \mid \int_{\mathbb{R}} |f(\lambda)|^2 \underbrace{d\langle u|P_\lambda^A u\rangle}_{\text{Bounded positive measure on } \mathbb{R}} < \infty \right\}$$

and

$$\forall (u,v) \in D(f(A)) \times \mathcal{H}, \ \langle v|f(A)u\rangle := \int_{\mathbb{R}} f(\lambda) \, d\langle v|P_\lambda^A u\rangle.$$

Theorem (form domain and quadratic form).

Let A be a self-adjoint operator on $\mathcal{H}$.

- **The set**

$$Q(A)) := \left\{ \psi \in \mathcal{H} \mid \int_{\mathbb{R}} |\lambda| \underbrace{d\langle \psi | P_\lambda^A \psi \rangle}_{\text{Bounded positive measure on } \mathbb{R}} < \infty \right\}$$

  is a vector space, called the form domain of A, and we have

$$D(A) \hookrightarrow Q(A) \hookrightarrow \mathcal{H}$$

  with dense embeddings.

- **The mapping defined by**

$$\forall \psi \in Q(A), \quad \langle \psi | A | \psi \rangle = \int_{\mathbb{R}} \lambda \underbrace{d\langle \psi | P_\lambda^A \psi \rangle}$$

  is called the quadratic form associated with A.

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- **B. Helffer, *Spectral theory and its applications*, Cambridge University Press 2013.**
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