Quantum Mechanics I

Mathematical Prerequisites

Linear Vector Spaces
Linear Self-Adjoint Operators

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Pink Floyd: "Another Brick in the Wall (Pt. II)"

Mathematical Prerequisites

Linear Vector Spaces

- The definition has a pre-requisite
- Ground field is a collection of numbers ($\alpha,\beta,\gamma,\ldots$) for which:
  - addition gives a group: $\alpha+\beta$, $\alpha+0=\alpha$, $\alpha+(-\alpha)=0$, $(\alpha+\beta)+\gamma=\alpha+(\beta+\gamma)$
  - multiplication ($\alpha\neq0$) gives a group: $\alpha\cdot\beta$, $\alpha\cdot1=\alpha$, $\alpha\cdot(1/\alpha)=1$, $(\alpha\cdot\beta)\cdot\gamma=\alpha\cdot(\beta\cdot\gamma)$
  - multiplication distributes accross addition: $\alpha\cdot(\beta+\gamma) = \alpha\cdot\beta + \alpha\cdot\gamma$
- For Quantum Mechanics, the ground field will be $\mathbb{C}$
- A $\mathbb{C}$-Linear vector space V is a collection of objects v_i,
  - such that all $\mathbb{C}$-linear combinations $\Sigma_i\, \alpha_i\, v_i$ are also in V.
  - E.g., solutions of linear differential equations form a vector space.
    - E.g., Maxwell's EM equations; superpositions of the E- and B-fields
- Linearly independent: $\alpha_1\, v_1 + \alpha_2\, v_2 = 0$ only if $\alpha_1 = 0 = \alpha_2$
- Basis: the smallest number of vectors $\{v_1, v_2,\ldots, v_d\}$ such that
  - $v = \Sigma_{1\leq i\leq d}\, \alpha_i\, v_i$ for each $v \in V$; $d = \dim(V)$.

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Linear Vector Spaces

- Example: V = all linear combinations of e^x, e^{2x} and $e^x(e^x-1)$
  - A basis: $\{e^x, e^{2x}\}$ since $\alpha_1 e^x + \alpha_2 e^{2x} = 0$ (for all x) only if $\alpha_1 = 0 = \alpha_2$
  - and $c_1 e^x + c_2 e^{2x} + c_3 e^x(e^x-1) = (c_1-c_3)e^x + (c_2+c_3)e^{2x}$.
- Linear vector spaces may be
  - Finite: dim(V) < ∞, e.g., 3D real vectors
  - Discrete: dim(V) = ∞ but V-bases are countable, e.g., guitar string
  - Continuous: dim(V) = ∞ but V-basis are uncountable, e.g., all differentiable functions
  - Also, span(v_1, v_2, v_3) = vector space of all linear combinations of v_1, v_2, v_3
- In QM, all three occur, and quite regularly
- We will write, formally:
  - $\{\phi_n\}$ for a basis of the linear vector space and $\Sigma_n\, c_n\, \phi_n$ of a superposition, regardless whether n is finite, discrete or continuous
  - Where necessary, remark on any subtleties incurred by this

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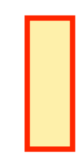
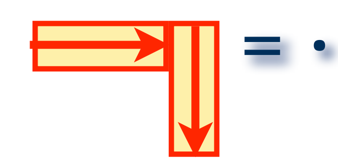
Linear Vector Spaces

- A scalar product (χ,ψ) is a 2-argument function such that:
  - a: (χ,ψ) is a complex scalar
  - b: $(\psi,\chi) = (\chi,\psi)^*$
  - c: $(\chi, c_1\psi_1 + c_2\psi_2) = c_1(\chi,\psi_1) + c_2(\chi,\psi_2)$
  - d: $(\psi,\psi) \geq 0$, and $(\psi,\psi) = 0$ only if $\psi = 0$
  - Together, (b) and (c) imply $(c_1\chi_1 + c_2\chi_2, \psi) = c_1^*(\chi_1,\psi) + c_2^*(\chi_2,\psi)$
- For discrete (countable) vector spaces,
  - a vector ψ is a column-vector with components ψ_i 
  - $(\chi,\psi) = (\text{row-}\chi)\cdot(\text{column-}\psi) = \sum_i \chi_i^* \psi_i$



- For continuous (uncountable) vector spaces,
  - a vector ψ is a function with "components" $\psi(x)$
  - $(\chi,\psi) = \int dx\, w(x)\, \chi^*(x)\, \psi(x)$, where $w(x) \geq 0$ is a weight-function
    - $w(x) > 0$, except $w(x) = 0$ at isolated points

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Linear Vector Spaces

- Using (*d*), we *define* the norm: $\|\psi\| \equiv (\psi,\psi)^{1/2}$
- Two vectors are orthogonal w.r. to a given scalar product
  - if the scalar product vanishes $(\chi,\psi) = 0$
  - May also define the angle $\measuredangle_{\chi,\psi} \equiv \cos^{-1}[(\chi,\psi)/(\|\chi\|\,\|\psi\|)]$
  - A set of vectors (or a basis) is orthogonal if $(\psi_i,\psi_j) = 0$ for $i \neq j$
  - A set of vectors (or a basis) is orthonormal if $(\psi_i,\psi_j) = \delta_{ij}$
    - The latter case implicitly requires a Dirac delta-symbol
- Two standard inequalities:
  - Schwarz's inequality: $|(\chi,\psi)| \leq \|\chi\|\,\|\psi\|$
  - Triangle inequality: $\|(\chi+\psi)\| \leq \|\chi\|+\|\psi\|$

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Linear Vector Spaces

- For each V, there is a *dual* space of linear functionals on V
  - A functional assigns to each vector a scalar $F[\psi] \in \mathbb{C}$
  - A functional is linear if $F[c_1\psi_1+c_2\psi_2] = c_1 F[\psi_1] + c_2 F[\psi_2]$
  - Functionals themselves form a vector space, $V°$, by defining
    - $(C_1 F_1 + C_2 F_2)[\psi] \equiv C_1 F_1[\psi] + C_2 F_2[\psi]$
- Riesz theorem: there is an isomorphism $V \leftrightarrow V°$ such that $X[\psi] = (\chi,\psi)$.
  - Clearly, χ defines $X[\ldots] = (\chi,\ldots)$
  - In turn, $X[\ldots]$ defines $\chi = \sum_i (F[\psi_i])^* \psi_i$ w.r.t. to any basis $\{\psi_i\}$
- Dirac notation: $\psi \to |\psi\rangle$ and $X[\ldots] = (\chi,\ldots) \to \langle\chi|$
  - Then $(\chi,\psi) = \langle\chi|\psi\rangle$
  - However, for infinite-dimensional vector spaces, subtleties may force us to consider rigged Hilbert space triples
  - where there are more bras than kets

Mathematical Prerequisites

Linear Self-Adjoint Operators

- An operator acts on a vector and produces a vector
  - Domain = all vectors on which an operator is defined to act
  - An operator is linear if $F(c_1\psi_1+c_2\psi_2) = c_1(F\psi_1) + c_2(F\psi_2)$
  - $A = B$ means that $A\psi = B\psi$ for all ψ in the common domain
- Operator algebra
  - Sum: $(A+B)\psi = A\psi + B\psi$
  - Product: $AB\psi = A\circ B\psi = A(B\psi)$; $A(BC) = (AB)C$ but $AB \neq BA$
  - In a discrete vector space, operators are matrices
  - Operatorial identities $\frac{\partial}{\partial x}x = \mathbb{1} + x\frac{\partial}{\partial x}$
  - mean $\frac{\partial}{\partial x}x\psi(x) = \mathbb{1}\psi(x) + x\frac{\partial}{\partial x}\psi(x)$
- Action to left: $(\langle\chi|A)|\psi\rangle := \langle\chi|A|\psi\rangle \quad \forall\langle\chi|,|\psi\rangle$

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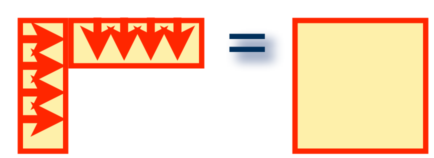
Linear Self-Adjoint Operators

- The trace: $\mathrm{Tr}(A) := \sum_j \langle\psi_i|A|\psi_i\rangle$
  - is cyclic: $\mathrm{Tr}(AB\cdots C) = \mathrm{Tr}(B\cdots CA)$ $\quad \mathrm{Tr}(AB) = \mathrm{Tr}(BA)$
  - For operators on finite vector spaces, Tr = sum of diagonal elements
  - For operators on infinite vector spaces, Tr = sum must converge
- Adjoint: $\langle\chi|\, A^\dagger \,|\psi\rangle := \langle\psi|\, A \,|\chi\rangle^* \quad \forall \langle\chi|, |\psi\rangle$
  - Properties: $(cA)^\dagger = c^* A^\dagger \quad c \in \mathbb{C}$ $\quad (A+B)^\dagger = A^\dagger + B^\dagger$ $\quad (AB)^\dagger = B^\dagger A^\dagger$
- Exterior product $|\psi\rangle\langle\chi|$  $\left(|\psi\rangle\langle\chi|\right)^\dagger = |\chi\rangle\langle\psi|$

  is an operator
- Self-Adjoint: $\langle\chi|\, A^\dagger \,|\psi\rangle \overset{!}{=} \langle\chi|\, A \,|\psi\rangle \quad \forall \langle\chi|, |\psi\rangle$

$$\langle\psi|\, A \,|\chi\rangle^* \overset{!}{=} \langle\psi|\, A^\dagger \,|\chi\rangle$$

Just like a Hermitian conjugate of a matrix $M_{ij} = (M_{ji})^*$

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Linear Self-Adjoint Operators

- Thm.1: $\langle\psi|A|\psi\rangle = \langle\psi|A|\psi\rangle^* \quad \Rightarrow \quad \langle\psi_1|A|\psi_2\rangle = \langle\psi_2|A|\psi_1\rangle^*$ (no dagger!)
- Definition: $A|\alpha_n\rangle = \alpha_n|\alpha_n\rangle$ ($|\alpha_n\rangle$: eigenvector, α_n: eigenvalue)
- Thm.2: If $A = A^\dagger$, then all eigenvalues are real.
- Thm.3: If $A = A^\dagger$, then eigenvectors of distinct eigenvalues are orthogonal.
- Definition: a set of vectors (w/prop.X) is complete, then all vectors (w/prop.X) can be written as a linear combination
- Formally: $\{|\psi_i\rangle\}$ complete $\Rightarrow \quad \sum_i |\psi_i\rangle\langle\psi_i| = \mathbb{1}$
  - Indeed:

$$|\chi\rangle = \mathbb{1}|\chi\rangle = \sum_i |\psi_i\rangle\langle\psi_i||\chi\rangle = \sum_i |\psi_i\rangle \underbrace{\langle\psi_i|\chi\rangle}_{:=c_i}$$

$$= \sum_i c_i|\psi_i\rangle \qquad c_i := \langle\psi_i|\chi\rangle$$

$\boldsymbol{\Pi}_i := |\psi_i\rangle\langle\psi_i|$

$\boldsymbol{\Pi}_i\boldsymbol{\Pi}_i = \boldsymbol{\Pi}_i$

projectors

The Fourier theorem, generalized

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Linear Self-Adjoint Operators

- Thm.π: If $A^\dagger = A \quad A|n\rangle = a_n|n\rangle, \quad \langle n|m\rangle = \delta_{nm} \quad \sum_n |n\rangle\langle n| = \mathbb{1}$
- then $$A = \sum_n a_n |n\rangle\langle n| \qquad f(A) := \sum_n f(a_n)|n\rangle\langle n|$$
- Caveat: The existence and completeness of eigenvectors strongly depends on boundary conditions. [p.18–20]
- How so?
  - Consider $\partial_x := \partial/\partial x$ and know that e^{ax} are eigenfunctions: $\partial_x e^{ax} = a\,e^{ax}$
  - Is ∂_x self-adjoint?
    No: $\int_a^b dx\, f^*(x)\,[\partial_x g(x)] = [f^*(x)g(x)]_a^b - \int_a^b dx\, [\partial_x f(x)]^*\, g(x)$
  - Sign: define $D_x := -i\partial_x$
  - Boundary terms: functions $f(x)$ and $g(x)$ must be restricted so it vanishes
  - They define the the domain self-adjointness of D_x
  - p.19–20 list four choices, only two of which make D_x self-adjoint

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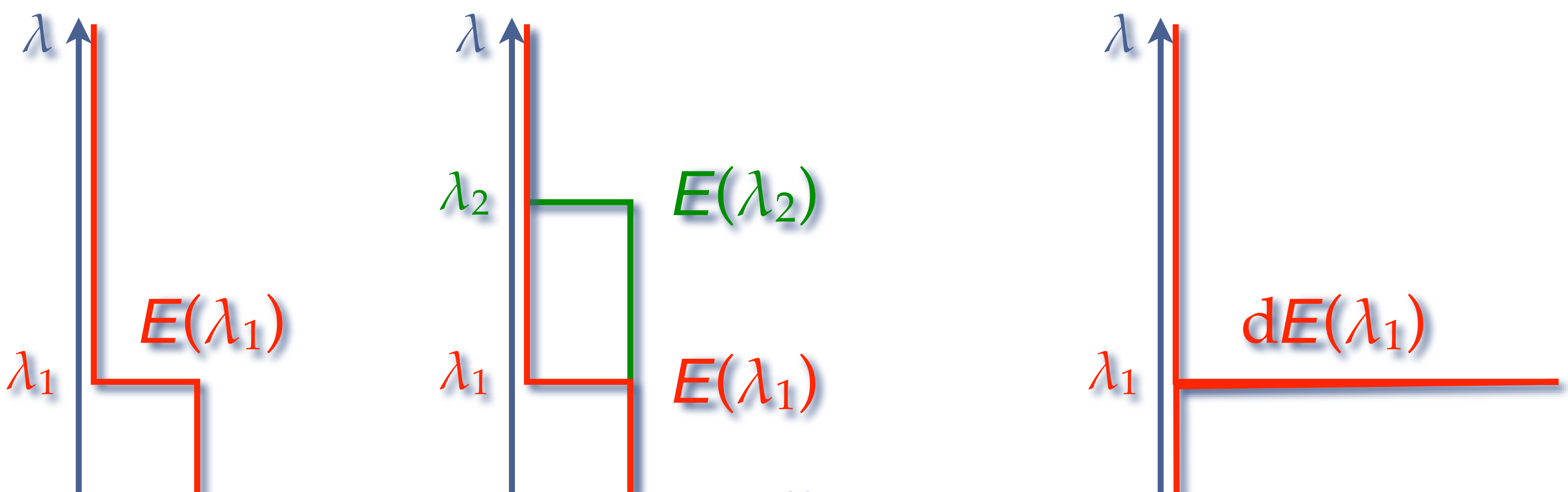
Linear Self-Adjoint Operators

- Thm.4 (spectral): Each self-adjoint operator has a unique family of projection operators $E(\lambda)$, for real λ, such that:

  1. If $\lambda_1 < \lambda_2$ then $E(\lambda_1)E(\lambda_2) = E(\lambda_2)E(\lambda_1) = E(\lambda_1)$.
  2. If $\epsilon > 0$ then $\lim_{\epsilon\to 0} E(\lambda+\epsilon)\,|\psi\rangle = E(\lambda)\,|\psi\rangle$.
  3. $\lim_{\lambda\to-\infty} E(\lambda)\,|\psi\rangle = 0$.
  4. $\lim_{\lambda\to+\infty} E(\lambda)\,|\psi\rangle = |\psi\rangle$.
  5. $\int_{-\infty}^{+\infty} \mathrm{d}E(\lambda)\,\lambda = A$. — reconstructs A

$E(\lambda)$ projects onto states with eigenvalue $\leq \lambda$



Mathematical Prerequisites

Linear Self-Adjoint Operators

- Thm.5: If A and B are self-adjoint operators, each with a complete set of eigenvectors and $AB = BA$, then they have a complete set of common (simultaneous) eigenvectors.
  - Define $[A,B] = AB - BA$, the commutator
  - If $[A,B] \neq 0$, there is no common eigenvector
- Thm.6: Any operator that commutes with all members A_i of a complete commuting set must itself be a function of A_i .
- Rigged Hilbert triple: $(\Omega \subset H \subset \Omega^\times)$
  - Start with Ξ, a countably infinite collection of vectors
  - $V \subset \Xi$ a collection of finite linear combinations
  - $H \subset \Xi$ completion of V, with limits of all norm-convergent sequences
  - $\Omega \subset H$ with some *stronger* convergence / functional requirement
  - $H^\times$ = conjugate: all vectors f such that $(f,h) < \infty$ for all $h \in H$
  - Then $V \subset \Omega \subset H = H^\times \subset \Omega^\times \subset V^\times = \Xi$. $\#[\Omega = \text{kets}] < \#[\Omega^\times = \text{bras}]$.

Quantum Mechanics I

Now, go forth and calculate!!

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