Quantum Mechanics I

Mathematical Prerequisites II

Linear Algebra Summary; Probability Theory

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

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Mathematical Prerequisites II

Linear Algebra Summary

- A ℂ-Linear vector space V is a collection of objects v_i,
  - such that all ℂ-linear combinations $\Sigma_i \, \alpha_i \, v_i$ are also in V.
- A scalar product (w,v) is a 2-argument function such that:
  - a: (w,v) is a complex scalar
  - b: $(v,w) = (w,v)^*$
  - c: $(w, c_1 v_1 + c_2 v_2) = c_1 (w, v_1) + c_2 (w, v_2)$
  - d: $(v,v) \geq 0$, and $(v,v) = 0$ only if $v = 0$
  - Together, (b) and (c) imply $(c_1 w_1 + c_2 w_2, v) = c_1^* \, (w_1, v) + c_2^* \, (w_2, v)$
  - Using (d), we *define* the norm: $\| v \| \equiv (v,v)^{1/2}$
- Linear functionals assigns to each vector a scalar $F[v] \in ℂ$
  - Linearity: $F[c_1 v_1 + c_2 v_2] = c_1 \, F[v_1] + c_2 \, F[v_2]$
  - Vector space $V°$: $(C_1 \, F_1 + C_2 \, F_2)[\psi] \equiv C_1 \, F_1[\psi] + C_2 \, F_2[\psi]$
  - Defined (also) by the scalar product: $W[\ldots] := (w, \ldots)$

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Mathematical Prerequisites II

Linear Algebra Summary

- An operator acts on a vector and produces a vector
  - An operator is linear if $A(c_1\psi_1+c_2\psi_2) = c_1(A\psi_1) + c_2(A\psi_2)$
- 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 $AB \neq BA$
  - Commutator: $[A,B] := A\circ B - B\circ A$
  - Adjoint: $(\chi, A^\dagger\psi) := (\psi, A\chi)^*$ for all ψ, χ
    - Just like the Hermitian conjugate of a matrix: $[M^\dagger]_{ij} = (M_{ji})^*$
  - Self-adjoint: $(\chi, A^\dagger\psi) = (\chi, A\psi) = (\psi, A\chi)^* = (\psi, A^\dagger\chi)$
    - Just like a Hermitiam matrix: $[M^\dagger]_{ij} = (M_{ji})^* = M_{ij}$
- Thm.1: If $(\psi, A\psi) = (\psi, A\psi)^*$, then $(\psi, A\chi) = (\chi, A\psi)^*$
- Definition: If $A\psi_a = a\psi_a$, then a is an eigenvalue, ψ_a the eigenfunction
- Thm.2 & 3: If $A^\dagger = A$, then all eigenvalues are real & $(\psi_a,\psi_b) = 0$ if $a \neq b$

Mathematical Prerequisites II

Linear Algebra Summary

- Thm.π: $A^\dagger = A \quad A\,|n\rangle = a_n\,|n\rangle\,, \quad \langle n|m\rangle = \delta_{nm} \quad \sum_n |n\rangle\,\langle n| = \mathbb{1}$

$$A = \sum_n a_n\,|n\rangle\,\langle n| \qquad f(A) := \sum_n f(a_n)\,|n\rangle\,\langle n|$$

- Thm.4: If $A^\dagger = A$, then there exist projection operators $E(\lambda)$, 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 $\leq \lambda$

- Thm.5: If $A{=}A^\dagger$, $B{=}B^\dagger$, and $[A,B]{=}0$, then they have a complete set of common eigenvectors, $|a,b\rangle$
- Thm.6: If $[A,B_i]{=}0$, $\{B_i\}$ a complete commuting set, $A{=}f(B_i)$

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Mathematical Prerequisites II

Linear Algebra Summary

- Note: $f(A) := \sum_n f(a_n)\,|n\rangle\langle n|, = \int_{-\infty}^{+\infty} \mathrm{d}E(\lambda)\, f(\lambda)$
- If $A = A^\dagger$ has a purely discrete spectrum

$$E(\lambda) = \sum_n \vartheta(\lambda - a_n)\ |a_n\rangle\langle a_n| \qquad \mathrm{d}E(\lambda) = \sum_n \mathrm{d}\lambda\, \delta(\lambda - a_n)\ |a_n\rangle\langle a_n|$$

$$f(A) = \int_{-\infty}^{+\infty} \sum_n \mathrm{d}\lambda\, \delta(\lambda - a_n)\, f(\lambda)\, |a_n\rangle\langle a_n| \ = \sum_n f(a_n)\, |a_n\rangle\langle a_n|$$

- For the continuous analogue, $Q\psi(x) := x\psi(x)$ for all $\psi(x)$
- Then, $Q\psi_\lambda(x) := \lambda\psi_\lambda(x)$ implies that $\psi_\lambda(x) = \delta(\lambda - x)$
  - …but $\delta(\lambda - x)$ is not square-normalizable, $\notin$ Hilbert space
  - $E(\lambda) = \vartheta(\lambda - x)$ and $\int_{-\infty}^{+\infty} \mathrm{d}E(\lambda)\, f(\lambda)\, \psi(x) = \int_{-\infty}^{+\infty} \mathrm{d}[\vartheta(\lambda - x)]\, f(\lambda)\, \psi(x)$

$$= \int_{-\infty}^{+\infty} \mathrm{d}\lambda\, \delta(\lambda - x)\, f(\lambda)\, \psi(x) \ = f(x)\, \psi(x)$$

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Mathematical Prerequisites II

Probability Theory

- Physics is concerned with describing the Nature
- …or, more accurately, our observations of Nature
  - Experiments are our questions posed to Nature,
  - …the experimental results are its (oft cryptic) answers
- Theoretical physics endeavors to model Nature
  - by creating mathematical models that faithfully reproduce Nature
  - …or, more accurately, its every answer to every conceivable question
- Every physical observation can be phrased in a binary form:
  - "The energy is 56.19 J" — T/F (= 1/0)
  - "The energy is 56.19 ± 0.50 J" — T/F (= 1/0)
  - "The energy is between 56.00 and 57.00 J" — T/F (= 1/0)
  - "(For x = 0 to 99) The energy is between x and x+1 J" — T/F (= 1/0)
  - *etc.*

Mathematical Prerequisites II

Probability Theory

- Experiments and experimental results are “events.”
  - Notation: A, B, C = “events”
  - “¬A” is the logical opposite / complement (= “not A”)
  - logical conjunction “A&B” (= “A and B”)
  - logical disjunction “AvB” (= “A or B”) vs. “AxB” (= “either A or B”)
  - logical ≠ chronological
  - Precedence: ¬ before &, v, and x
    “¬A&B” means “(¬A)&B,” “¬AvB” means “(¬A)vB”
  - Dependence: AvB = ¬((¬A)&(¬B)), AxB = (AvB)&¬(A&B)
    - Also, “A => B” = (¬A)vB implication (= “if A then B”)
  - Both & and v are:
    - idempotent [A&A=A], associative [A&(B&C) = (A&B)&C]
    - commutative A&B = B&A, absorbing A&(AvB) = A = Av(A&B)
  - Distributive: A&(BvC) = (A&B)v(A&C) and Av(B&C) = (AvB)&(AvC)

Mathematical Prerequisites II

Probability Theory

- $P(A|B)$ = "The probability that A, provided/assuming B"
  - 1. Reality: $0 \le P(A|B) \le 1$
  - 2. Certainty: $P(A|A) = 1$
  - 3a. Complementarity: $P(\neg A|B) = 1 - P(A|B)$ "Av(¬A), no third option"
  - 4. $P(A\&B|C) = P(A|C) \cdot P(B|A\&C) = P(B|C) \cdot P(A|B\&C)$ (Bayes' Thm.)
    - 2 & 3: $P(\neg A|A) = 0$
  - Equivalently 3b. $P(A \vee B|C) = P(A|C) + P(B|C) - P(A\&B|C)$
    - Substitute $B = \neg A$, this reads $P(1|C) = P(A|C)+P(\neg A|C) - P(0|C)$ which reproduces Axiom 3 since $P(1|C) = 1$ and $P(0|C) = 0$
- Bayes' Thm.: $P(B|A\&C) = P(B|C) \cdot P(A|B\&C) / P(A|C)$
- Independence: If AiB then $P(B|A\&C) = P(B|C)$
  - Then, Axiom 4: $P(A\&B|C) = P(A|C) \cdot P(B|C)$
- Probability as "limit frequency" or as "propensity"

Mathematical Prerequisites II

Probability Theory

- Probability distributions
- Binomial probability distribution
  - Individual experiments (E) have two possible outcomes, A or $\neg A$
  - $P(A \mid E) = p$ then $P(\neg A \mid E) = 1-p$

$$P(\#_A \mapsto k|E^n) = \binom{n}{k} p^k (1-p)^{n-k}$$

  - Note:

$$\binom{n}{k} := \frac{n!}{k!\,(n-k)!} = \frac{n(n-1)\cdots(n-k+1)(n-k)!}{k!\,(n-k)!}$$

$$= \frac{n}{1}\cdot\frac{n-1}{2}\cdots\frac{n-k+1}{k}$$

$$(p+q)^n = \sum_{k=0}^{n} \binom{n}{k} p^k q^{n-k}$$

binomial formula

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Probability Theory

- Average (=expectation value) of a probable quantity A

$$\langle A \rangle := \sum_{k=0}^{n} A_k \, P(A_k | E^n)$$

- For example, average $\#_A$

$$\langle \#_A \rangle := \sum_{k=0}^{n} k \, P(\#_A \mapsto k | E^n)$$

- For the binomial distribution

$$\langle \#_A \rangle = \sum_{k=0}^{n} k \binom{n}{k} p^k q^{n-k} = \sum_{k=0}^{n} \binom{n}{k} \left(\frac{\partial p^k}{\partial p}\right) q^{n-k}$$

$$= \frac{\partial}{\partial p} \sum_{k=0}^{n} \binom{n}{k} p^k q^{n-k} = \frac{\partial}{\partial p} (p+q)^n = np$$

- So the frequency of A becomes $\langle f(A;n) \rangle = \dfrac{\langle \#_A \rangle}{n} = p$

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Mathematical Prerequisites II

Probability Theory

- Continuous probability: X has continuous values x, $g(x) \geq 0$
- Then (for $X \geq 0$):

$$\langle X \rangle = \int_0^\infty g(x)\,\mathrm{d}x\,x \geqslant \int_\epsilon^\infty g(x)\,\mathrm{d}x\,x \geqslant \epsilon \int_\epsilon^\infty g(x)\,\mathrm{d}x\,x$$
$$= \epsilon\, P(X \mapsto x \geqslant \epsilon | E)$$

$$P(X \mapsto x \geqslant \epsilon | E) \leqslant \frac{\langle X \rangle}{\epsilon}$$

- Then, for $X \to |X - c|^\alpha$, for $\alpha > 0$,

$$P(|X-c| \geqslant \epsilon | E) = P(|X-c|^\alpha \geqslant \epsilon^\alpha | E) \leqslant \frac{\langle |X-c|^\alpha \rangle}{\epsilon^\alpha}$$

- is the Chebyshev inequality.
- Since $\langle |X-c|^2 \rangle = \sigma^2$ is the variance and $\langle X \rangle = c$ the mean, setting $\epsilon = k\sigma$,

$$P\big(|X - \langle X \rangle| \geqslant k\sigma | E\big) \leqslant \frac{1}{k^2}$$

- The probability of X being $k\sigma$-fold away from c is $\leq 1/k^2$.

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Mathematical Prerequisites II

Probability Theory

- Back to the binomial probability distribution
- Similar results:

$$P(A|E) = p \qquad P(|\#_A - np| \geqslant \epsilon | E^n) \leqslant \frac{\langle (\#_A - np)^2 \rangle}{\epsilon^2}$$

$$\langle (\#_A - np)^2 \rangle = \left\langle \sum_{i=1}^{n} \left(\delta_{E_i \mapsto A} - p\right)^2 \right\rangle \leq n$$

- and for the relative frequency

$$f(A;n) := \frac{\#_A}{n} \qquad P\big(|f(A;n) - p| \geqslant \delta | E^n\big) \leqslant \frac{1}{n\delta^2}$$

- known as the *law of large numbers*.
- It doesn't say that $f(A;n)$ *limits* to p or is close to p
  - but that the deviations of $f(A;n)$ from p become increasingly improbable
  - probability of deviation of $f(A;n)$ from p becomes arbitrarily small

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Mathematical Prerequisites II

Probability Theory

- Inductive inference, prior and posterior probability
- Estimate the propensity p of the experiment E to yield A.
- Repeating E independently n times, A occurs r times.
- Bayes:

$$P(p \mapsto \theta \pm \delta | (\#_A \mapsto r) \& E^n) = \frac{P(\#_A \mapsto r | (p \mapsto \theta \pm \delta) \& E^n) \cdot P(p \mapsto \theta \pm \delta | E^n)}{P(\#_A \mapsto r | E^n)}$$

- Binomial distribution:

$$P(p \mapsto \theta \pm \delta | (\#_A \mapsto r) \& E^n) = \left(\binom{n}{r} \theta^r (1-\theta)^{n-r} \right) \cdot P(p \mapsto \theta \pm \delta | E^n)$$

posterior probability — prior probability

- …still does not determine p.
- If we (1) choose a uniform prior probability
- …and (2) maximize with respect to θ, then:

$$p = \max(\theta) = \frac{r}{n}$$

Quantum Mechanics I

Now, go forth and calculate!!

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