Quantum Machine Learning Seminars

Week 1: Foundations of Quantum Mechanics for Quantum Computing

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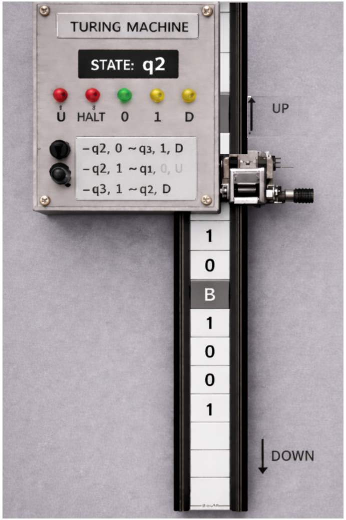
Outline

1. Classical Computability Theory
2. Conceptual Introduction to QM
3. Linear Algebra

Classical Computability Theory

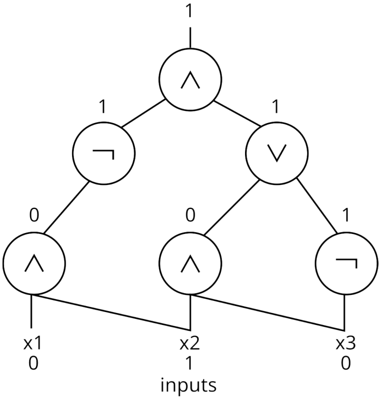
What is computability?

- It's a branch of mathematical logic that studies the limits of what can be computed by algorithms; it classifies problems as solvable (computable) or unsolvable (uncomputable) by theoretical models.
- An algorithm is a step-by-step procedure (the order matters) or rules to accomplish a specific task or solve a problem.
- Theoretical computational models comprehend how the output is obtained from the input, e.g., Turing machine, RAM, decision tree, logic gates, recursive function ... etc.



Limitations of Classical Computability

- Polynomial-time or Polynomial-sized circuit: $T(n) = \mathcal{O}(n^k)$ where $k \neq n$ or its multiples.
- $\boxed{\text{Shannon}}$ $f : \{0,1\}^n \to \{0,1\}$ needs $T(n) \geq \mathcal{O}(2^n/n)$.
- A decision problem that can be solved "efficiently" by a deterministic Turing machine is in class $\mathcal{P}$.
- A decision problem that can be solved by a non-deterministic Turing machine is in class $\mathcal{NP}$.
- Non-deterministic does NOT mean probabilistic, i.e. $\mathcal{BPP} \subset \mathcal{NP}$
- $\boxed{\mathcal{P} \subset \mathcal{NP} \quad \text{but} \quad \mathcal{P} \neq \mathcal{NP}??}$

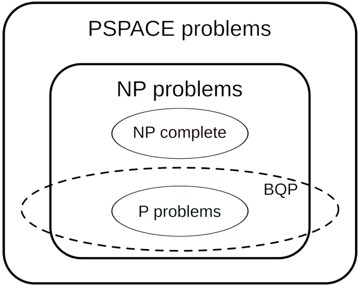


https://en.wikipedia.org/wiki/Boolean_circuit

Classical Computability Theory

$\mathcal{BQP}$

- It has an error probability of at most 1/3 for all instances.
- They explore many possibilities at the same time using superposition.
- The outcome has a tiny chance of error as interference enforces correct paths and cancels wrong ones.
- Solving integer factorization in polynomial time is a $\mathcal{BQP}$ not $\mathcal{BPP}$.



https://en.wikipedia.org/wiki/BQP

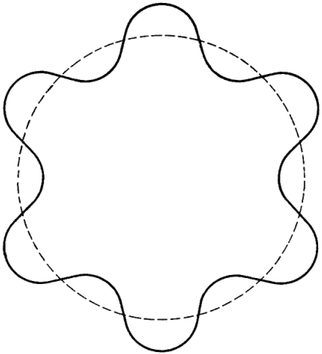
Adiabatic Invariant

- (Einstein-Ehrenfest-Bohr): $E = nhf \Rightarrow nh = E/f$ is invariant under changing any variable ξ.
- e.g. $E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}kx^2$

  Define $p = \sqrt{2m(E - \frac{1}{2}kx^2)}$ such that

  $$I = \int_0^{\sqrt{2E/k}} p dx = E/f = 2\pi E/\omega = 2\pi E\sqrt{\frac{m}{k}}$$
- $\frac{dI}{dk} = 0 \Rightarrow E/f =$ constant, i.e., any I with periodic limits and of units $[J.s]$ is defined as $I = nh$.
- C.f. M. Jammer, The Conceptual Development of Quantum Mechanics.

  J. Mehra, H. Rechenberg, The Historical Development of Quantum Theory.



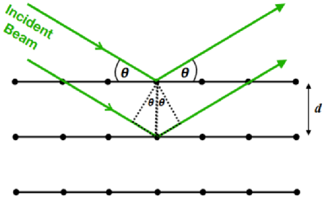
Conceptual Introduction to QM

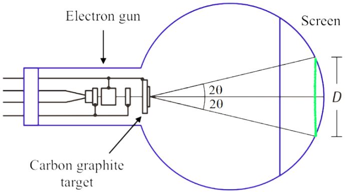
de Broglie Matter Wave

- Hamilton's least action: particles and mechanical waves are governed by the same law. (Snell's law)
- X-ray diffraction experiment: wave has momentum! (Laue then Bragg then de Broglie(s))
- Electrons scattering as a diffraction phenomena.

$$\boxed{\lambda = \frac{h}{p}}$$

- Recall $D(x) = A\sin(kx \pm \omega t)$ from PHYS 32, $\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \xLeftrightarrow{\text{Debye}} ||\frac{dS}{dx}|| = \kappa n$ iff $\Psi = Ae^{iS}$.

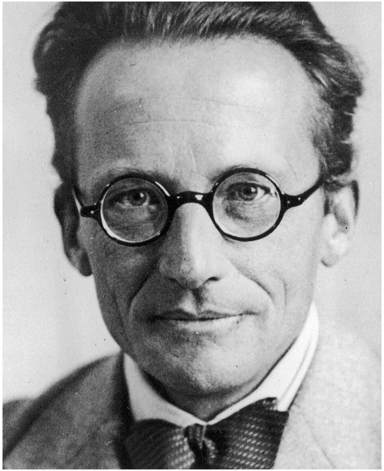




Conceptual Introduction to QM

Schrödinger Equation

- Schrödinger replaced S by $-i\hbar \ln \psi$ then asked: what is equivalent to p in $I = nh$?
- It is $\dfrac{dS}{dx} = -i\hbar \dfrac{\psi'}{\psi}$ or $\boxed{p\psi = -i\hbar \dfrac{d\psi}{dx}}$
- For a free particle with $K = p^2/2m$ we have
$$\frac{1}{2m}\left(-i\hbar\frac{d\psi}{dx}\right)^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = K\psi.$$
And for bounded with potential $V(x)$ it becomes
$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi = E\psi}$$
- This is called an eigenvalue/eigenvector problem!

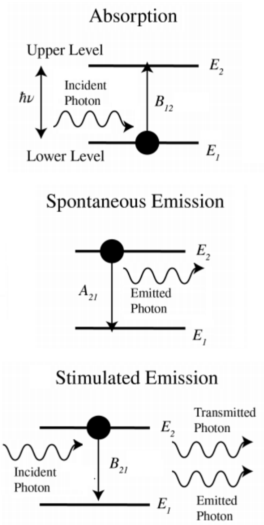


https://en.wikipedia.org/wiki/Erwin_Schrödinger

Conceptual Introduction to QM

Einstein coefficients

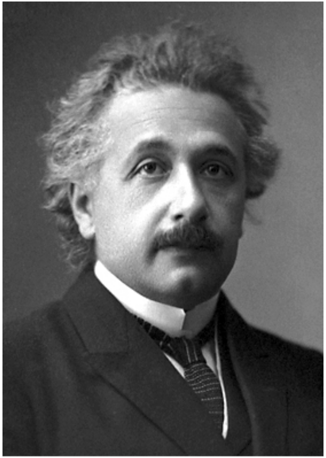
- Spontaneous absorption $dN_j/dt = B_{ij}N_i\rho(\epsilon_j - \epsilon_i)$.
- Spontaneous emission $dN_j/dt = -A_{ji}N_j$.
- Stimulated emission $dN_i/dt = B_{ji}N_j\rho(\epsilon_j - \epsilon_i)$.
- Absorption/emission rates $A_{ij} \propto B_{ij} \propto |D_{ij}|^2$.
- Fourier transform $D_{ij} = qx_{ij}$ of dipole $d = qx$.
- $I_P \propto \omega^4 |D_{ij}|^2 \xLeftrightarrow{\text{Experiment}} A_{ij} \propto I_P \Rightarrow A_{ij} \propto |x_{ij}|^2$.
- $\dfrac{dN_j}{dt} = -\dfrac{dN_i}{dt} \xRightarrow{\text{prove}} N_i \propto e^{|x_{ij}|^2 t}$.



Conceptual Introduction to QM

Probability and Transition Amplitude

- The probability no particle is emitted in time t is $P(t, N_0)$, and that of some are emitted is $P(t, N_{\neq 0})$.
- And for $t+dt$ (mutually independent) it's $P(t+dt, N_0) = P(t, N_0) \times P(dt, N_0)$
- The change $dP(t, N_0) = P(t+dt, N_0) - P(t, N_0) = -P(t, N_0)\Big[1 - P(dt, N_0)\Big] = -P(t, N_0) \times P(dt, N_{\neq 0})$
- $dP(t, N_0) = -P(t, N_0) \times -dN_j/N_j = -P(t, N_0) \times A_{ij} dt.$ (Why $-dN_j/N_j$ not $+dN_j/N_j$?)
- $P(t, N_0) \propto e^{-|x_{ij}|^2 t} \Rightarrow P(t, N_{\neq 0}) = 1 - e^{-|x_{ij}|^2 t}$
- $P(t, N_{\neq 0}) \sim 1 - (1 - |x_{ij}|^2 t) \Rightarrow \boxed{P(t, N_{\neq 0}) \propto |x_{ij}|^2}$



https://en.wikipedia.org/wiki/Albert_Einstein

Conceptual Introduction to QM

Heisenberg Matrix Mechanics

- Periodic motion:

$$x_n = \sum_{\alpha=-\infty}^{\infty} a_{n\alpha} e^{i\alpha\omega_n t} \xRightarrow{k=n-\alpha} x_n = \sum_{k=-\infty}^{\infty} a_{nk} e^{i\omega_{nk} t}$$

where from $E_a - E_b = \hbar\omega_{ab}$ we must impose $\boxed{\omega_{nk} = \omega_{nj} + \omega_{jk}}$ for $n > j > k$, and $a_{nk} = a^*_{kn}$.

- $I = \int p_n dx_n = m \int \dot{x}_n dx_n = m \int (\dot{x}_n)^2 dt \Rightarrow$

$$\hbar = m \sum_\alpha \left(|a_{n,n+\alpha}|^2 \omega_{n,n+\alpha} - |a_{n,n-\alpha}|^2 \omega_{n,n-\alpha} \right)$$

- In addition, $I = \int p_n dx_n - \int x_n dp_n = -i\hbar$.

https://en.wikipedia.org/wiki/Werner_Heisenberg

Linear Algebra

Summary

- Vector addition:

$$(\vec{v}+\vec{w})_j = v_j + w_j$$

- Vector scalar multiplication:

$$(c\vec{v})_j = cv_j$$

- Matrix addition:

$$(M+N)_{ij} = M_{ij} + N_{ij}$$

- Matrix scalar multiplication:

$$(cM)_{ij} = c(M_{ij})$$

Summary

- Matrix multiplication:

$$(MN)_{ij} = \sum_k M_{ik} N_{kj}$$

- Matrix/vector complex conjugate:

$$(M^*)_{ij} = (M_{ij})^*$$

- Matrix/vector transpose:

$$(M^T)_{ij} = M_{ji}$$

- Matrix/vector conjugate transposed:

$$(M^\dagger)_{ij} = ((M^*)^T)_{ij} = (M_{ji})^*$$

Summary

- Inner / Scalar / Dot product:

$$\vec{v} \bullet \vec{w} = \vec{v}^{\dagger} \vec{w} = \sum_{j=1}^{n} v_j^{T*} w_j$$

- Norm of a vector:

$$\|\vec{v}\| = \sqrt{\vec{v} \bullet \vec{v}}$$

- Projection of $\vec{v}$ onto $\vec{w}$:

$$P_{\vec{v},\vec{w}} = \frac{1}{\|\vec{w}\|} \vec{w} \bullet \vec{v}$$

Summary

- Eigenvectors and eigenvalues:

$$M\vec{v} = \lambda\vec{v}$$

$$[M - \lambda\mathbb{I}]\vec{v} = \vec{0}$$

$$\det[M - \lambda\mathbb{I}] = 0$$

- Matrix diagonaliztion

$$P^{-1}MP = D$$

where $P = [v_1\ v_2\ \cdots]$ for linearly independent v_i.

Thank You!