Quantum Machine Learning Seminars

Week 1: Foundations of Quantum Mechanics for Quantum Computing

Dr. Hassan Alshal

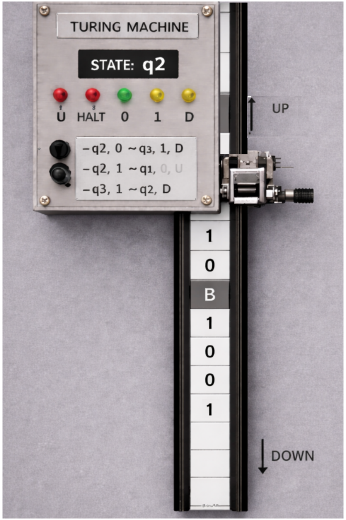
Outline

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

Classical Computability Theory

What is computability?

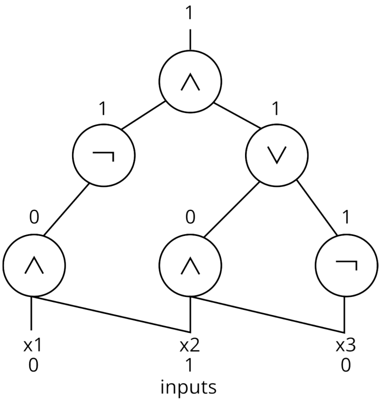
- It's a branch of mathematical logic that studies the limits of what can be computed by <u>algorithms</u>; it classifies problems as solvable (computable) or unsolvable (uncomputable) by <u>theoretical models</u>.
- An algorithm is a step-by-step procedure (the order matters) or rules to accomplish 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.



Classical Computability Theory

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. $\mathcal{BPP} \subset \mathcal{NP}$
- $\boxed{\mathcal{P} \subset \mathcal{NP} \quad \text{but} \quad \mathcal{P} \neq \mathcal{NP}??}$

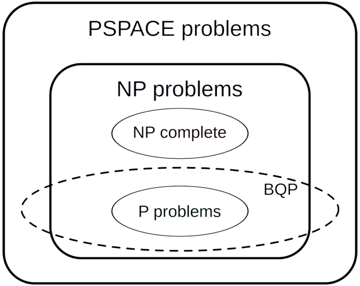


https://en.wikipedia.org/wiki/Boolean_circuit

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

Conceptual Introduction to QM

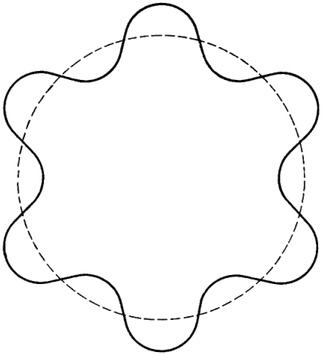
Adiabatic Invariant

- (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

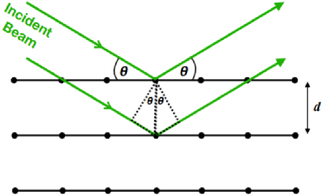
  $$I = \int_0^{\sqrt{2E/k}} pdx = E/f = 2\pi E/\omega = 2\pi E\sqrt{\frac{m}{k}}$$
- $\frac{dI}{dk} = 0 \Rightarrow E/f =$ constant, i.e., any I with periodic limits and of units $[J.s]$ is defined as $I = nh$.
- C.f. M. Jammer, The Conceptual Development of Quantum Mechanics.

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



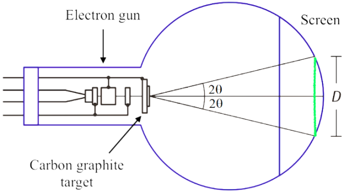
Conceptual Introduction to QM

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.

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



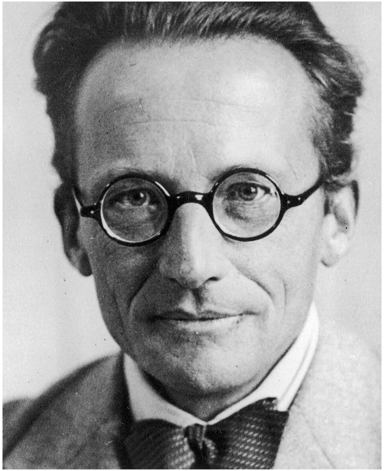
- Recall $D(x) = A\sin(kx \pm \omega t)$ from PHYS 32,

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \overset{\text{Debye}}{\Longleftrightarrow} ||\frac{dS}{dx}|| = \kappa n \text{ iff } \Psi = Ae^{iS}.$$

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 $\frac{dS}{dx} = -i\hbar \frac{\psi'}{\psi}$ or $\boxed{p\psi = -i\hbar \frac{d\psi}{dx}}$
- For a free particle with $K = p^2/2m$ we have $\frac{1}{2m}(-i\hbar \frac{d}{dx})^2 \psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = K\psi.$ 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!

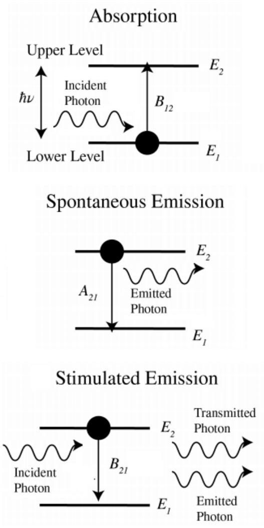


https://en.wikipedia.org/wiki/Erwin_Schrödinger

Conceptual Introduction to QM

Einstein coefficients

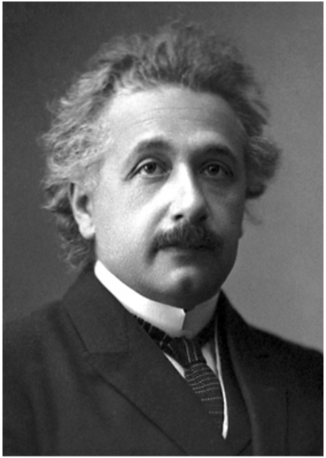
- Spontaneous absorption $dN_j/dt = B_{ij}N_i\rho(\epsilon_j - \epsilon_i)$.
- Spontaneous emission $dN_j/dt = -A_{ji}N_j$.
- Stimulated emission $dN_i/dt = B_{ji}N_j\rho(\epsilon_j - \epsilon_i)$.
- Absorption/emission rates $A_{ij} \propto B_{ij} \propto |D_{ij}|^2$.
- Fourier transform $D_{ij} = qx_{ij}$ 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:

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

Linear Algebra

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:

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

Linear Algebra

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!