

Some of the Big Ideas in Quantum Mechanics

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Part I

Quantum Mechanics

Chapter 1

Measurement theory

Chapter 2

Postulates

Chapter 3

Quantum theory

3.1 Quantum statistics

3.2 Time evolution

3.2.1 Schrödinger and Heisenberg pictures

Lemma I.1. *Let \mathcal{H} be a Hilbert space and $\{e_i\}$ an orthonormal basis. Let U be a unitary operator on \mathcal{H} . Then $\{Ue_i\}$ is also an orthonormal basis for \mathcal{H} .*

$\{e_i\}$ gives Schrödinger and $\{Ue_i\}$ gives Heisenberg.

3.2.2 Adiabatic theorem

Chapter 4

Approximations

4.1 Approximating eigenvectors

4.1.1 Power series expansion of a non-degenerate level

4.2 Approximating evolutions

Chapter 5

Investigations of systems

5.1 Stepped potentials

(Use density to solve general potentials?)

5.2 Coulomb interaction

5.3 Harmonic oscillator

Part II

Quantum Information and computation

Chapter 1

Circuit model

1.1 Qubits

A qubit is an element of $\mathbb{C}P^2$.

1.1.1 $\mathfrak{su}(2)$ and the Pauli matrices

The qubit Hamiltonians are elements of $\mathfrak{su}(2)$. Getting rid of the arbitrary global phase gives us elements of $\mathfrak{su}(2)$.

Lemma II.1. *For all $\sigma \in \mathfrak{su}(2)$, the eigenvalues λ_1, λ_2 are real and $\lambda_1 = -\lambda_2$.*

Proof. For all $\sigma \in \mathfrak{su}(2)$, σ is self-adjoint and $\text{Tr}[\sigma] = \lambda_1 + \lambda_2 = 0$. \square

Corollary II.1.1. *For all $\sigma \in \mathfrak{su}(2)$, we have $\|\sigma\|_2 = \sqrt{2}\|\sigma\|$, where $\|\cdot\|_2$ is the Hilbert-Schmidt norm.*

Proof. We have $\|\sigma\|_2 = \sqrt{\lambda_1^2 + \lambda_2^2} = \sqrt{2}|\lambda_1| = \sqrt{2}\|\sigma\|$. \square

Corollary II.1.2. *The inner product*

$$\langle \cdot, \cdot \rangle : (\sigma_1, \sigma_2) \mapsto \frac{1}{2} \text{Tr}[\sigma_1 \sigma_2]$$

on $\mathfrak{su}(2)$ yields the operator norm as the norm associated with this inner product.

Corollary II.1.3. *Let σ be a unit vector in $\mathfrak{su}(2)$. Then σ has eigenvalues ± 1 . This means σ is unitary.*

Corollary II.1.4. *There is a bijection between the unit vectors in $\mathfrak{su}(2)$ and the rank-1 projections on \mathbb{C}^2 given by $\mathfrak{su}(2)/\mathbb{R} \rightarrow \sigma \mapsto E_1^\sigma$, where E_1^σ is the eigenspace of σ associated with eigenvalue $+1$.*

Proof. We construct an inverse of the map. Let P_1 be the orthogonal projector on E_1^σ . Then $\sigma = 2P_1 - \text{id}$. \square

Proposition II.2. *Let $\sigma \in \mathfrak{su}(2)$. Then $\sigma^2 = \|\sigma\|^2 \mathbf{1}$.*

Proof. We have

$$\sigma^2 = \|\sigma\|^2 \left(\frac{\sigma}{\|\sigma\|} \right)^2 = \|\sigma\|^2 \frac{\sigma}{\|\sigma\|} \left(\frac{\sigma}{\|\sigma\|} \right)^* = \|\sigma\|^2 \mathbf{1},$$

where we have used that $\frac{\sigma}{\|\sigma\|}$ is unitary by II.1.3. \square

Corollary II.2.1. *The real algebra generated by $\mathfrak{su}(2)$ is the Clifford algebra $\text{Cl}_{3,0}$. The unit pseudoscalar is $i\mathbf{1}$.*

Note that $\mathfrak{su}(2)$ is a Lie algebra and thus closed under the Lie bracket, but not an algebra under operator composition. Thus the algebra generated by $\mathfrak{su}(2)$ is larger than $\mathfrak{su}(2)$ (indeed $\sigma^2 = \|\sigma\|^2 \mathbf{1} \notin \mathfrak{su}(2)$).

Proposition II.3 (Pauli matrices). *The Clifford algebra $\mathfrak{su}(2)$ has an orthonormal basis*

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

1.1.2 The Bloch sphere

Because $\mathfrak{su}(2)$ is the Clifford algebra $\text{Cl}_{3,0}$, we can use the unit sphere in \mathbb{R}^3 to represent the unit vectors in $\mathfrak{su}(2)$. By II.1.4 we can also use it to represent the rank-1 projections on \mathbb{C}^2 . The unit sphere with as x, y, z axes the Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ is called the Bloch sphere.
 TODO image of Bloch sphere.

TODO spherical coordinates: $\cos \theta/2 |0\rangle + e^{i\phi} \sin \theta/2 |1\rangle$

Lemma II.4.

$$e^{\phi/2i\sigma} e^{\theta/2i\sigma^\perp} |1\rangle = \cos \theta/2 |0\rangle + e^{i\phi} \sin \theta/2 |1\rangle$$

1.2 Gates

1.2.1 Controlled gates

Let H_1, H_2 be two Hilbert spaces. Let P be a projector on H_1 and L an operator on H_2 . The operation of L controlled by P is the operation $P \otimes L + (\text{id}_{H_1} - P) \otimes \text{id}_{H_2}$ in $H_1 \otimes H_2 \rightarrow H_1 \otimes H_2$.

Chapter 2

Eigenpath traversal

2.1 Quantum Zeno effect

Proposition II.5. *Consider a path of states $|\psi(s)\rangle$ where $s \in [0, 1]$. Assume that, for fixed d and all δ ,*

$$|\langle\psi(s)|\psi(s+\delta)\rangle|^2 \geq 1 - d^2\delta^2.$$

Then

2.2 Adiabatic quantum computation

2.3 Evolution through measurement

2.3.1 Phase randomisation

$$|\psi_0\rangle = |E_0(0)\rangle = \sum_i \alpha_i |E_i(s_1)\rangle$$

$$\begin{aligned} \rho(s_1) &= \frac{1}{T} \int_0^T e^{-iH(s_1)t} |\psi_0\rangle \langle\psi_0| e^{iH(s_1)t} dt \\ &= \sum_{i,j} \alpha_i \alpha_j^* \frac{1}{T} \left(\int_0^T e^{-i(E_i - E_j)t} dt \right) |E_i\rangle \langle E_j| \\ &= \sum_{i,j} \alpha_i \alpha_j^* \left(\frac{i(e^{-i(E_i - E_j)T} - 1)}{T(E_i - E_j)} \right) |E_i\rangle \langle E_j| \end{aligned}$$

Theorem II.6 (Randomised dephasing). *Let $|\psi(s)\rangle$ be a nondegenerate eigenstate of $H(s)$ and $\{\omega_j\}$ the energy differences to the other eigenstates $|\psi_j(s)\rangle$. Let T be a random variable. Then, for all states ρ , we have*

$$\left\| (M_l - e^{-iH(s)T} \rho e^{-iH(s)T}) \right\|_{tr} \leq \epsilon = \sup_{\omega_j} |\Phi(\omega_j)|$$

Chapter 3

Variational quantum algorithms

Chapter 4

Algorithms

4.1 Deutsch's problem

4.2 Grover's search algorithm

Suppose we have a set \mathcal{N} of N items, some of which are marked. WLOG we can take \mathcal{N} to be the set of bit strings of length ν . The marked items form a subset \mathcal{M} of size M . Suppose we have an oracle that tells us whether an object is marked or not:

$$f : \mathcal{N} \rightarrow \{0, 1\} : x \mapsto \begin{cases} 0 & (x \in \mathcal{M}) \\ 1 & (x \notin \mathcal{M}) \end{cases}$$

Now we want to find a marked item. Classically we need to check $\Theta(N/M)$ items on average.

4.2.1 Circuit model

Let $\{|n\rangle \mid n \in \mathcal{N}\}$ be a basis of a Hilbert space \mathcal{H}_N and let \mathcal{H}_2 be a qubit space.

4.2.1.1 The oracle

We would like to use the operator

$$U_f : \mathcal{H}_N \rightarrow \mathcal{H}_N : |n\rangle \mapsto (-1)^{f(n)} |n\rangle.$$

This can be constructed from the oracle

$$O_f : \mathcal{H}_N \otimes \mathcal{H}_2 \rightarrow \mathcal{H}_N \otimes \mathcal{H}_2 : |n\rangle \otimes |q\rangle \mapsto |n\rangle \otimes |f(n) \oplus q\rangle,$$

where \oplus is addition modulo 2, by preparing the qubit in the superposition $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Then

$$\begin{aligned} O_f \left(|n\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \right) &= |n\rangle \otimes \frac{1}{\sqrt{2}}(|f(n)\rangle - |f(n) \oplus 1\rangle) \\ &= (-1)^{f(n)} |n\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \end{aligned}$$

The operator U_f can also be written

$$U_f = \text{id}_{\mathcal{H}_N} - 2 \sum_{m \in \mathcal{M}} |m\rangle \langle m|.$$

4.2.1.2 The algorithm

We construct the an initial state which is a superposition of all possible solutions

$$|\mathcal{N}\rangle = \frac{1}{\sqrt{N}} \sum_{n \in \mathcal{N}} |n\rangle.$$

This can be prepared by applying a Hadamard gate W to each qubit in the register. We also define the state

$$|\mathcal{M}\rangle = \frac{1}{\sqrt{M}} \sum_{m \in \mathcal{M}} |m\rangle.$$

We define the operation

$$U_0 = W^{\otimes \nu} (\text{id} - 2|0\rangle\langle 0|) W^{\otimes \nu} = \text{id} - 2|\mathcal{N}\rangle\langle \mathcal{N}|.$$

Now both U_0 and U_f leave $\text{span}\{\}$

4.2.2 Analogue Grover

Why does analogue Grover work?

4.2.3 Adiabatic Grover

$$H_0 = \mathbf{1} - |\mathcal{N}\rangle\langle \mathcal{N}| = \mathbf{1} - \mathbb{J}/N$$

$$H_f = \mathbf{1} - \sum_{m \in \mathcal{M}} |m\rangle\langle m| = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix}.$$

Then

$$H(s) = (1-s)H_0 + sH_f = \begin{pmatrix} (1-s)\mathbb{1} + \frac{s-1}{N}\mathbb{J} & \frac{s-1}{N}\mathbb{J} \\ \frac{s-1}{N}\mathbb{J} & \mathbb{1} + \frac{s-1}{N}\mathbb{J} \end{pmatrix} = \begin{pmatrix} (1-s)\mathbb{1}_M & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix} + \frac{s-1}{N}\mathbb{J}.$$

Then, setting $A = \begin{pmatrix} (1-s-\lambda)\mathbb{1}_M & 0 \\ 0 & (1-\lambda)\mathbb{1}_{N-M} \end{pmatrix}$

$$\begin{aligned} \det(H(s) - \lambda) &= \det\left(A + \frac{s-1}{N}\mathbb{J}^{n \times 1} \mathbb{J}^{1 \times n}\right) \\ &= \det(A) \det\left(\mathbb{1}_N + \frac{s-1}{N}A^{-1}\mathbb{J}^{n \times 1} \mathbb{J}^{1 \times n}\right) \\ &= \det(A) \det\left(1 + \frac{s-1}{N}\mathbb{J}^{1 \times n} A^{-1} \mathbb{J}^{n \times 1}\right) \\ &= (1-s-\lambda)^M (1-\lambda)^{N-M} \left(1 + \frac{M(s-1)}{(1-s-\lambda)N} + \frac{(N-M)(s-1)}{(1-\lambda)N}\right) \\ &= (1-s-\lambda)^{M-1} (1-\lambda)^{N-M-1} \left(\lambda^2 - \lambda + s(1-s)\frac{N-M}{N}\right), \end{aligned}$$

where we have used the matrix determinant lemma to simplify the calculation.

We see that there are four distinct eigenvalues:

$$\begin{aligned}\lambda_{0,1} &= \frac{1}{2} \left(1 \pm \frac{\sqrt{N + 4(Ns^2 - Ns - Ms^2 + Ms)}}{\sqrt{N}} \right) && \text{with multiplicity } 1 \\ \lambda_2 &= 1 - s && \text{with multiplicity } M - 1 \\ \lambda_3 &= 1 && \text{with multiplicity } N - M - 1.\end{aligned}$$

Next we are interested in the eigen vectors associated to $\lambda_{0,1}$. Let Q_1 be a unitary transfor-

mation that maps $\mathbb{J}^{M \times 1}$ to $\begin{pmatrix} \sqrt{M} \\ 0 \\ 0 \\ \vdots \end{pmatrix} \in \mathbb{C}^M$. Similarly let Q_2 be a unitary transformation that maps $\mathbb{J}^{(N-M) \times 1}$ to $\begin{pmatrix} \sqrt{N-M} \\ 0 \\ 0 \\ \vdots \end{pmatrix} \in \mathbb{C}^{(N-M)}$ and define $Q = \begin{pmatrix} Q_1 & 0 \\ 0 & Q_2 \end{pmatrix}$, which is also unitary.

Then we have

$$\begin{aligned}QH(s)Q^{-1} &= \begin{pmatrix} (1-s)\mathbb{1}_M & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix} + \frac{s-1}{N} Q \mathbb{J}^{N \times 1} (\mathbb{J}^{N \times 1})^* Q^* \\ &= \begin{pmatrix} (1-s)\mathbb{1}_M & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix} + \frac{s-1}{N} \begin{pmatrix} \sqrt{M} \\ 0 \\ \vdots \\ 0 \\ \sqrt{N-M} \\ 0 \\ \vdots \end{pmatrix} \begin{pmatrix} \sqrt{M} \\ 0 \\ \vdots \\ 0 \\ \sqrt{N-M} \\ 0 \\ \vdots \end{pmatrix}^*.\end{aligned}$$

All but two of the eigenvectors are just elements of \mathcal{N} . To study the other two we can simplify by “removing the zeros”. Now the eigenvalue problem becomes

$$\left(\begin{pmatrix} 1-s-\lambda_{0,1} & 0 \\ 0 & 1-\lambda_{0,1} \end{pmatrix} + \frac{s-1}{N} \begin{pmatrix} \sqrt{M} \\ \sqrt{N-M} \end{pmatrix} \begin{pmatrix} \sqrt{M} \\ \sqrt{N-M} \end{pmatrix}^* \right) \mathbf{v} = 0.$$

Setting $\mathbf{v} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ gives us the equations

$$\begin{aligned}0 &= (1-s-\lambda_{0,1})x_1 + \frac{s-1}{N}(Mx_1 + \sqrt{M}\sqrt{N-M}x_2) \\ 0 &= (1-\lambda_{0,1})x_2 + \frac{s-1}{N}(\sqrt{M}\sqrt{N-M}x_1 + (N-M)x_2)\end{aligned}$$

reshuffling and dividing these equations gives

$$\frac{(1-s-\lambda_{0,1})x_1}{(1-s-\lambda_{0,1})x_2} = \frac{-\frac{s-1}{N}(Mx_1 + \sqrt{M}\sqrt{N-M}x_2)}{-\frac{s-1}{N}(\sqrt{M}\sqrt{N-M}x_1 + (N-M)x_2)} = \frac{\sqrt{M}(\sqrt{M}x_1 + \sqrt{N-M}x_2)}{\sqrt{N-M}(\sqrt{M}x_1 + \sqrt{N-M}x_2)} = \frac{\sqrt{M}}{\sqrt{N-M}}.$$

So we have eigenvectors $\mathbf{v}_{0,1} = (\sqrt{M}(1 - \lambda_{0,1}), \sqrt{N - M}(1 - s - \lambda_{0,1}))^T$ of $QH(s)Q^{-1}$. The corresponding eigenvectors of $H(s)$ are then given by

$$Q^* \mathbf{v}_{0,1} = \begin{pmatrix} (1 - \lambda_{0,1}) \mathbb{J}^{M \times 1} \\ (1 - s - \lambda_{0,1}) \mathbb{J}^{(N-M) \times 1} \end{pmatrix}.$$

For computational ease we will keep on working with the eigenvectors $\mathbf{v}_{0,1}$ of $QH(s)Q^{-1}$. We denote by $|0\rangle$ and $|1\rangle$ the normalisation of $\mathbf{v}_{0,1}$.

4.2.3.1 Poisson projective measurement

The dynamics of the system is governed by the differential equation

$$\frac{d\rho}{ds} = \Lambda(|0\rangle\langle 0|\rho|0\rangle\langle 0| + |1\rangle\langle 1|\rho|1\rangle\langle 1| - \rho).$$

Now we can rewrite $\frac{d\rho}{ds}$ in the basis $|0\rangle, |1\rangle$: let $i, j, k, l = 0, 1 \pmod 2$ with implicit summation

$$\begin{aligned} \frac{d\rho}{ds} &= \frac{d}{ds} (|i\rangle\langle i|\rho|j\rangle\langle j|) \\ &= \frac{d}{ds} (\langle i|\rho|j\rangle) |i\rangle\langle j| + \langle i|\rho|j\rangle \frac{d}{ds} (|i\rangle\langle j|) \\ &= \frac{d}{ds} (\langle i|\rho|j\rangle) |i\rangle\langle j| + \langle i|\rho|j\rangle |k\rangle\langle k| \frac{d}{ds} |i\rangle\langle j| - \langle i|\rho|j\rangle |i\rangle\langle j| \frac{d}{ds} |l\rangle\langle l| \\ &= \frac{d}{ds} (\langle i|\rho|j\rangle) |i\rangle\langle j| + \langle i|\rho|j\rangle |i+1\rangle\langle i+1| \frac{d}{ds} |i\rangle\langle j| - \langle i|\rho|j\rangle |i\rangle\langle j| \frac{d}{ds} |j+1\rangle\langle j+1| \\ &= \left(\frac{d}{ds} (\langle i|\rho|j\rangle) + \langle i+1|\rho|j\rangle \langle i| \frac{d}{ds} |i+1\rangle - \langle i|\rho|j+1\rangle \langle j+1| \frac{d}{ds} |j\rangle \right) |i\rangle\langle j|. \end{aligned}$$

For each $|i\rangle\langle j|$ we get an equation, four in total. One of these is redundant by the zero trace requirement. Writing $y_{i,j} := \langle i|\rho|j\rangle$ and $\omega_{ij} := \langle i| \frac{d}{ds} |j\rangle$ the three remaining equations are

$$\begin{aligned} \frac{d\rho_{00}}{ds} &= -\rho_{10}\omega_{01} + \rho_{01}\omega_{10} \\ \frac{d\rho_{01}}{ds} &= -\Lambda\rho_{01} - (1 - \rho_{00})\omega_{01} + \rho_{00}\omega_{01} \\ \frac{d\rho_{10}}{ds} &= -\Lambda\rho_{10} - \rho_{00}\omega_{10} + (1 - \rho_{00})\omega_{10} \end{aligned}$$

Setting $\omega = \omega_{10} = -\omega_{01}$ and $y = \rho_{00} - 1/2$ we obtain the equation

$$\frac{d^2 y}{ds^2} = \left(\frac{\frac{d\omega}{ds}}{\omega} - \Lambda \right) \frac{dy}{ds} - 4\omega^2 y.$$

Setting $\mathbf{y} = \begin{pmatrix} y \\ y' \end{pmatrix}$ this second order differential equation is equivalent to the first order system

$$\begin{pmatrix} y \\ y' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -4 & -\Lambda/\omega \end{pmatrix} \mathbf{y},$$

which is in the form $\mathbf{y}' = A\mathbf{y}$. Now A is similar to $\begin{pmatrix} \omega/\Lambda & 0 \\ -4 & -\Lambda/\omega \end{pmatrix}$, so it is bounded if both Λ and Λ^{-1} are bounded functions.

Then by the Picard-Lindelöf theorem the initial value problem has a unique solution on $[0, 1]$. In addition let y_1 be the solution obtained using Λ_1 and y_2 using Λ_2 . Then

$$\Lambda_1 \leq \Lambda_2 \implies y_1 \leq y_2.$$

To see this, we may first remark that

$$\{t \in [0, 1] \mid y_1(t) \leq y_2(t) \wedge y'_1(t) \leq y'_2(t)\} = (y_2 - y_1)^{-1}[[0, +\infty[] \cap (y'_2 - y'_1)^{-1}[[0, +\infty[]$$

is a closed and bounded set that contains 0. Let t_1 be its supremum. This means that $y_1(t_1) \leq y_2(t_1)$ and $y'_1(t_1) \leq y'_2(t_1)$, but $y_1(t) > y_2(t)$ or $y'_1(t) > y'_2(t)$ on some open set $]t_1, t_1 + \delta[$.