

# 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  $\mathbb{C}P^2$ .

**Lemma II.1.** *Each equivalence class in  $\mathbb{C}P^2$  contains an element of the form  $\begin{pmatrix} a \\ e^{i\varphi}b \end{pmatrix}$  where  $a, b, \varphi \in \mathbb{R}_+$  and  $a^2 + b^2 = 1$ .*

**Corollary II.1.1** (Bloch sphere). *There is a bijection  $\mathbb{C}P^2 \rightarrow S^2$  given by*

$$\begin{pmatrix} a \\ e^{i\varphi}b \end{pmatrix} = \begin{pmatrix} \cos(\theta/2) \\ e^{i\varphi} \sin(\theta/2) \end{pmatrix} \rightarrow (\theta, \varphi).$$

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

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

*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.3** (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  $\rho$ , 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  $\nu$ . 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

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

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  $\Lambda$  and  $\Lambda^{-1}$  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  $\Lambda_1$  and  $y_2$  using  $\Lambda_2$ . 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  $]t_1, t_1 + \delta[$ .