

Some of the Big Ideas in Quantum Mechanics

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Contents

I	Quantum Mechanics	3
1	Measurement theory	4
2	Postulates	5
2.1	States, observables and measurement	5
2.1.1	States	5
2.1.2	Effects	5
3	Quantum theory	6
3.1	Quantum statistics	6
3.1.1	Uncertainty relations	7
3.2	Time evolution	7
3.2.1	The Schrödinger equation	7
3.2.2	Schrödinger and Heisenberg pictures	8
3.2.3	Adiabatic theorem	8
4	Approximations	11
4.1	Approximating eigenvectors	11
4.1.1	Power series expansion of a non-degenerate level	11
4.2	Approximating evolutions	11
5	Investigations of systems	12
5.1	Stepped potentials	12
5.2	Coulomb interaction	12
5.3	Harmonic oscillator	12
II	Quantum Information and computation	13
1	Bras and kets	14
2	Circuit model	15
2.1	Qubits	15
2.1.1	$\mathfrak{su}(2)$ and the Pauli matrices	15
2.1.2	The Bloch sphere	16
2.2	Gates	16
2.2.1	One-qubit gates	16
2.2.1.1	Hadamard gate	16

2.2.1.2	Pauli gates	17
2.2.2	Controlled gates	17
3	Eigenpath traversal	18
3.1	Quantum Zeno effect	18
3.2	Adiabatic quantum computation	18
3.3	Evolution through measurement	18
3.3.1	Phase randomisation	18
4	Variational quantum algorithms	19
5	Algorithms	20
5.1	Some building blocks	20
5.1.1	Preparing states	20
5.1.1.1	Uniform superposition	20
5.1.2	Quantum Fourier transform	20
5.2	Quantum oracle querying	20
5.2.1	Oracle set-up	20
5.2.2	Deutsch's problem	21
5.2.3	Grover's search algorithm	22
5.2.3.1	The algorithm	22
5.2.3.2	Analogue Grover	23
5.2.3.3	Adiabatic Grover	24
5.2.3.4	Poisson projective measurement	25
A	Bibliography	27

Part I

Quantum Mechanics

Chapter 1

Measurement theory

Chapter 2

Postulates

2.1 States, observables and measurement

2.1.1 States

[A state on a Hilbert space is a positive trace class operator with trace 1.

Proposition I.1. *Let ρ be a state. The following are equivalent:*

1. ρ is extremal;
2. ρ is a projector;
3. $\rho = \rho^2$;
4. $\text{Tr}[\rho^2] = 1$;
5. $\|\rho\| = 1$;
6. $S(\rho) := -\text{Tr}[\rho \ln \rho] = 0$.

The quantity $S(\rho) := -\text{Tr}[\rho \ln \rho]$ is called the von Neumann entropy.

2.1.2 Effects

[An effect on a Hilbert space is a bounded operator in $[0, \text{id}]$.

Chapter 3

Quantum theory

3.1 Quantum statistics

Let \mathcal{H} be a Hilbert space, A a symmetric operator on \mathcal{H} and ψ a unit vector in $\text{dom}(A)$. Then we define

- the expectation value of A at ψ is defined as $\langle A \rangle_\psi := Q_A(\psi) = \langle \psi | A | \psi \rangle$;
- the uncertainty or standard deviation of A at ψ is defined as

$$\Delta_\psi A := \left\| (A - \langle A \rangle_\psi \text{id}) \psi \right\|.$$

The expectation value $\langle A \rangle_\psi$ is always real (by XVI.46.1).

Lemma I.2. $\langle A \rangle_\psi = \langle \psi | A | \psi \rangle = \text{Tr} (A | \psi \rangle \langle \psi |)$.

Lemma I.3. Let \mathcal{H} be a Hilbert space, A a symmetric operator on \mathcal{H} and ψ a unit vector in $\text{dom}(A)$. Then $\Delta_\psi A = 0$ if and only if ψ is an eigenvalue of A . In this case the eigenvalue of ψ is $\langle A \rangle_\psi$.

Proof. Assume $\Delta_\psi A = \left\| (A - \langle A \rangle_\psi \text{id}) \psi \right\| = 0$. Then $(A - \langle A \rangle_\psi \text{id}) \psi = 0$, or $A\psi = \langle A \rangle_\psi \psi$, which means that ψ is an eigenvector with eigenvalue $\langle A \rangle_\psi$.

Conversely, suppose ψ is an eigenvector of A with eigenvalue λ , i.e. $A\psi = \lambda\psi$. Then

$$\langle A \rangle_\psi = \langle \psi, A\psi \rangle = \langle \psi, \lambda\psi \rangle = \lambda \langle \psi, \psi \rangle = \lambda.$$

Thus $A\psi = \langle A \rangle_\psi \psi$ and $\Delta_\psi A = 0$. □

Lemma I.4. Let \mathcal{H} be a Hilbert space, A a symmetric operator on \mathcal{H} and ψ a unit vector in $\text{dom}(A)$. Then

$$(\Delta_\psi A)^2 = \left\langle (A - \langle A \rangle_\psi \text{id}) \psi, (A - \langle A \rangle_\psi \text{id}) \psi \right\rangle = \langle A\psi, A\psi \rangle - \langle A \rangle_\psi^2.$$

If ψ is also in $\text{dom}(A^2)$, then

$$(\Delta_\psi A)^2 = \left\langle (A - \langle A \rangle_\psi \text{id})^2 \psi, \psi \right\rangle = \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2.$$

Proof. We calculate (using symmetry, the fact that $\langle A \rangle_\psi$ is real and the fact that ψ is a unit vector)

$$\begin{aligned}
(\Delta_\psi A)^2 &= \left\langle (A - \langle A \rangle_\psi \text{id})\psi, (A - \langle A \rangle_\psi \text{id})\psi \right\rangle \\
&= \langle A\psi, A\psi \rangle - \left\langle A\psi, \langle A \rangle_\psi \psi \right\rangle - \left\langle \langle A \rangle_\psi \psi, A\psi \right\rangle + \left\langle \langle A \rangle_\psi \psi, \langle A \rangle_\psi \psi \right\rangle \\
&= \langle A\psi, A\psi \rangle - \langle A \rangle_\psi \langle \psi, A\psi \rangle - \langle A \rangle_\psi \langle \psi, A\psi \rangle + \langle A \rangle_\psi^2 \langle \psi, \psi \rangle \\
&= \langle A\psi, A\psi \rangle - \langle A \rangle_\psi^2 - \langle A \rangle_\psi^2 + \langle A \rangle_\psi^2 \\
&= \langle A\psi, A\psi \rangle - \langle A \rangle_\psi^2.
\end{aligned}$$

Now assume $\psi \in \text{dom}(A^2)$. Then $\psi \in \text{dom}((A - \langle A \rangle_\psi \text{id})^2)$ and thus $(A - \langle A \rangle_\psi \text{id})\psi \in \text{dom}(A - \langle A \rangle_\psi \text{id})$. The first equality follows by symmetry. For the second equality we have a similar reasoning starting from the equation above. \square

3.1.1 Uncertainty relations

Theorem I.5 (Heisenberg's uncertainty principle). *Let \mathcal{H} be a Hilbert space and A, B symmetric operators on \mathcal{H} . Let ψ be a unit vector in $\text{dom}(AB) \cap \text{dom}(BA)$. Then*

$$(\Delta_\psi A)(\Delta_\psi B) \geq \frac{1}{2} |\langle [A, B] \rangle_\psi|.$$

Proof. By the Cauchy-Schwarz inequality, XVI.8, we have

$$\begin{aligned}
(\Delta_\psi A)(\Delta_\psi B) &= \left\| (A - \langle A \rangle_\psi \text{id})\psi \right\| \left\| (B - \langle B \rangle_\psi \text{id})\psi \right\| \\
&\geq \left| \left\langle (A - \langle A \rangle_\psi \text{id})\psi, (B - \langle B \rangle_\psi \text{id})\psi \right\rangle \right| \\
&\geq |\Im \langle (A - \langle A \rangle_\psi \text{id})\psi, (B - \langle B \rangle_\psi \text{id})\psi \rangle| \\
&= |\Im \left(\langle A\psi, B\psi \rangle - \langle A\psi, \langle B \rangle_\psi \psi \rangle - \langle \langle A \rangle_\psi \psi, B\psi \rangle + \langle \langle A \rangle_\psi \psi, \langle B \rangle_\psi \psi \rangle \right)| \\
&= |\Im \left(\langle A\psi, B\psi \rangle - \langle A \rangle_\psi \langle B \rangle_\psi \right)| \\
&= \frac{1}{2} |\langle A\psi, B\psi \rangle - \overline{\langle A\psi, B\psi \rangle}| = \frac{1}{2} |\langle A\psi, B\psi \rangle - \langle B\psi, A\psi \rangle|.
\end{aligned}$$

Since $\psi \in \text{dom}(AB)$, we have $B\psi \in \text{dom}(A)$. Similarly $A\psi \in \text{dom}(B)$. Thus, by symmetry, we have

$$\frac{1}{2} |\langle A\psi, B\psi \rangle - \langle B\psi, A\psi \rangle| = \frac{1}{2} |\langle \psi, AB\psi \rangle - \langle \psi, BA\psi \rangle| = \frac{1}{2} |\langle \psi, [A, B]\psi \rangle| = \frac{1}{2} |\langle [A, B] \rangle_\psi|.$$

\square

3.2 Time evolution

3.2.1 The Schrödinger equation

$$H = i\hbar \frac{d}{dt}$$

Lemma I.6. $U = e^{Ht/i\hbar} = e^{-iHt/\hbar}$.

3.2.2 Schrödinger and Heisenberg pictures

Lemma I.7. *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.

3.2.3 Adiabatic theorem

Theorem I.8. *Let \mathcal{H} be a Hilbert space and consider a path $H : [0, 1] \rightarrow \mathcal{SA}(\mathcal{H}) : s \mapsto H(s)$ of self-adjoint operators on the Hilbert space.*

Take $\epsilon > 0$. If the Hamiltonian of a system is given by $H(\epsilon t)$ for times $t \in [0, \epsilon^{-1}]$. Then the state ρ of the system satisfies

$$i\epsilon \frac{d\rho(s)}{ds} = [H(s), \rho(s)],$$

where $s = \epsilon t \in [0, 1]$.

Assume $\lambda(s) \in \sigma(H(s))$ is an isolated point of the spectrum for all $s \in [0, 1]$. It is an eigenvalue and let $P(s)$ be the orthogonal projector onto the eigenspace. Set $\Delta(s) := \inf d(\lambda, \sigma(H(s)) \setminus \{\lambda(s)\})$.

Assume $\rho(0) \leq P(0)$. Consider the fidelity $F(s) := \text{Tr}(P(s)\rho(s))$. Then

$$F(1) \geq 1 - \epsilon O\left(\frac{\|H'\|^2}{\Delta^3} + \frac{\|H''\|}{\Delta^2}\right).$$

Proof. We first write down a differential equation for the fidelity (where $\iota = \frac{d}{ds}$)

$$\frac{dF(s)}{ds} = \text{Tr}(P' \rho) + \text{Tr}(P \rho').$$

The second term is zero because P commutes with H :

$$\begin{aligned} \text{Tr}(P \rho') &= -\epsilon^{-1} i \text{Tr}\left(P[H, \rho]\right) \\ &= -\epsilon^{-1} i \text{Tr}\left(P(H\rho - \rho H)\right) \\ &= -\epsilon^{-1} i \text{Tr}\left(PH\rho\right) + \epsilon^{-1} i \text{Tr}\left(\rho HP\right) \\ &= -\epsilon^{-1} i \text{Tr}\left(PH\rho\right) + \epsilon^{-1} i \text{Tr}\left(\rho PH\right) \\ &= -\epsilon^{-1} i \text{Tr}\left([PH, \rho]\right) = 0, \end{aligned}$$

by XVI.162.

Now set $Q(s) = \text{id} - P(s)$ and consider the pseudoinverse $(H - \lambda \text{id})^+$ (TODO by continuous functional calculus?). Then $(H - \lambda \text{id})(H - \lambda \text{id})^+ = Q = (H - \lambda \text{id})^+(H - \lambda \text{id})$ by continuous

functional calculus (TODO ref). Now we can expand $P' = PP'Q + QP'P$ (by XIV.72.2), so

$$\begin{aligned}
\frac{dF(s)}{ds} &= \text{Tr}(P'\rho) \\
&= \text{Tr}(PP'Q\rho + QP'P\rho) \\
&= \text{Tr}\left(PP'(H - \lambda \text{id})^+(H - \lambda \text{id})\rho + (H - \lambda \text{id})(H - \lambda \text{id})^+P'P\rho\right) \\
&= \text{Tr}\left(P'(H - \lambda \text{id})^+(H - \lambda \text{id})\rho P + (H - \lambda \text{id})^+P'P\rho(H - \lambda \text{id})\right) \\
&= \text{Tr}\left(P'(H - \lambda \text{id})^+(H\rho P - \rho\lambda P) + (H - \lambda \text{id})^+P'(P\rho H - \lambda P\rho)\right) \\
&= \text{Tr}\left(P'(H - \lambda \text{id})^+(H\rho - \rho H)P + (H - \lambda \text{id})^+P'P(\rho H - H\rho)\right) \\
&= \text{Tr}\left(P'(H - \lambda \text{id})^+[H, \rho]P - (H - \lambda \text{id})^+P'P[H, \rho]\right) \\
&= \text{Tr}\left(PP'(H - \lambda \text{id})^+[H, \rho] - (H - \lambda \text{id})^+P'P[H, \rho]\right) \\
&= \text{Tr}\left(P'Q(H - \lambda \text{id})^+[H, \rho] - (H - \lambda \text{id})^+QP'[H, \rho]\right) \\
&= \text{Tr}\left(P'(H - \lambda \text{id})^+[H, \rho] - (H - \lambda \text{id})^+P'[H, \rho]\right) \\
&= \text{Tr}\left([P', (H - \lambda \text{id})^+] \cdot [H, \rho]\right) \\
&= i\epsilon \text{Tr}\left([P', (H - \lambda \text{id})^+]\rho'\right)
\end{aligned}$$

Integrating this w.r.t. s gives

$$F(1) - F(0) = i\epsilon \int_0^1 \text{Tr}\left([P', (H - \lambda \text{id})^+]\rho'\right) ds.$$

We fill in that $F(0) = 1$ and perform integration by parts to obtain

$$\begin{aligned}
F(1) &= 1 + i\epsilon \int_0^1 \text{Tr}\left([P', (H - \lambda \text{id})^+]\rho'\right) ds \\
&= 1 + i\epsilon \text{Tr}\left([(H - \lambda \text{id})^+, P']\rho\right)_0^1 - i\epsilon \int_0^1 \text{Tr}\left([(H - \lambda \text{id})^+, P']'\rho\right) ds
\end{aligned}$$

□

Proposition I.9. *Let \mathcal{H} be a Hilbert space, $H : [0, 1] \rightarrow \mathfrak{SA}(\mathcal{H})$ and $P(s)$ the projector on an eigenspace associated to some subset of the spectrum σ' that is separated from the rest by a gap $g(s)$. Let $\rho(s)$ be the solution the the Heisenberg equation*

$$i\epsilon \frac{d\rho(s)}{ds} = [H(s), \rho(s)] \quad \rho(0) = P(0).$$

Then we can write

$$\rho(s) = \sum_{n=0}^N \epsilon^n B_n(s) - \epsilon^N \int_0^s U_\epsilon(s, r) \dot{B}_N(r) U_\epsilon(r, s) dr,$$

where the B_n satisfy the recursion relation

$$\begin{cases} B_0(s) = P(s) \\ B_n(s) = \frac{1}{2\pi} \int_\Gamma R_H(z) [P, \dot{B}_{n-1}] R_H(z) dz + S_n - 2PS_nP \end{cases},$$

where Γ is some Jordan curve that contains σ' , but not the rest of the spectrum,

$$S_n := \sum_{m=1}^{n-1} B_m B_{n-m}$$

and $U_\epsilon(s, t)$ is the propagator that satisfies

$$\begin{cases} i\epsilon \frac{\partial}{\partial s} U_\epsilon(s, r) = H U_\epsilon(s, r) \\ U_\epsilon(r, r) = \text{id} . \end{cases}$$

Lemma I.10. *Let \mathcal{H} be a Hilbert space and $H : [0, 1] \rightarrow \mathcal{SA}(\mathcal{H})$ a function that belongs to the Gevrey class $G^\alpha(R)$. Then*

$$\left\| \frac{d^k B_n(s)}{ds^k} \right\| \leq L(n, k) := \frac{1}{(10n + 0.3)^2} g^{-2n-k} (2CR(k + 3n))^{k+3n} .$$

Proof.

□

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

Bras and kets

Let A be some set. We denote the Hilbert space $\ell^2(A)$ by \mathcal{H}_A and define the ket function

$$|-\rangle : A \rightarrow \ell^2(A) : a \mapsto |a\rangle$$

by

$$|a\rangle(x) = \delta_{ax}.$$

In particular $\mathcal{H}_n \cong \mathbb{C}^n$ for all $n \in \mathbb{N}$.

The set $\{|a\rangle\}_{a \in A}$ forms a Hilbert basis of \mathcal{H}_A .
In particular $\{|0\rangle, |1\rangle\}$ is a basis of \mathbb{C}^2 .

Chapter 2

Circuit model

2.1 Qubits

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

2.1.1 $\mathfrak{su}(2)$ and the Pauli matrices

The qubit Hamiltonians are elements of $\mathfrak{u}(2)$. 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*

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

We call

- the eigenbasis of σ_z the Z-basis or computational basis and write the elements

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix};$$

- the eigenbasis of σ_x the X-basis or coherence basis and write the elements

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \quad |-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{|0\rangle - |1\rangle}{\sqrt{2}}.$$

2.1.2 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.

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

2.2 Gates

2.2.1 One-qubit gates

2.2.1.1 Hadamard gate

The Hadamard gate or Walsh-Hadamard gate W is the linear operation determined by

the following matrix:

$$W = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We have the following mappings

$$\begin{aligned} W|0\rangle &= |+\rangle & W|+\rangle &= |0\rangle \\ W|1\rangle &= |-\rangle & W|-\rangle &= |1\rangle \end{aligned}$$

Lemma II.5. *The Hadamard gate is its own inverse: $W^2 = \mathbb{1}$.*

2.2.1.2 Pauli gates

Each of the Pauli matrices determines an operation on \mathbb{C}^2 . In this context we often write X, Y and Z for σ_x, σ_y and σ_z .

Lemma II.6. *The Pauli gates are their own inverses: $X^2 = Y^2 = Z^2 = \mathbb{1}$.*

2.2.2 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 3

Eigenpath traversal

3.1 Quantum Zeno effect

Proposition II.7. *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

3.2 Adiabatic quantum computation

3.3 Evolution through measurement

3.3.1 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.8 (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 4

Variational quantum algorithms

Chapter 5

Algorithms

5.1 Some building blocks

5.1.1 Preparing states

5.1.1.1 Uniform superposition

Lemma II.9. *Consider the Hilbert space $\mathcal{H}_{\mathbb{F}_2^k}$. We can generate a uniform superposition of computational basis states by applying a Hadamard gate to each register, initialised to zero:*

$$\frac{1}{2^k} \sum_{b \in \mathbb{F}_2^k} |b\rangle = W^{\otimes k} |0\rangle^{\otimes k}.$$

Projection on the n -dimensional uniform superposition is given by $\frac{1}{n} \mathbb{J}_{n \times n}$.

5.1.2 Quantum Fourier transform

5.2 Quantum oracle querying

5.2.1 Oracle set-up

For any finite set A , we define a mapping

$$O : (A \rightarrow \mathbb{F}_2) \rightarrow \text{End}(\mathcal{H}_A \otimes \mathcal{H}_{\mathbb{F}_2}) : f \mapsto O_f$$

where

$$O_f(|k\rangle \otimes |q\rangle) := |k\rangle \otimes |f(k) + q\rangle.$$

We call O_f the quantum oracle of f .

Lemma II.10. *We can convert an oracle O_f to a unitary operator $U_f : \mathcal{H}_A \rightarrow \mathcal{H}_A : |k\rangle \mapsto (-1)^{f(k)} |k\rangle$ using only a constant number of Hadamard and NOT gates: If A is finite, then $U_f = \text{id} - 2 \sum_{k \in f^{-1}(1)} |k\rangle\langle k|$, which is a Householder matrix.*

Proof. We show that the circuit transforms $|k\rangle$ into $(-1)^{f(k)} |k\rangle$.

Given input $|k\rangle$, the oracle acts on $|k\rangle \otimes |-\rangle = |k\rangle \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = \frac{|k\rangle \otimes |0\rangle}{\sqrt{2}} - \frac{|k\rangle \otimes |1\rangle}{\sqrt{2}}$ and produces

$$\begin{aligned} \frac{|k\rangle \otimes |f(k)\rangle}{\sqrt{2}} - \frac{|k\rangle \otimes |f(k) + 1\rangle}{\sqrt{2}} &= \begin{cases} |k\rangle \otimes |-\rangle & (f(k) = 0) \\ -|k\rangle \otimes |-\rangle & (f(k) = 1) \end{cases} \\ &= (-1)^{f(k)} |k\rangle \otimes |-\rangle. \end{aligned}$$

Given that XW is the inverse of WX , the output $U_f |k\rangle$ is equal to $(-1)^{f(k)} |k\rangle$. The second register is left in the state $|0\rangle$, thus we can either measure or just discard it. Finally, assume A finite. Then

$$\begin{aligned} U_f &= U_f \text{id} = U_f \sum_{k \in A} |k\rangle \langle k| = \sum_{k \in f^{-1}(0)} U_f |k\rangle \langle k| + \sum_{k \in f^{-1}(1)} U_f |k\rangle \langle k| \\ &= \sum_{k \in f^{-1}(0)} |k\rangle \langle k| - \sum_{k \in f^{-1}(1)} |k\rangle \langle k| \\ &= \sum_{k \in f^{-1}(0)} |k\rangle \langle k| - \sum_{k \in f^{-1}(1)} |k\rangle \langle k| + \sum_{k \in f^{-1}(1)} |k\rangle \langle k| - \sum_{k \in f^{-1}(1)} |k\rangle \langle k| \\ &= \left(\sum_{k \in f^{-1}(0)} |k\rangle \langle k| + \sum_{k \in f^{-1}(1)} |k\rangle \langle k| \right) - 2 \sum_{k \in f^{-1}(1)} |k\rangle \langle k| \\ &= \text{id} - 2 \sum_{k \in f^{-1}(1)} |k\rangle \langle k| \end{aligned}$$

□

5.2.2 Deutsch's problem

Problem statement

Suppose we have a 1-bit to 1-bit function $f : \{0, 1\} \rightarrow \{0, 1\} : x \mapsto f(x)$. Determine whether f is

- constant, i.e. $f(0) = f(1)$; or
- balanced, i.e. $f(0) \neq f(1)$.

Proposition II.11. *The classical query complexity of Deutsch's problem is 2. The quantum query complexity is 1.*

Proof. The classical case is clear.

In the quantum case, we have access to the unitary $U_f : \mathcal{H}_{\mathbb{F}_2} \rightarrow \mathcal{H}_{\mathbb{F}_2}$ from II.10. The state

$WU_fW|0\rangle$ is as follows:

$$\begin{aligned}
WU_fW|0\rangle &= WU_f|+\rangle = WU_f\left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \\
&= W\left(\frac{(-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle}{\sqrt{2}}\right) \\
&= W\begin{cases} (-1)^{f(0)}\frac{|0\rangle + |1\rangle}{\sqrt{2}} = (-1)^{f(0)}|+\rangle & (f(0) = f(1)) \\ (-1)^{f(0)}\frac{|0\rangle - |1\rangle}{\sqrt{2}} = (-1)^{f(0)}|-\rangle & (f(0) \neq f(1)) \end{cases} \\
&= \begin{cases} (-1)^{f(0)}|0\rangle & (f(0) = f(1)) \\ (-1)^{f(0)}|1\rangle & (f(0) \neq f(1)) \end{cases}
\end{aligned}$$

If we measure this state, then we will certainly measure 0 if f is constant and 1 if f is balanced. \square

5.2.3 Grover's search algorithm

Problem statement

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:

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

The problem is to find any marked item.

Classically we need to check $\Theta(N/M)$ items on average. Grover's algorithm has a query complexity of $O(\sqrt{N/M})$.

5.2.3.1 The algorithm

Define the states

$$|\mathcal{N}\rangle := \frac{1}{\sqrt{N}} \sum_{n \in \mathcal{N}} |n\rangle \langle n|, \quad \text{and} \quad |\mathcal{M}\rangle := \frac{1}{\sqrt{M}} \sum_{m \in \mathcal{M}} |m\rangle \langle m|.$$

Using II.10, construct the unitary $U_f = \text{id}_{\mathcal{H}_N} - 2 \sum_{m \in \mathcal{M}} |m\rangle \langle m|$. Also construct the Householder matrix

$$U = W^{\otimes \nu} (\text{id} - 2|0\rangle \langle 0|) W^{\otimes \nu} = \text{id} - \mathbb{J}_{2 \times 2}^{\otimes \nu} = \text{id} - \mathbb{J}_{2\nu \times 2\nu} = \text{id} - 2|\mathcal{N}\rangle \langle \mathcal{N}|.$$

(TODO Householder circuit).

Now consider the subspace $S := \text{span}\{|\mathcal{M}\rangle, |\mathcal{N}\rangle\}$. We take an orthonormal basis $\{|\mathcal{M}\rangle, |\mathcal{M}'\rangle\}$ of S where

$$|\mathcal{M}'\rangle := \sqrt{\frac{N}{N-M}} |\mathcal{N}\rangle - \sqrt{\frac{M}{N-M}} |\mathcal{M}\rangle = \frac{1}{\sqrt{N-M}} \sum_{k \in \mathcal{N} \setminus \mathcal{M}} |k\rangle.$$

Then we can write

$$|\mathcal{N}\rangle = \sqrt{\frac{N-M}{N}} |\mathcal{M}'\rangle + \sqrt{\frac{M}{N}} |\mathcal{M}\rangle$$

and (using $\text{id} = |\mathcal{M}\rangle\langle\mathcal{M}| + |\mathcal{M}'\rangle\langle\mathcal{M}'|$)

$$\begin{aligned} U_f &= \text{id} - 2|\mathcal{M}\rangle\langle\mathcal{M}| = -|\mathcal{M}\rangle\langle\mathcal{M}| + |\mathcal{M}'\rangle\langle\mathcal{M}'| \\ U &= \text{id} - 2 \left(\sqrt{\frac{N-M}{N}} |\mathcal{M}'\rangle + \sqrt{\frac{M}{N}} |\mathcal{M}\rangle \right) \left(\sqrt{\frac{N-M}{N}} \langle\mathcal{M}'| + \sqrt{\frac{M}{N}} \langle\mathcal{M}| \right) \\ &= \frac{N-2M}{N} |\mathcal{M}\rangle\langle\mathcal{M}| + \frac{2M-N}{N} |\mathcal{M}'\rangle\langle\mathcal{M}'| - 2 \left(\frac{\sqrt{M}\sqrt{N-M}}{N} \right) (|\mathcal{M}\rangle\langle\mathcal{M}'| + |\mathcal{M}'\rangle\langle\mathcal{M}|) \end{aligned}$$

So S is invariant under both U and U_f and we can write the matrix G of $-UU_f$ in this basis:

$$G = \begin{pmatrix} 1 - \frac{2M}{N} & -2\frac{\sqrt{M}\sqrt{N-M}}{N} \\ 2\frac{\sqrt{M}\sqrt{N-M}}{N} & 1 - \frac{2M}{N} \end{pmatrix}.$$

We note that $1 - \frac{2M}{N}$ is some number between -1 and 1 , so we can write it as $\cos \alpha$. Then

$$\sin \alpha = \sqrt{1 - \cos^2 \alpha} = \sqrt{1 - \left(1 - 2\frac{M}{N}\right)^2} = \sqrt{4\frac{M}{N} - 4\frac{M^2}{N^2}} = 2\sqrt{\frac{M}{N}} \sqrt{1 - \frac{M}{N}} = 2\frac{\sqrt{M}\sqrt{N-M}}{N}.$$

Thus

$$G = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} = R_\alpha.$$

We now want to apply G a certain number of times, say k , such that

$$G^k |\mathcal{N}\rangle = G^k \begin{pmatrix} \sqrt{M/N} \\ \sqrt{1-M/N} \end{pmatrix} = R_{k\alpha} R_{\tan^{-1}(\sqrt{N/M-1})} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \approx \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\mathcal{M}\rangle.$$

TODO:

$$\sqrt{\frac{N}{M}} \approx T_k(\cos \alpha) - \sqrt{\frac{N}{M} - 1} U_{k-1}(\cos \alpha)$$

or

$$0 \approx \sqrt{\frac{N}{M} - 1} T_k(\cos \alpha) + U_{k-1}(\cos \alpha) \sin \alpha$$

and

$$(\cos \alpha + \sin \alpha)^k = T_k(\cos \alpha) + \sin \alpha U_{k-1}(\cos \alpha).$$

We also have $\cos \alpha + \sin \alpha = \frac{(\sqrt{N-M} - \sqrt{M})^2 + 2M}{N}$.

5.2.3.2 Analogue Grover

Consider the Hamiltonian $H = |\mathcal{M}\rangle\langle\mathcal{M}| + |\mathcal{N}\rangle\langle\mathcal{N}|$, which we can rewrite in terms of $|\mathcal{M}\rangle$ and $|\mathcal{M}'\rangle$:

$$H = \left(1 + \frac{M}{N}\right) |\mathcal{M}\rangle\langle\mathcal{M}| + \left(1 - \frac{M}{N}\right) |\mathcal{M}'\rangle\langle\mathcal{M}'| + \frac{\sqrt{M}\sqrt{N-M}}{M} (|\mathcal{M}\rangle\langle\mathcal{M}'| + |\mathcal{M}'\rangle\langle\mathcal{M}|),$$

This operator is self-adjoint and leaves the subspace S invariant, so S has a basis of eigenvectors for it.

By XVIII.11.2, all elements of $e^{-iHt}|\mathcal{N}\rangle$ lie in S . W.r.t. the basis $\{|\mathcal{M}\rangle, |\mathcal{M}'\rangle\}$, we have

$$e^{-iHt}|\mathcal{N}\rangle = \begin{pmatrix} \sqrt{M/N} \cos(\sqrt{M/N}t) - i \sin(\sqrt{M/N}t) \\ \sqrt{1-M/N} \cos(\sqrt{M/N}t) \end{pmatrix}.$$

Thus $\langle \mathcal{M} | e^{-iHt} | \mathcal{N} \rangle = \frac{M}{N} \cos^2(\sqrt{M/N}t) + \sin^2(\sqrt{M/N}t)$. This is equal to 1 when $t = \frac{\pi}{2} \sqrt{\frac{N}{M}}$.

Thus we can produce $|\mathcal{M}\rangle$ in $O(\sqrt{N/M})$ time.

TODO: optimality.

5.2.3.3 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 $\mathbf{v}_{0,1}$.

5.2.3.4 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 $\frac{d\rho}{dt}$ 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

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

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 $]t_1, t_1 + \delta[$.

Appendix A

Bibliography

- Quantum Theory - Peres
- QM - Schwabl