Some of the Big Ideas in Quantum Mechanics

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Part I

Quantum Mechanics

Chapter 1

Measurement theory

Chapter 2

Postulates

2.1 States, observables and measurement

2.1.1 States

A <u>state</u> 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. *$\mathrm{Tr}[\rho^2] = 1$;*
5. *$\|\rho\| = 1$;*
6. *$S(\rho) := -\mathrm{Tr}[\rho \ln \rho] = 0$.*

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

2.1.2 Effects

An <u>effect</u> on a Hilbert space is a bounded operator in $[0, \mathrm{id}]$.

Chapter 3

Quantum theory

3.1 Quantum statistics

3.2 Time evolution

3.2.1 The Schrödinger equation

$$H = i\hbar \frac{\mathrm{d}}{\mathrm{d}t}$$

Lemma I.2. *$U = e^{Ht/i\hbar} = e^{-iHt/\hbar}$.*

3.2.2 Schrödinger and Heisenberg pictures

Lemma I.3. *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.4. *Let $\mathcal{H}$ be a Hilbert space and consider a path $H : [0,1] \to \mathcal{SA}(\mathcal{H}) : s \mapsto H(s)$ 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

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

where $s = \epsilon t \in [0,1]$.
Assume $\lambda(s) \in \sigma\big(H(s)\big)$ 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 $\Delta(s) \coloneqq \inf d\big(\lambda, \sigma(H(s)) \setminus \{\lambda(s)\}\big)$.
Assume $\rho(0) \leq P(0)$. Consider the fidelity $F(s) \coloneqq \operatorname{Tr}\big(P(s)\rho(s)\big)$. 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 $\prime = \frac{\mathrm{d}}{\mathrm{d}s}$)

$$\frac{\mathrm{d}F(s)}{\mathrm{d}s} = \mathrm{Tr}(P'\rho) + \mathrm{Tr}(P\rho').$$

The second term is zero because P commutes with H:

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

by XV.161.

Now set $Q(s) = \mathrm{id} - P(s)$ and consider the pseudoinverse $(H - \lambda\,\mathrm{id})^+$ (TODO by continuous functional calculus?). Then $(H-\lambda\,\mathrm{id})(H-\lambda\,\mathrm{id})^+ = Q = (H-\lambda\,\mathrm{id})^+(H-\lambda\,\mathrm{id})$ by continuous functional calculus (TODO ref). Now we can expand $P' = PP'Q + QP'P$ (by XIII.18.2), so

$$\begin{aligned}
\tfrac{\mathrm{d}F(s)}{\mathrm{d}s} &= \mathrm{Tr}(P'\rho) \\
&= \mathrm{Tr}(PP'Q\rho + QP'P\rho) \\
&= \mathrm{Tr}\left(PP'(H-\lambda\,\mathrm{id})^+(H-\lambda\,\mathrm{id})\rho + (H-\lambda\,\mathrm{id})(H-\lambda\,\mathrm{id})^+P'P\rho\right) \\
&= \mathrm{Tr}\left(P'(H-\lambda\,\mathrm{id})^+(H-\lambda\,\mathrm{id})\rho P + (H-\lambda\,\mathrm{id})^+P'P\rho(H-\lambda\,\mathrm{id})\right) \\
&= \mathrm{Tr}\left(P'(H-\lambda\,\mathrm{id})^+\big(H\rho P - \rho\lambda P\big) + (H-\lambda\,\mathrm{id})^+P'\big(P\rho H - \lambda P\rho\big)\right) \\
&= \mathrm{Tr}\left(P'(H-\lambda\,\mathrm{id})^+\big(H\rho - \rho H\big)P + (H-\lambda\,\mathrm{id})^+P'P\big(\rho H - H\rho\big)\right) \\
&= \mathrm{Tr}\left(P'(H-\lambda\,\mathrm{id})^+\big[H,\rho\big]P - (H-\lambda\,\mathrm{id})^+P'P\big[H,\rho\big]\right) \\
&= \mathrm{Tr}\left(PP'(H-\lambda\,\mathrm{id})^+\big[H,\rho\big] - (H-\lambda\,\mathrm{id})^+P'P\big[H,\rho\big]\right) \\
&= \mathrm{Tr}\left(P'Q(H-\lambda\,\mathrm{id})^+\big[H,\rho\big] - (H-\lambda\,\mathrm{id})^+QP'\big[H,\rho\big]\right) \\
&= \mathrm{Tr}\left(P'(H-\lambda\,\mathrm{id})^+\big[H,\rho\big] - (H-\lambda\,\mathrm{id})^+P'\big[H,\rho\big]\right) \\
&= \mathrm{Tr}\left(\big[P',(H-\lambda\,\mathrm{id})^+\big]\cdot\big[H,\rho\big]\right) \\
&= i\epsilon\,\mathrm{Tr}\left(\big[P',(H-\lambda\,\mathrm{id})^+\big]\rho'\right)
\end{aligned}$$

Integrating this w.r.t. s gives

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

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

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

□

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

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

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 $\mathrm{Tr}[\sigma] = \lambda_1 + \lambda_2 = 0$. $\square$

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*

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

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 $\mathfrak{su}(2)/\mathbb{R} \to \sigma \mapsto E_1^\sigma$, 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 $\sigma = 2P_1 - \mathrm{id}$. $\square$

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. □

Corollary II.2.1. *The real algebra generated by* $\mathfrak{su}(2)$ *is the Clifford algebra* $\mathrm{Cl}_{3,0}$*. 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*

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

We call

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

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

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

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

2.1.2 The Bloch sphere

Because $\mathfrak{su}(2)$ is the Clifford algebra $\mathrm{Cl}_{3,0}$, 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

$$W|0\rangle = |+\rangle \qquad\qquad W|+\rangle = |0\rangle$$
$$W|1\rangle = |-\rangle \qquad\qquad W|-\rangle = |1\rangle$$

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 $P \otimes L + (\mathrm{id}_{H_1} - P) \otimes \mathrm{id}_{H_2}$ in $H_1 \otimes H_2 \to H_1 \otimes H_2$.

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

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

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

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

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

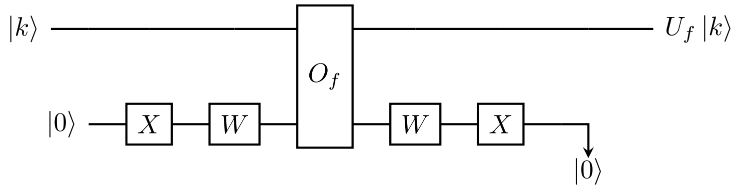
where

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

We call O_f the quantum oracle of f.

Lemma II.10. *We can convert an oracle O_f to a unitary operator $U_f : \mathcal{H}_A \to \mathcal{H}_A : |k\rangle \mapsto$*

$(-1)^{f(k)}\,|k\rangle$ *using only a constant number of Hadamard and NOT gates:*



If A is finite, then $U_f = \mathrm{id} - 2\sum_{k\in f^{-1}(1)} |k\rangle\langle k|$, 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 of just discard it.
Finally, assume A finite. Then

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

□

5.2.2 Deutsch's problem

Problem statement

Suppose we have a 1-bit to 1-bit function $f : \{0,1\} \to \{0,1\} : x \mapsto f(x)$.
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 Deutch'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 $U_f : \mathcal{H}_{\mathbb{F}_2} \to \mathcal{H}_{\mathbb{F}_2}$ 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 is f is constant and 1 if f is balanced. □

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:

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

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

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

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

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

(TODO Householder circuit).
Now consider the subspace $S := \mathrm{span}\{|\mathcal{M}\rangle, |\mathcal{N}\rangle\}$. 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 $\mathrm{id} = |\mathcal{M}\rangle\langle\mathcal{M}| + |\mathcal{M}'\rangle\langle\mathcal{M}'|$)

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

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 $|\mathcal{M}'\rangle$:

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

This operator is self-adjoint and leaves the subspace S invariant, so S has a basis of eigenvectors for it.
By XVII.11.2, all elements of $e^{-iHt}\left|\mathcal{N}\right\rangle$ lie in S. W.r.t. the basis $\{\left|\mathcal{M}\right\rangle, \left|\mathcal{M}'\right\rangle\}$, we have

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

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 $\left|\mathcal{M}\right\rangle$ in $O(\sqrt{N/M})$ time.
TODO: optimality.

5.2.3.3 Adiabatic Grover

$$H_0 = \mathbf{1} - |\mathcal{N}\rangle\langle\mathcal{N}| = \mathbb{1} - \mathbb{J}/N$$
$$H_f = \mathbf{1} - \sum_{m\in\mathcal{M}} |m\rangle\langle m| = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1}_{N-M} \end{pmatrix}.$$

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 transformation 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 $\mathbf{v}_{0,1} = (\sqrt{M}(1-\lambda_{0,1}), \sqrt{N-M}(1-s-\lambda_{0,1}))^{\mathrm{T}}$ 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

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

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

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

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

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

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

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

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