PHY682 Special Topics in Solid-State Physics: Quantum Information Science

Lecture time: 2:40-4:00PM Monday & Wednesday

Today 9/21:

1. Will discuss Grover's algorithm
2. Next Week 5's topics: VQE, QAOA, Hybrid Q-Classical Neural Network, Application to Molecules

Comments: Clifford gates and Gottesman-Knill no go theorem*

- Clifford gates U_C are those that transform a Pauli product σ to another Pauli product operator σ':

$$U_C \, \sigma \, U_C^\dagger = \sigma'$$

- Theorem 10.7: (Gottesman–Knill theorem) Suppose a quantum computation is performed which involves only the following elements: **state preparations in the computational basis, Hadamard gates, phase gates, controlled-NOT gates, Pauli gates, and measurements of observables in the Pauli group** (which includes measurement in the computational basis as a special case), together with the possibility of classical control conditioned on the outcome of such measurements.

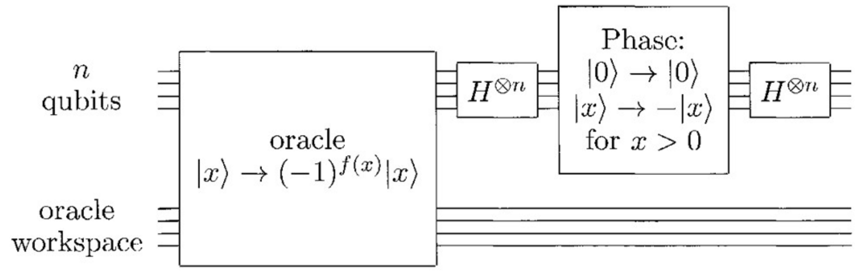
➔ Such a computation may be efficiently simulated on a classical computer.

Quick overview of Grover searching

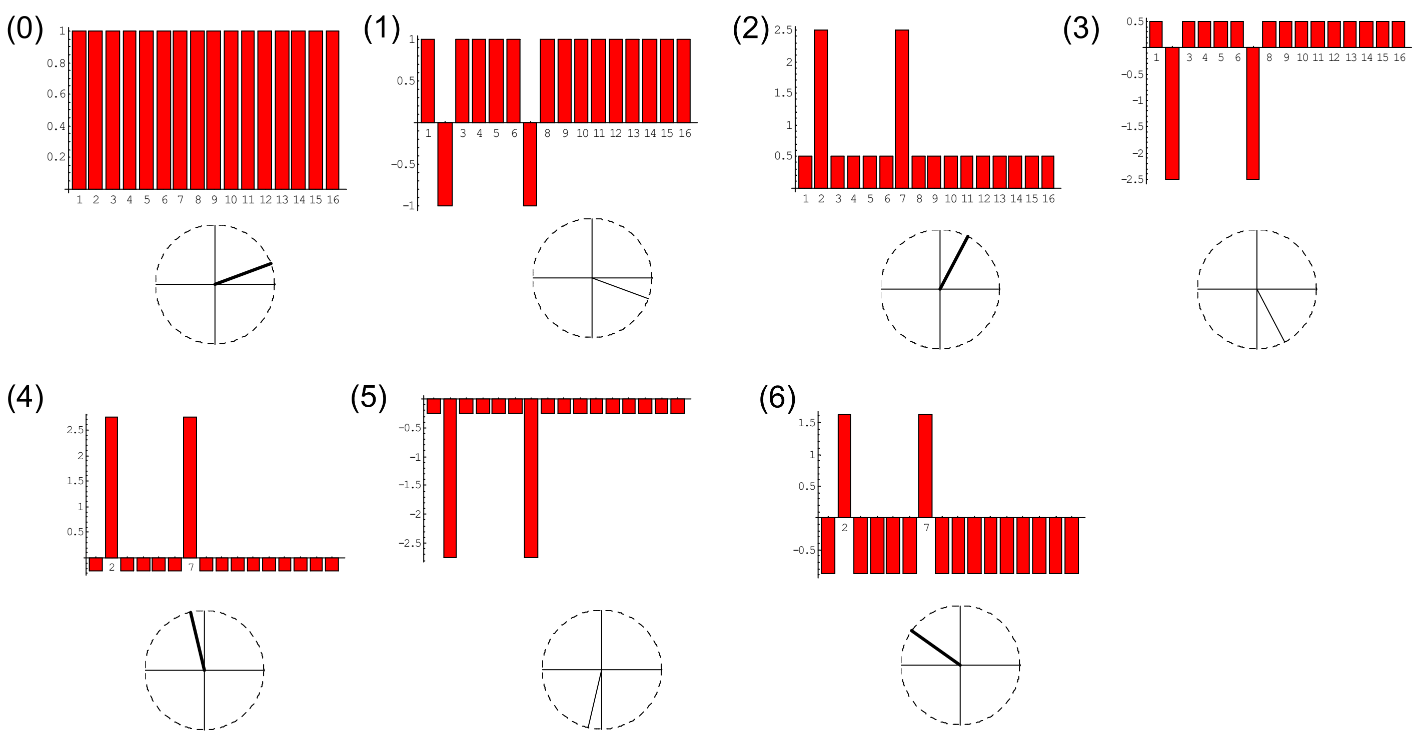
Perform iteration:

(i) Sign on marked targets

(ii) Reflection w.r.t mean



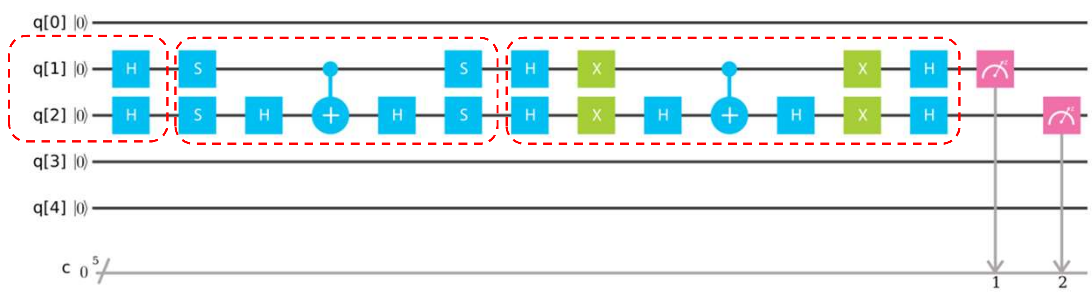
Suppose: items 2 and 7 marked



One-step Grover

4 items (use 2 qubits) with marked item 00

- Web-based interface:



1.initialize

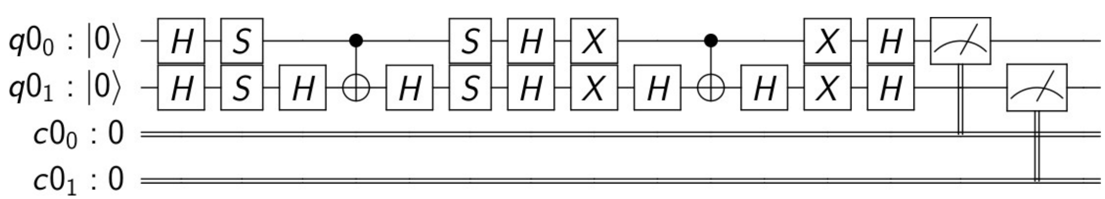
2. Multiply 00 by (-1)

3. Reflect about mean

$$U_s = 2|s\rangle\langle s| - I$$

$$|s\rangle = |++\rangle$$

- Can use python codes (on right) and draw circuit:




```
q = QuantumRegister(2)
c = ClassicalRegister(2)
qc = QuantumCircuit(q, c)

# initialize
qc.h(q[0])
qc.h(q[1])

# mark item 0 (or $|00\rangle$)
qc.s(q[0])
qc.s(q[1])
qc.h(q[1])
qc.cx(q[0], q[1])
qc.h(q[1])
qc.s(q[0])
qc.s(q[1])

# apply reflection around average
qc.h(q[0])
qc.h(q[1])
qc.x(q[0])
qc.x(q[1])

qc.h(q[1])
qc.cx(q[0], q[1])
qc.h(q[1])

qc.x(q[0])
qc.x(q[1])
qc.h(q[0])
qc.h(q[1])

# measure
qc.measure(q,c)
```

See IBM Q userguide or my IPython Notebook:

[Note this is a very old notebook]

https://nbviewer.jupyter.org/url/insti.physics.sunysb.edu/~twei/Notebook/GroverExample.ipynb

Analysis of one Grover step

(i) Sign on marked targets
[equivalent to reflection w.r.t. the unmarked "plane"]

$$\hat{O}_f = \sum_x (-1)^{f(x)} |x\rangle\langle x| = I - 2 \sum_{x \in \text{marked}} |x\rangle\langle x|$$

(ii) Reflection w.r.t mean

$$U_s = 2|s\rangle\langle s| - I = H^{\otimes n}(2|0\ldots 0\rangle\langle 0\ldots 0| - I)H^{\otimes n}$$

$$|s\rangle = |++\cdots+\rangle = \frac{1}{\sqrt{N = 2^n}} \sum_{x=0}^{2^n-1} |x\rangle$$

$$|\alpha\rangle \equiv \sum_k \alpha_k |k\rangle \longrightarrow 2|s\rangle\langle s|\alpha\rangle - |\alpha\rangle \qquad \alpha_k \longrightarrow 2\frac{1}{N}\sum_j \alpha_j - \alpha_k = 2\langle\alpha\rangle - \alpha_k$$

- One Grover iteration is a unitary operation that is equivalent to a rotation:

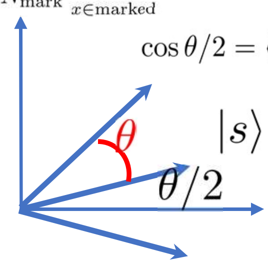
$$\hat{G} \equiv U_s \hat{O}_f$$

with the angle satisfying

$$\sin\theta = 2\frac{\sqrt{N_{\text{mark}}(N - N_{\text{mark}})}}{N}$$

$$|\psi_{\text{marked}}\rangle \equiv \frac{1}{\sqrt{N_{\text{mark}}}} \sum_{x \in \text{marked}} |x\rangle$$

$$\cos\theta/2 = \langle s|\psi_{unmarked}\rangle = \frac{\sqrt{(N - N_{\text{mark}})}}{\sqrt{N}}$$



$$|\psi_{\text{unmarked}}\rangle \equiv \frac{1}{\sqrt{N - N_{\text{mark}}}} \sum_{x \in \text{unmarked}} |x\rangle$$

Time complexity of Grover Algorithm

- One Grover iteration is a unitary operation that is equivalent to a rotation:

$$\hat{G} \equiv U_s \hat{O}_f$$

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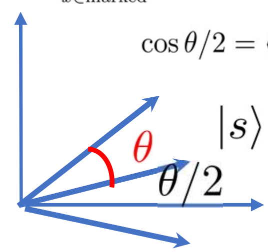


$$|\psi_{\mathrm{unmarked}}\rangle \equiv \frac{1}{\sqrt{N - N_{\mathrm{mark}}}} \sum_{x \in \mathrm{unmarked}} |x\rangle$$

- Assume number of marked items smaller than N/2, and approximate

$$\theta \approx 2\frac{\sqrt{N_{\mathrm{mark}}(N - N_{\mathrm{mark}})}}{N}$$

➔ Number of iterations to reach an angle π/2:

$$N_{\mathrm{iter}}\,\theta + \frac{\theta}{2} \approx \frac{\pi}{2} \qquad N_{\mathrm{iter}} \approx \frac{\pi}{2\theta} - \frac{1}{2} \approx \left\lceil \frac{1}{4}\sqrt{\frac{N}{N_{\mathrm{mark}}}} \right\rceil$$

➔ For N=4, only one marked item: θ=π/3, one iteration reaches the target with probability 1

What if number of marked items is unknown?

- One Grover iteration is a unitary operation that is equivalent to a rotation:

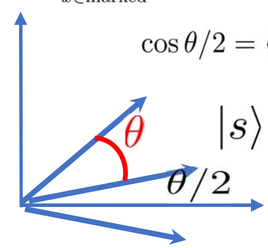
$$\hat{G} \equiv U_s \, \hat{O}_f$$

$$|\psi_{\text{marked}}\rangle \equiv \frac{1}{\sqrt{N_{\text{mark}}}} \sum_{x \in \text{marked}} |x\rangle$$

$$\cos\theta/2 = \langle s|\psi_{unmarked}\rangle = \frac{\sqrt{(N - N_{\text{mark}})}}{\sqrt{N}}$$

with the angle satisfying

$$\sin\theta = 2\frac{\sqrt{N_{\text{mark}}(N - N_{\text{mark}})}}{N}$$



$$|\psi_{\text{unmarked}}\rangle \equiv \frac{1}{\sqrt{N - N_{\text{mark}}}} \sum_{x \in \text{unmarked}} |x\rangle$$

- Need to estimate θ first, using the quantum phase estimation (later lecture)

➔ Grover operator has two eigenvalues $e^{\pm i\theta}$

Generalization: Amplitude amplification*

- Recall one Grover:

$$\hat{G} \equiv U_s \hat{O}_f$$
$$= H^{\otimes n} U_{|0\rangle^\perp} H^{\otimes n} \hat{O}_f$$

$$\hat{O}_f = \sum_x (-1)^{f(x)} |x\rangle\langle x|$$
$$U_s = H^{\otimes n}(2|0\ldots0\rangle\langle 0\ldots0| - I)H^{\otimes n}$$
$$= H^{\otimes n} U_{|0\rangle^\perp} H^{\otimes n}$$

With initial state: $|\psi_{\rm ini}\rangle = H^{\otimes n}|0\ldots0\rangle$

- Generalize above form to

$$\hat{G}_A = A\, U_{|0\rangle^\perp} A^{-1} \hat{O}_f$$
$$= U_{|\psi\rangle^\perp} \hat{O}_f$$

With initial state: $|\psi\rangle = A|0\ldots0\rangle$

$$= \sin(\theta/2)|\psi_{\rm good}\rangle + \cos(\theta/2)|\psi_{\rm bad}\rangle$$

|0…0> can contain extra work qubits

➔ Action of G_A is a rotation of angle θ in the 2D space spanned by $\{|\psi_{\rm good}\rangle, |\psi_{\rm bad}\rangle\}$

Or equivalently $\{|\psi\rangle, |\bar{\psi}\rangle \equiv \cos(\theta/2)|\psi_{\rm good}\rangle - \sin(\theta/2)|\psi_{\rm bad}\rangle\}$

$$(\hat{G}_A)^k|\psi\rangle = \sin(k\,\theta + \theta/2)|\psi_{\rm good}\rangle + \cos(k\theta + \theta/2)|\psi_{\rm bad}\rangle$$