Unit 04: Grinding Gates in Quantum Computers

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In this unit, we discuss the standard circuit-based quantum computation and introduce the Qiskit software developed by IBM.

Learning outcomes: (1) You'll be able to know elementary single-qubit and two-qubit quantum gates. (2) You'll be able to understand what quantum computation is and the specific quantum algorithm on searching. (3) You'll be able to get started in IBM Qiskit and run simple Jupyter notebooks of quantum circuits.

I. INTRODUCTION

We will now give an overview of quantum computation in terms of the standard circuit model. You have seen all the necessary ingredients before, and these are: (1) Initialization, (2) Gate operations and (3) Measurement/Readout. The schematic circuit is shown in Fig. 1.

In the initialization, we usually assume that all qubits are initialized to $|0\rangle$, unless stated otherwise. The specific layout of gate operations does not need to resemble that shown in the figure and it may depend on how an n-qubit unitary U is decomposed into a sequence of one-qubit and two-qubit gates. This second ingredient is the crux of quantum computation. To read out results, we need to perform measurement and it is usually assumed that each qubit is measured in the 0/1 or equivalently Z basis. If we need to measure in $+/-$ basis, we can apply a Hadamard gate H right before the 0/1 measurement.

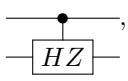
Universal gate set. In classical computation, AND and NOT gates or just NAND gates are sufficient to build any Boolean functions. They are regarded as universal gate sets. In quantum computation, we also have the similar notion of universality. You may have heard people say that H, T and CNOT constitute a universal gate set, where we have seen H and CNOT, and T gate is

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix},$$

which can be regarded as a $\pi/4$ rotation about the z-axis: $T = e^{i\pi/8} e^{-i(\pi/4)(Z/2)}$. However, there are two fine-grained details. First, these three gates together *cannot* exactly constitute an arbitrary unitary U, but *can approximate* it as close as possible. This is the approximate universality. There are two other examples of such approximate universal gate sets.

- Example 2:

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \text{Controlled} - \text{HZ} =$$



$$, \quad \text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} =$$

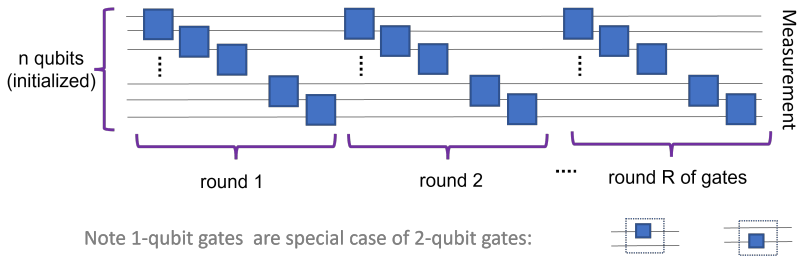


FIG. 1. Illustration of quantum computation in terms of the standard circuit model. We also note that one-qubit gates are a special case of two-qubit gates.

- Example 3:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{Toffoli} = \text{C}^2 - X \text{ (Control-Control-NOT)} =$$

The last two examples show universal gates but achieve arbitrary gates in an approximate way. They also illustrate that universal quantum computation can be done with real-valued gates only.

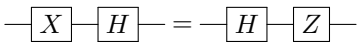
The exact universal set of gates includes all the one-qubit gates $u3(\theta, \phi, \lambda)$ and the CNOT gate (or equivalently C-Z gate for the latter); the specific form of u_3 is

$$u3(\theta,\phi,\lambda) = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & e^{i\lambda+i\phi}\cos(\theta/2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix} = e^{i(\phi+\lambda)/2} e^{-i\phi Z/2} e^{-i\theta Y/2} e^{-i\lambda Z/2}, \tag{1}$$

which is a rotation using Euler angles: first around z by λ, then around y by θ, followed by rotation around z by ϕ.

II. GATE IDENTITIES AND MULTIQUBIT GATE DECOMPOSITION

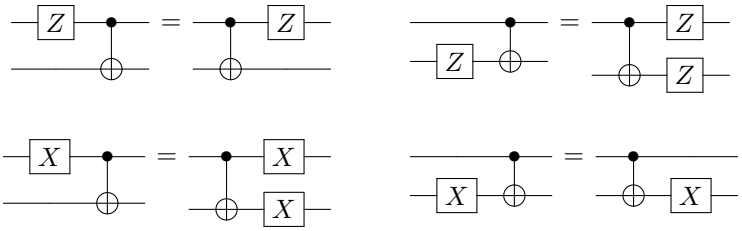
Gate identities. The first one we have seen earlier is the transformation between x and z bases via the Hadamard gate,



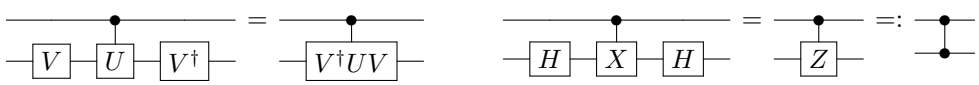
How do we transform between x and y bases? It is done via the phase gate,

$$S \equiv \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \quad SXS^\dagger = Y.$$

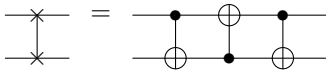
Given CNOT's importance as a two-qubit gate, we examine how it commutes with X and Z gates.



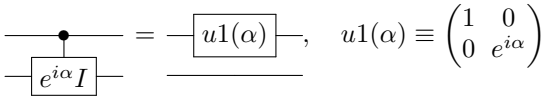
We can also conguate controlled gates by a single-qubit unitary at the target,



To build a swap gate between two qubits requires three CNOTs,

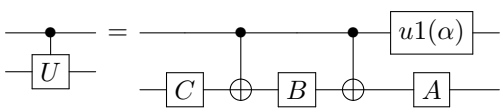


A controlled phase gate is similar to the phase kickback,



$$u1(\alpha) \equiv \begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix}$$

Multiqubit gates from the standard set. There are a few useful identities for us to construct multiqubit gates. But first we look at the two-qubit gate,



(2)

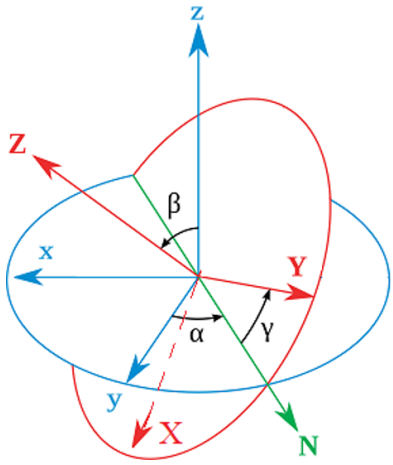
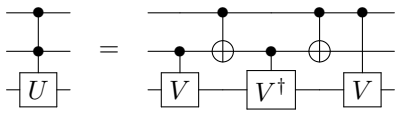


FIG. 2. Illustration of Euler rotations: how two sets of coordinate frames can be rotated to each other. The two x-y and X-Y planes intersect along the N axis. It is thus clear that the two axes z and Z are orthogonal to N. To align the two frames, one rotate y axis around z axis (by an angle α) so that y axis aligns with the N axis. Then one rotate z axis about N to align with the Z axis by an angle β. Finally, one rotates the y axis (now with N) around the Z axis by an angle γ to align with the Y axis. The x and X axes will then be aligned automatically.

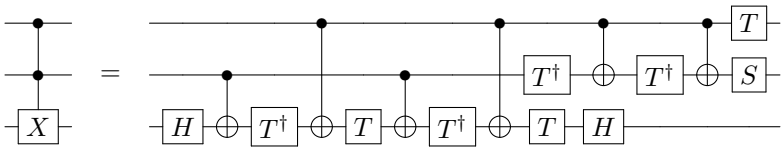
This is based on the single-qubit U being decomposed to $U = e^{i\alpha}AXBXC$, with $ABC = I$. The next is a three-qubit controlled gate,



where $V^2 = U$. For Toffoli gate: U=X, so can choose the following V and then the controlled-V,

$$V = \frac{1-i}{2}(I + iX) \Rightarrow V^2 = X.$$

This requires 8 CNOT gates. But there is a decomposition with 6 CNOT gates



This is left as an exercise. We note that there is a proof that there must be at least 5 two-qubit gates for the Toffoli gate [1].

In the book by Nielsen and Chuang, there is some discussion on n-qubit controlled unitary, but we will not cover it here.

Euler rotation. According to the steps in Fig. 2, the overall rotation is described by

$$U(\alpha, \beta, \gamma) = R_Z(\gamma)R_N(\beta)R_z(\alpha).$$

We will need the two identities

$$R_Z(\gamma) = R_N(\beta)R_z(\gamma)R_N(\beta)^{-1}, \quad R_N(\beta) = R_z(\alpha)R_y(\beta)R_z(\alpha)^{-1},$$

which simply come from the fact that a rotation by one axis can be done by first rotating the vector to a second axis, then rotating around this axis by the desired angle, and finally rotating from the second axis back to the firist. We then rewrite the above U with mixed axes to one with the fixed axes,

$$U(\alpha, \beta, \gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma).$$

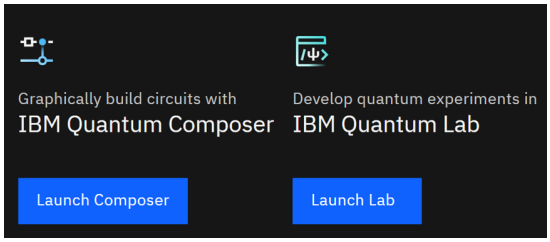


FIG. 3. Illustration of part of the view in a Qiskit account. Two key components to write and run codes are: (1) IBM Quantum Composer and (2) IBM Quantum Lab.

We also include an arbitrary overall phase in the unitary group and for one qubit we have

$$e^{\imath\delta}U(\alpha,\beta,\gamma) = e^{i\delta}R_z(\alpha)R_y(\beta)R_z(\gamma).$$

The IBM's $u3$ gate (see above Eq. 1) is related to this via $\delta = \frac{\alpha+\gamma}{2},\ \beta=\theta,\ \alpha=\phi,\ \gamma=\lambda$.

Relating back to the decomposition of control-U in Eq. (2), for the above Euler decomposition, one can verify that $A = R_z(\alpha)R_y(\beta/2)$, $B = R_y(-\beta/2)R_z\big(-(\gamma+\alpha)/2\big)$ and $C = R_z\big((\gamma-\alpha)/2\big)$.

III. IBM QISKIT: AN INTRODUCTION

A. Register for an account

Please go to `https://quantum-computing.ibm.com/` to register an account. After loginning to your account, you will see (1) IBM Quantum Composer and (2) IBM Quantum Lab among other things, as illustrated in Fig. 3.

B. Qiskit gate set

Here, we list a gates that are available on IBM Qiskit [2]. (We note that some conventions have changed, e.g. gates u3 and u2, will be lumped into a single u gate and u1 gate is renamed as 'p' gate. This also affect their controlled versions.)

u gates.

- u3(angle1,angle2,angle3):

$$u3(\theta,\phi,\lambda) = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & e^{i\lambda+i\phi}\cos(\theta/2) \end{pmatrix}$$

- u2(angle1,angle2):

$$u2(\phi,\lambda) = u3(\pi/2,\phi,\lambda) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\phi} & e^{i(\phi+\lambda)} \end{pmatrix}$$

- u1(angle1):

$$u1(\lambda) = u3(0,0,\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}$$

Identity gate: iden = u0(angle),

$$u0(\delta) = u3(0,0,0)$$

Hadamard gate: h.

Phase gate and its inverse: s and sdg.

T gate and its inverse: t and tdg.

Rotations about X,Y,Z axes: rx(angle,qubit), ry(angle,qubit) and rz(angle,qubit).

There are multiple qubit gates.

Controlled-NOT gate: cx(control,target).

Controlled-Y and -Z gates: cy(control,target) and cz(control,target).

Controlled-Hadamard gate: ch(control,target).

Controlled-Rotation gates: crx(angle,control,target), cry(angle,control,target) and crz(angle,control,target).

Controlled-U1 gate: cu1(angle,control,target).

Controlled-U3 gate: cu3(angle1,angle2,angle3,control,target).

Swap gate: swap(qubit1,qubit2).

Toffoli gate: ccx(control1,control2,target).

Controlled swap gate (Fredkin gate): cswap(control,qubit2,qubit3).

The following are not unitary operations. **Measurement**: measure(qubit, classical bit).

Reset qubit to 0: reset(qubit).

Conditional operation (on classical outcome):

```
qc.measure(q, c)
qc.x(q[0]).c_if(c, 0)#apply X to q[0] if c is 0
```

C. Measurement

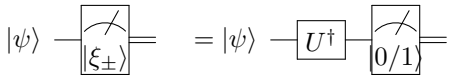
In IBM, Google or Rigetti, the measurement is done in 0/1 basis, e.g.

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

In order to measure in arbitrary basis defined by $|\xi(0)\rangle$ and $|\xi(1)\rangle$:

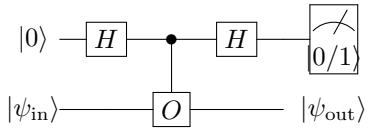
$$|\xi_+\rangle = U_\xi|0\rangle,\ |\xi_-\rangle = U_\xi|1\rangle,$$

we first apply inverse of U (i.e. $U^\dagger$) before measuring in 0/1 basis,



Note if one cares about the exact post-measurement state being in the $\xi\rangle$ basis, one should apply U after the measurement to undo the basis change $U^\dagger$ done earlier.

How to measure a single-qubit operator O (unitary and Hermitian, thus $O^2 = I$) and leave the output in the eigenstate? It can be done with the following circuit (a kind of Hadamard test),



Principle of deferred measurement. In principle, measurement can be moved to the end of the circuit; if measurement results are used to classically control some operation, it can be replaced by a corresponding controlled operation.

IV. CLIFFORD GATES AND GOTTESMAN-KNILL NO-GO THEOREM

Clifford gates UC are those that transform a Pauli product σ to another Pauli product operator σ' (up to ± 1):

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

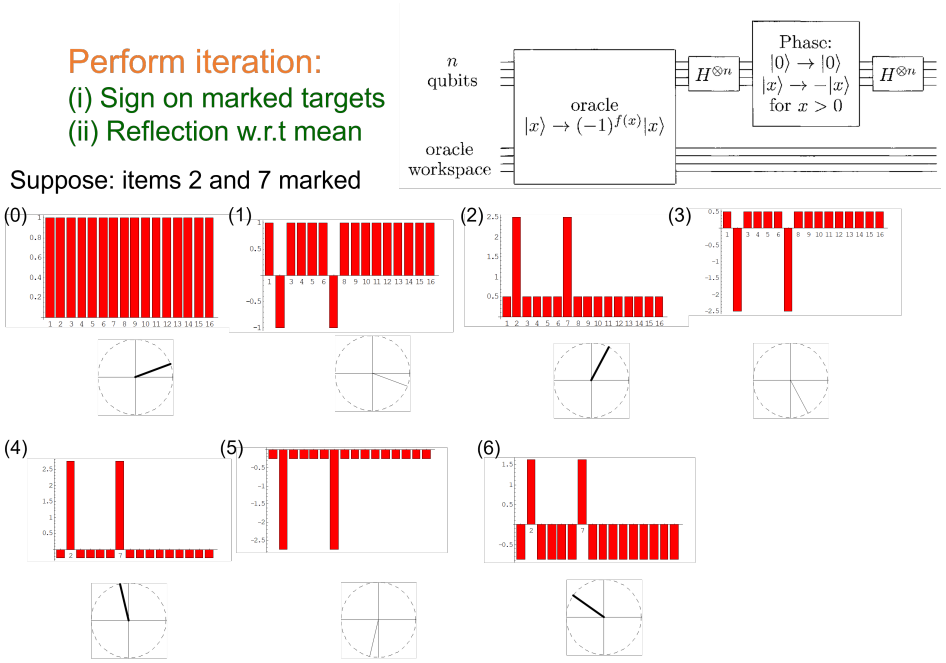


FIG. 4. Illustration of Grover's algorithm on 16 objects with 2 marked items.

For one qubit, we have seen example gates that do this: $\{H, S\}$. Of course, Pauli gates X, Y, Z are also other examples, albeit trivial, as they commute or any commute with each other. In fact, the Pauli gates can be generated by $\{H, S\}$, e.g. $Z = S^2$, and $X = HS^2H$. It turns one-qubit Clifford group is generated by H and S, i.e. $\mathcal{C}_1 = \langle\langle H, S\rangle\rangle$. Moreover, for multiple qubit Clifford group, we need additionally CNOT gates.

Given that the transformation by the Clifford group can be identified by how Pauli products are transformed, quantum computation using only these gates (and simple measurements) can be efficiently simulated.

Theorem 10.7 [of Nielsen and Chuang]: (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.

V. GROVER'S SEARCH ALGORITHM

Let us refer to Fig. 4 for an illustration of Grover's search algorithm [3–5]. The algorithm invovles these following steps ,

(i) Flip the 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) Relfection w.r.t. to the mean:

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

where

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

Under this,

$$|\alpha\rangle \equiv \sum_k \alpha_k |k\rangle \longrightarrow 2|s\rangle\langle s|\alpha\rangle - |\alpha\rangle,$$

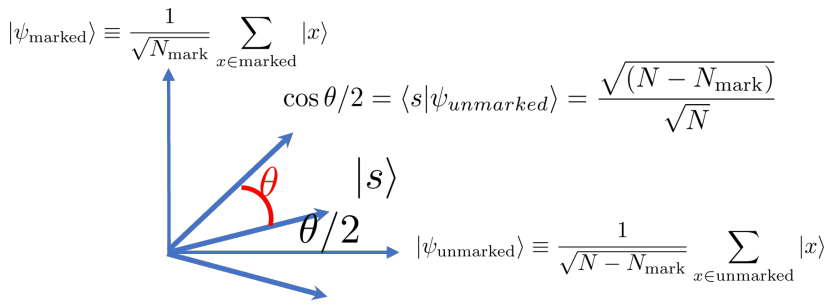


FIG. 5. Illustration of the geometric picture of the Grover's search algorithm.

in terms of the components,

$$\alpha_k \longrightarrow 2\frac{1}{N}\sum_j \alpha_j - \alpha_k = 2\langle\alpha\rangle - \alpha_k.$$

These two steps are reflections. One Grover iteration is a combination of the two and is thus a unitary operation that is equivalent to a rotation:

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

with the angle θ satisfying

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

This is illustrated in Fig. 5. The goal is to reach $\theta = \pi/2$ as close as possible, and the mumber of iterations to reach the angle $\pi/2$ is

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

When there is just one marked item $N_{\rm mark} = 1$,

$$N_{\rm iter} \approx \left\lceil \frac{\sqrt{N}}{4} \right\rceil,$$

meaning that there is a speedup compared to classical search that needs to examine on average $N/2$ items.

Note that for $N = 4$ with only one marked item: $\theta = \pi/3$, one iteration reaches the target with probability 1.

When the number of marked items is unknown. How do we know when to stop? This requires the knowledge of the angle θ, which can be estimated using the quantum phase estimation algorithm, which we will discuss in a later lecture. Essentially, the Grover operator $\hat{G}$ has two eigenvalues $e^{\pm i\theta}$. If one can imprint the phase to a quantum register then we can read it out using the so-called quantum Fourier transform, which is part of the quantum phase estimation algorithm.

VI. GENERALIZATION: AMPLITUDE AMPLIFICATION

Amplitude amplication [6] generalizes the Grover's algorithm and we do not need to create an equal superposition of all objects. Let us recall the case for Grover.

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

where

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

The algorithm iteratively applies $\hat{G}$ to an initial state

$$|\psi_{\rm ini}\rangle = H^{\otimes n}|0\ldots 0\rangle.$$

With such a picture, we can generalize the above form

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

The initial state is generated by A,

$$|\psi\rangle = A|0\ldots 0\rangle = \sin(\theta/2)|\psi_{\rm good}\rangle + \cos(\theta/2)|\psi_{\rm bad}\rangle,$$

where $|\psi_{\rm good}\rangle$ is a superposition of all marked items and $|\psi_{\rm bad}\rangle$ contains no marked item in the superposition. Note that $|00...0\rangle$ can contain extra work qubits. The action of $\hat{G}_A$ is a rotation of θ in the 2D space spanned by $\{|\psi_{\rm good}\rangle, |\psi_{\rm bad}\rangle\}$, or equivalently, spanned by

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

Then the action of $\hat{G}_A$ on $|\psi\rangle$ leads to

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

The goal is to get as close to $k\theta + \theta/2 = \pi/2$ for some integer k.

Note that similar to Grover's search, the operator $\hat{G}_A$ also has eigenvalues $e^{\pm i\theta}$, which, in principle, can be calculated from the so-called quantum phase estimation (to be covered in a later lecture).

Hadamard test and generalization. This part combines ideas from Hadamard test, amplitude amplification and quantum phase estimation; see, e.g., Section II of Ref. [7] for a summary. But given useful applications require the use of the quantum phase estimation, we are not yet prepared to discuss the details at this point.

VII. CONCLUDING REMARKS

In this unit, we have discussed the standard circuit-based quantum computation and introduced the Qiskit software developed by IBM.

It is a good time to check whether you have achieved the following Learning Outcomes:

After this Unit, (1) You'll be able to know elementary single-qubit and two-qubit quantum gates. (2) You'll be able to understand what quantum computation is and the specific quantum algorithm on searching. (3) You'll be able to get started in IBM Qiskit and run simple Jupyter notebooks of quantum circuits.

Suggested reading: N&C chap 4; KLM chap 4; Qb 1.4; 2.4, 2.5. A. Barenco et al., Elementary gates for quantum computation [8].

[1] N. Yu, R. Duan, and M. Ying, Five two-qubit gates are necessary for implementing the toffoli gate, Physical Review A **88**, 010304 (2013).

[2] M. S. ANIS, Abby-Mitchell, H. Abraham, *et al.*, Qiskit: An open-source framework for quantum computing (2021).

[3] L. K. Grover, A fast quantum mechanical algorithm for database search, in *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing* (1996) pp. 212–219.

[4] L. K. Grover, Quantum mechanics helps in searching for a needle in a haystack, Phys. Rev. Lett. **79**, 325 (1997).

[5] L. K. Grover, Quantum computers can search rapidly by using almost any transformation, Phys. Rev. Lett. **80**, 4329 (1998).

[6] G. Brassard, P. Hoyer, M. Mosca, and A. Tapp, Quantum amplitude amplification and estimation, Contemporary Mathematics **305**, 53 (2002).

[7] J. Zhao, Y.-H. Zhang, C.-P. Shao, Y.-C. Wu, G.-C. Guo, and G.-P. Guo, Building quantum neural networks based on a swap test, Phys. Rev. A **100**, 012334 (2019).

[8] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. A. Smolin, and H. Weinfurter, Elementary gates for quantum computation, Phys. Rev. A **52**, 3457 (1995).