



Lectures 31-33: Grover's Algorithm

CS 401: Quantum Computing
Dr. Kell, Spring 2023

Grover's Algorithm



(Discovered in 1996 by Lov Grover)



Problem: “unstructured” search problem, where we can efficiently verify if we’ve found a target solution (i.e., a problem in NP).

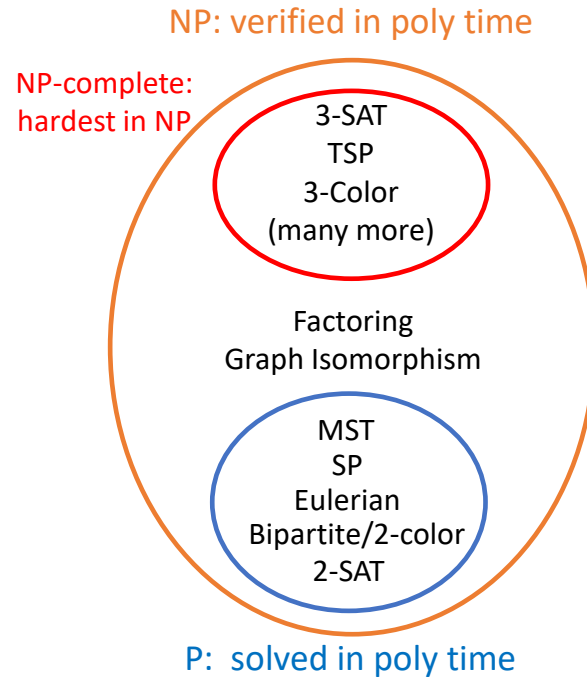
Input: list L, target value
Output: index of target in L

$L = [2, 1, 10, 4, 7, 9, 3] \rightarrow 4$
target = 7 (index of 7)



Many applications in cloud quantum computing, databases, etc.

Best Possible Classical Algorithm: $O(n)$
Grover's Quantum Algorithm: $O(n^{1/2})$



Punchline: N total solutions that can be verified in $O(T)$ time then:

Best Possible Classical Algo: $O(NT)$ time

↓ quadratic speed-up

Best Possible Quantum Algo: $O(\sqrt{NT})$ time

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NP: verified in poly time

NP-complete:
hardest in NP

3-SAT
TSP
3-Color
(many more)

Factoring
Graph Isomorphism

MST
SP
Eulerian
Bipartite/2-color
2-SAT

P: solved in poly time

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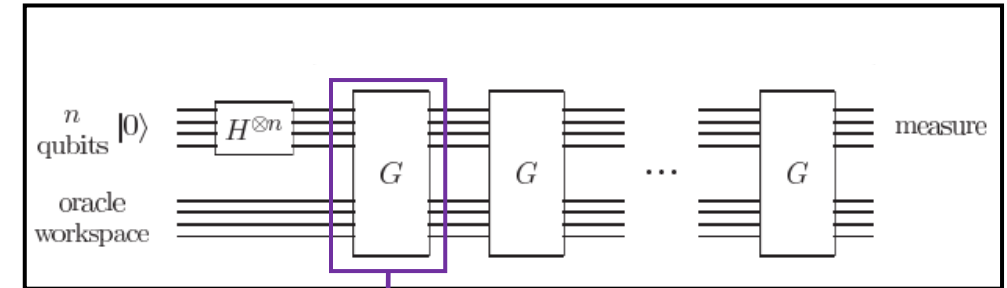
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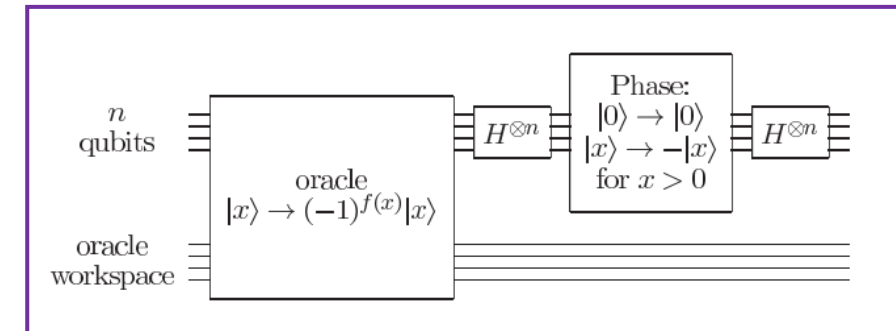
Best Possible Quantum Algo: $O(\sqrt{NT})$ time

Grover's Algorithm Circuit Outline

Top-level



Grover Iteration



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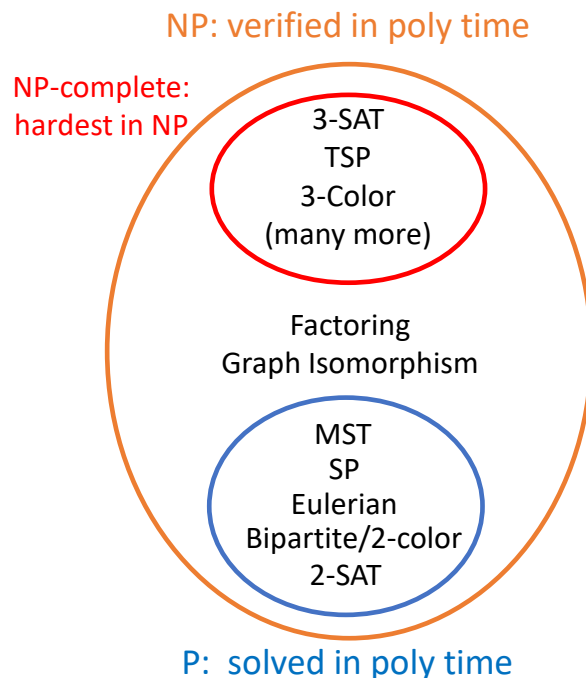
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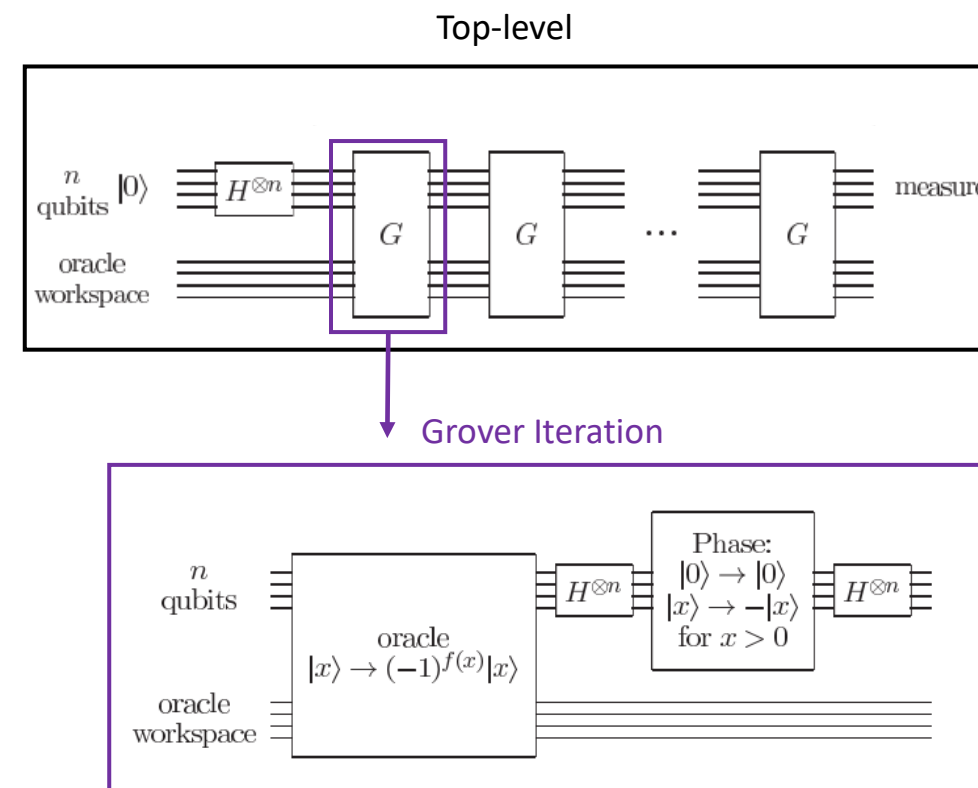


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Grover's Algorithm Circuit Outline



Essentially: oracle = U_f gate with $|-\rangle$ qubit
 $f(x) = 0 \rightarrow$ not a solution $f(x) = 1 \rightarrow$ is a solution

$$\begin{bmatrix} x & & x \\ & U_f & \\ y & & y \oplus f(x) \end{bmatrix} \text{ on } |x\rangle \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}} \right] = (-1)^{f(x)} |x\rangle \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}} \right]$$

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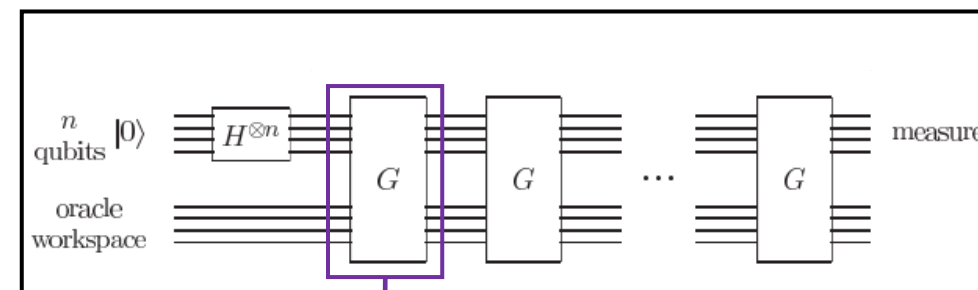
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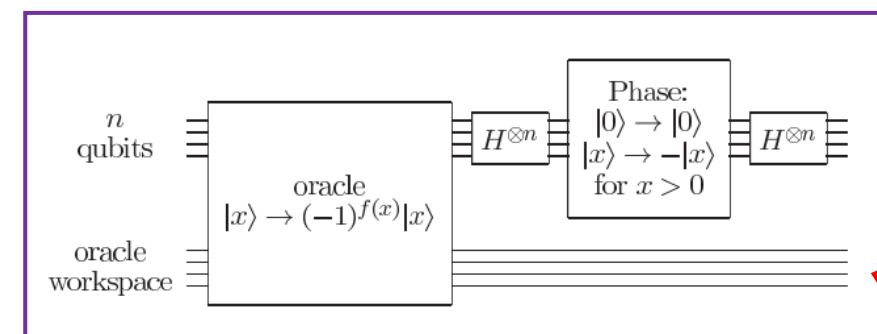
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Grover's Algorithm Circuit Outline

Top-level



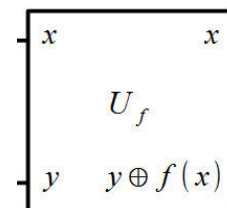
Grover Iteration



... can think of it belonging to workspace

Essentially: oracle = U_f gate with $|-\rangle$ qubit

$f(x) = 0 \rightarrow$ not a solution $f(x) = 1 \rightarrow$ is a solution



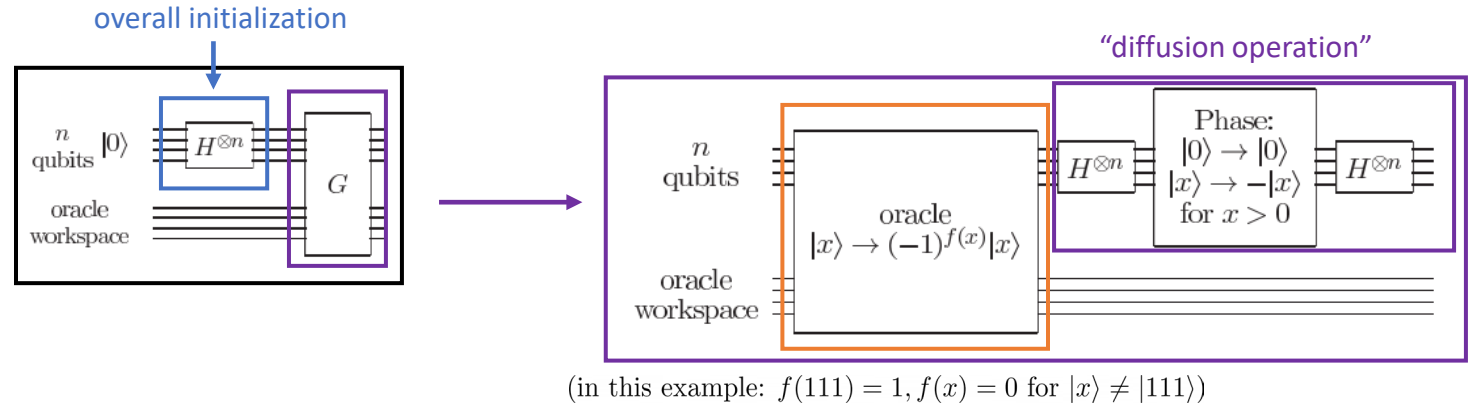
$$\text{on } |x\rangle \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}} \right] = (-1)^{f(x)} |x\rangle \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}} \right]$$

Just like Deutsch-Jozsa: y qubit won't be changed throughout

Geometric Interpretation of a Grover Iteration

Example: 3-qubits, target = $|111\rangle$

solution to instance



Hadamard on n-qubit 0 state

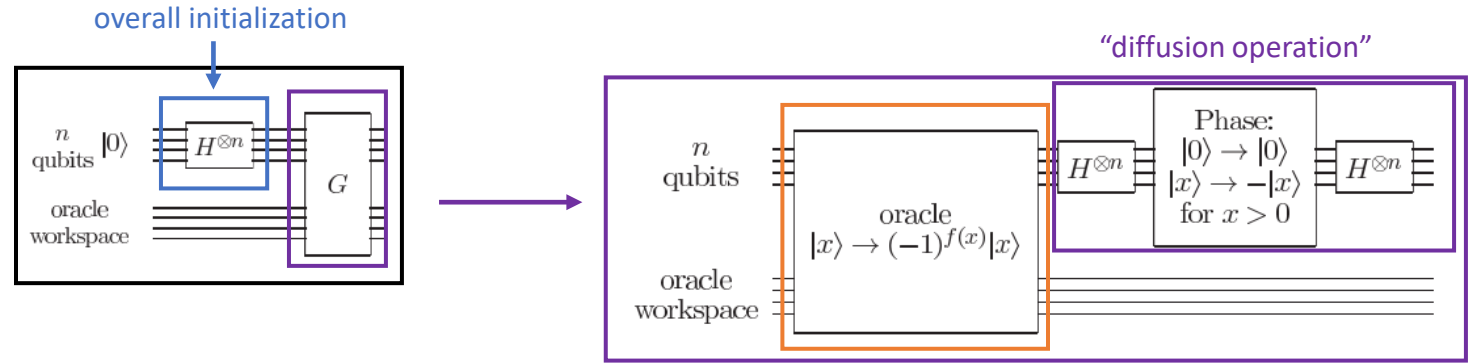
“unit vector in direction of all non-solutions”

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solution to instance

$$|\beta\rangle = |111\rangle$$



(in this example: $f(111) = 1, f(x) = 0$ for $|x\rangle \neq |111\rangle$)

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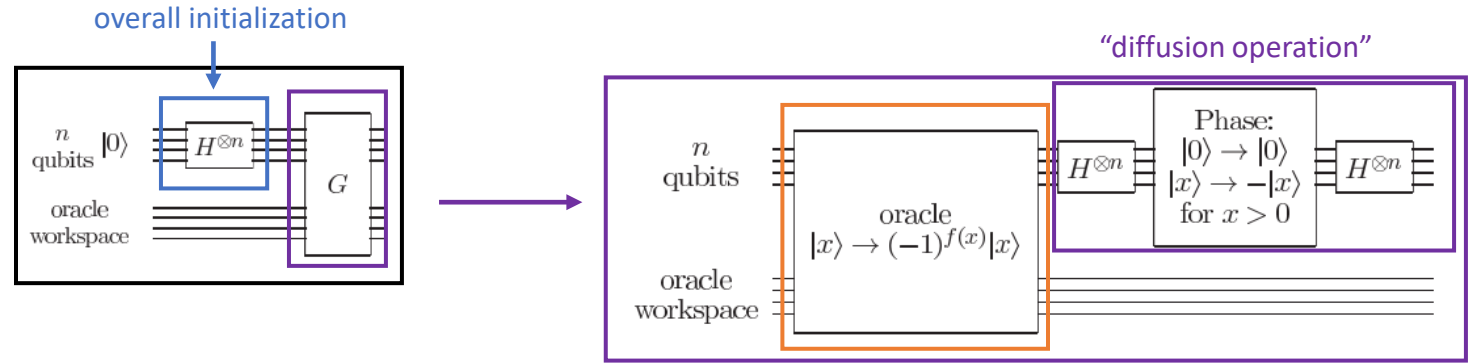
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$$|\psi\rangle = H|000\rangle = \frac{1}{\sqrt{8}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle \right]$$

Hadamard on n-qubit 0 state

“unit vector in direction of all non-solutions”

$$|\alpha\rangle = \frac{1}{\sqrt{7}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle \right]$$

Geometric Interpretation of a Grover Iteration

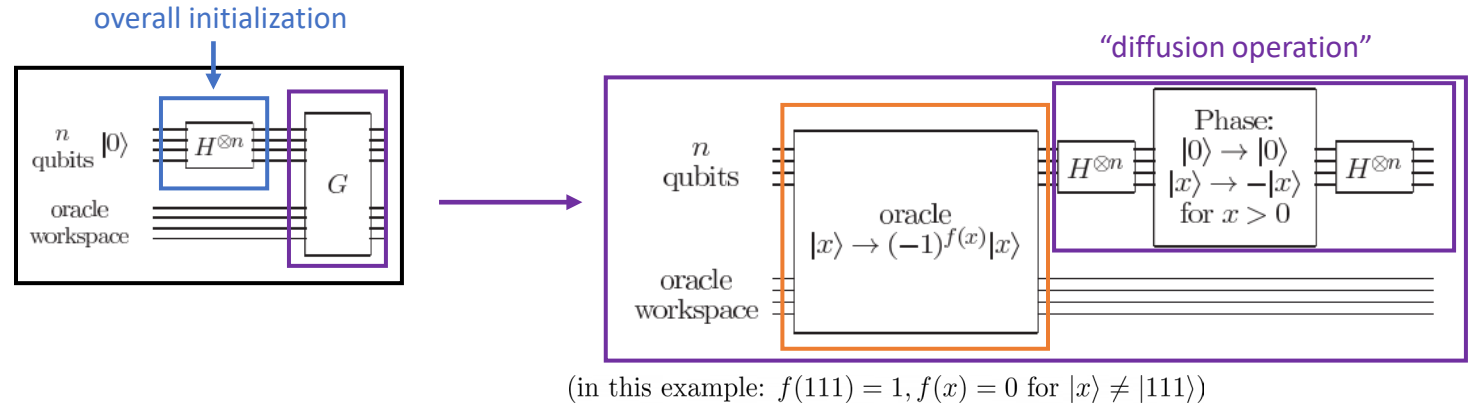
Example: 3-qubits, target = $|111\rangle$

solution to instance

no instance

▲

$$|\beta\rangle = |111\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$



$$|\psi\rangle = H|000\rangle = \frac{1}{\sqrt{8}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle \right] =$$

Hadamard on n-qubit 0 state

[illegible]

“unit vector in direction of all non-solutions”

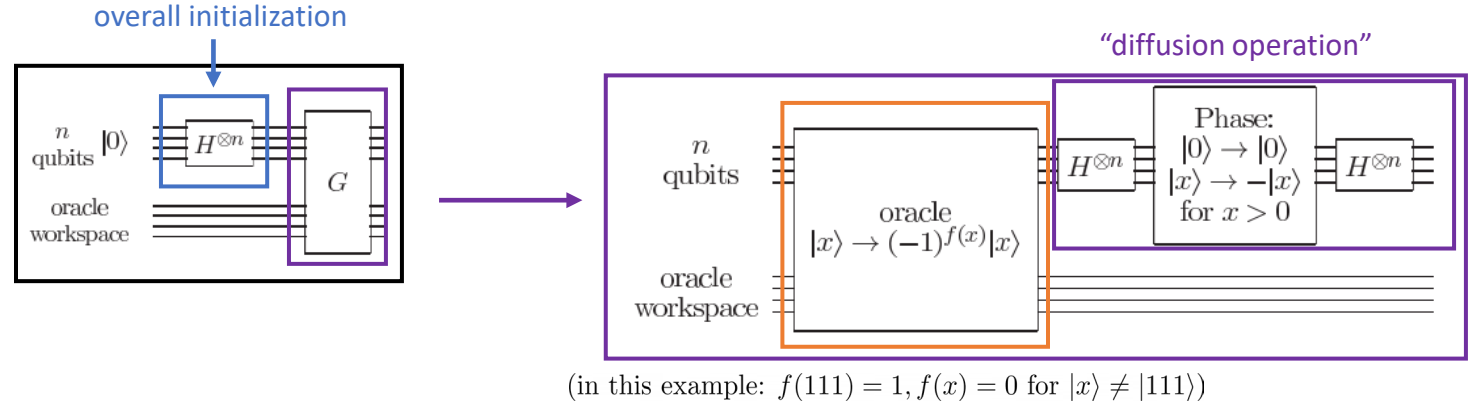
$$|\alpha\rangle = \frac{1}{\sqrt{7}} \begin{bmatrix} |000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle \end{bmatrix} = \begin{bmatrix} \frac{\sqrt{7}}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ 0 \end{bmatrix}$$

Geometric Interpretation of a Grover Iteration

Example: 3-qubits, target = $|111\rangle$

solution to instance

$$|\beta\rangle = |111\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$



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$$\begin{bmatrix} \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \end{bmatrix}$$

reflection across $|\alpha\rangle$

“unit vector in direction of all non-solutions”

$$|\alpha\rangle = \frac{1}{\sqrt{7}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle \right] =$$

$$\begin{bmatrix} \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ \frac{1}{\sqrt{7}} \\ 0 \end{bmatrix}$$

$$\frac{1}{\sqrt{8}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle - |111\rangle \right]$$

Identical vector but now negative direction along beta axis

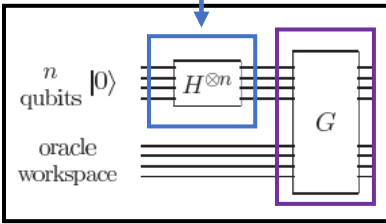
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Example: 3-qubits, target = $|111\rangle$

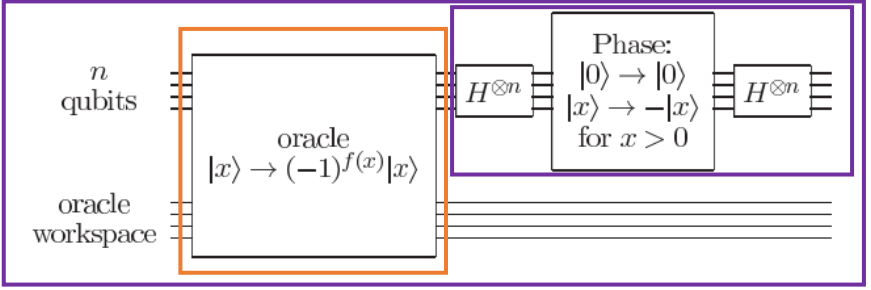
solution to instance

$$|\beta\rangle = |111\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

overall initialization



“diffusion operation”



(in this example: $f(111) = 1, f(x) = 0$ for $|x\rangle \neq |111\rangle$)

High-level: brings current state “back up” above $|\psi\rangle$

$$|\psi\rangle = H|000\rangle = \frac{1}{\sqrt{8}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle \right] =$$

Hadamard on n-qubit 0 state

$$\begin{bmatrix} \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{8}} \end{bmatrix}$$

reflection across $|\alpha\rangle$

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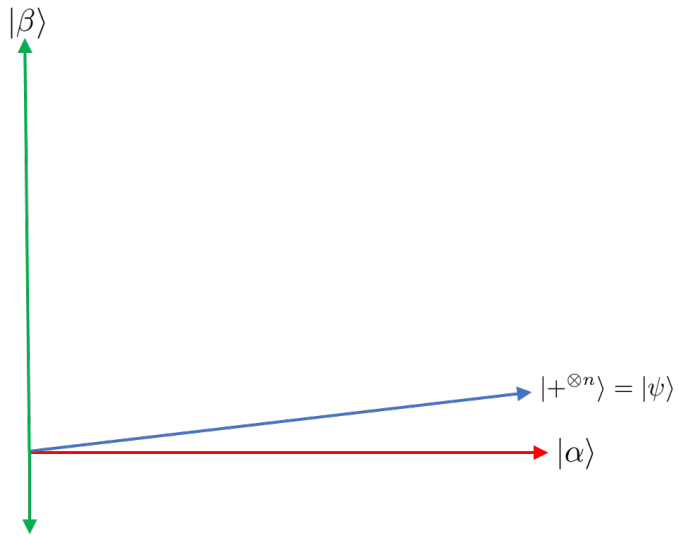
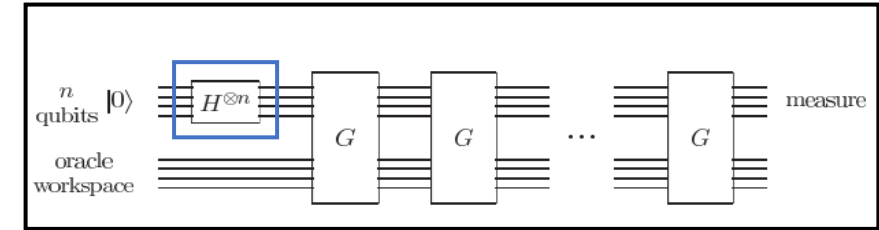
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Identical vector but now negative direction along beta axis

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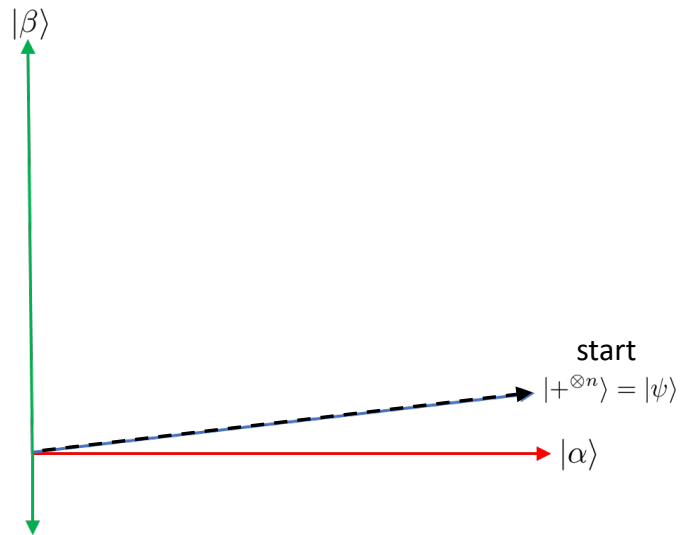
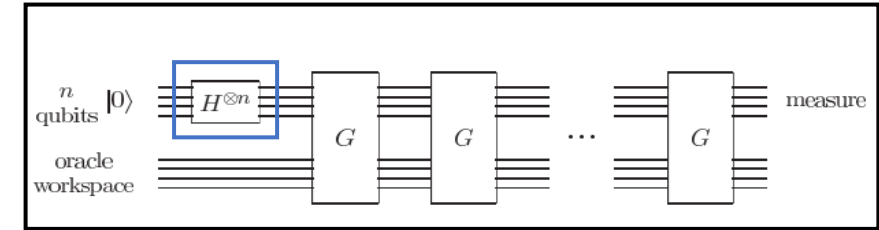
Geometric Interpretation of a Grover Iteration

Thus: state of circuit makes progress toward beta with each application of G.



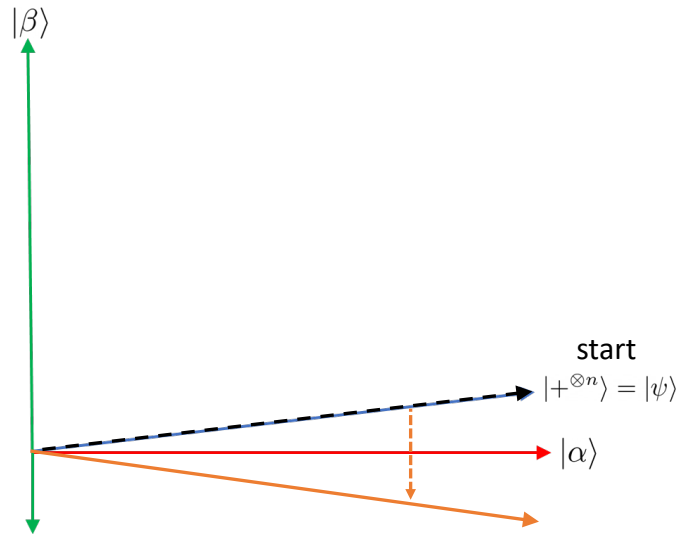
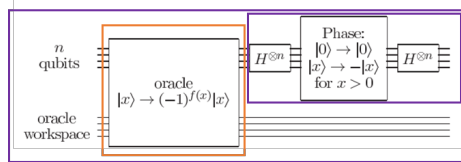
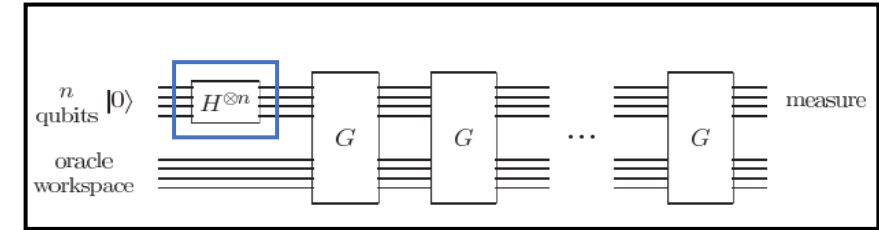
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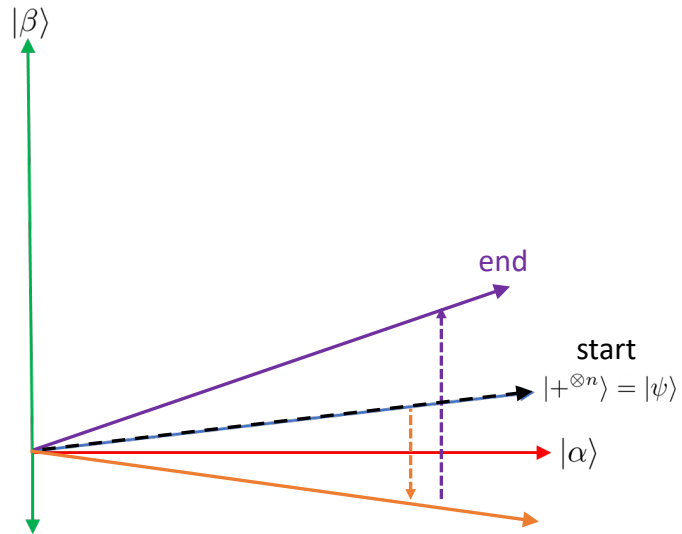
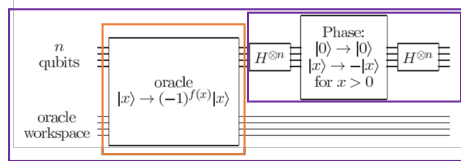
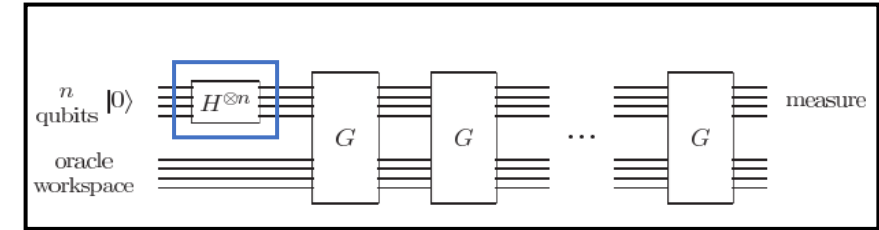
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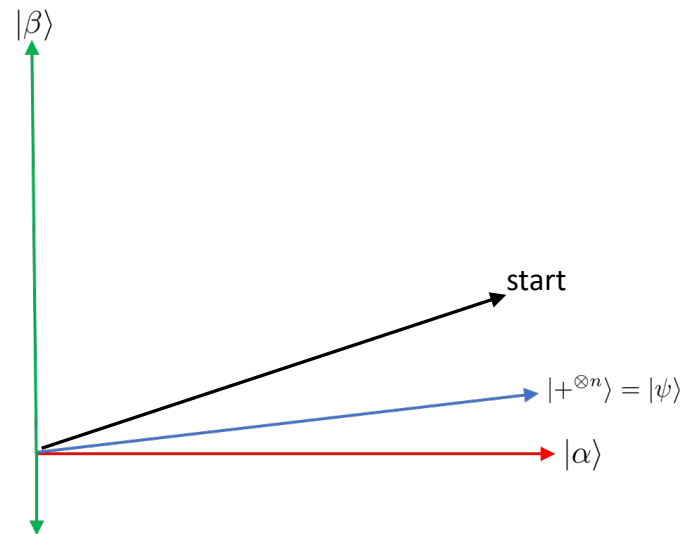
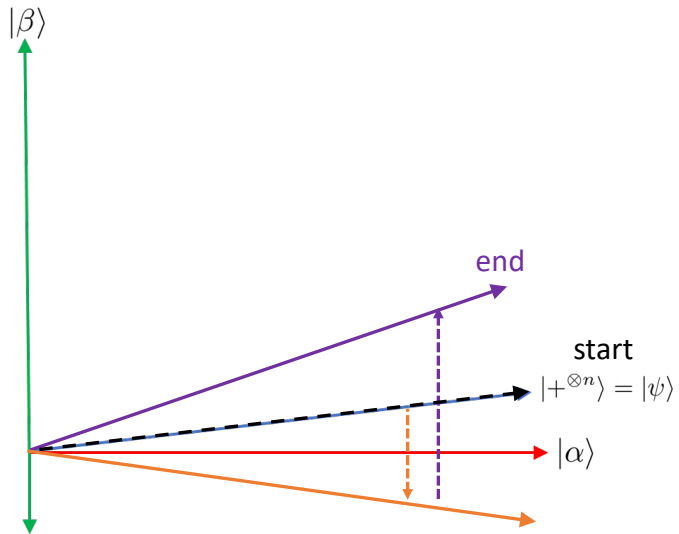
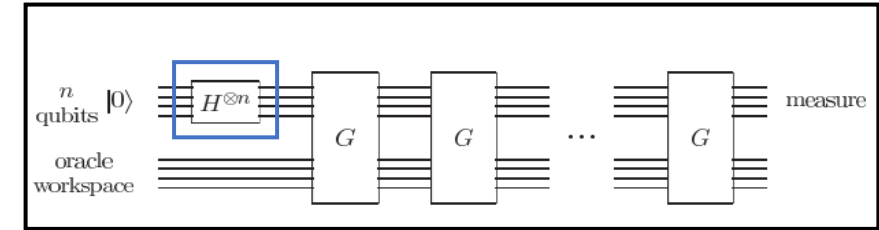
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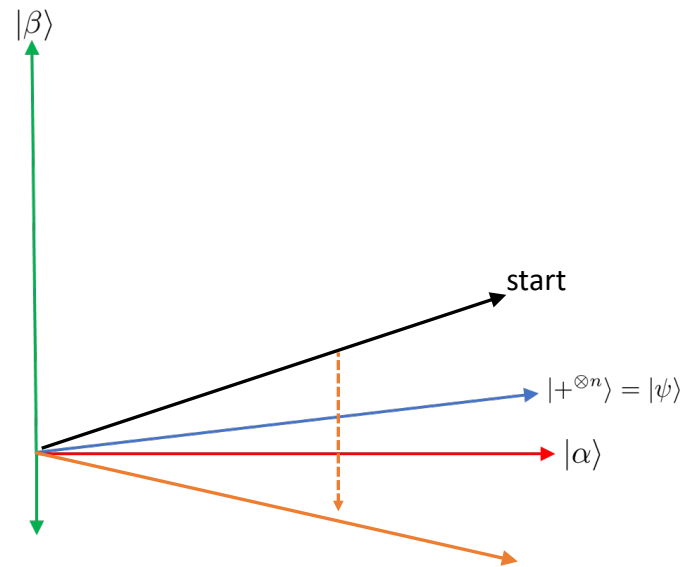
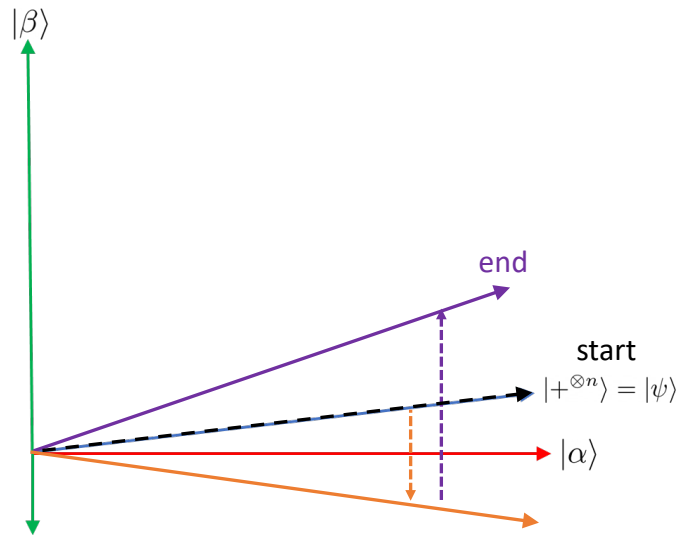
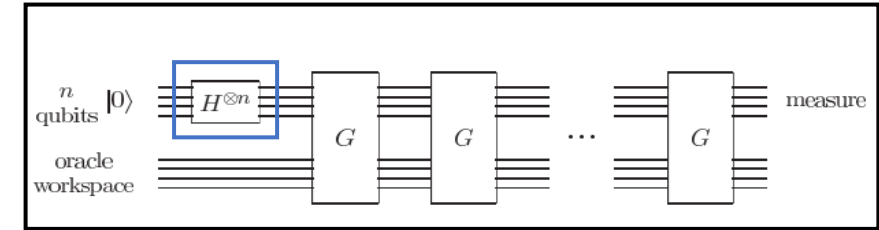
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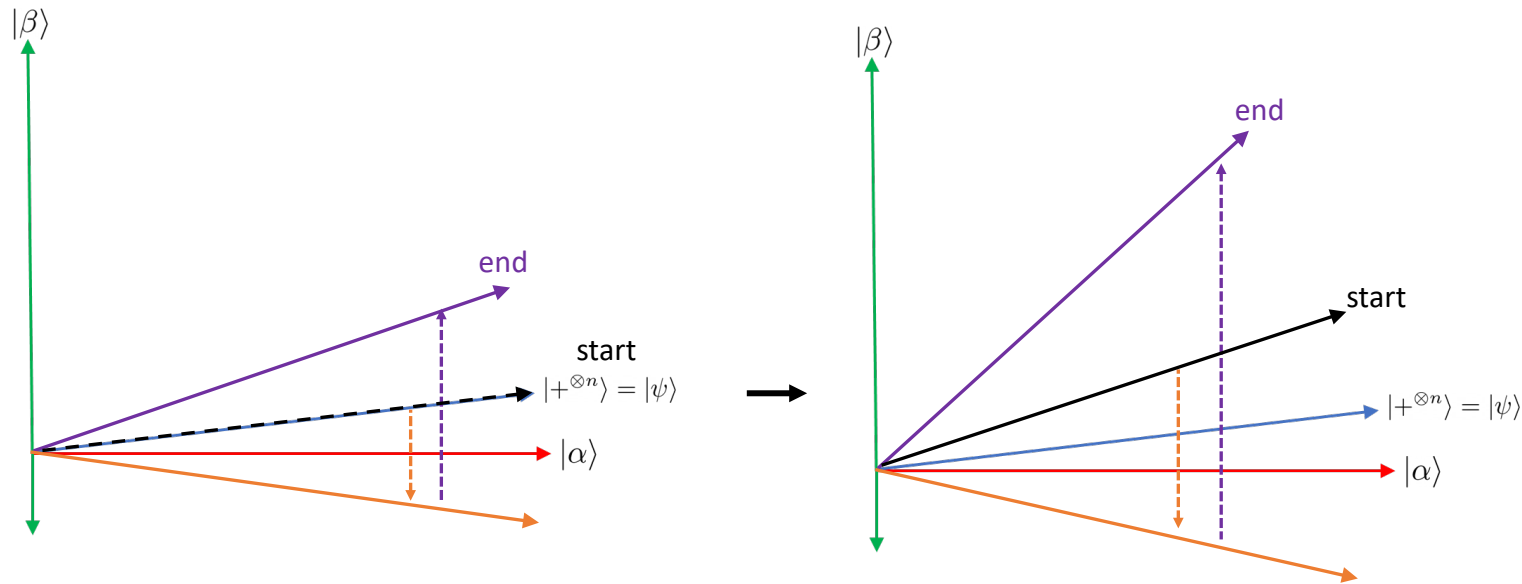
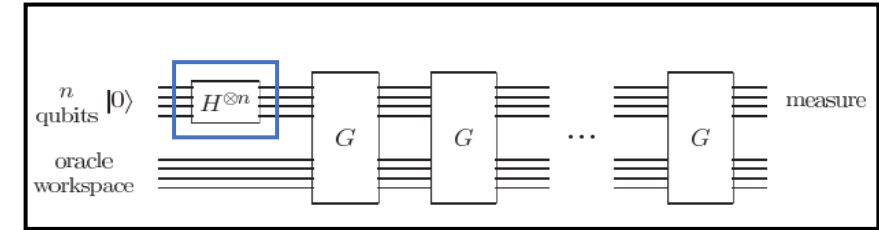
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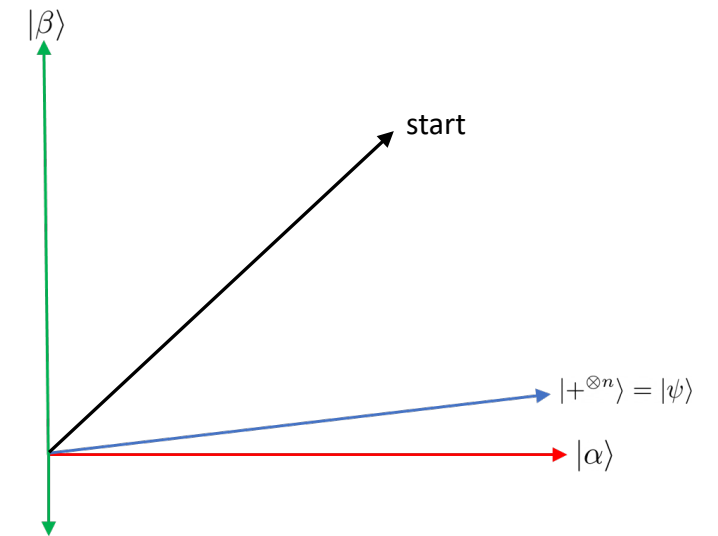
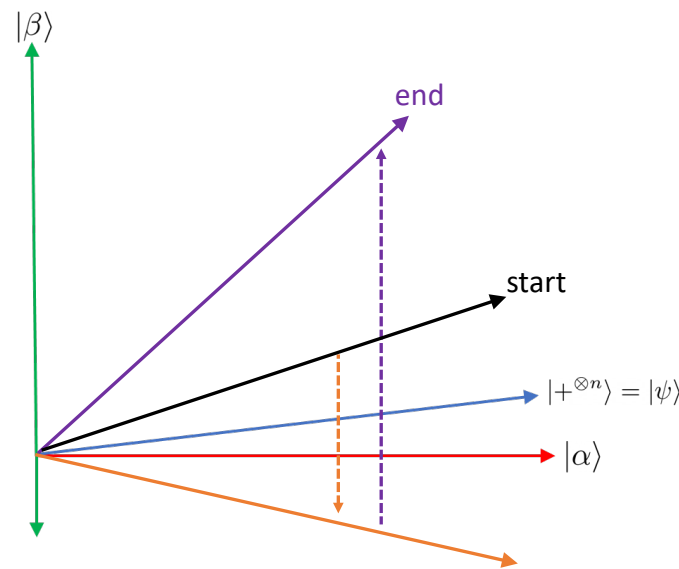
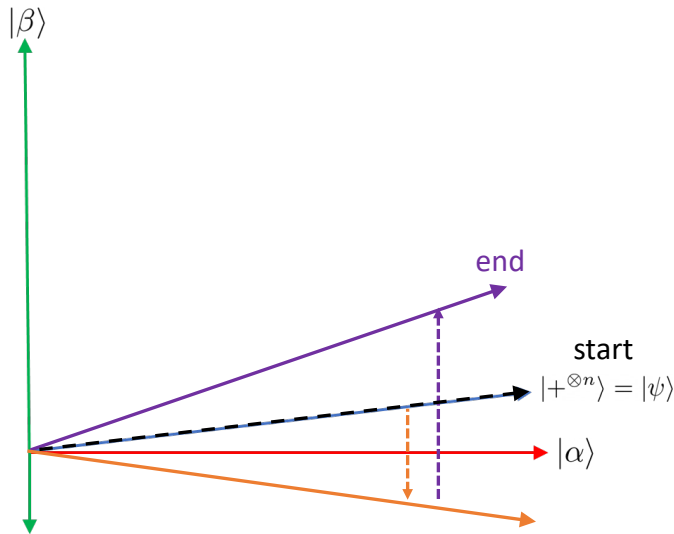
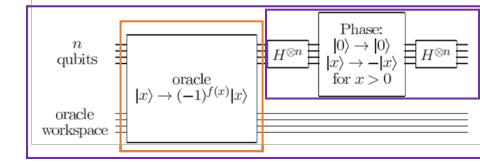
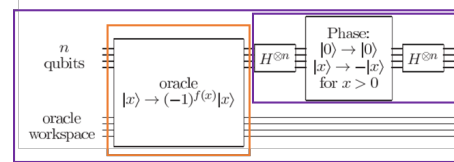
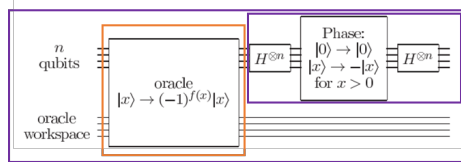
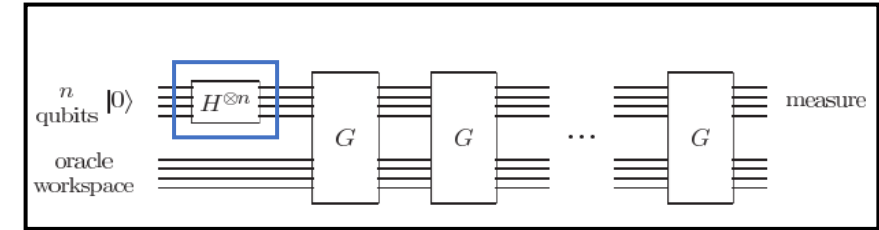
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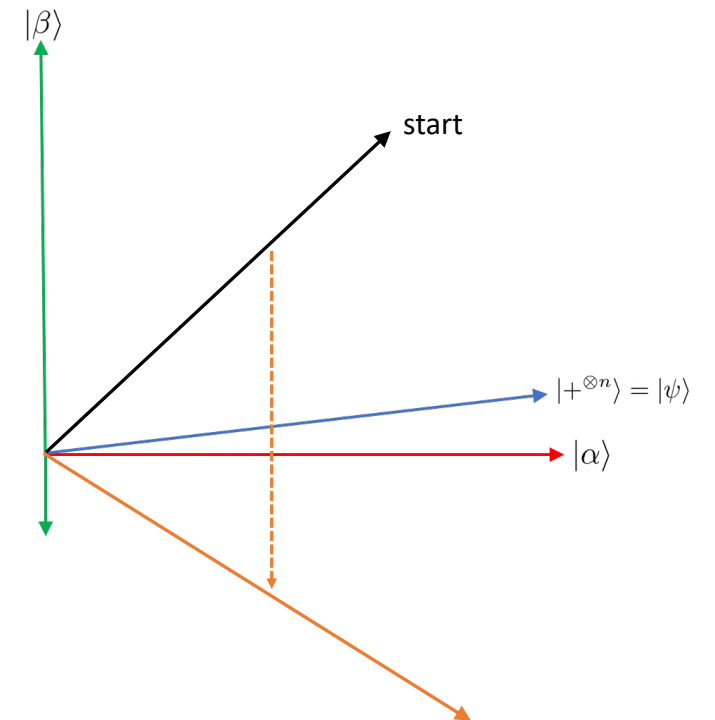
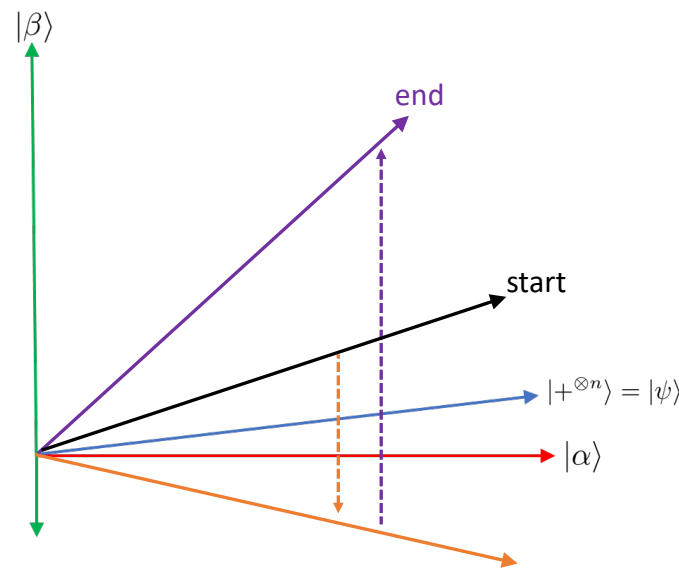
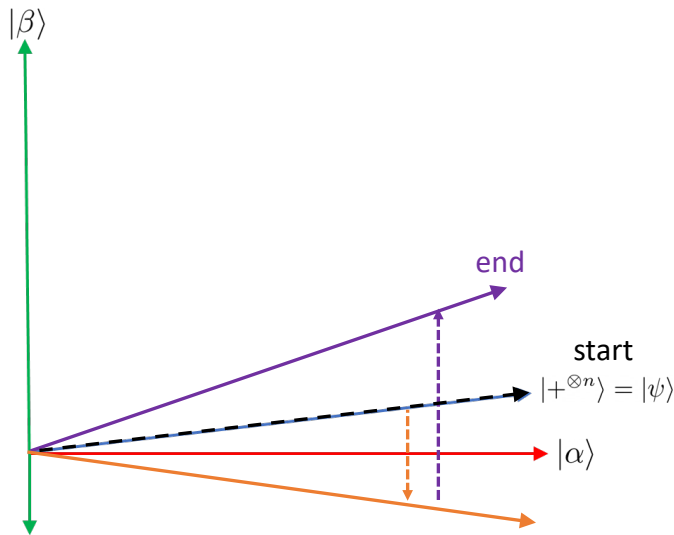
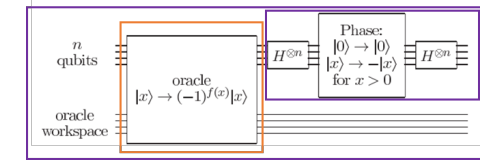
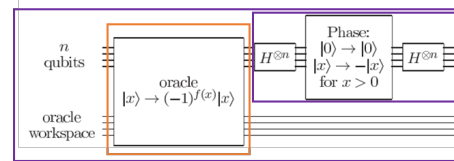
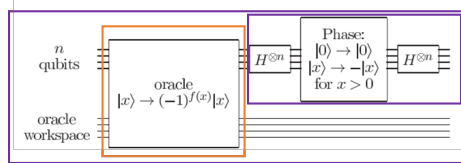
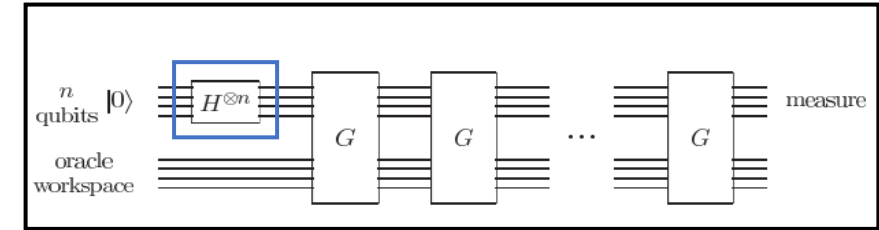
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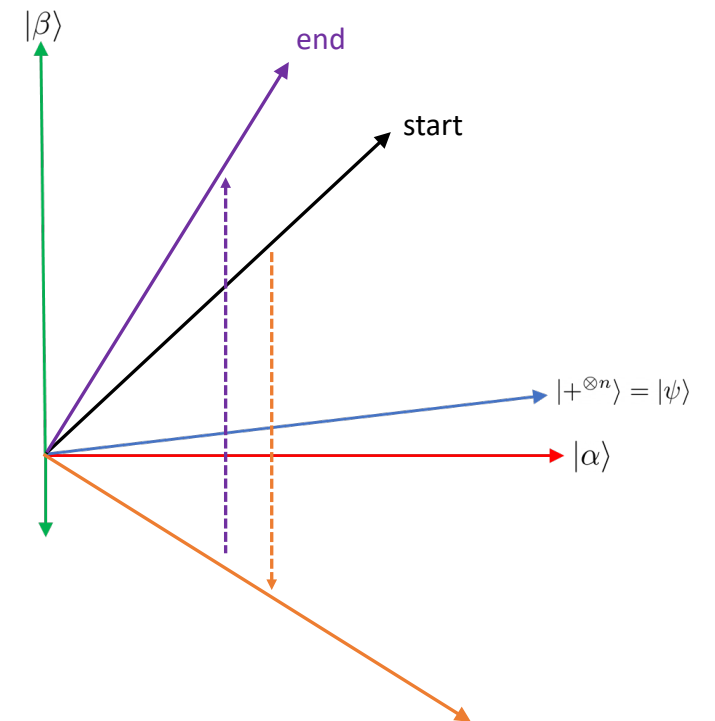
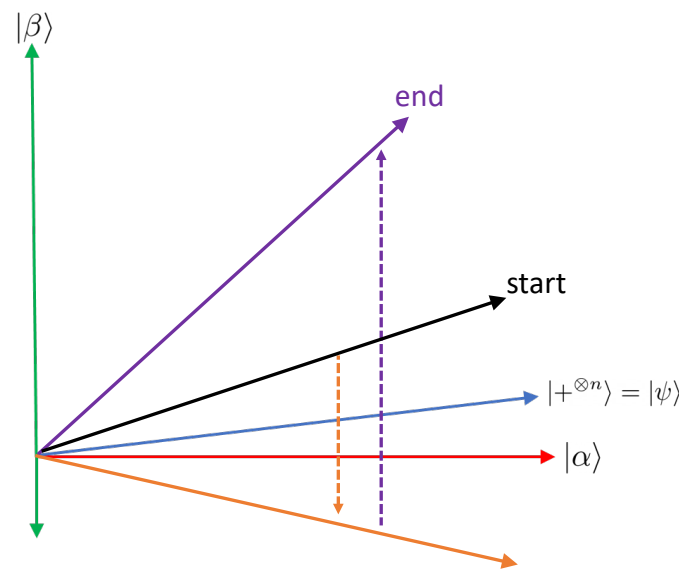
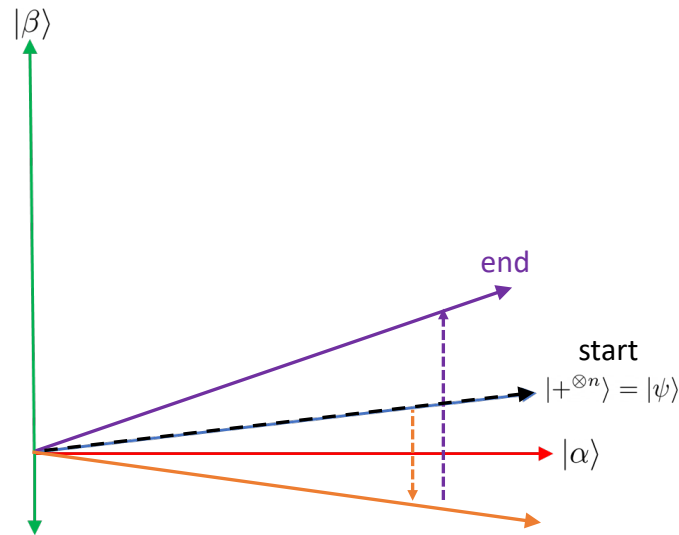
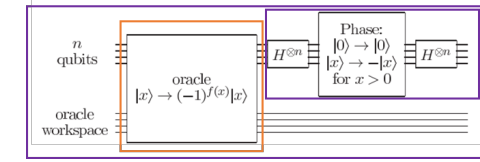
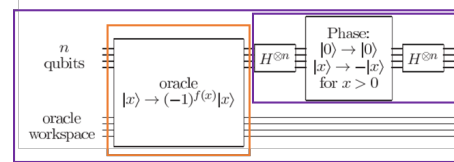
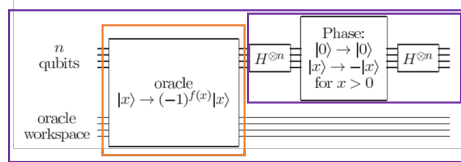
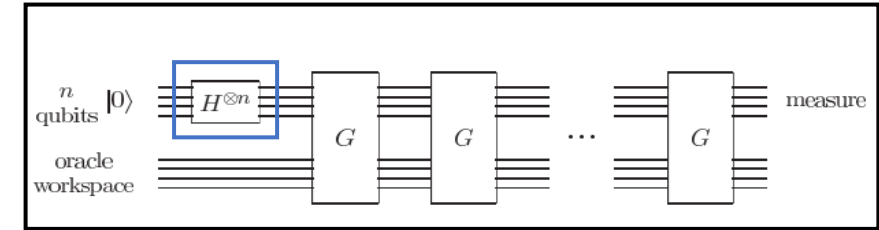
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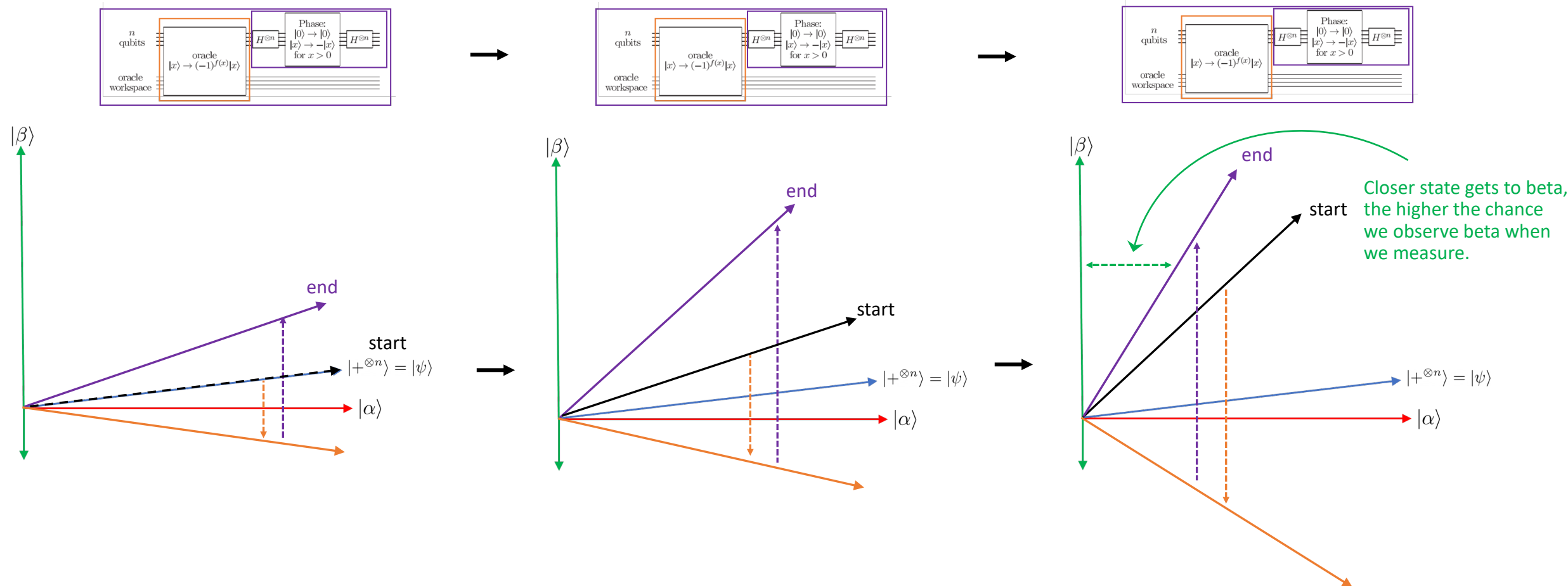
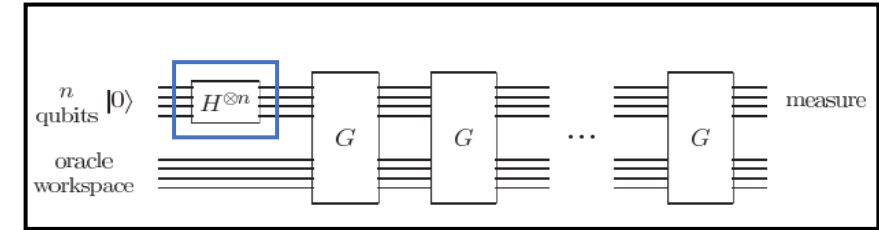
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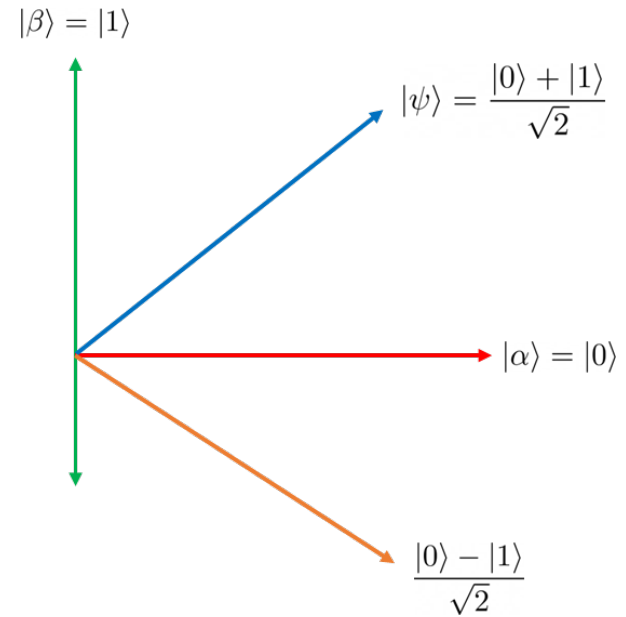
Geometric Interpretation of a Grover Iteration

Thus: state of circuit makes progress toward beta with each application of G.



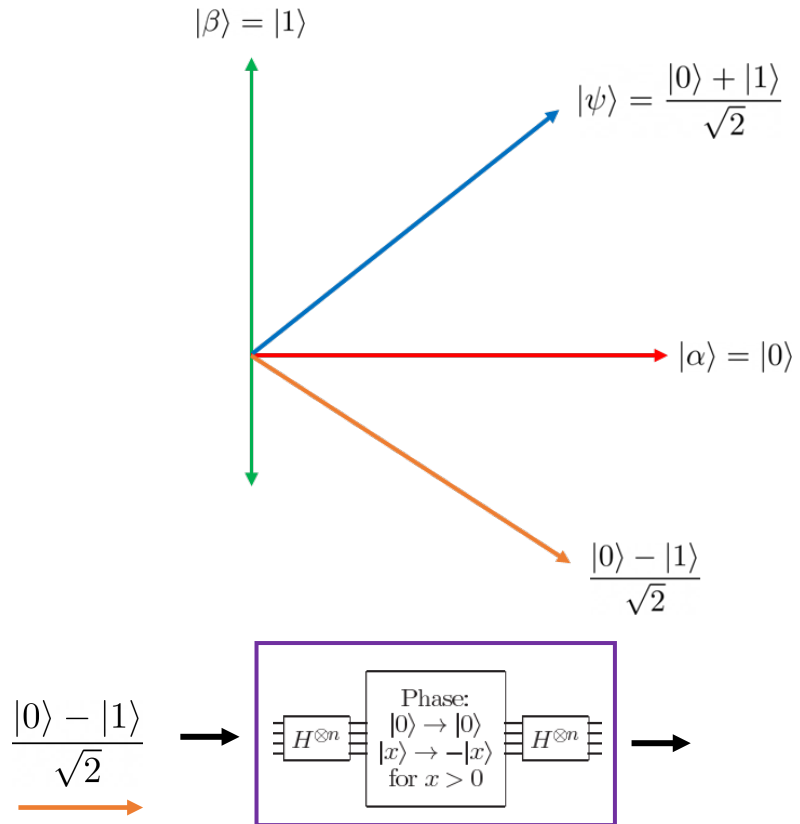
Geometric Interpretation of Diffusion Operator

one qubit, target = $|1\rangle$



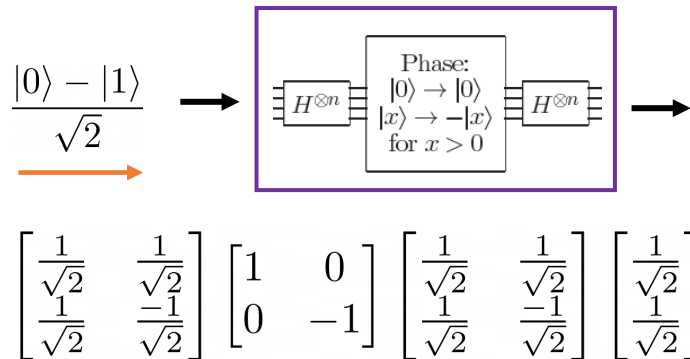
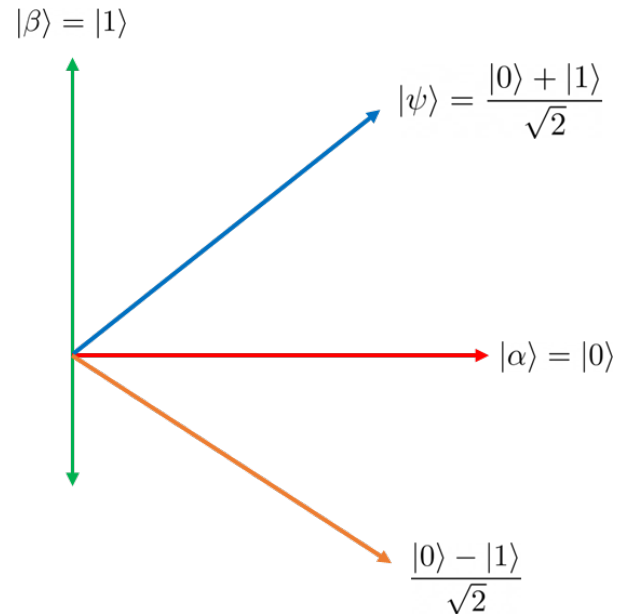
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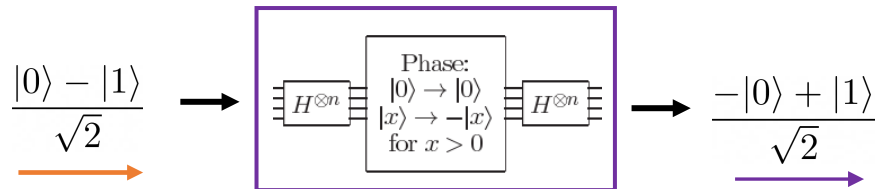
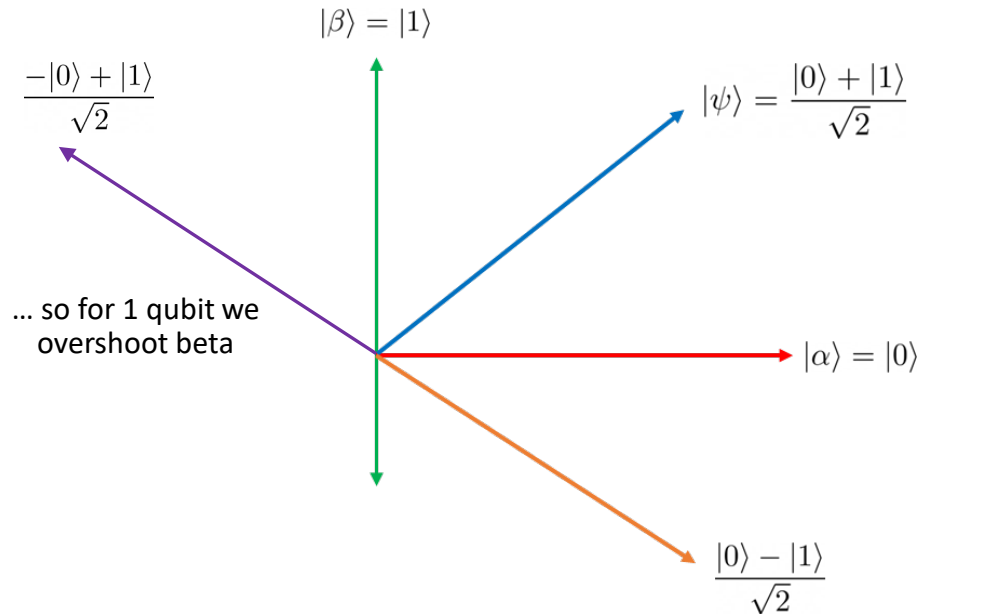
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Geometric Interpretation of Diffusion Operator

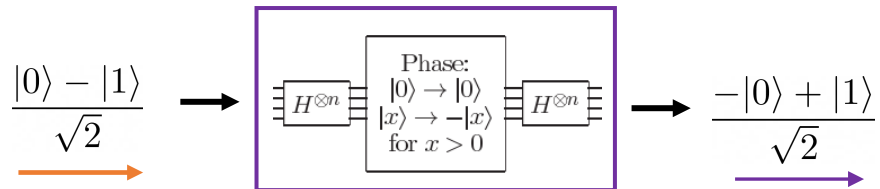
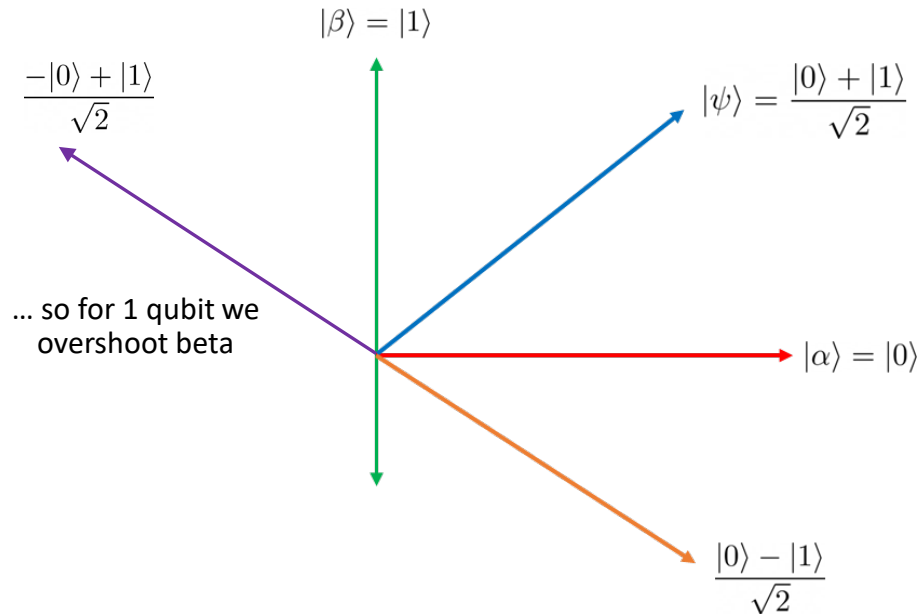
one qubit, target = $|1\rangle$



$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

Geometric Interpretation of Diffusion Operator

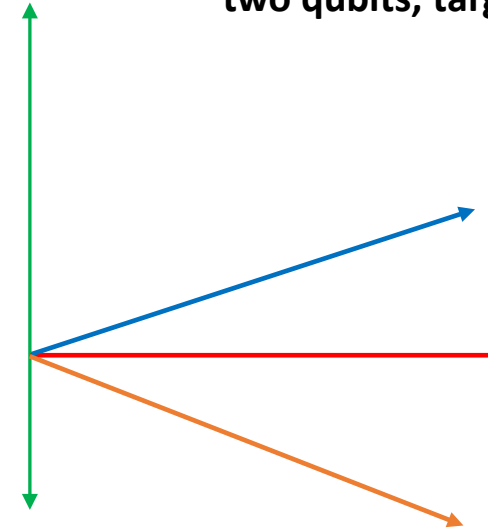
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$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

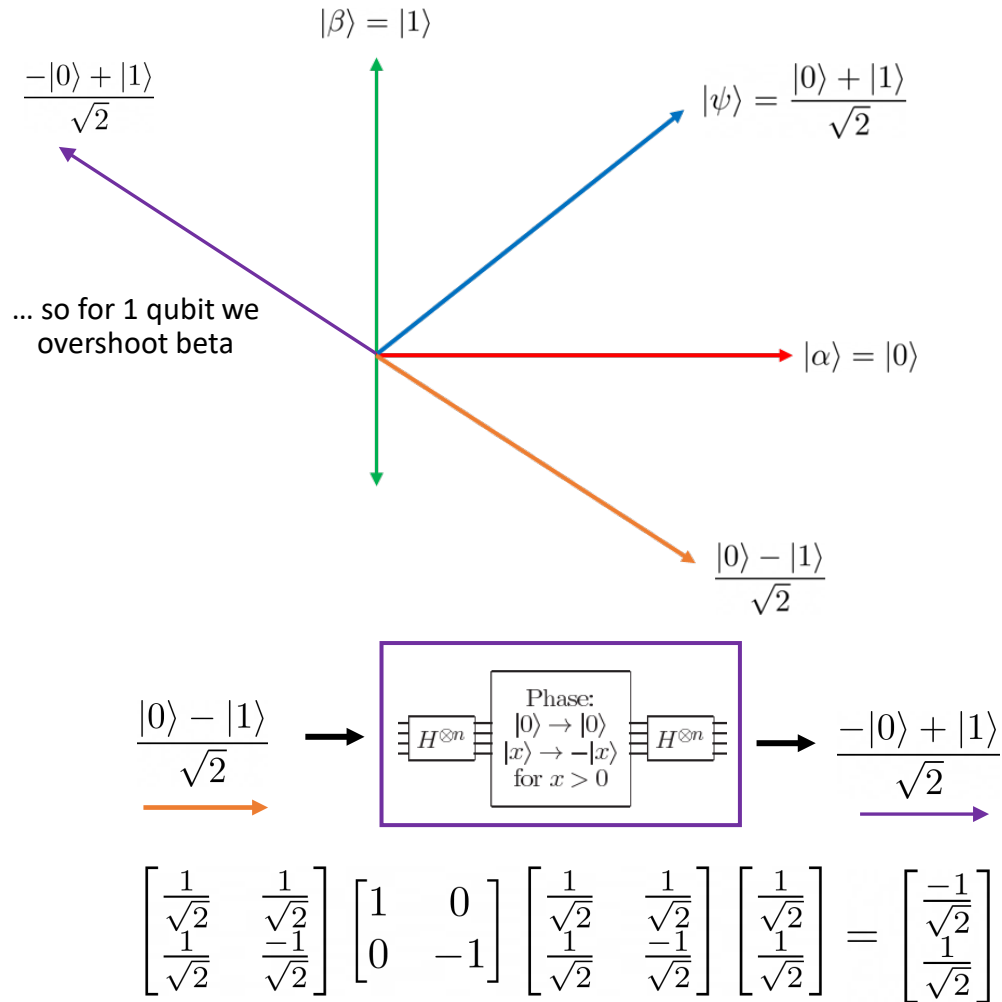
$|\beta\rangle = |11\rangle$

two qubits, target = $|11\rangle$

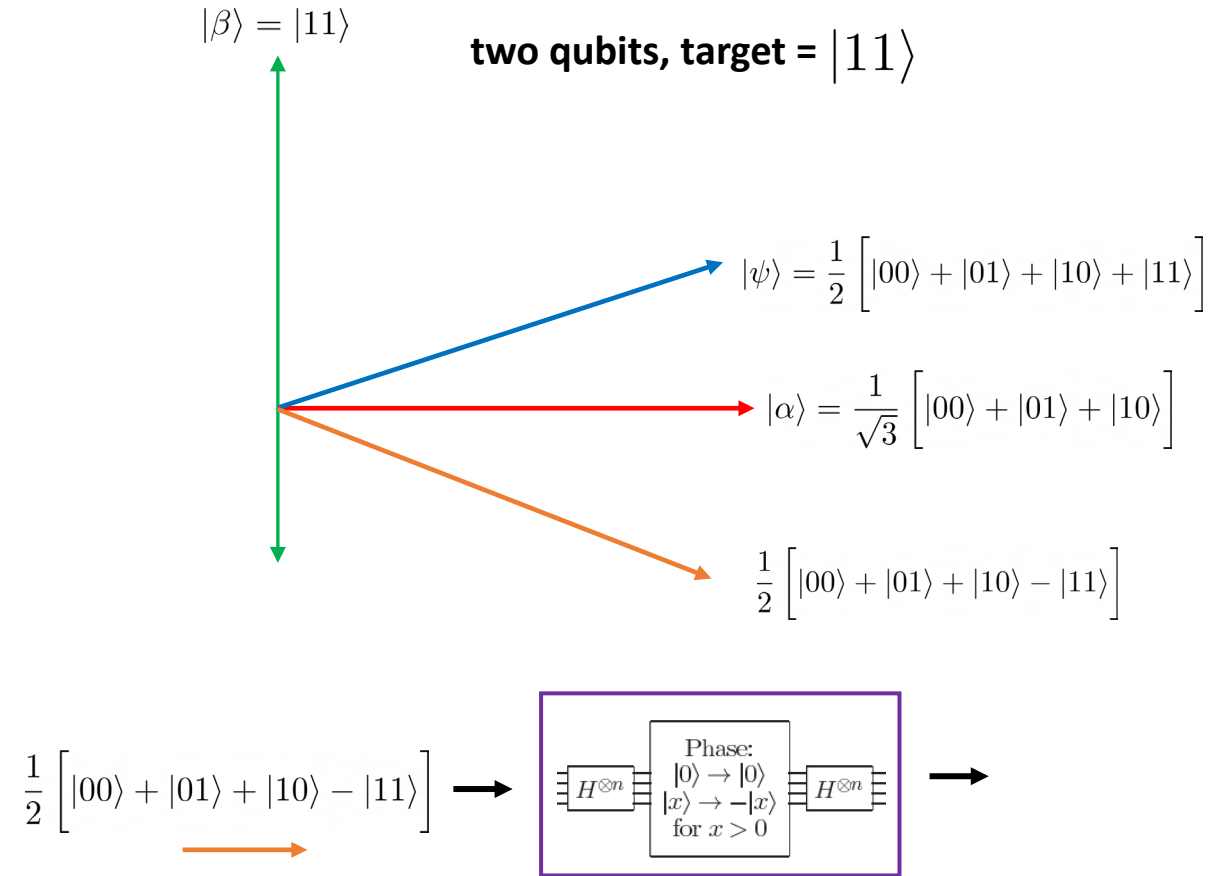


Geometric Interpretation of Diffusion Operator

one qubit, target = $|1\rangle$

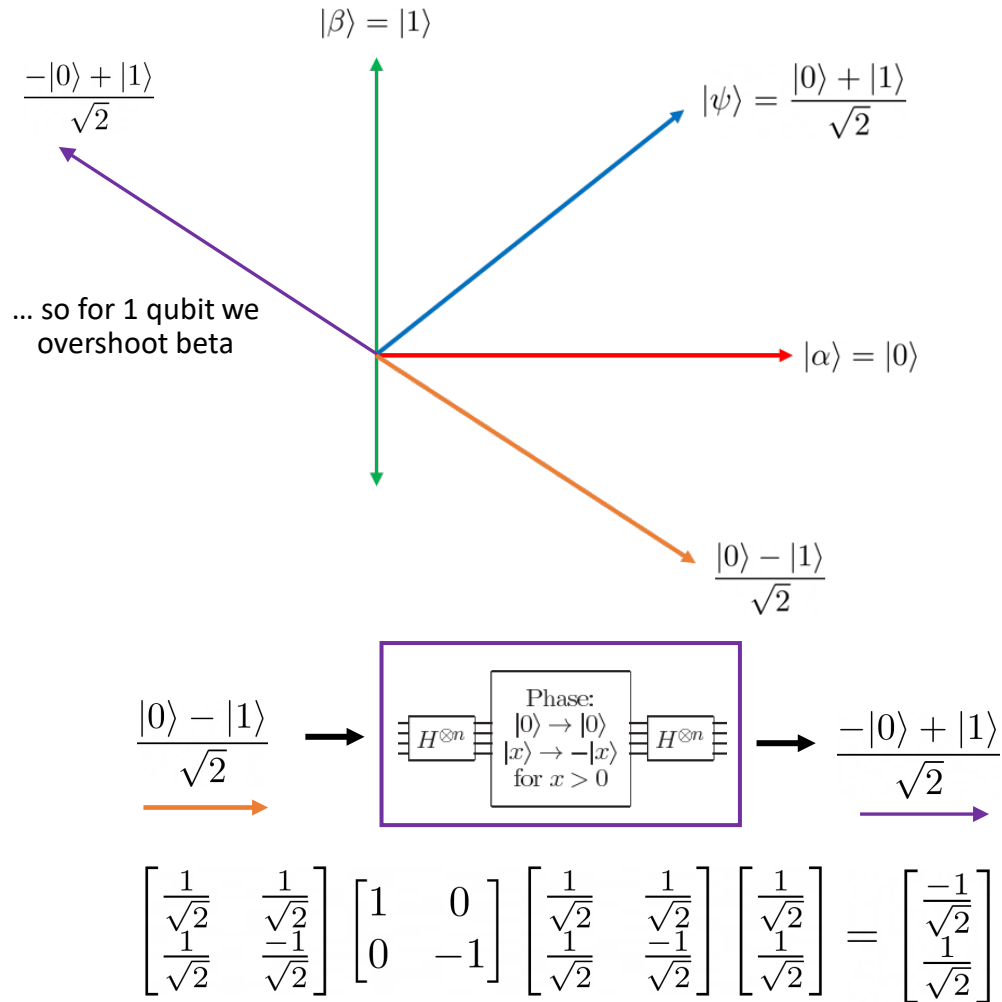


two qubits, target = $|11\rangle$

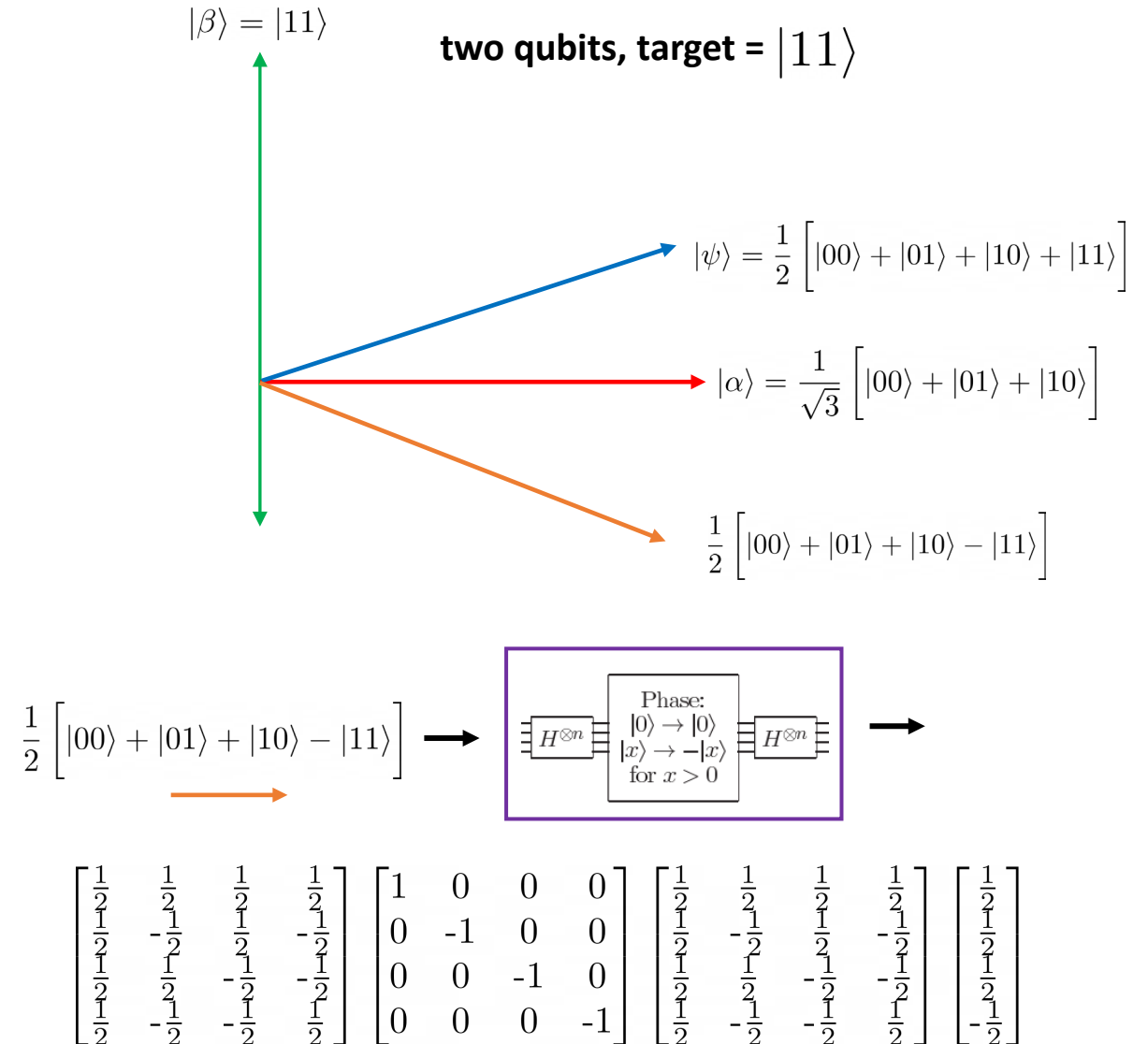


Geometric Interpretation of Diffusion Operator

one qubit, target = $|1\rangle$

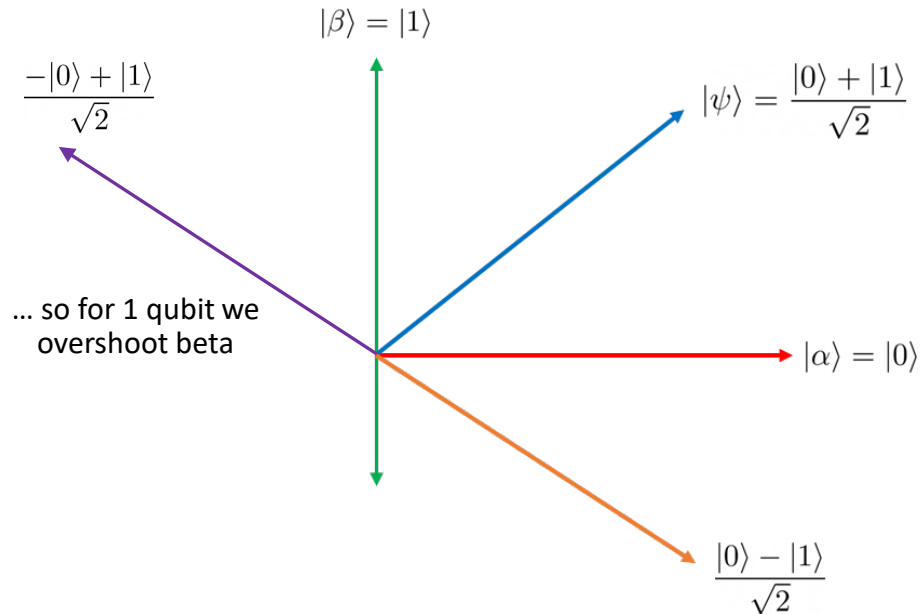


two qubits, target = $|11\rangle$



Geometric Interpretation of Diffusion Operator

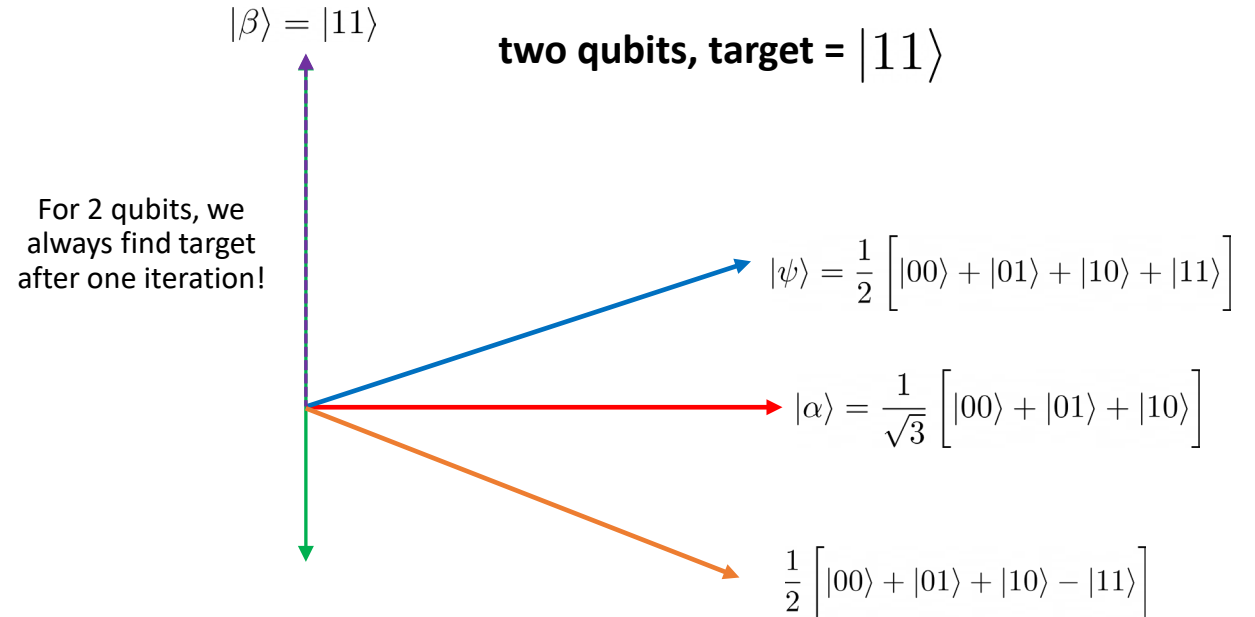
one qubit, target = $|1\rangle$



$$\frac{|0\rangle - |1\rangle}{\sqrt{2}} \xrightarrow{\text{Phase: } |0\rangle \rightarrow |0\rangle, |x\rangle \rightarrow -|x\rangle \text{ for } x > 0} \frac{-|0\rangle + |1\rangle}{\sqrt{2}}$$

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

two qubits, target = $|11\rangle$

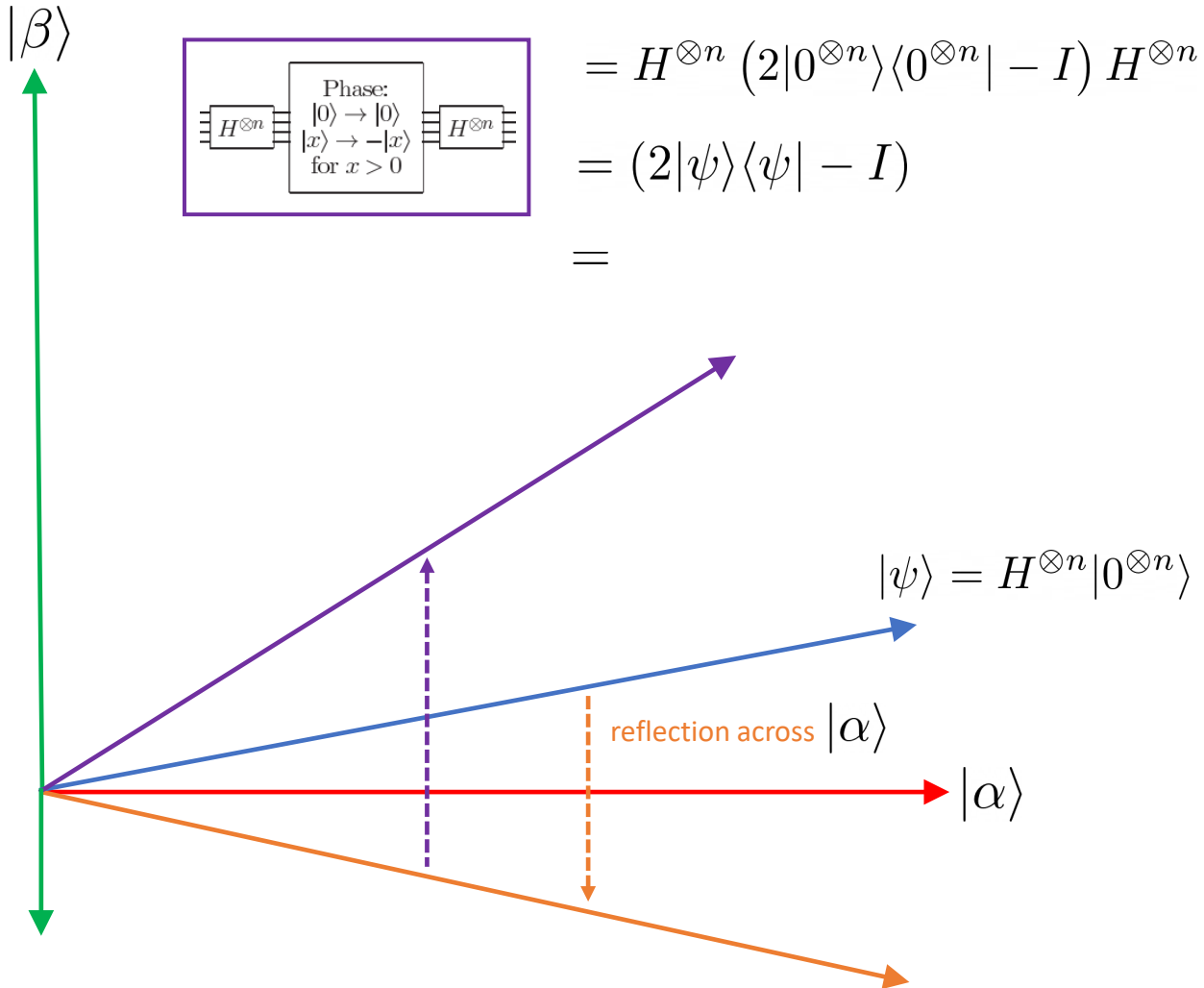


$$\frac{1}{2} [|00\rangle + |01\rangle + |10\rangle - |11\rangle] \xrightarrow{\text{Phase: } |0\rangle \rightarrow |0\rangle, |x\rangle \rightarrow -|x\rangle \text{ for } x > 0} |11\rangle$$

$$\begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

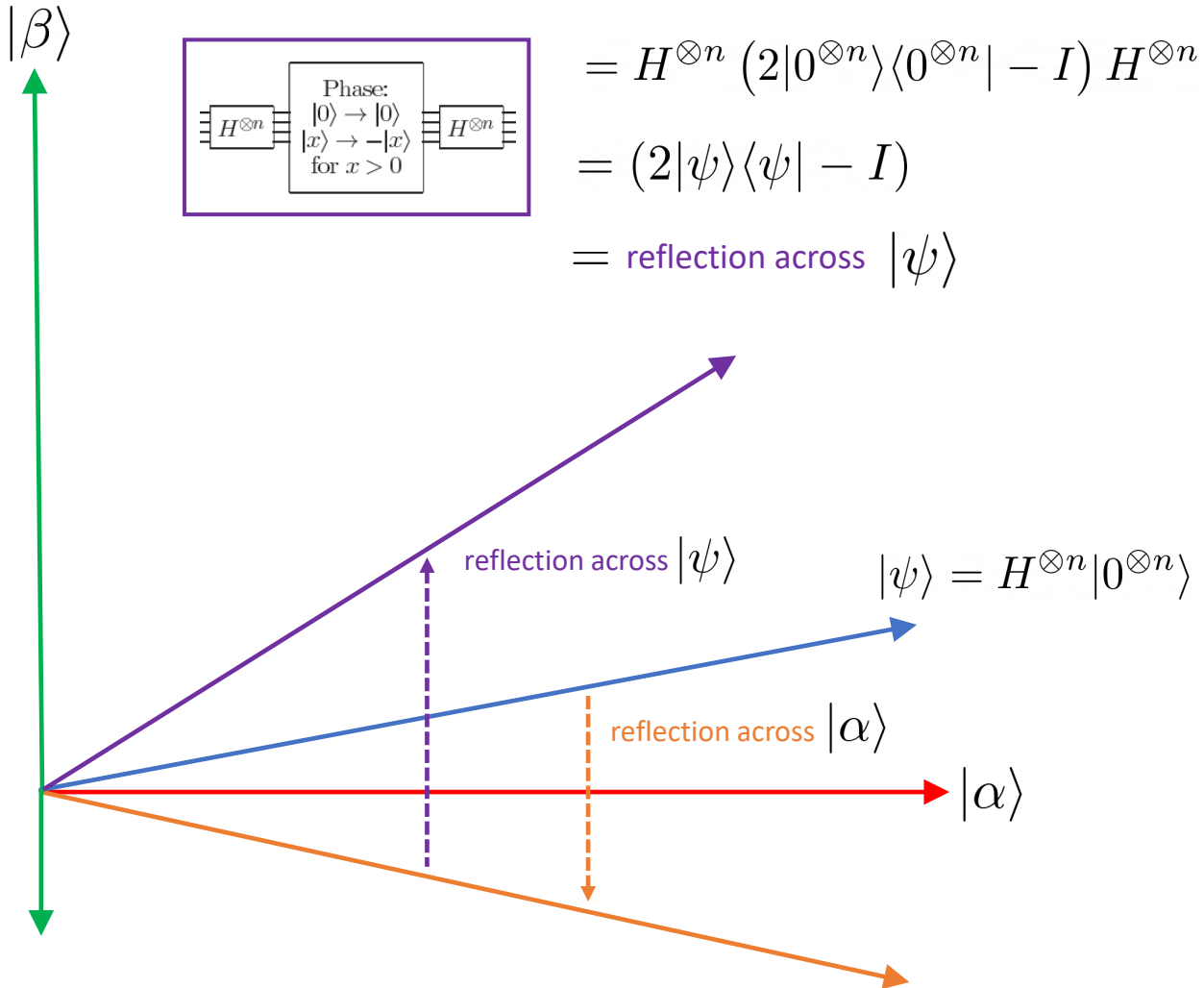
Geometric Interpretation of Diffusion Operator

In General



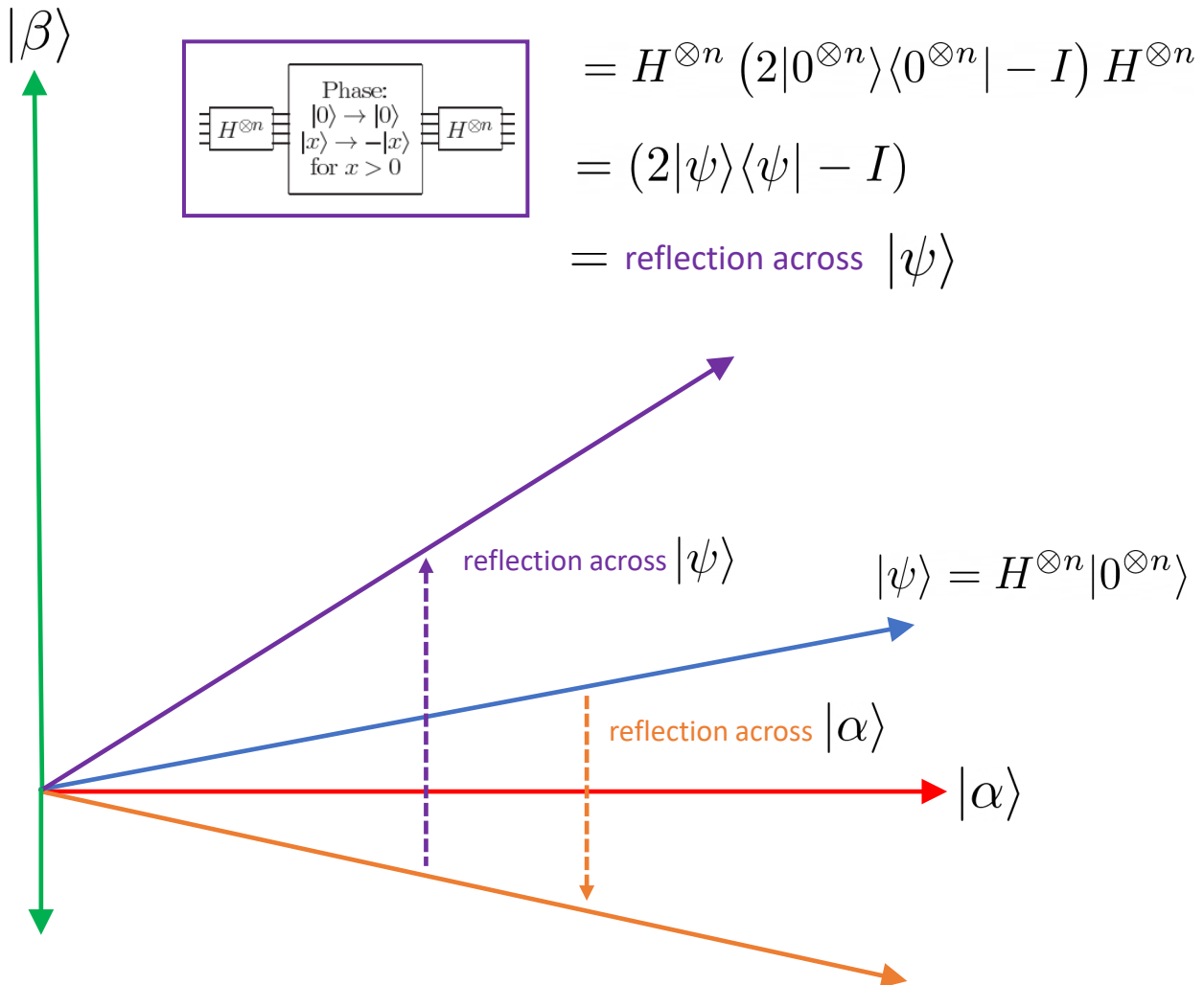
Geometric Interpretation of Diffusion Operator

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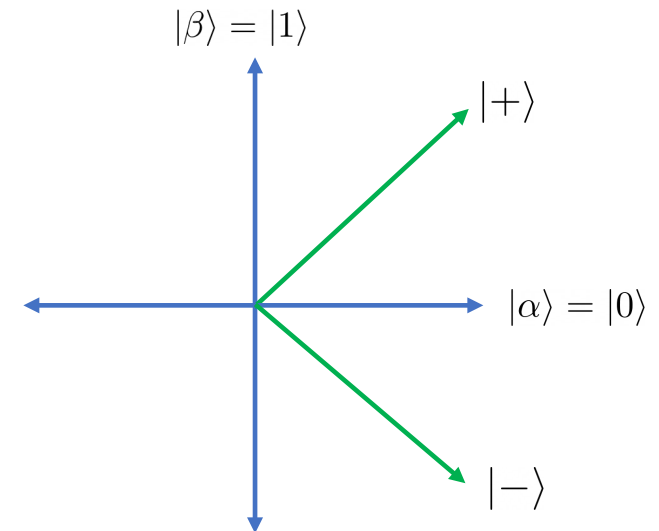
Geometric Interpretation of Diffusion Operator

In General



Easiest way to see why: Change of Basis

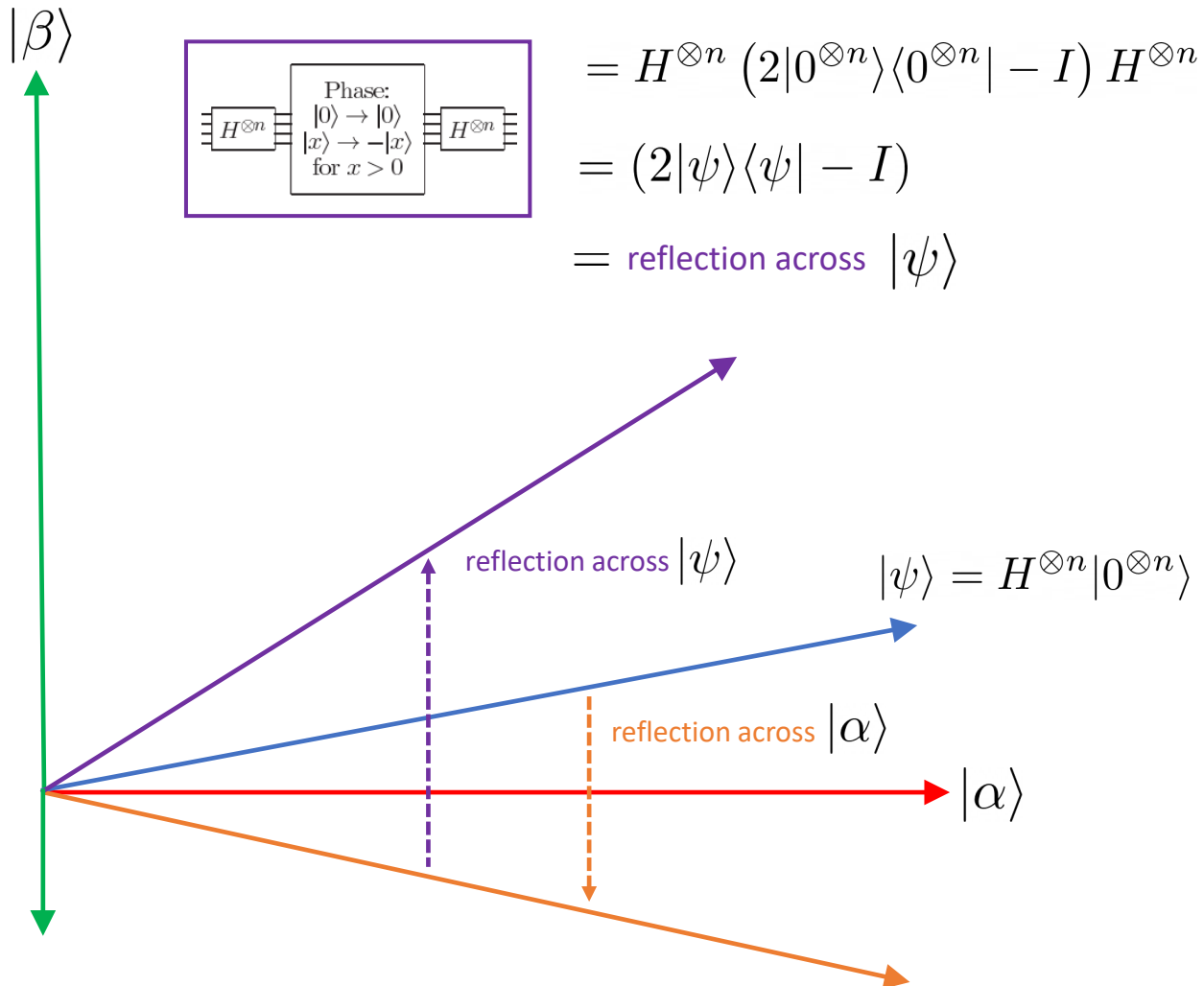
Recall: one qubit picture (using color scheme from CHSH game)



$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

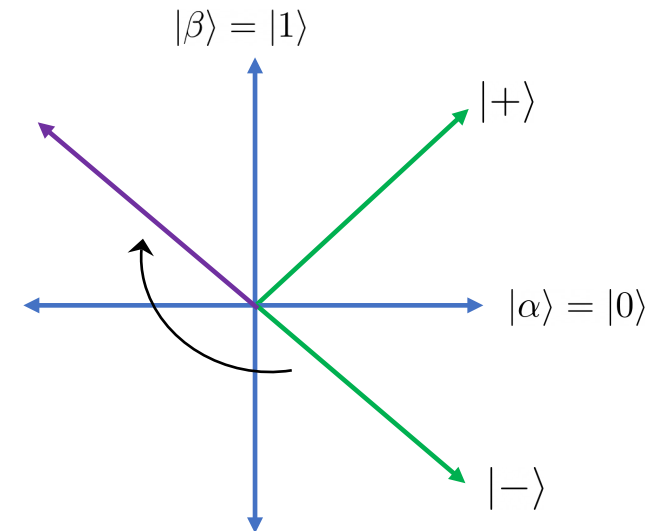
Geometric Interpretation of Diffusion Operator

In General



Easiest way to see why: Change of Basis

Recall: one qubit picture (using color scheme from CHSH game)



change back

"reflect over x-axis"

change to H basis

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

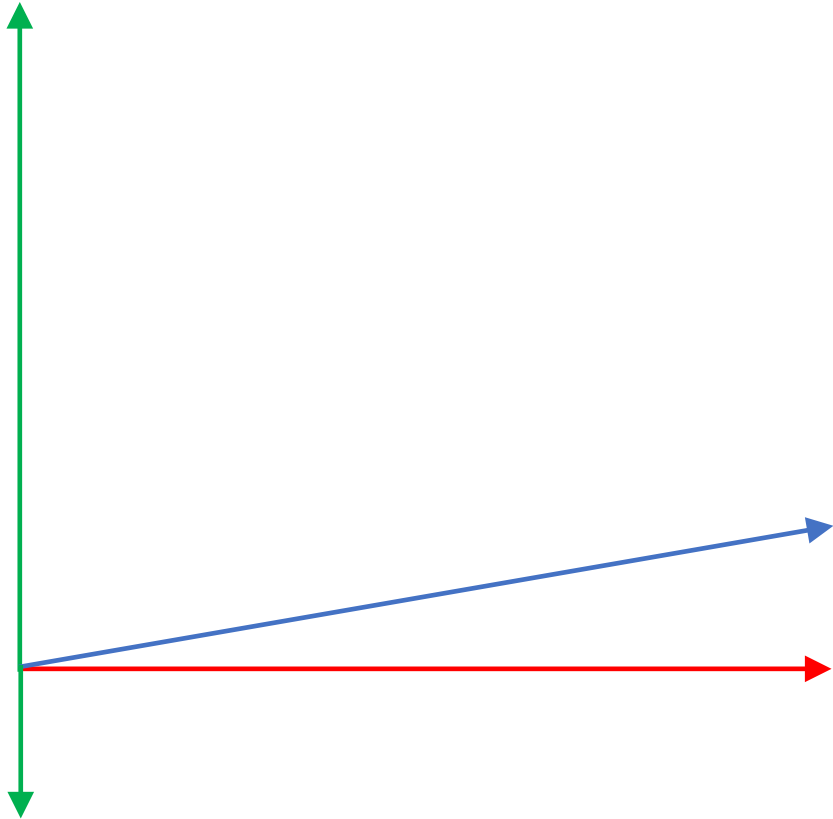
$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

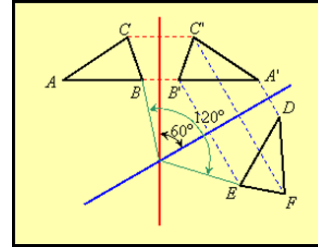
Number of Iterations: Finding Rotation Angle

$$|\beta\rangle = |1^{\otimes n}\rangle$$

$$(|\beta\rangle = |x\rangle : f(x) = 1)$$

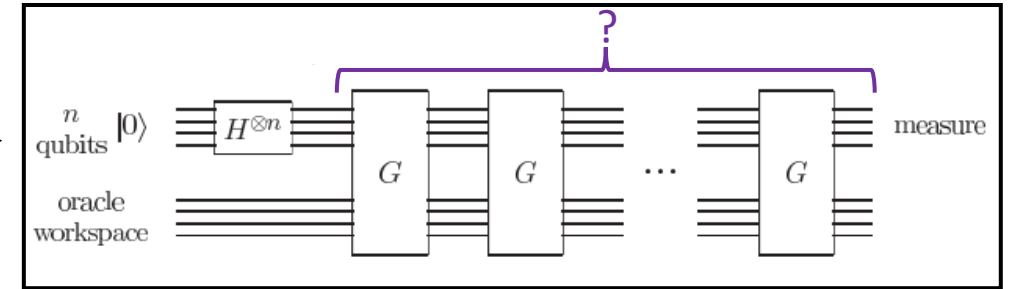


Fact: two reflections \rightarrow rotation



(figure courtesy of ceemrr.com)

Thus: number Grover iterations \sim angle of rotation



Number of Iterations: Finding Rotation Angle

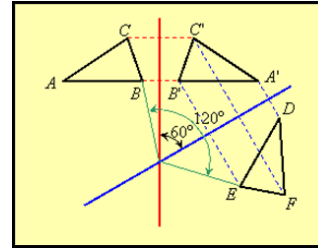
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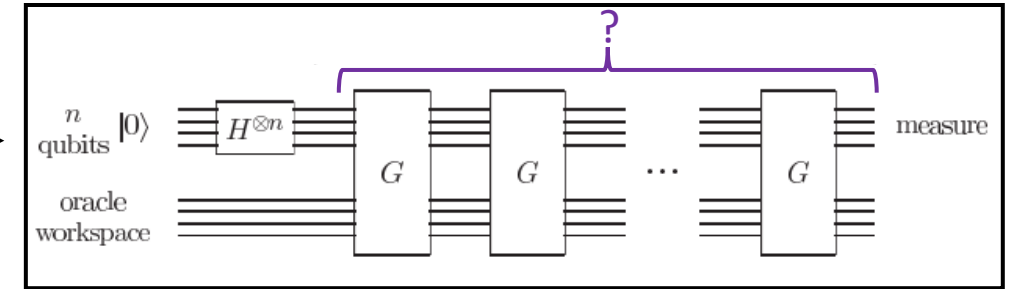


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(figure courtesy of ceemrr.com)



Let $N = 2^n$

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} |x\rangle$$



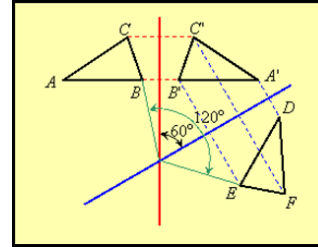
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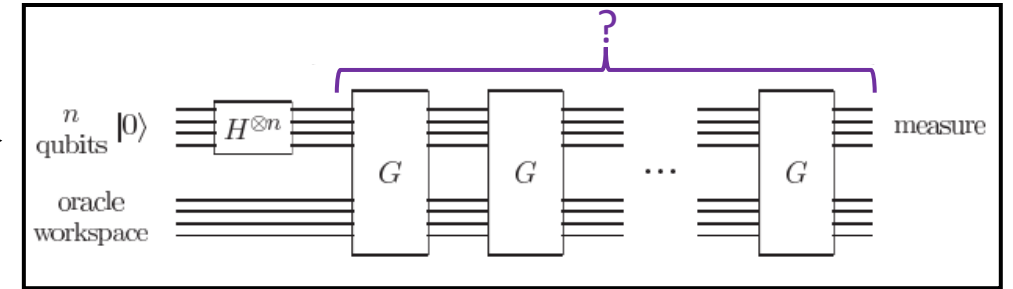
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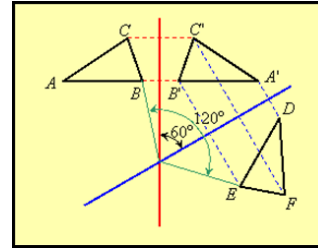
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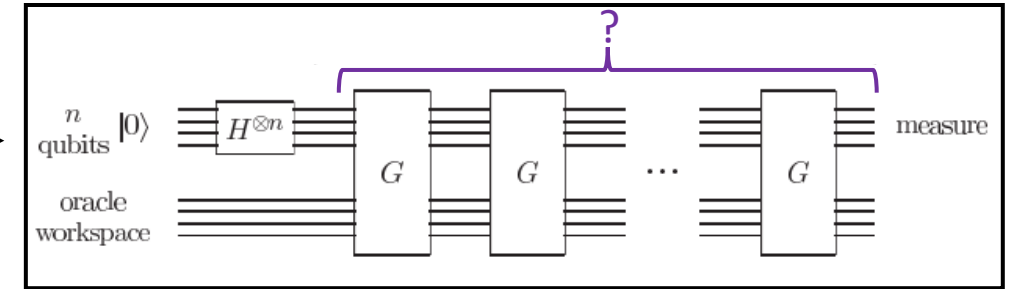
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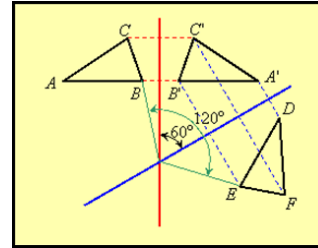
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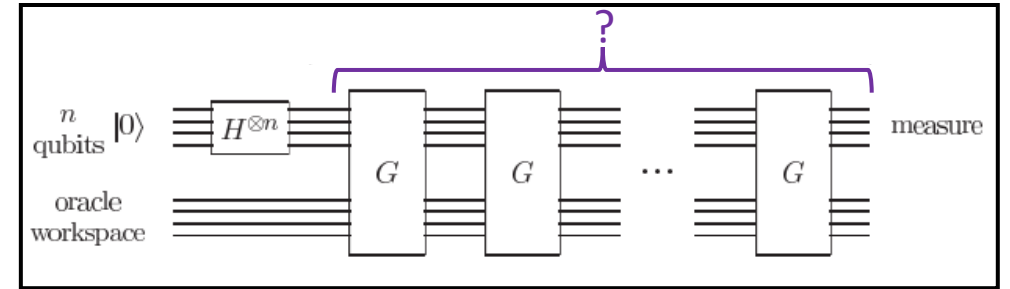
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1

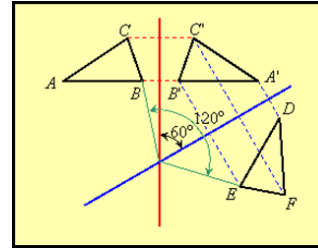
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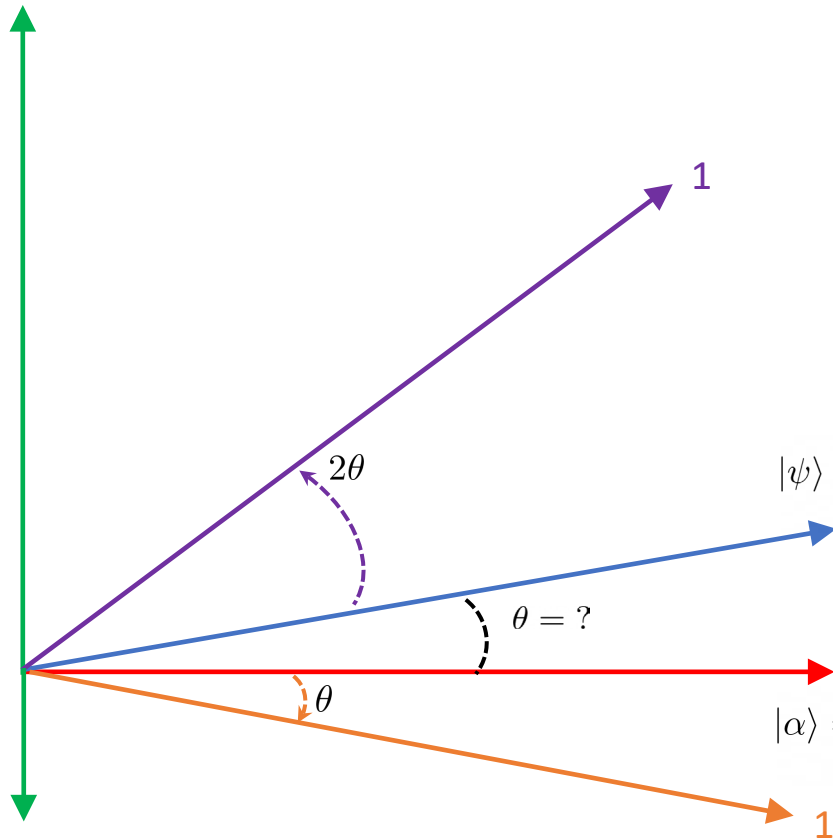
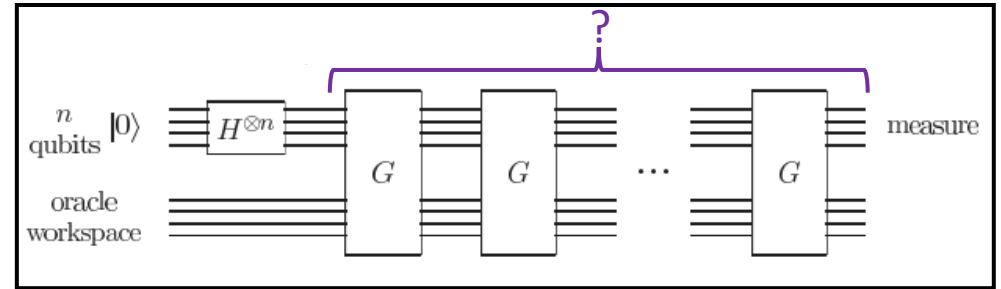
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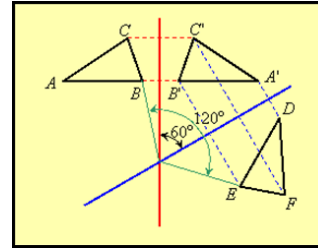
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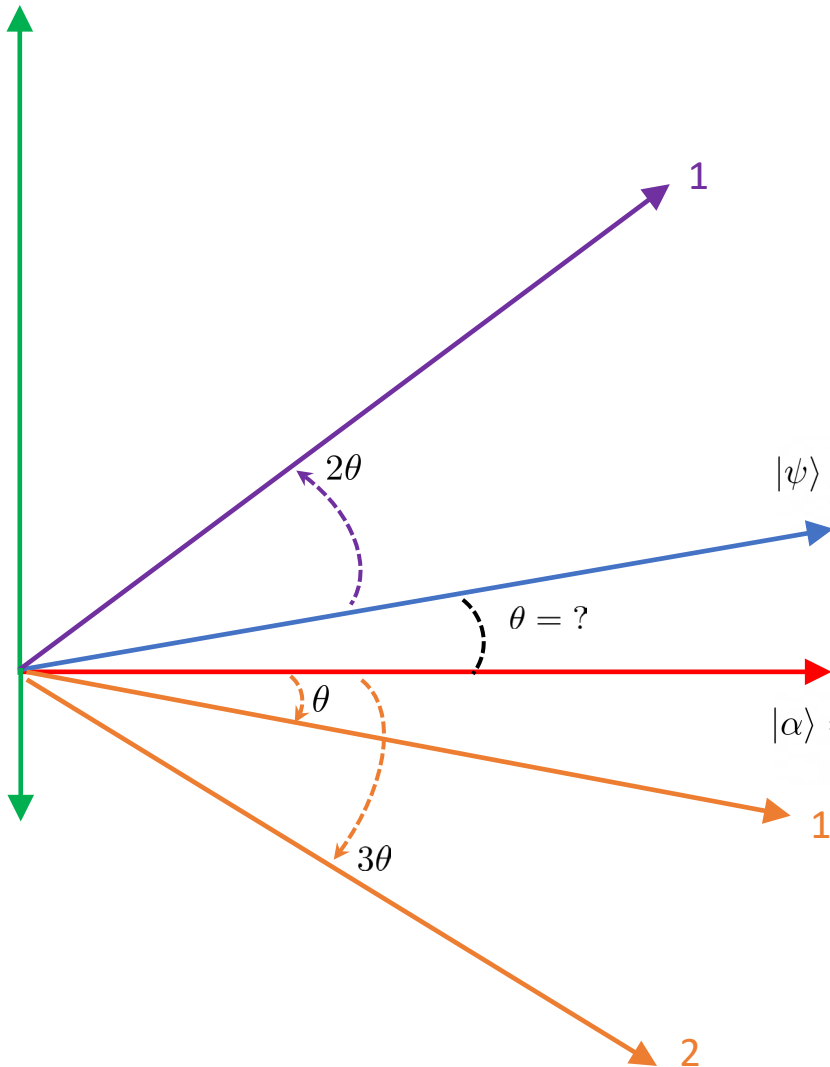
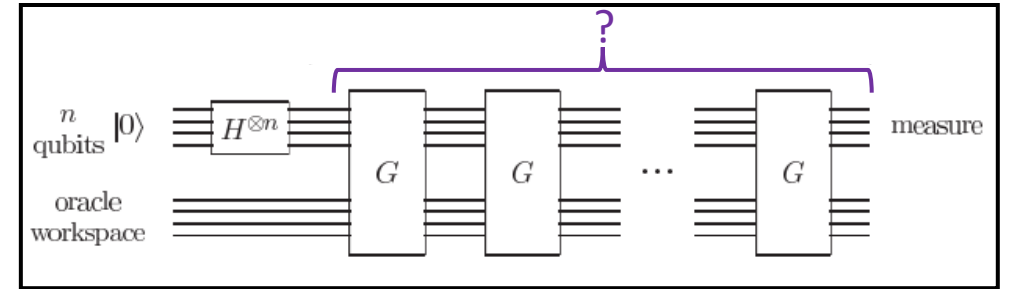
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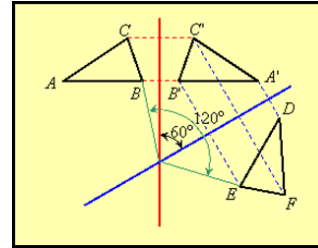
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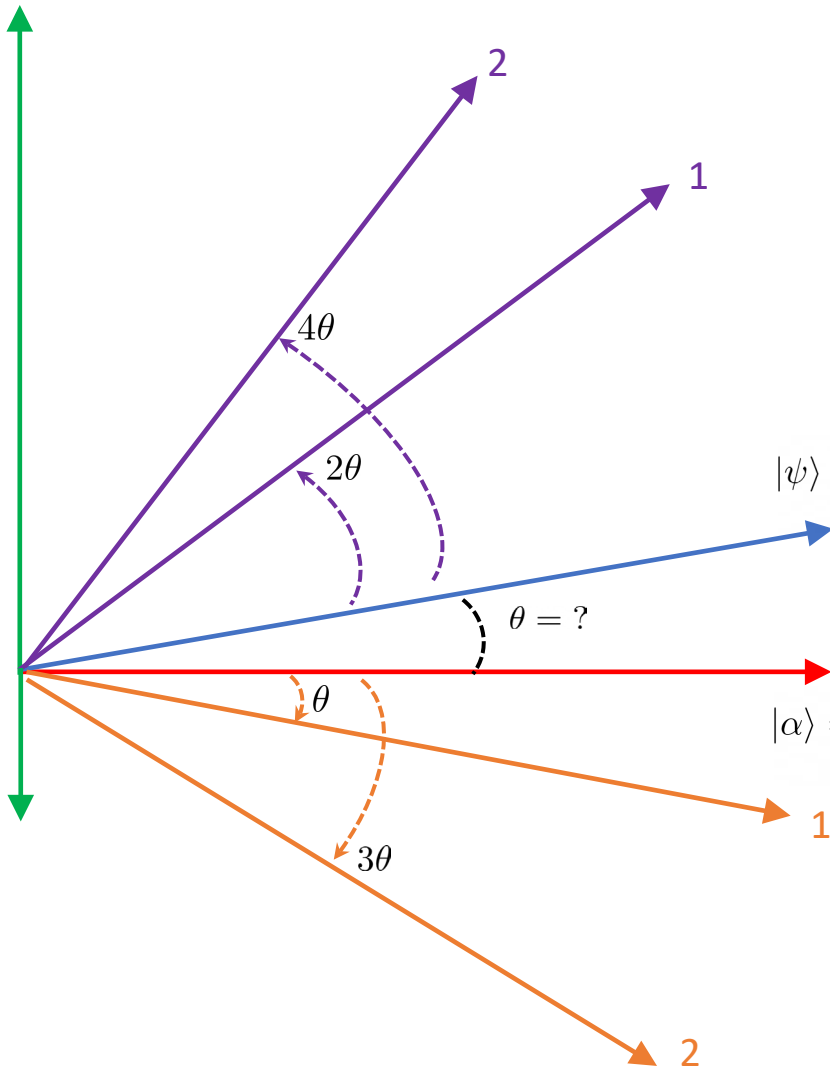
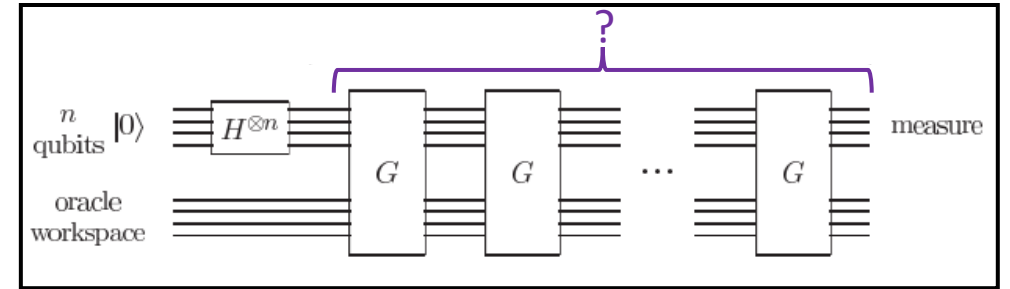
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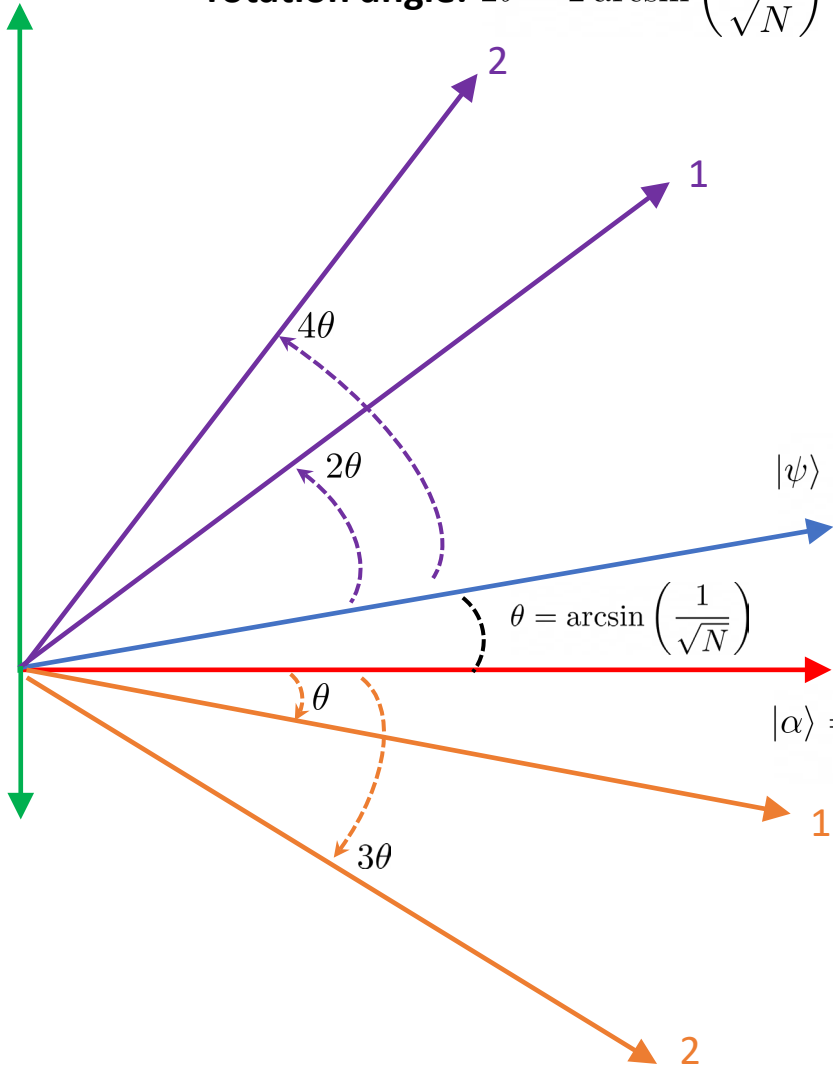
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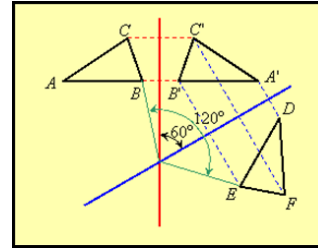
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rotation angle: $2\theta = 2 \arcsin\left(\frac{1}{\sqrt{N}}\right)$

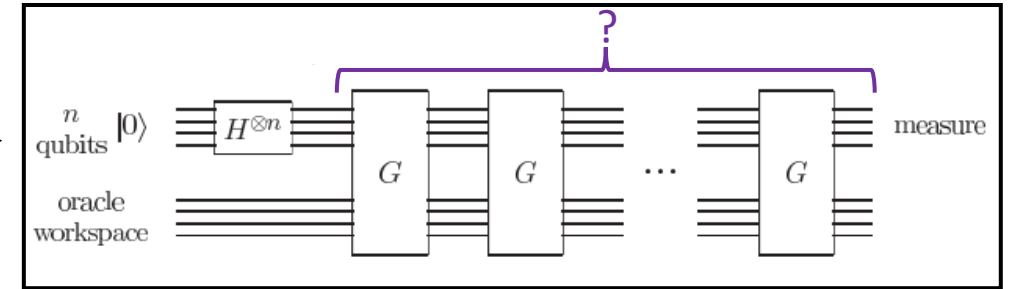


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(figure courtesy of ceemrr.com)

Thus: number Grover iterations \sim angle of rotation



Let $N = 2^n$

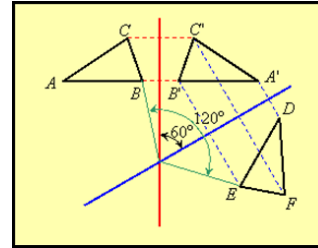
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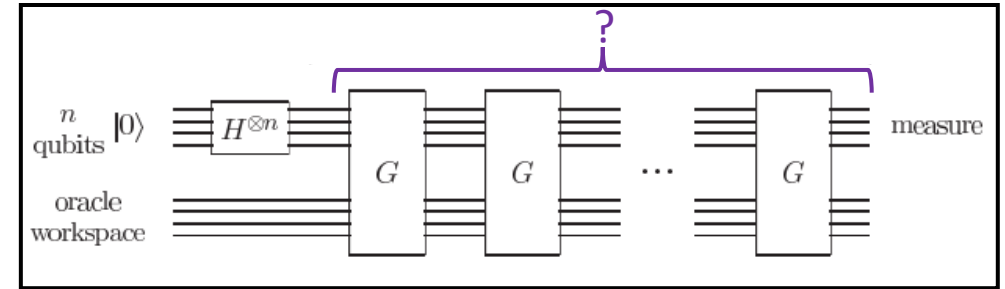
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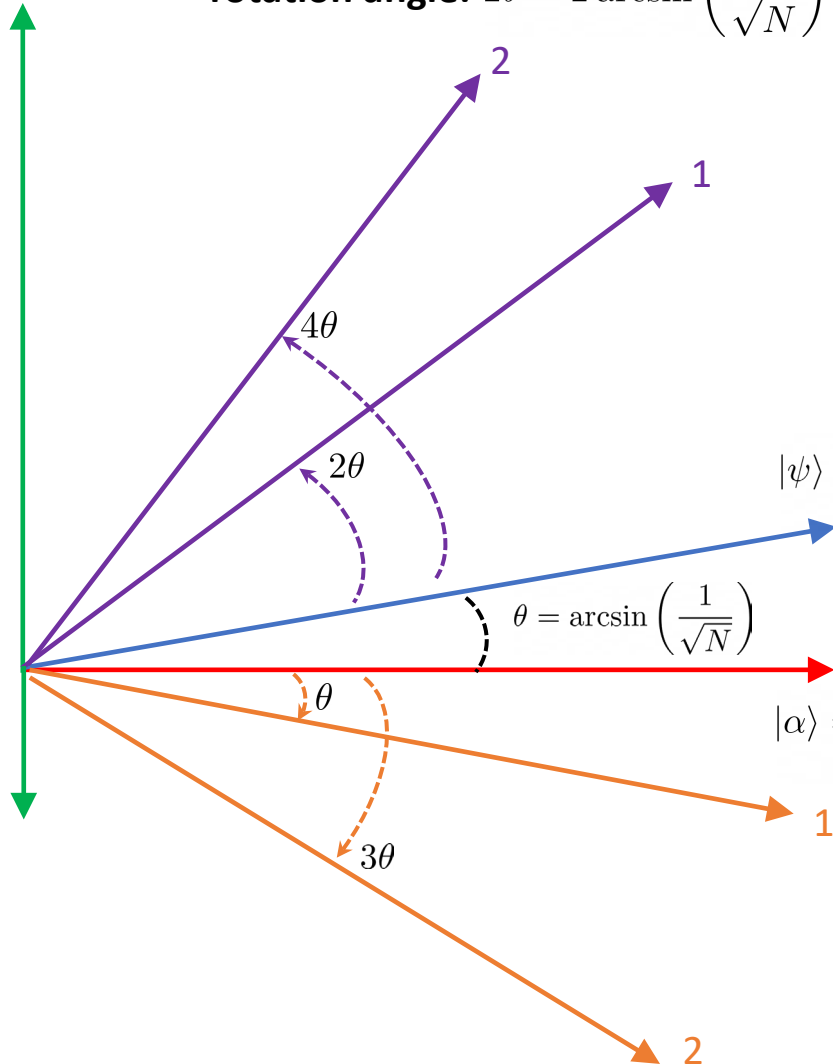
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(figure courtesy of ceemrr.com)



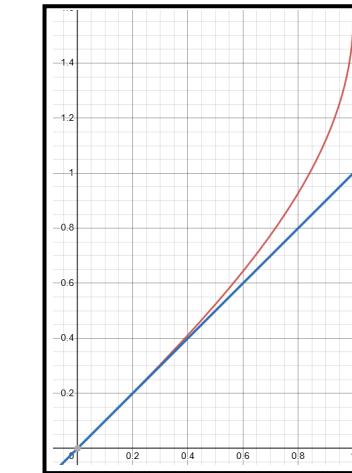
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$\arcsin(x)$: — red — x : — blue —

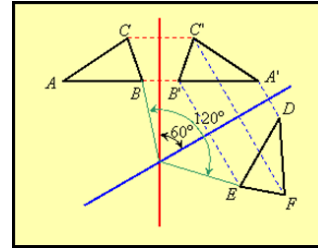
since
 $\arcsin(x) \geq x$ for $x \in [0, 1]$
and
 need to rotate at most $\frac{\pi}{2}$ radians

\rightarrow required iterations:

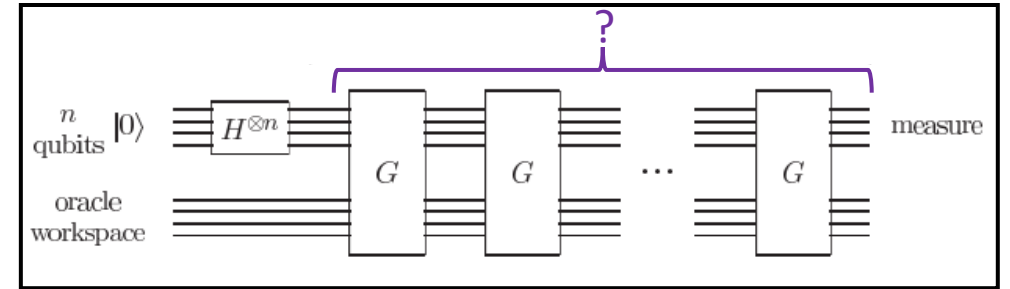
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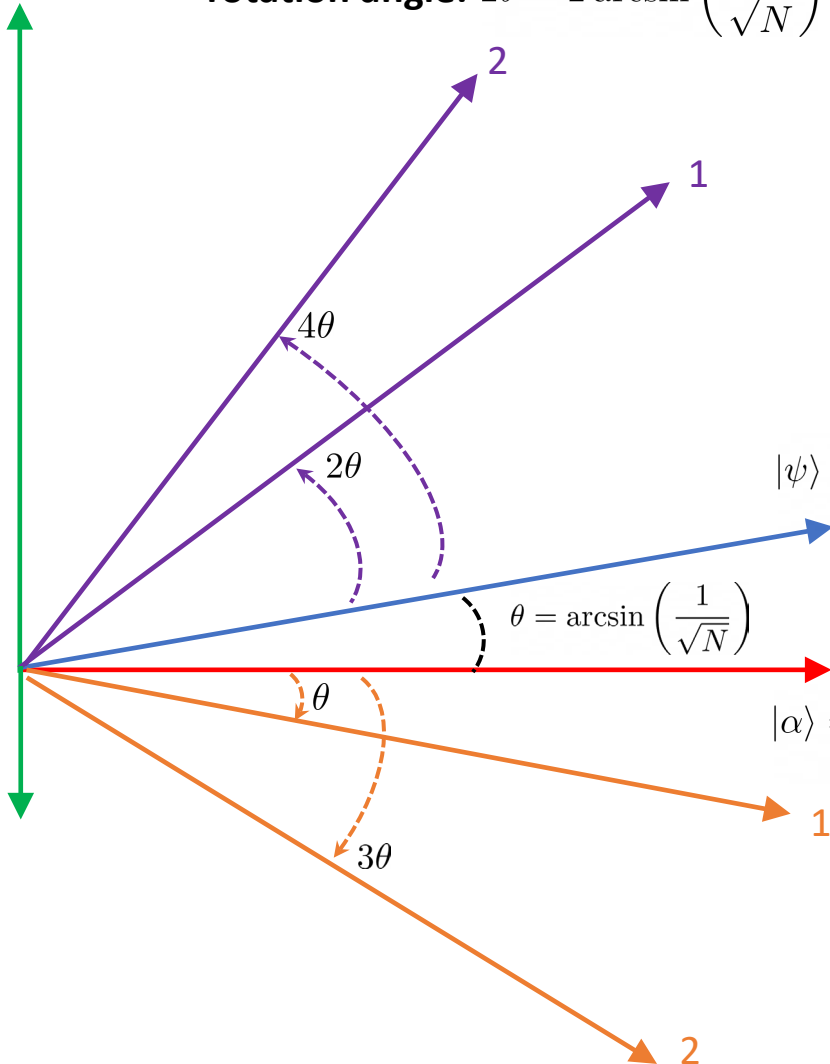
Thus: number Grover iterations \sim angle of rotation



(figure courtesy of ceemrr.com)



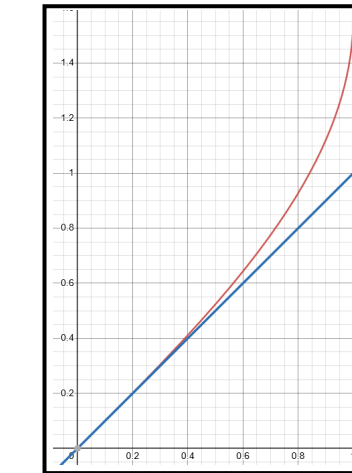
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since
 $\arcsin(x) \geq x$ for $x \in [0, 1]$
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 need to rotate at most $\frac{\pi}{2}$ radians

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$$\leq \frac{\frac{\pi}{2}}{2\theta} \leq \frac{\frac{\pi}{2}}{2 \arcsin\left(\frac{1}{\sqrt{N}}\right)} \leq \frac{\frac{\pi}{2}}{\frac{2}{\sqrt{N}}} = \frac{\pi}{4} \sqrt{N} = O(\sqrt{N})$$