# Grover Algorithm and Gutzwiller Ansatz

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# 1. Introduction to Grover Algorithm

## 1.1. To what classes of problems does it apply?

N P problems

Polynomial-bound: a given state can be checked to be a solution in polynomial time.

Non-deterministic: there is no known algorithm to find solution in polynomial time.

What does "polynomial time" mean? It means that the time required to solve problem or check solution scales with the size of the problem (e.g. number of states in search space, number of lattice sites, number of atoms in molecule) according to polynomial function.

e.g. NP problems: Search in unstructured database

Boolean satisfiability problem (e.g. 3-SAT)

Traveling Salesman problem.

## 1.2. How are such problems solved on a classical computer? How fast?

Generic approach is trial and error: pick a state from the search space and check if it is the/an answer to the problem. In some cases, there might exist an heuristic that, though not efficient (i.e. their scaling is superpolynomial), may nonetheless outperform trial and error.

## 1.3. What is the quantum speedup achieved by the Grover algorithm?

Case 1: Single solution in search space comprising N states

Trial and error requires $O(N)$ queries to have at least 50% probability of finding solution. Grover algorithm finds solution with high probability in $O(\sqrt{N})$ queries.

Case 2: $k$ solutions in search space comprising $N \gg k$ states

Trial and error: $O(N/k)$ queries

Grover algorithm: $O\left(\sqrt{N/k}\right)$ queries.

$\therefore$ Quadratic speed-up.

## 2. Derivation of Grover Algorithm Inspired by Quantum Simulation

In this derivation I shall assume there is a single solution to the problem. The generalization to the case where there are multiple solutions is straightforward. Let the solution be $|u\rangle$.

Suppose we can initialize a quantum processor in a state $|\psi\rangle$ that has nonzero overlap with the solution $|u\rangle$, i.e. $\langle u|\psi\rangle \neq 0$. The goal is to find some Hamiltonian $\mathcal{H}$ such that time evolving the state $|\psi\rangle$ under $\mathcal{H}$ over a given time $t$ yields the solution $|u\rangle$:

$$|\psi\rangle \xrightarrow{e^{-i\mathcal{H}t}} |u\rangle .$$

In principle, we should be able to find a suitable Hamiltonian in terms of $\{|\psi\rangle\langle\psi|, |u\rangle\langle u|, |\psi\rangle\langle u|, |u\rangle\langle\psi|\}$. It is therefore useful to define an appropriate Bloch sphere. The problem is that $|u\rangle$ and $|\psi\rangle$ are not orthogonal, so let us define $|\tilde{\psi}\rangle$ such that:

$$|\tilde{\psi}\rangle = \frac{|\psi\rangle - \langle u|\psi\rangle |u\rangle}{\sqrt{1-|\langle u|\psi\rangle|^2}}$$

$\langle\tilde{\psi}|u\rangle = 0$ by construction, so $\{|u\rangle, |\tilde{\psi}\rangle\}$ span the Bloch sphere. Now, $\mathcal{H}$ should have some term of the form $X = |u\rangle\langle\tilde{\psi}| + |\tilde{\psi}\rangle\langle u|$ so that some part of the initial state $|\psi\rangle$ is converted into $|u\rangle$, as desired. A natural guess is

$$\mathcal{H} = |u\rangle\langle\psi| + |\psi\rangle\langle u| .$$

There is a problem with this Hamiltonian, though: although $\mathcal{H}$ is Hermitian, the two terms individually are not. This makes it harder to implement the propagator via a quantum circuit, as Trotterization is not an option. Instead, let us take:

$$\mathcal{H} = |\psi\rangle\langle\psi| + |u\rangle\langle u|$$

Let us check that it works. Taking $a \equiv \langle u|\psi\rangle \in \mathbb{R}$ WLOG and $b = \sqrt{1-a^2}$, we have $|\psi\rangle = a|u\rangle + b|\tilde{\psi}\rangle$, in which case:

$$\begin{aligned}
\mathcal{H} &= |u\rangle\langle u| + |\psi\rangle\langle\psi| = \\
&= |u\rangle\langle u| + a^2|u\rangle\langle u| + ab\left(|u\rangle\langle\tilde{\psi}| + |\tilde{\psi}\rangle\langle u|\right) + b^2|\tilde{\psi}\rangle\langle\tilde{\psi}| = \\
&= \begin{pmatrix} 1+a^2 & ab \\ ab & b^2 \end{pmatrix} = \begin{pmatrix} 1+a^2 & ab \\ ab & 1-a^2 \end{pmatrix} \equiv \mathbb{1} + a\left(bX + aZ\right).
\end{aligned}$$

Hence, the corresponding propagator is

$$e^{-i\mathcal{H}t} = e^{-it}\left[\cos(at)\,\mathbb{1} - i\sin(at)\left(bX + aZ\right)\right]$$

Ignoring the global phase $e^{-it}$ and noting that $(bX + aZ)|\psi\rangle = |u\rangle$, we get the state $\cos(at)|\psi\rangle - i\sin(at)|u\rangle$ after a time $t$. To maximize the probability of reaching $|u\rangle$, we set $at = \frac{\pi}{2} \Leftrightarrow t = \frac{\pi}{2a}$.

There is a caveat: $a = \langle u|\psi\rangle$, which in principle depends on the solution $|u\rangle$, which we do not know. This can be addressed by taking $|\psi\rangle$ to be a linear combination of all states in the search space, in which case $a = \frac{1}{\sqrt{N}}$ regardless of $|u)$, as desired. Hence, the initial state of the answer register in the Grover algorithm is

$$|\psi) = \frac{1}{\sqrt{N}} \sum_{y=0}^{N-1} |y) = H^{\otimes n} |0), \quad N = 2^n .$$

Now that we have found the Hamiltonian $\mathcal{H} = |\psi)\langle\psi| + |u)\langle u|$ and the time required to do the time evolution under $\mathcal{H}$, $t = \frac{\pi}{2a} = \frac{\pi\sqrt{N}}{2}$, we must figure out how to implement $e^{-i\mathcal{H}t}$ as a quantum circuit. The natural starting point is to decompose $e^{-i\mathcal{H}t}$ into $M$ elementary steps $e^{-i\mathcal{H}t} = \left(e^{-i\mathcal{H}\Delta t}\right)^M$, with $M\Delta t = t$. Since all elements commute with each other, this decomposition is exact. A second decomposition will be adopted in order to treat the terms $|u)\langle u|$ and $|\psi)\langle\psi|$ separately. This is the (first-order) Trotter-Suzuki expansion

$$e^{i(A+B)\Delta t} = e^{iA\Delta t} e^{iB\Delta t} + \mathcal{O}\left(\|[A,B]\|\Delta t^2\right).$$

Notice the dependence on $\|[A,B]\|$, which is normally taken to be $\mathcal{O}(1)$. In this instance, let us take $M = \frac{\sqrt{N}}{2}$, in which case $\Delta t = \pi$. Clearly, $\Delta t \ll 1$ is not satisfied, so it would seem the $1^{st}$ order Trotter-Suzuki expansion does not work. However, $[|u)\langle u|, |\psi)\langle\psi|] = |u)\langle u|\psi)\langle\psi| - |\psi)\langle\psi|u)\langle u| = \frac{1}{\sqrt{N}}\left(|u)\langle\psi| - |\psi)\langle u|\right)$, and therefore $\|[|u)\langle u|, |\psi)\langle\psi|]\| = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$, in which case it follows that

$$e^{-i\pi\left(|u)\langle u| + |\psi)\langle\psi|\right)} = e^{-i\pi|u)\langle u|} e^{-i\pi|\psi)\langle\psi|} + \mathcal{O}\left(1/\sqrt{N}\right).$$

Provided that $N$ is large, which is certainly the case if the problem is hard, this approximation should hold. This is to say that, if $N \gg 1$, the overlap between the projectors

$|\psi\rangle\langle\psi|$ and $|n\rangle\langle n|$ should be small, in which case they essentially commute and we can treat them separately.

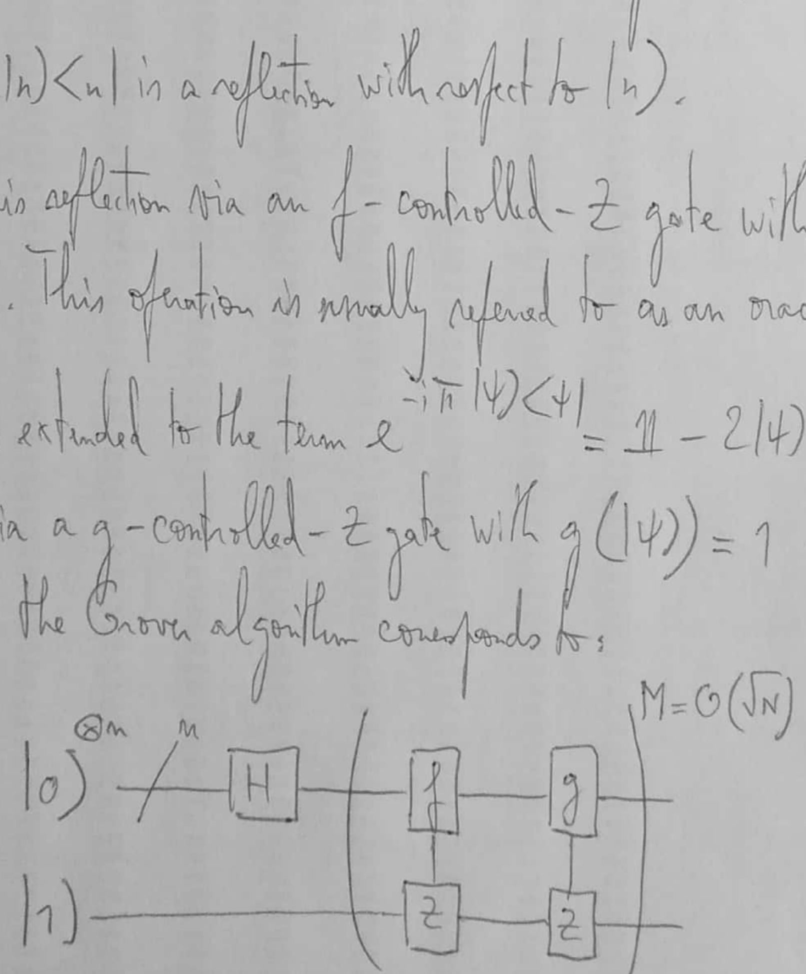
Let us now consider the term $e^{-i\pi|n\rangle\langle n|}$ in the $\{|n\rangle, |\tilde{\psi}\rangle\}$ basis. Clearly, $e^{-i\pi|n\rangle\langle n|}|n\rangle = e^{-i\pi}|n\rangle = -|n\rangle$ and $e^{-i\pi|n\rangle\langle n|}|\tilde{\psi}\rangle = \left(\mathbb{1} - i\pi|n\rangle\langle n| + \frac{1}{2!}(-i\pi)^2|n\rangle\langle n| + \dots\right)|\tilde{\psi}\rangle = |\tilde{\psi}\rangle$, since $|n\rangle$ and $|\tilde{\psi}\rangle$ are orthogonal. Hence:

$$e^{-i\pi|n\rangle\langle n|} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = -Z = \mathbb{1} - 2|n\rangle\langle n|$$

In words, given some state that overlaps with $|n\rangle$, $e^{-i\pi|n\rangle\langle n|}$ will swap the sign of the amplitude of the $|n\rangle$ term and leave all the other amplitudes unchanged. That is, $e^{-i\pi|n\rangle\langle n|} = \mathbb{1} - 2|n\rangle\langle n|$ is a reflection with respect to $|n\rangle$.

We can implement this reflection via an $f$-controlled-$Z$ gate with $f(n) = 1$ and $f(y \neq n) = 0$ otherwise. This operation is usually referred to as an oracle $O$.

This analysis can be extended to the term $e^{-i\pi|\psi\rangle\langle\psi|} = \mathbb{1} - 2|\psi\rangle\langle\psi|$. Again, this can be implemented via a $g$-controlled-$Z$ gate with $g(|\psi\rangle) = 1$ and $g(|y\rangle \neq |\psi\rangle) = 0$ otherwise. In summary, the Grover algorithm corresponds to:




1) Initializing $n$-qubit register in linear combination of all $N = 2^n$ states in search space via Walsh-Hadamard transform $H^{\otimes n}$

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2) Repeating two-step iteration $M = O(\sqrt{N})$ times:

a) Oracle call, corresponding to $f$-controlled-$Z$ gate, that marks solution $|u\rangle$ with a minus sign, $U = \mathbb{1} - 2|u\rangle\langle u|$.

b) Amplitude amplification, corresponding to $g$-controlled-$Z$ gate, that reflects state resulting from oracle call about linear combination of all states $|\psi\rangle$, $A = \mathbb{1} - 2|\psi\rangle\langle\psi|$.

Although it should now be clear how the Grover algorithm works at a qualitative level, there are still two crucial elements missing. First, the circuit still seems to lack a detailed structure, in that we do not quite know how to implement the $f/g$-controlled gates. For the moment, I am treating them as black boxes that can be implemented in some way. Later, I will fill this gap by providing explicit methods to implement them. Second, it is still unclear how the algorithm amplifies the amplitude of the solution $|u\rangle$. This will become clear in the next section, where a geometric description of the Grover algorithm is provided.

## 3. Geometric Interpretation of Grover Algorithm

Noting that the oracle call $U = \mathbb{1} - 2|u\rangle\langle u|$ and the amplitude amplification $A = \mathbb{1} - 2|\psi\rangle\langle\psi|$ are both reflections, their product should amount to a rotation. Hence, the Grover algorithm can be visualized as a rotation in the plane defined by $|u\rangle$, $|\tilde{\psi}\rangle$.

$$U = \mathbb{1} - 2|u\rangle\langle u| = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$A = \mathbb{1} - 2|\psi\rangle\langle\psi| = \mathbb{1} - 2\left(a|u\rangle + b|\tilde{\psi}\rangle\right)\left(a\langle u| + b\langle\tilde{\psi}|\right) =$$

$$= \begin{pmatrix} 1-2a^2 & -2ab \\ -2ab & 2a^2-1 \end{pmatrix} = \begin{pmatrix} 1-\frac{2}{N} & -\frac{2}{\sqrt{N}}\sqrt{1-\frac{1}{N}} \\ -\frac{2}{\sqrt{N}}\sqrt{1-\frac{1}{N}} & \frac{2}{N}-1 \end{pmatrix} =$$

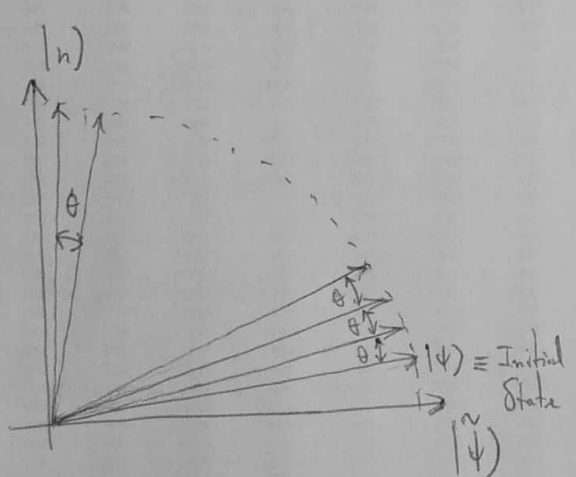
$$= \begin{pmatrix} \frac{N-2}{N} & -\frac{2\sqrt{N-1}}{N} \\ -\frac{2\sqrt{N-1}}{N} & -\frac{N-2}{N} \end{pmatrix}, \quad a \equiv \langle u|\psi\rangle = \frac{1}{\sqrt{N}}, \quad b = \sqrt{1-a^2}$$

A single step of the Grover algorithm therefore corresponds to:

$$AO = \begin{pmatrix} \frac{N-2}{N} & -\frac{2\sqrt{N-1}}{N} \\ -\frac{2\sqrt{N-1}}{N} & -\frac{N-2}{N} \end{pmatrix}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{2-N}{N} & -\frac{2\sqrt{N-1}}{N} \\ \frac{2\sqrt{N-1}}{N} & \frac{2-N}{N} \end{pmatrix} \equiv$$

$$\equiv \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \equiv \exp\left(i2\theta\frac{\sigma_y}{2}\right)$$

where $\theta \equiv \arctan\left(\frac{2\sqrt{N-1}}{N-2}\right) \simeq 2/\sqrt{N}$ for $N \gg 1$.




The number of iterations required to maximize the probability of measuring the solution $|u\rangle$ is:

$$M\theta \simeq \frac{\pi}{2} \Leftrightarrow M \simeq \frac{\pi/2}{2/\sqrt{N}} = \sqrt{N}\frac{\pi}{4} = O(\sqrt{N})$$

A similar derivation applies to the case where there are $k>1$ solutions, except that the orthogonal states that define the plane of rotation are:

$$|u\rangle = \frac{1}{\sqrt{k}}\sum_{i=1}^{k}|u_i\rangle$$

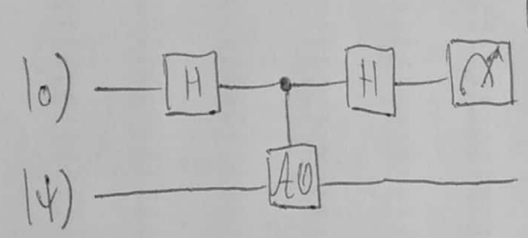
$$|\tilde{\psi}\rangle = \frac{\sqrt{N}|\psi\rangle - \sum_{i=1}^{k}|u_i\rangle}{\sqrt{N-k}}$$

$$\mathcal{O} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \mathcal{A} = \begin{pmatrix} N-2k & -\frac{2\sqrt{k(N-k)}}{N} \\ -\frac{2\sqrt{k(N-k)}}{N} & -\frac{N-2k}{N} \end{pmatrix}$$

$$\mathcal{A}\mathcal{O} = \begin{pmatrix} \frac{2k-N}{N} & -\frac{2\sqrt{k(N-k)}}{N} \\ \frac{2\sqrt{k(N-k)}}{N} & \frac{2k-N}{N} \end{pmatrix} \equiv \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \quad \theta \equiv \arctan\left(\frac{2\sqrt{k(N-k)}}{N-2k}\right) \simeq 2\sqrt{\frac{k}{N}}.$$

Hence, the number of required iterations is $M = \frac{\pi/2}{2\sqrt{\frac{k}{N}}} = \mathcal{O}\left(\sqrt{\frac{N}{k}}\right)$.

Notice, however, that, in this case, we need to know the number of solutions to the problem, $k$, in order to find the optimal number of iterations. $k$ can be found by adapting the Hadamard test or the Quantum Phase Estimation algorithm. Let us consider the former for the sake of simplicity.




$$p_0 = \cos^2\left(\frac{\theta}{2}\right), \quad \theta = \arctan\left(\frac{2\sqrt{k(N-k)}}{N-2k}\right).$$

Hence, by repeating this circuit multiple times, the probability of measuring the ancilla qubit in state $|0\rangle$ gives $\theta$, which in turn yields $k$, since $N$ is known. Of course, if $N \gg k$, this phase will be very tiny, so it will take many measurements to resolve it via the Hadamard test. The natural alternative is quantum phase estimation, where $U = e^{-i\hat{H}t/\hbar}$ is replaced by the Grover element $\mathcal{A}\mathcal{O}$.

Alternatively, the Grover algorithm for $k > 1$ solutions can be implemented without the need to count the number of solutions in advance. This is accomplished via the following algorithm [cf. Boyer et al., arXiv: quant-ph/9605034]:

1. Initialize $m = 1$ and set $\lambda = 6/5$ [Any $\lambda \in (1, \frac{4}{3})$ will do.]
2. Choose $j$ uniformly at random among the nonnegative integers smaller than $m$.

3. Apply $j$ iterations of Grover algorithm starting from initial state $|\psi\rangle = \sum_{i=0}^{N-1} \frac{1}{\sqrt{N}} |y\rangle$.
4. Measure the answer register; let $|y\rangle$ be the outcome.
5. If $f(|y\rangle) = 1$, the problem is solved: exit.
   Else, set $m = \min(\lambda m, \sqrt{N})$ and go back to step 2.

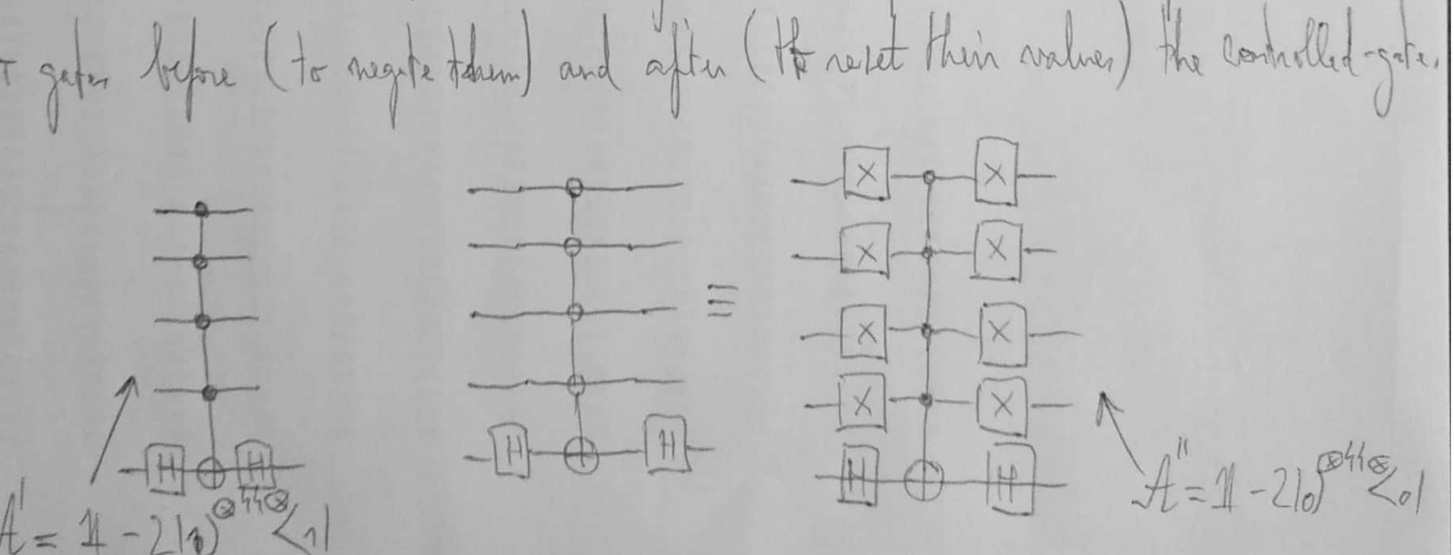
It can be shown that this method finds a solution in $O\left(\sqrt{\frac{N}{k}}\right)$ iterations, as required.

## 4. Implementation of Grover Algorithm

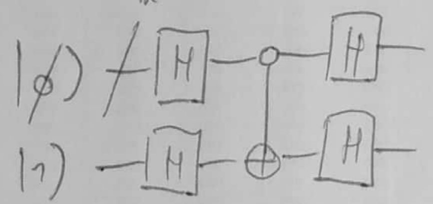
### 4.1. Quantum Circuit for Amplitude Amplification

We want to implement $A = \mathbb{1} - 2|\psi\rangle\langle\psi|$, where $|\psi\rangle = H^{\otimes n}|0\rangle$.

Suppose that, instead, we wanted to prepare $A' = \mathbb{1} - 2|1\rangle^{\otimes n}\,{}^{n\otimes}\langle 1|$. This corresponds to a quantum gate that does nothing unless the controls are all $|1\rangle$, in which case it applies a phase shift of $\pi$ (i.e. a minus sign) to the target qubit if this is in state $|1\rangle$. In other words, $A'$ is quite simply a controlled-$Z$ gate with $n$ control qubits. If, instead, we wanted to find the quantum circuit for $A'' = \mathbb{1} - 2|0\rangle^{\otimes n}\,{}^{n\otimes}\langle 0|$, we would just need to pad the control qubits with NOT gates before (to negate them) and after (to reset their values) the controlled-gate.



What if we replace the X gates by Hadamard gates? In that case, the controlled gate will only be triggered by $H^{\otimes n}|0\rangle = |\psi\rangle$, which is precisely what we want. Let us prove this generally. Suppose the state before this controlled gate is $|\phi\rangle = \sum_i c_i |i\rangle$, where $\{|i\rangle\}$ is the computational basis. Clearly, we can also express $|\phi\rangle$ in the basis $\{H^{\otimes n}|i\rangle\}$, which gives $|\phi\rangle = \sum_i c_i' \, H^{\otimes n}|i\rangle$. There is a one-to-one correspondence between the two bases, because $H^{\otimes n}$ is invertible.




After the action of the first $H^{\otimes n}$, we get $H^{\otimes n}|\phi\rangle = \sum_i c_i' \left(\cancelto{\mathbb{1}}{H^{\otimes n} H^{\otimes n}}\right)|i\rangle = \sum_i c_i' |i\rangle$.
Now comes the controlled-Z gates, which applies a minus sign to the $|0\rangle$ state: $\sum_{i \neq 0} c_i' |i\rangle - c_0' |0\rangle$. The final Walsh-Hadamard transform gives:

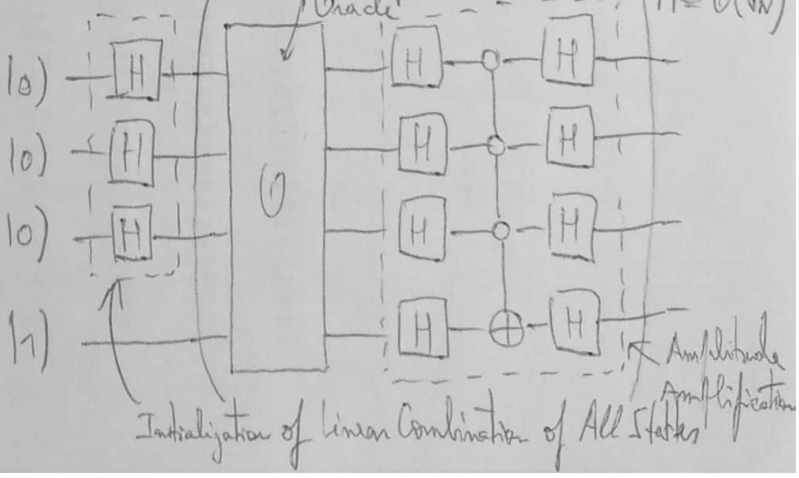
$$\sum_{i \neq 0} c_i' H^{\otimes n} |i\rangle - c_0' H^{\otimes n} |0\rangle =$$

$$= |\phi\rangle - 2 c_0' |\psi\rangle =$$

$$= \left(\mathbb{1} - 2|\psi\rangle\langle\psi|\right)|\phi\rangle.$$

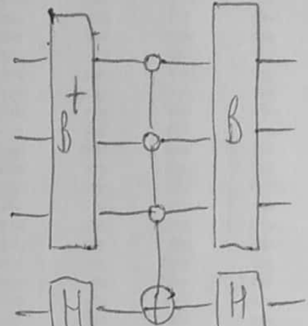
Since $|\phi\rangle$ was an arbitrary state, this proves the circuit above implements $A = \mathbb{1} - 2|\psi\rangle\langle\psi|$.

Example of Quantum Circuit for Grover Algorithm in Search Space with $N = 2^3 = 8$ States



## 4.2. Quantum Circuit for Oracle Call

At first glance, one might think that the same strategy used for $A$ could be applied to $O$, since $A$ and $O$ are identical — they both amount to reflections, $A = \mathbb{1} - 2|\psi\rangle\langle\psi|$, and $O = \mathbb{1} - 2|u\rangle\langle u|$. Instead of applying the Walsh-Hadamard transform before and after the controlled-gate, one would simply apply some operator $B$ such that $B|0\rangle = |u\rangle$:




$\leftarrow \mathbb{1} - 2|u\rangle\langle u|$
if $B|0\rangle = |u\rangle$

The problem with this method is that it assumes one can find such a $B$, which is to say one can initialize the solution state $|u\rangle$. But if that is the case, then the problem is already solved from the start, so why bother apply the Grover algorithm?

The reality is that there is no generic recipe to implement the oracle call, contrary to the amplitude amplification. This is not to say, however, that an oracle cannot be found for a particular problem. In general, it can, and, importantly, it can be implemented in polynomial time for NP problems.

The simplest strategy to find the quantum circuit for the oracle call of the Grover algorithm for a given NP problem is to translate the classical logical circuit into a quantum circuit. This is immediate by noting that any classical circuit can be implemented in terms of NOT and AND gates, and these gates can be implemented in a quantum circuit via the X and CCX (or Toffoli), respectively.

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# 5. Application of Grover Algorithm to Gutzwiller Ansatz

Before I introduce the Gutzwiller ansatz, I should motivate its application by discussing Hubbard interactions. In condensed matter physics, particularly in the study of strongly correlated phenomena, it is common practice to study toy models describing itinerant electrons in a lattice of positively-charged ions, which describes the crystal structure of materials. Each electron is assumed to be, at a given time, on a lattice site, but it is allowed to hop to other sites. The leading-order term describing this motion of the electrons comprises only hopping between nearest-neighbor sites. This mobility of the electrons gives rise to electric conductivity, and hence to metallic behavior (as opposed to insulating).

In addition to this hopping, electrons interact with each other via the Coulomb repulsion. To leading order, we can describe this electron-electron Coulomb interaction as an on-site repulsive term, meaning that two electrons in the same site (with opposite spin) repel each other, which is energetically costly. Of course, electrons at different sites also repel each other, but, since the Coulomb interaction goes like $1/r$, we can restrict this to only on-site interactions. Combined with the hopping terms, we get a minimal model of strongly correlated matter that goes by the name of Hubbard model:

$$\underbrace{\mathcal{H}}_{\text{Hubbard Hamiltonian}} = -t \sum_{\substack{\mu=\uparrow,\downarrow \\ \langle i,j \rangle}} \underbrace{\left( c^{\dagger}_{i\mu} c_{j\mu} + \text{H.c.} \right)}_{\text{Nearest-neighbor hopping}} + \frac{U}{2} \sum_{i} \underbrace{n_{i\uparrow} n_{i\downarrow}}_{\text{On-Site Coulomb Repulsion}}$$

Although this may seem like an overly simplified model, it turns out to be extremely rich in physical phenomena, and extremely hard to solve as well. In one dimension, an exact solution can be found via analytical methods (cf. Bethe Ansatz), but no exact solution is known in two or three dimensions. In any case, it is widely conjectured that the two-dimensional Hubbard model contains the physics of copper-based high-temperature superconductors (the so-called cuprates), for which the microscopic mechanism that accounts for their superconductivity is unknown.

More generally, the on-site Hubbard interaction can be added to any condensed matter model as a simplified description of electron-electron repulsion. This is a common practice in condensed matter theory, so methods to solve models involving Hubbard interactions are very useful.

Another important class of models in condensed matter physics that usually include Hubbard interactions are the so-called impurity models. The most famous one is the Single-Impurity Anderson model, which describes an impurity site connected to the conduction band of a metal

$$\mathcal{H}_{SIAM} = \underbrace{\varepsilon_d \sum_\sigma d_\sigma^\dagger d_\sigma + \frac{U}{2} n_\uparrow n_\downarrow}_{\text{Impurity with single-particle energy } \varepsilon_d \text{ and Hubbard repulsion } U} + \underbrace{\sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma}}_{\text{Noninteracting metal with dispersion } \varepsilon_k} + \underbrace{\sum_{k,\sigma} V_k \left( c_{k\sigma}^\dagger d_\sigma + \text{H.c.} \right)}_{\text{Coupling of metal to impurity}}$$

but in principle there can be more impurities. Besides being useful to describe real metals with defects, these impurity models are extremely important because there exist embedding theories, the most famous example of which is Dynamical Mean-Field Theory (DMFT), that map realistic models of materials to impurity models within some controllable approximations. Hence, coming up with efficient methods to solve impurity problems is very useful.

## 5.1. The Gutzwiller Ansatz

The Gutzwiller ansatz is one of the most widely used trial states in classical variational methods of models comprising Hubbard interactions. The logic behind it is very simple: as the Hubbard parameter U increases, the repulsion between two electrons in the same site increases as well, so it becomes more energetically unfavorable to have two electrons in the same site. Hence, if we start from the ground state of the non-interacting system (i.e. $U=0$), a good approximation of the ground state at $U>0$ corresponds to decreasing the amplitude of the states that involve doubly-occupied sites, followed by the renormalization of the wave-function. This is exactly what the Gutzwiller ansatz amounts to:

Free parameter (increases with U)

$$|\Psi_G) = \prod_i \left(1 - g\, n_{i\uparrow} n_{i\downarrow}\right) |\Psi_0)$$

Gutzwiller Wavefunction

Projecting out doubly occupied states

Non interacting Ground State

To find exactly by how much the states with doubly occupied sites should be mitigated for a given U, one minimizes the energy $\langle \Psi_G | \mathcal{H}(U) | \Psi_G)$ with respect to the free parameter $g$. The greater U, the greater $g$. At $U=0$, $g=0$. At $U \to +\infty$, $g \to +\infty$.

For the sake of clarity, let us consider a simple example: the Hubbard dimer, i.e. the Hubbard model applied to a chain of two sites. Assuming half-filling (i.e. the number of electrons equals the number of lattice sites, 2), there are 6 possible basis states:

$$\{ |\uparrow\downarrow, 0), |0, \uparrow\downarrow), |\uparrow, \downarrow), |\downarrow, \uparrow), |\uparrow, \uparrow), |\downarrow, \downarrow) \}$$

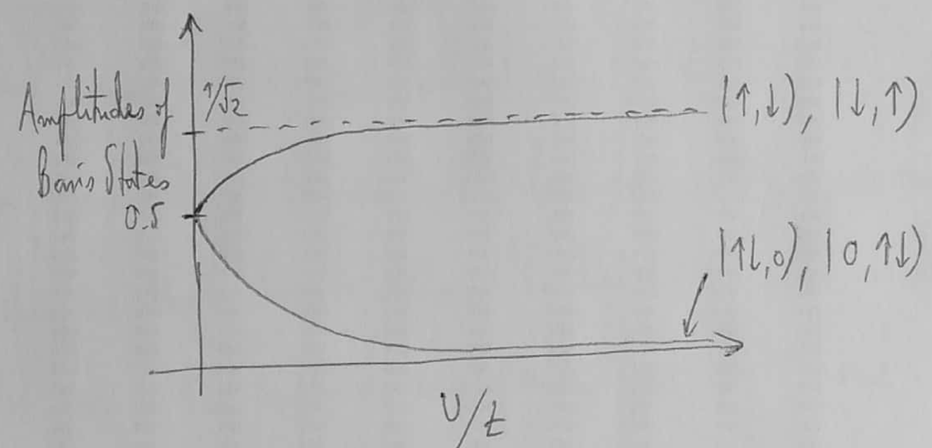
We can ignore the states $|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$ because they have spin $+1$ and $-1$, respectively, and we know that the ground state of the Hubbard dimer must have spin $0$ (cf. Lieb's Theorem). Hence, we are left with four states, $\{|\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle\}$, two of which have a doubly occupied site while the other two don't.

The ground state at $U=0$ is

$$|\psi_0\rangle = \frac{1}{2}\Big(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle + |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\Big)$$

As $U$ increases, the amplitudes of $|\uparrow\downarrow,0\rangle$ and $|0,\uparrow\downarrow\rangle$ decrease, and the amplitudes of the other two states must ~~decrease~~ increase to maintain the normalization. In the limit, $U\to+\infty$, having a doubly occupied site is infinitely costly (i.e. forbidden), and the ground state is:

$$|\psi_\infty\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\Big)$$




## 5.2. Implementing the Gutzwiller Ansatz on Quantum Hardware

Implementing the Gutzwiller ansatz on a quantum computer is not immediately obvious: the projector is nonunitary, and quantum circuits are all unitary. Hence, we have to come up with an indirect way of preparing the Gutzwiller ansatz.

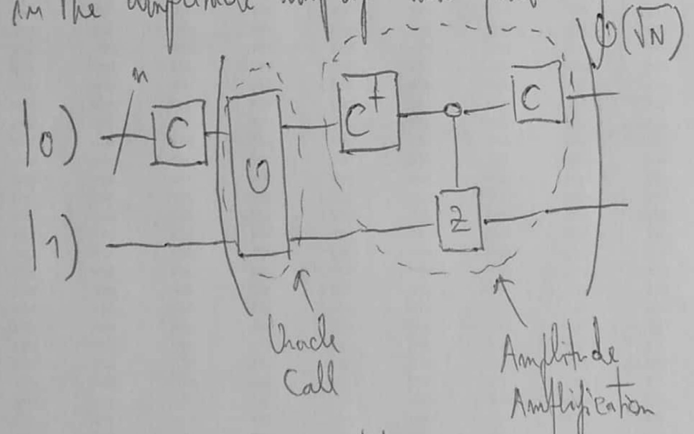
The approach that I will explore henceforth is an adaptation of the Grover algorithm: the rationale is as follows: much as the Grover algorithm can be used to amplify the amplitudes of the states that encode the solution(s) to a search problem to the detriment of the remaining states in the Hilbert space, it can also be used to mitigate the amplitude of some basis states within a given wave function. This requires, however, two changes: 

- The amplitude amplification must be restricted to the subspace comprising only the basis states of the given wave function. In other words, no extra states are supposed to be added to the wavefunction.
- The oracle must mark the targeted states (in the case of the Gutzwiller projector, the basis states with doubly occupied sites) as opposed to the solutions to a search problem.

Let us consider each of these issues in turn.

5.2.1. Restricting Amplitude Amplification to Subspace

Let us assume that, instead of starting from the uniform linear combination of all states in the search space, $H^{\otimes n}|0\rangle = \frac{1}{\sqrt{2^n}}\sum_{i=0}^{2^n-1}|i\rangle$, we start from some wave function (e.g. the noninteracting ground state of the Hubbard model) $|\psi_0\rangle = C|0\rangle$. Now, we want the amplitude amplification to be confined to the basis states with nonzero amplitude in $|\psi_0\rangle$. To accomplish this, we simply have to replace the Walsh-Hadamard transforms on either side of the controlled-gate in the amplitude amplification part by $C^\dagger$ and $C$:




Let us confirm that no extra basis states are added. Let us define $|\psi_0\rangle = \sum_s \varphi_s|s\rangle + \sum_d \varphi_d|d\rangle$, where $\{|d\rangle\}$ are the states we want to mitigate and $\{|s\rangle\}$ are the remaining ones. In principle, the Hilbert space can include more states, i.e. $H^{\otimes n}|0\rangle = \frac{1}{\sqrt{2^n}}\left(\sum_s|s\rangle + \sum_d|d\rangle + \sum_m|m\rangle\right)$.

The action of the oracle is:

$$O|\psi_0\rangle = \sum_s \varphi_s |s\rangle - \sum_d \varphi_d |d\rangle$$

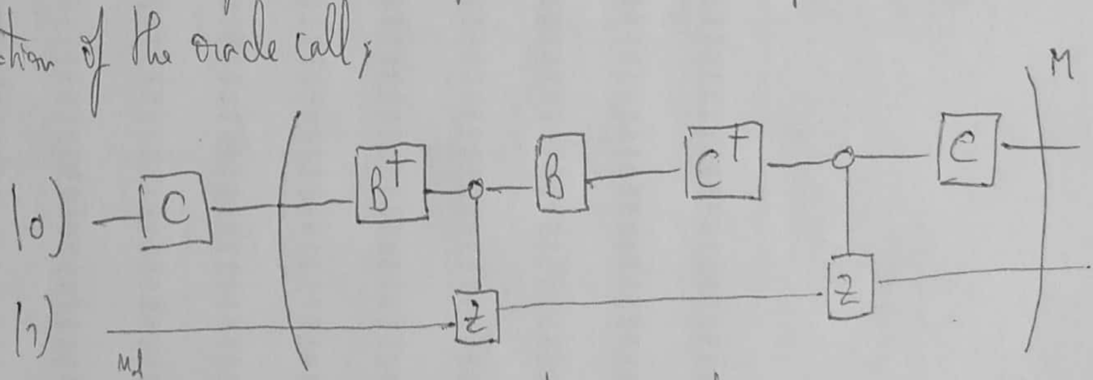
The action of the amplitude amplification is:

$$A\left(O|\psi_0\rangle\right) = (-1)\times\Big[\sum_s \varphi_s\Big(2\Big(\sum_s|\varphi_s|^2-\sum_d|\varphi_d|^2\Big)-1\Big)|s\rangle + \sum_d\varphi_d\Big(2\Big(\sum_s|\varphi_s|^2-\sum_d|\varphi_d|^2\Big)+1\Big)|d\rangle\Big].$$

As desired, no extra basis states are added and the amplitude amplification works as usual. If the initial weight of the targeted states is greater than that of the remaining ones, $\sum_d |\varphi_d|^2 > \sum_s |\varphi_s|^2$, then the amplitudes of $\{|d\rangle\}$ are reduced and those of $\{|s\rangle\}$ are increased. If instead $\sum_s |\varphi_s|^2 > \sum_d |\varphi_d|^2$, if we want to reduce the amplitude of the $\{|d\rangle\}$ states, we should target the $\{|s\rangle\}$ states with the oracle instead. If $\sum_s |\psi_s|^2 = \sum_d |\varphi_d|^2$, nothing happens. This shows the Grover algorithm behaves like a see-saw.

### 5.2.2. Deriving Quantum Circuit for Oracle Call

In this case, we are not solving a search problem. In fact, we know a priori what the targeted states are, therefore we can replicate the structure of the amplitude amplification in the construction of the oracle call:




where $B|0\rangle = \frac{1}{\sqrt{M_d}}\sum_{d=1}^{M_d}|d\rangle$ is a linear combination of the targeted states.

### 5.2.3. Example of Application: Anderson Dimer

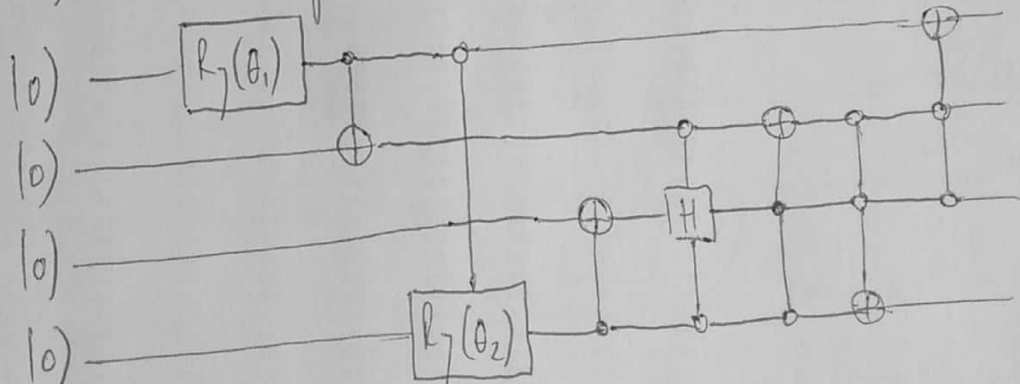
Let us consider the Anderson dimer, which involves a site with on-site Hubbard repulsion and negative single-particle energy, and another site with 0 single-particle energy. There is hopping between the two sites:

$$\mathcal{H} = \varepsilon_1 \sum_{\mu=\uparrow,\downarrow} c_{1\mu}^{\dagger} c_{1\mu} + \frac{U}{2} n_{1\uparrow} n_{1\downarrow} + (-t) \sum_{\mu=\uparrow\downarrow} \left( c_{1\mu}^{\dagger} c_{2\mu} + c_{2\mu}^{\dagger} c_{1\mu} \right)$$

The noninteracting ground state is:

$$|\psi_0) = N_0 \left[ \alpha^2 |\uparrow\downarrow, 0) + \alpha \left( |\uparrow, \downarrow) + |\downarrow, \uparrow) \right) + |0, \uparrow\downarrow) \right]$$

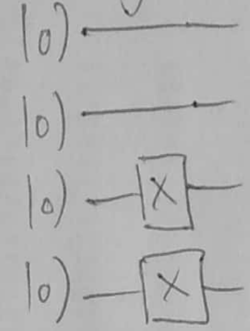
with $\alpha = \dfrac{2t}{|\varepsilon_1| + \sqrt{\varepsilon_1^2 + 4t^2}}$ and $N_0 = \dfrac{1}{1+\alpha^2}$. Notice that the labelling is $|2,1)$, that is, the impurity site is the rightmost site. The subcircuit $C$ must therefore prepare this state $|\psi_0)$. It can be found to be:




Where $\theta_1 \equiv 2 \arcsin N_0$, $\theta_2 = 2 \arcsin \left( N_0 \alpha / \sqrt{1 - N_0^2} \right)$ and the top two qubits store the normal site and the bottom two store the impurity site. In this mapping to qubits, the noninteracting ground state $|\psi_0)$ prepared by this circuit is:

$$|\psi_0) = N_0 \left[ \alpha^2 |1100) + \alpha \left( |1001) + |0110) \right) + |0011) \right].$$

In this case, there is a single state to mitigate, $|0,\uparrow\downarrow\rangle = |0011\rangle$. Hence, the circuit that implements B is trivially:




Plugging these two subcircuits, B and C onto the circuit shown at the bottom of page 17 allows to change the amplitudes of the doubly-occupied impurity state. By performing multiple runs of the algorithm and measuring the energy of the resulting states, one can find the optimal amplitude for $|0,\uparrow\downarrow\rangle$, i.e. the one that yields the lowest energy.

### 5.2.4. Generalizing to Arbitrarily Large Systems

Let us now consider how hard it is to apply this method to an arbitrarily large system. Finding the circuit C is not trivial, but it can be done efficiently: there are methods in the literature to initialize noninteracting ground states efficiently on a quantum computer. Hence, finding out how to implement C as a quantum circuit should not be an issue.

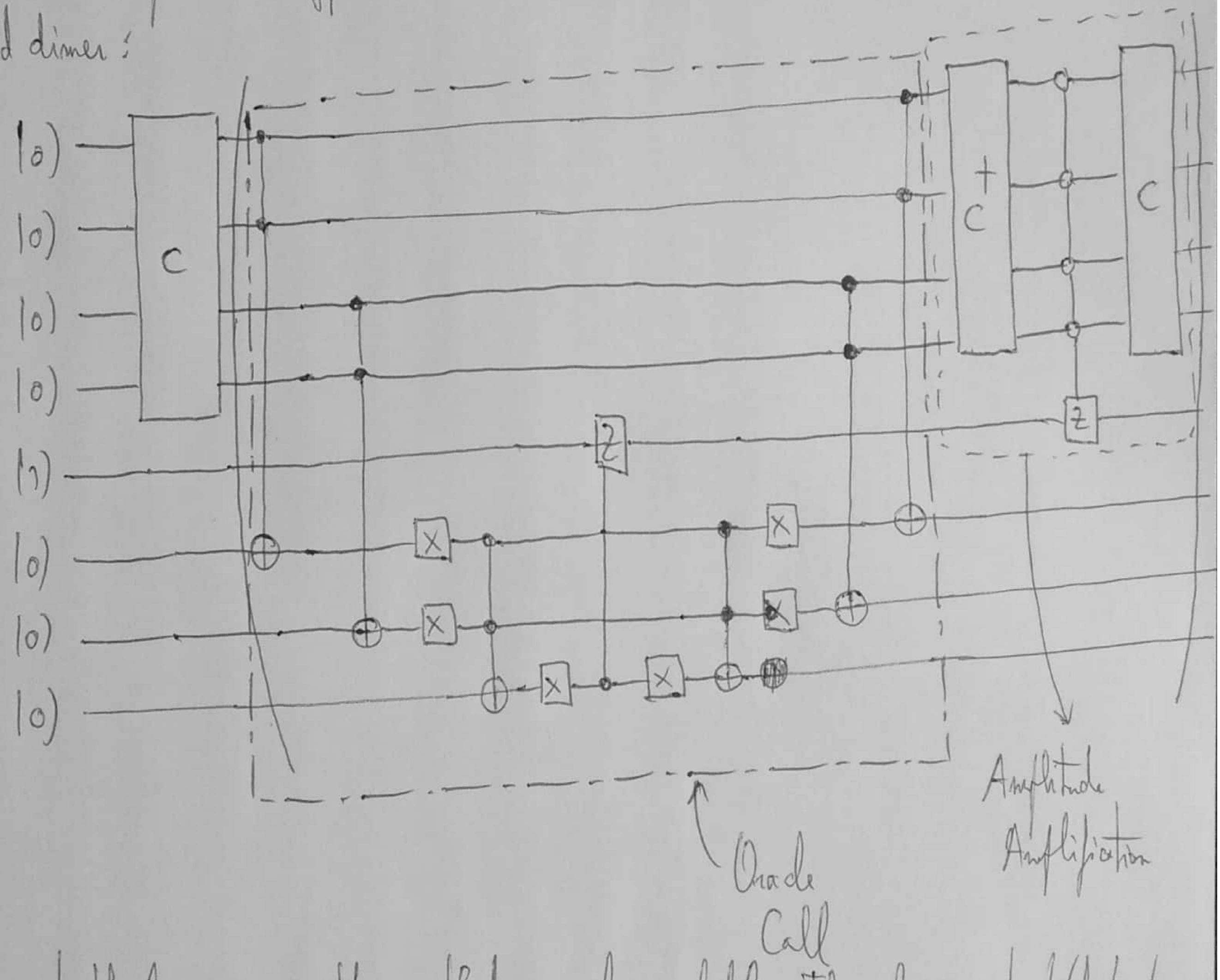
The problem lies in implementing B. Contrary to the simple example above, there should in general exist many states with doubly-occupied sites. Finding the circuit B that prepares a linear combination of only those states does not seem to be obvious.

We can, however, implement the oracle call in a different way, one that resembles more the classical design of oracles. Basically, we apply a Toffoli with the two qubits that store the occupation of the $\{|\uparrow\rangle, |\downarrow\rangle\}$ states for a given site as control qubits and an ancilla initialized in $|0\rangle$ as target: if the site is doubly occupied, the ancilla becomes $|1\rangle$, otherwise it remains $|0\rangle$. Once we do this for all sites, we have to determine if there is at least one doubly-occupied state; in other words, we need to perform a logic OR gate on all N ancillas (where N is the number of lattice sites with Hubbard interactions).

How does one implement an OR gate on a quantum computer? Given that a Toffoli gate implements a AND gate, we can use the De Morgan rules:

$$\neg(A \vee B) = (\neg A)\wedge(\neg B)$$

Finally, we need to reset all the ancillas so we can reuse them in the next iteration, so we have to repeat all Toffolis. All this is illustrated in the circuit below for a Hubbard dimer:




Contrary to the previous one, this method is easily scalable. The only caveat is that it requires additional ancilla qubits. For the Hubbard model in a system with N sites, the previous method required 2N+1 qubits, while this method need a total of 3N+1 qubits. //