

+ Caltech

**Shubh Agrawal, Gianluca Delgado, Wenyan Guan, Ananth Malladi, Aditi Venkatesh**

# Task 1: Divisibility by 4

- $a_1 a_2 a_3 \dots a_N$  is our binary number in little endian form
  - base 10 equivalent is:  $n = 1 * a_1 + 2 * a_2 + 4 * a_3 + 8 * a_4 \dots = a_1 + 2a_2 + 4(\dots)$ , divisible by 4 when  $a_1$  and  $a_2$  are 0.
- 
- ★ Flip the first two bits
  - ★ Controlled X from these 2 onto the target
  - ★ Target is 1 iff the first 2 bits are 0

## Task 2 and 3: Are all 3 bits the same?

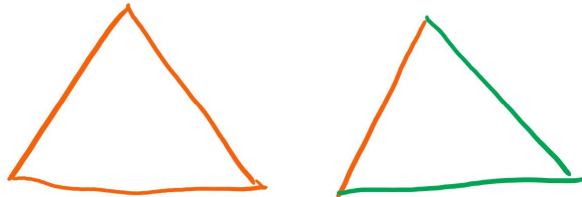
- Imagine a Controlled X gate from all 3 bits to the target.
  - ★ If there are one 0 and two 1, we want to flip that 0 to get target = 1
  - ★ If there are two 0s and two 1, we want to flip both the 0s to get target = 1

```
operation Task2_ValidTriangle (inputs : Qubit[], output : Qubit) : Unit is Adj+Ctl {  
    for i in 0 .. (Length(inputs)-1) {  
        X(inputs[i]);  
        Controlled X(inputs, output);  
        X(inputs[i]);  
    }  
    X(inputs[0]);  
    X(inputs[1]);  
    Controlled X(inputs, output);  
    X(inputs[0]);  
  
    X(inputs[2]);  
    Controlled X(inputs, output);  
    X(inputs[1]);  
  
    X(inputs[0]);  
    Controlled X(inputs, output);  
    X(inputs[0]);  
    X(inputs[2]);  
}
```

```
operation Task3_ValidTriangle (inputs : Qubit[], output : Qubit) : Unit is Adj+Ctl {  
    X(inputs[0]);  
    CNOT(inputs[0], inputs[1]);  
    CNOT(inputs[0], inputs[2]);  
    CCNOT(inputs[1], inputs[2], output);  
    X(output);  
    CNOT(inputs[0], inputs[2]);  
    CNOT(inputs[0], inputs[1]);  
    X(inputs[0]);  
}
```

## Task 4: Triangle Free Graph Coloring

- Task: Determine if a graph colouring has a triangle with all three edges having the same colour.
- Step 1: Find all triangles (this can be done classically)
  - Iterate over all possible edge triplets (this is  $O(n^3)$ ).
- Step 2: For each triangle, run the oracle from task 3
  - Notice that when all three edges have the same parity, this is identical to the task 3 case where all three qubits have the same value.
  - And similarly when the edges have different parity.



## 7.2 Independent Electron Model

We will be interested in solving the Schrödinger equation for electrons in a condensed matter system with some fixed set of positions of the nuclei. In particular, when the system is in the crystalline state the nuclei are located on lattice sites  $\{\vec{R}_I\}$ . Neglecting for the moment the spin degree of freedom of the electrons, the Schrödinger equation for the  $n$ th eigenfunction is

$$\mathcal{H}\Phi_n(\vec{r}_1, \dots, \vec{r}_N) = E_n\Phi_n(\vec{r}_1, \dots, \vec{r}_N), \quad (7.25)$$

where the Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^N \left( \frac{-\hbar^2 \nabla_i^2}{2m_e} - \sum_I \frac{e^2 Z}{|\vec{r}_i - \vec{R}_I|} \right) + \frac{1}{2} \sum_{i \neq j}^N \frac{e^2}{|\vec{r}_i - \vec{r}_j|}. \quad (7.26)$$

The presence of the (last) electron–electron Coulomb interaction term couples the degrees of freedom of different electrons and makes this many-body Schrödinger equation difficult to solve. Fortunately, it is frequently (but not always!) a good approximation to replace  $\mathcal{H}$  by an effective independent-particle Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N H_i = \sum_{i=1}^N \left( \frac{-\hbar^2 \nabla_i^2}{2m_e} + v_{\text{eff}}(\vec{r}_i) \right). \quad (7.27)$$

There are (at least) two different approaches leading to effective independent-particle Hamiltonians of this form. We will discuss these approaches and their limitations in Chapter 15. It is clear that  $v_{\text{eff}}(\vec{r})$  is some sort of effective potential which includes the interaction of an electron with the nuclei and represents in some average way the interaction of an electron with all other electrons. The most naive approximation to a condensed matter system is one where  $v_{\text{eff}}(\vec{r})$  is replaced by a constant, which we can take to be the zero of energy. This leaves us with the so-called free-electron-gas model. In this model the single-particle states are plane waves, which can be labeled by a wave vector,

$$\langle \vec{r} | \vec{k} \rangle = \frac{1}{\sqrt{L^3}} \exp(i \vec{k} \cdot \vec{r}), \quad (7.28)$$

where  $L^3$  is the normalization volume. These plane waves have eigenenergy

$$\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m_e} \quad (7.29)$$

and are eigenstates of the velocity operator

$$\vec{V} = \frac{d\vec{r}}{dt} = \frac{i}{\hbar} [H, \vec{r}] = \frac{i}{2m_e \hbar} [\vec{p} \cdot \vec{p}, \vec{r}] = \frac{i}{m_e \hbar} \vec{p} (-i\hbar) = \frac{\vec{p}}{m_e} = \frac{-i\hbar \nabla}{m_e} \quad (7.30)$$

with eigenvalue  $\hbar \vec{k} / m_e$ . Because the velocity is a constant of motion, the electrical resistance is strictly zero, since a current does not decay in the free-electron model.

The next-simplest model (and one which we will now study extensively), sometimes called the **independent-particle model**, uses

$$v_{\text{eff}}(\vec{r}) = V(\vec{r}), \quad (7.31)$$

where  $V$  is a periodic potential with the symmetries of the crystalline lattice:

$$V(\vec{r} + \vec{R}_j) = V(\vec{r}), \quad (7.32)$$

where  $\vec{R}_j$  is a lattice vector of the crystal. Amazingly, as we will see shortly, one is able to make many concrete statements about the electronic structure that are based on this symmetry property *alone*, without additional information on the detailed form of  $V(\vec{r})$ . Recall that in Drude's classical model it was scattering from the periodic potential that produced a very short mean free path (on the order of the lattice spacing) and hence was responsible for the finite electrical resistance. We now need to learn how to solve this problem quantum mechanically. We will find from a powerful result known as **Bloch's theorem** that quantum coherence makes the mean free path infinite. Hence the electrical resistance is actually zero in this model for metals with perfectly ordered crystalline lattices. In the end, we will find that Drude's transport formulas are still very useful, provided that we compute the scattering time  $\tau$  (due to impurities or phonons which disturb the perfect crystalline order) quantum mechanically rather than classically.



# Grover's Algorithm

- Input to the Algorithm:
  - a Hamiltonian, implemented using qDRIFT == our black box oracle
  - a set of initial possible states of the system (for example, positions of the nuclei with electrons in a condensed matter system) == our database, use Born Oppenheimer approximation)
- Output of the Algorithm:
  - possible initial conditions that work == solution for the condensed matter system

