Errata for "Quantum Algorithms for solving Hard Constrained Optimization Problems"

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NOTE: The most significant changes that this version of the thesis has undergone has been the unification of the upper limits N and rewriting some paragraphs so that the work that has been done is better understood. However, the most critical point that could affect the reader was section 2, where the weight matrix c_{ij} was not defined, and an equal one was missing.

Section 2: Travelling Salesman Problem

Before: It was necessary to define the variables c_{ij} and standardise the upper limit n to N.

The *Travelling Salesman Problem* known as TSP is defined as follows: *Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?*

For this problem we can associate each possible solution p to a permutation $(x_1, ..., x_N)$ of the numbers $\{1, ..., N\}$ that affects the order in which they are going to be tour the cities, and taking as function $f(p) = d_{x_1,x_2} + ... + d_{x_{n-1},x_n}$, where $d_{x_i,x_{i+1}}$ corresponds to the distance between the cities x_i and x_{i+1}, we have that our goal will be to find the minimum of f in the set of permutations of $\{1, ..., N\}$.

TSP is an NP-Hard problem within combinatorial optimization. The problem was first formulated in 1930 and is one of the most studied optimization problems. Although the situation is computationally complex, many exact heuristics and methods are known so that some instances from one hundred to thousands of cities can be solved.

In the TSP formulation (5) to (8), there are $N!$ Possible routes (for the exact calculation). However, it can be simplified since, given a path, the starting point does not matter, and this reduces the number of routes to be examined by a factor N, leaving $(N-1)!$. Since the direction in which the traveller is travelling does not matter, the number of routes to be examined is again reduced by a factor of 2. Therefore, it is necessary to consider $\frac{(N-1)!}{2}$ possible routes.

The number of routes is multiplied by the N factor for each new city, and its growth is factorial. So, the TSP belongs to the NP-complete complexity class.

$$min \sum_{i=0}^{n} \sum_{i \neq j j=0}^{n} c_{ij} x_{ij}, \tag{1}$$

$$0 \leq x_{ij} \leq 1. \tag{2}$$

Where x_{ij} is an integer and could take the following value $i, j = 0, 1, \ldots n$

$$\sum_{i=0 i \neq j}^{n} x_{ij} = 1, \tag{3}$$

$$\sum_{j=0 i \neq j}^{n} x_{ij}, \tag{4}$$

After:
We have redefined the TSP to solve the previously mentioned problems.

In section 2: Travelling Salesman Problem

The *Travelling Salesman Problem* known as TSP is defined as follows: *Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?*

For this problem we can associate each possible solution p to a permutation $(x_1, ..., x_N)$ of the numbers $\{1, ..., N\}$ that affects the order in which they are going to be tour the cities, and taking as function $f(p) = d_{x_1,x_2} + ... + d_{x_{N-1},x_N}$, where $d_{x_i,x_{i+1}}$ corresponds to the distance between the cities x_i and x_{i+1}, we have that our goal will be to find the minimum of f in the set of permutations of $\{1, ..., N\}$.

TSP is an NP-Hard problem within combinatorial optimization. The problem was first formulated in 1930 and is one of the most studied optimization problems. Although the situation is computationally complex, many exact heuristics and methods are known so that some instances from one hundred to thousands of cities can be solved.

In the TSP formulation (5) to (9), in this case, the distance matrix of the TSP will be determined by the elements c_{ij} indicating the distance (cost) between node i and node j. The decision variables are $x_{ij} = 1$, if the solution to the TSP goes from city i to city j, $x_{ij} = 0$, otherwise. Then the solution of the problem is found by solving. This formulation is known as MTZ [23].

$$\min \sum_{i=1}^{N} \sum_{j=1}^{N} c_{ij} x_{ij}, \tag{5}$$

$$\sum_{i=1}^{N} x_{ij} = 1 \quad \forall j \in \{1, ..., N\} \tag{6}$$

$$\sum_{j=1}^{N} x_{ij} = 1 \quad \forall i \in \{1, ..., N\} \tag{7}$$

$$\begin{aligned} x_{i,j} \in \{0, 1\} \quad & \forall i \in \{0, \ldots, N\} \\ & \forall j \in \{0, ..., N\} \end{aligned}. \tag{8}$$

$$u_i - u_j + N x_{i,j} \leq N - 1 \quad 1 \leq i \neq j \leq N. \tag{9}$$

In this formulation, the objective function equation (5) minimizes the cost function. The restrictions equations (6) and (7) declare that each salesman can only be one node at any time. The restriction (8) describes that x_{ij}, are binary variables. The constraint (9) are the route of continuity and the elimination of sub-courses, which ensure that the solution does not contain a sub-route disconnected from the exchange.

There are $N!$ possible routes (for the exact calculation). However, it can be simplified since, given a path, the starting point does not matter, and this reduces the number of routes to be examined by a factor N, leaving $(N-1)!$. Since the direction in which the traveller is travelling does not matter, the number of routes to be examined is again reduced by a factor of 2. Therefore, it is necessary to consider $\frac{(N-1)!}{2}$ possible routes.

The number of routes is multiplied by the N factor for each new city, and its growth is factorial. So, the TSP belongs to the NP-complete complexity class.

Before: Without a mathematical formulation of the VRP
Section: 2.4 Vehicle Routing Problem

After: We have added the formulation of the VRP to help the reading of the document.

Section: 2.4 Vehicle Routing Problem

Let $G = (V, E)$ be a complete graph directed with $V = \{0, 1, 2, .., N\}$, as the set of nodes and $E = \{(i, j) : i, j \in V, i \neq j\}$ as the set of arcs, where node 0 represents the central, for the K vehicles with the same capacity q and n remaining nodes that represent geographically dispersed cities/locations. In this case, the distance matrix of the VRP will be determined by the elements c_{ij} indicating the distance (cost) between node i and node j. The VRP formulation is described as follow:

$$\min \sum_{i=1}^{N} \sum_{j=1}^{N} c_{ij} x_{ij}, \tag{10}$$

$$\sum_{i=1}^{N} x_{ij} = 1 \quad \forall j \in \{1, ..., N\} \tag{11}$$

$$\sum_{j=1}^{N} x_{ij} = 1 \quad \forall i \in \{1, ..., N\} \tag{12}$$

$\sum_{j=1}^{N} x_{0j} = K \quad \forall i \in 1, \ldots, N, (13)$

$\sum_{j=1}^{N} x_{j0} \ = K, \quad \forall i \in 1, \ldots, N, (14)$

$\sum_{i=1}^{N} \sum_{j=1}^{N} x_{ij} c_{ij} \leq q, (15)$

$$u_i - u_j + N x_{i,j} \leq N - 1 \quad 1 \leq i \neq j \leq N. \tag{16}$$

$$x_{i,j} \in \{0, 1\} \quad \begin{matrix} \forall i \in \{0, \ldots, N\} \\ \forall j \in \{0, ..., N\} \end{matrix}. \tag{17}$$

In this formulation, the objective function equation (10) minimizes the new cost function. The restrictions equations (11) and (12) declare that each vehicle can only be one node at any time. The constraint () establishes that all the vehicles start from Depot and () establishes that all the vehicles end at the Depot. The restriction () establishes that any vehicle can travel more distance than allowed. In the case of wanting to measure the time, here, what we would do is change the matrix c_{ij} for a matrix of the maximum contract time. The constraints (16) are the route of continuity and the elimination of sub-courses, which ensure that the solution does not contain a sub-route disconnected from the exchange. Restrictions (17) describes that x_{ij}, are binary variables.

It is also observed that the Vehicle Routing Problem can serve to encode the difficulty of finding the optimal schedules of the n social assistants (vehicles) who visit the m patients (locations).

Up to this point, the mathematical formulation of equations (10) to (17) represents a conventional CVRP. To solve a scheduling problem, we will need a time variable. The introduction of time (schedule) into the QUBO formulations of the CVRP is a significant obstacle to formulating several important VRP restrictions associated with the VRPTW time window [27].

During the state of the art of these formulations carried out, we have found several articles [27, 12, 16] that solve the TSP and VRP for annealing computers [7, 6, 11]. However, the number of variables is still intractable for the current size of quantum computers. The **number of qubits** of

the TSPTW[27], is proportional to $N^3 + N^2 \log_2 N$, and for this VRPTW[16], is N^4. For this reason, we will propose a new VRPTW formulation ((194) and (195)) with a heuristic function executed by an classical algorithm that generates a description of a quantum circuit as advocate the following reference [13]. With this strategy, we aim to reduce the number of the qubits from N^4 to $N2$ for our proposed VRPTW for solving our SWP.

The new formulation of the VRPTW will be developed in section (11).

Before: In the summary of section 2.

Summary In this section, we have introduced some classical combinatorial algorithms on which we will base the design of our SWP. We have reviewed state of the art, both the definition and the formulations of the TSP with its techniques of constructive heuristics. We also analysed the $JSSP$, which despite being an algorithm designed for factories, can be used to model combinatorial planning problems and finally, the VRP.

To summarise, we observed that even with the best restrictions, heuristics or programming techniques, depending on the size of the data considerably high, the best TSP, $JSSP$ or VRP requires a very high computational cost for classical computing and would continue to approach an exponential cost. When the number of the input increases, any polynomial algorithm is more efficient than any exponential [15]. Another positive feature of polynomial algorithms is that, in a sense, they take better advantage of technological advances.

In these cases, another approach would be needed, such as using the power of quantum computing to solve the problem of this magnitude.

Now we have to relate these classical algorithms with the usual concepts that can be of great help in the development of this thesis.

After: In the summary of section 2. We emphasize the problem of qubits/variable numbers so that the reader sees our motivation.

Summary In this section, we have introduced some classical combinatorial algorithms on which we will base the design of our SWP. We have reviewed state of the art, both the definition and the formulations of the TSP with its techniques of constructive heuristics. We also analysed the $JSSP$, which despite being an algorithm designed for factories, can be used to model combinatorial planning problems and finally, the VRP. We have also realized that since we want to implement this SWP with the VRPTW, we will need to define a strategy since the number of qubits of the VRPTW is proportional to N^4, which makes it intractable to implement in a gate-based quantum computer.

To summarise, we observed that even with the best restrictions, heuristics or programming techniques, depending on the size of the data considerably high, the best TSP, $JSSP$ or VRP requires a very high computational cost for classical computing and would continue to approach an exponential cost. When the number of the input increases, any polynomial algorithm is more efficient than any exponential [15]. Another positive feature of polynomial algorithms is that, in a sense, they take better advantage of technological advances.

In these cases, another approach would be needed, such as using the power of quantum computing to solve the problem of this magnitude.

Now we have to relate these classical algorithms with the usual concepts that can be of great help in the development of this thesis.

Before:
Section 3.4 Hamiltonian of a TSP
These are encoded in the Hamiltonian:

$$H_A = A\sum_{v=1}^{n}(1-\sum_{j=1}^{N}x_{v,j})^2 + A\sum_{j=1}^{n}(1-\sum_{v=1}^{N}x_{v,j})^2 + A\sum_{(u,v)\notin E}\sum_{j=1}^{N}x_{u,j}x_{v,j+1}. \tag{18}$$

After: We have set all limits to N instead of having some at n.
Section 3.4 Hamiltonian of a TSP
These are encoded in the Hamiltonian:

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Before:
Section 3.5 The Hamiltonian of a VRP
We can write the Hamiltonian of the vehicle routing problem defined by the sum of (22) and (23):

$$\begin{aligned} H_A = {} & A\sum_{i=1}^{n}\left(1-\sum_{j\in\delta(i)^+}^{N}x_{i,j}\right)^2 + A\sum_{i=1}^{n}\left(1-\sum_{j\in\delta(i)^-}^{N}x_{ji}\right)^2 + A\left(k-\sum_{i\in\delta(0)^+}^{N}x_{0,i}\right)^2 \\ & + A\left(k-\sum_{j\in\delta(0)^+}^{N}x_{j,0}\right)^2. \end{aligned} \tag{20}$$

$$H_B = B\sum_{ij\in E}W_{ij}x_{i,j}. \tag{21}$$

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Section 3.5 The Hamiltonian of a VRP
We can write the Hamiltonian of the vehicle routing problem defined by the sum of (22) and (23):

$$\begin{aligned} H_A = {} & A\sum_{i=1}^{N}\left(1-\sum_{j\in\delta(i)^+}^{N}x_{i,j}\right)^2 + A\sum_{i=1}^{N}\left(1-\sum_{j\in\delta(i)^-}^{N}x_{ji}\right)^2 + A\left(K-\sum_{i\in\delta(0)^+}^{N}x_{0,i}\right)^2 \\ & + A\left(K-\sum_{j\in\delta(0)^+}^{N}x_{j,0}\right)^2. \end{aligned} \tag{22}$$

$$H_B = B \sum_{ij \in E}^{N} W_{ij} x_{i,j}. \tag{23}$$

Before:
Section 4.4.1: The Objective function, decision variables and the constraints If these options were not given, the following restrictions (26) and (27) would be established:

$$\sum_{i=0 i \neq j}^{n} x_{ij} \leq 1, \tag{24}$$

$$\sum_{j=0 i \neq j}^{n} a_{ij} x_{ij} \leq b_i. \tag{25}$$

After: We have set all limits to N instead of having some at n.
Section 4.4.1: The Objective function, decision variables and the constraints

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$$\sum_{i=0 \ i \neq j}^{N} x_{ij} \leq 1, \tag{26}$$

$$\sum_{j=0 \ i \neq j}^{N} a_{ij} x_{ij} \leq b_i. \tag{27}$$

Before:
Finally, the last limitation (29) forces a single road to cover all the cities, and it is not two or more disjoint roads that include all the towns together.

$$u_i - u_j + n x_{ij} \leq n - 1. \tag{28}$$

After: We have set all limits to N instead of having some at n.
Finally, the last limitation (29) forces a single road to cover all the cities, and it is not two or more disjoint roads that include all the towns together.

$$u_i - u_j + N x_{ij} \leq N - 1. \tag{29}$$

Before:
Section 4.2.2: Formulation of linear programming of binary integers
Let us introduce a *linear programming of binary integers* as follows: If $z_1 z_2 z_3 \dots z_n$ are N binary variables, which are ordered in a vector z, what is the most substantial value of cx, for some vector c, given a constraint?

$$Sx = b. \tag{30}$$

From (35) with S an $m \times N$ matrix and b a vector with m components, it is known that the resolution of this equation has an NP-hard complexity, with a corresponding NP-complete decision problem. As discussed above, almost most daily challenges are combinatorial optimisation problems,

and many of them can be posed as ILP [33]. In our case, a social worker must maximise visits to a home patient, given the regulatory restrictions of her/his contract.

Let $H = H_A + H_B$ be the Hamiltonian (mathematical and physical model introduced above) defined by (36).

$$H_A = A\sum_{j=1}^{m}\left[b_j - \sum_{i=1}^{N} S_{ji}x_i\right]^2. \tag{31}$$

With $A \in R^+$. The ground states of $H_A = 0$ enforce the constraint that $Sx = b$. Then you get that

$$H_B = -B\sum_{i=1}^{N} C_i x_i. \tag{32}$$

With $A \gg B$ and B is a positive constant.

To find restrictions on the required A/B ratio, we can proceed similarly as before. In many cases, for simplicity, it is assumed that the constraint of the equation $Sx = b$ can be satisfied with a selection of x. For such a choice, the most substantial possible value of $-\Delta H_B$ is, in principle, constraint limits, where:

$$C = \sum_{i=1}^{N} max(Ci, 0). \tag{33}$$

The smallest possible value of ΔH_A is related to the properties of the matrix S and would occur if only a single constraint were violated, and that constraint was broken by the least amount possible, given by (39)

$$S \equiv \min_{\sigma_i \,\epsilon 0,1,j} \left(\max\left[1, \frac{1}{2}\sum_{i}(-1)^{\sigma_i} S_{ji}\right]\right). \tag{34}$$

This limit could be improved if more specific properties of S and b are known.

It can be concluded that if the coefficients C_i and S_{ji} are integers $O(1)$, we have that $C \leq N$ $\max(C_i)$ and $S \geq 1$, so it is concluded that A/B.

After: We have set all limits to N instead of having some at n. We have also put some parentheses to make it easier to read. We also put C_{ij} in lowercase.

Section 4.2.2: Formulation of linear programming of binary integers

Let us introduce a *linear programming of binary integers* as follows: If $z_1, z_2, z_3, \ldots z_N$ are N binary variables, which are ordered in a vector z, what is the most substantial value of $c \cdot z$, for some vector c, given a constraint?

$$Sz = b. \tag{35}$$

From (35) with S an $m \times N$ matrix and b a vector with m components, it is known that the resolution of this equation has an NP-hard complexity, with a corresponding NP-complete decision problem. As discussed above, almost most daily challenges are combinatorial optimisation problems, and in many cases, the framework use to model these problems is the ILP [33]. In our case, a social worker must maximise visits to a home patient, given the regulatory restrictions of her/his contract.

Let $H = H_A + H_B$ be the Hamiltonian (mathematical and physical model introduced above) defined by (36).

$$H_A = A\sum_{j=1}^{m}\left[b_j - \sum_{i=1}^{N} S_{ji}z_i\right]^2. \tag{36}$$

With $A \in R^+$. The ground states of $H_A = 0$ enforce the constraint that $Sz = b$. Then you get that

$$H_B = -B\sum_{i=1}^{N} c_i z_i. \tag{37}$$

With $A \gg B$ and B is a positive constant.

To find restrictions on the required A/B ratio, Let us proceed as follow. It is assumed that the constraint of the equation $Sz = b$ can be satisfied with a selection of z. Taking this in account, the most meaningful possible value of $-\Delta H_B = BC$ is shown as the constraint limits where:

$$C = \sum_{i=1}^{N} \max(c_i, 0). \tag{38}$$

One way of adjusting the Lagrange multiplier is given as described as the following. The lowest value of ΔH_A is leveraged on the properties of the matrix S and would occur if only a single constraint were violated. That constraint was broken by the least amount possible, given by (39).

$$S \equiv \min_{\sigma_i \in \{0,1\}, j}\left(\max\left[1, \frac{1}{2}\sum_i (-1)^{\sigma_i} S_{ji}\right]\right). \tag{39}$$

This limit could be improved if more specific properties of S and b are known.

It can be concluded that if the coefficients c_i and S_{ji} are integers $O(1)$, we have that $C \leq N \max(c_i)$ and $S \geq 1$, so it is concluded that $A/B \geq N$.

Before:
Section 4.3.2: Change of variables to simplify the quadratic formulation

In some cases, to simplify the objective function and therefore simplify the programming of the algorithm, it is required to make some variable changes (see Fig. (2)). This contribution is analysed below.

Next, the change of variables is studied to simplify quadratic programming. These variable changes and some linear algebra tricks will help with quantum programming.

When a variable change is made for any matrix $P \in R^{nxn}\varepsilon$ coordinates to B coordinates, it is to make the quadratic function easier.

$$\overrightarrow{x} = P\overrightarrow{y} \leftrightarrow \overrightarrow{y}P^{-1}\overrightarrow{x} \leftrightarrow [\overrightarrow{y}]_B = [\overrightarrow{x}]_\varepsilon. \tag{40}$$

The idea is:

$$\overrightarrow{x}^T Ax = (P\overrightarrow{y})^T A (P\overrightarrow{y}) = \overrightarrow{y}^T P^T AP\overrightarrow{y} = \overrightarrow{y}^T \left(P^T AP\right)\overrightarrow{y} = \overrightarrow{y}^T (D)\overrightarrow{y}. \tag{41}$$

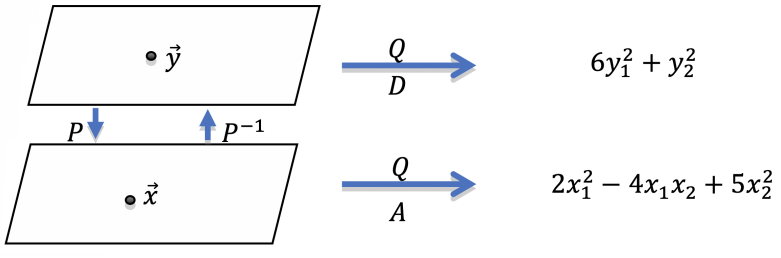

Figure 1: Variable change to simplify quadratic programming

Given the quadratic function $Q(x) = 2x_1^2 - 4x_1x_2 + 5x_2^2$ we will perceive what happens with the variable changes. Let us imagine for a moment that the function $Q(x)$ is the Ising Hamiltonian of the TSP.

Let us find the matrix A. $A = \begin{bmatrix} 2 & 5 \\ -2 & 5 \end{bmatrix}$ How is A found? Following this trick:

$$A = \begin{bmatrix} a & c \\ d & b \end{bmatrix}. \tag{42}$$

If we consider that of the function $Q(x)$, a is the constant that multiplies x_1^2 and b is the term that multiplies x_2^2; $a = 2$ and $a = 5$. So far, relatively easy. How are c and d determined? c and d are half the coefficient of x_1x_2. So, $c = \frac{4}{2} = d$. From here are the values and eigenvectors to be able to change the variables.

Given the characteristic polynomial $P(\lambda) = det(A - \lambda I_n)$ if we want to calculate the eigenvalues, the characteristic polynomial must be zero. This translates to $\det(A - \lambda I_n) = 0$, where I_n is the identity matrix of rank n and λ the eigenvalue. Mathematically speaking, if we want the characteristic polynomial of matrix A to be null, the following linear equation must be solved. The characteristic polynomial is of rank n, and its roots are the eigenvalues of matrix A. Since in our case matrix A is of rank 2, it will not be necessary to apply the Laplace expansion formula. Starting from a square matrix of degree n.

$$\det(A - \lambda I_n) = 0. \tag{43}$$

According to Laplace's theorem, the value of its determinant is equal to the sum of the products of the elements of a row or column by their attachments, thus taking any row f, the determinant is:

$$\det(P) = \sum_{j=1}^{n} a_{f,j} P_{f,j}. \tag{44}$$

And taking a column c, it will be:

$$\det(P) = \sum_{i=1}^{n} a_{i,c} P_{i,c}. \tag{45}$$

Solving the equation of the characteristic polynomial we get:

$$\det \begin{pmatrix} 2-\lambda & -2 \\ -2 & 5-\lambda \end{pmatrix} = 0. \tag{46}$$

Since it is a rank two matrix, the calculation of the determinant is direct and is shown through the following quadratic expression:

$$\lambda^2 - 7\lambda + 6 = 0. \tag{47}$$

Where the roots of the equation are $\lambda_1 = 1$ and $\lambda_2 = 6$. If the eigenvectors are now calculated to matrix A , this definition is fulfilled.

$$\exists v \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} \neq 0 / \exists \lambda \in C / A \cdot v = \lambda \cdot v. \tag{48}$$

Where λ is the eigenvalue and v is the eigenvector. And, if this definition is applied, it arrives at (65)

$$\begin{bmatrix} 2 & 5 \\ -2 & 5 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{49}$$

With this expression $-2x_1 = x_2$, we can find the two eigenvectors associated with matrix A.

$$v_1 \begin{pmatrix} 1 \\ -2 \end{pmatrix} and\ v_2 \begin{pmatrix} 2 \\ 1 \end{pmatrix}. \tag{50}$$

Once this point has been reached, if the quadratic form is rewritten, the reader can understand how simple it is and, consequently, its resolution or programming will also be more straightforward.

$$P(y) = \lambda_1 y_1^2 + \lambda_2 y_2^2. \tag{51}$$

If we remember that we came from the expression $Q(x) = 2x_1^2 - 4x_1x_2 + 5x_2^2$, we can find the matrix P.

$$P = \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}. \tag{52}$$

If the matrix P is normalized, the following expression is reached,

$$P = \frac{1}{dist} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}. \tag{53}$$

With $dist = \sqrt{1^2 + -2^2}$ as the distance.

$$P = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}. \tag{54}$$

Retrieving the expression, $A = PDP^T$ takes us to $D = P^T AP$, where D is the following matrix:

$$D = \begin{bmatrix} 6 & 0 \\ 0 & 1 \end{bmatrix}. \tag{55}$$

These variable changes help simplify the objective function by undoing the crossed variables.

After: We have rewritten a paragraph to understand the text, given the importance of developing this idea during this thesis. We have also rewritten a mathematical expression to make it easier to read.

Section 4.3.2: Change of variables to simplify the quadratic formulation
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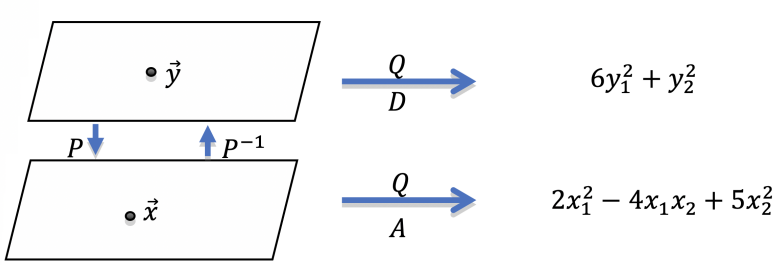

Figure 2: Variable change to simplify quadratic programming

Next, the change of variables is studied to simplify quadratic programming. These variable changes and linear algebra tricks will help model our problem into "quantum" programming.

The matrix that defines an arbitrary quadratic problem can be expressed as a symmetric matrix A. Because it is symmetric, it will be diagonalizable. That is, there will be an invertible matrix P and another diagonal D such that:

$$A = PDP^{-1}. \tag{56}$$

The matrix P acts as a base change, and if A represents the quadratic problem in the initial base, D will define the problem for the new base. Said matrix D drastically simplifies the formulation and, therefore, the computation.

Given the quadratic function $Q(x) = 2x_1^2 - 4x_1x_2 + 5x_2^2$ we will perceive what happens with the variable changes. Let us imagine for a moment that the function $Q(x)$ is the Ising Hamiltonian of the TSP.

Let us find the matrix A.

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And taking a column c, it will be:

$$\det(P) = \sum_{i=1}^{n} a_{i,c} P_{i,c}. \tag{61}$$

Returning to our case, solving the equation of the characteristic polynomial we get:

$$\det \begin{pmatrix} 2-\lambda & -2 \\ -2 & 5-\lambda \end{pmatrix} = 0. \tag{62}$$

Since it is a rank two matrix, the calculation of the determinant is direct and is shown through the following quadratic expression:

$$\lambda^2 - 7\lambda + 6 = 0. \tag{63}$$

Where the roots of the equation are $\lambda_1 = 1$ and $\lambda_2 = 6$. Now let us calculated the eingenvectors of the matrix A.

$$\exists\ v \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} \neq 0 \quad / \quad \exists\ \lambda \in \mathbf{C}: \quad A \cdot v = \lambda \cdot v. \tag{64}$$

Where λ is the eigenvalue, v is the eigenvector, and, if this definition is applied, it arrives at (65):

$$\begin{bmatrix} 2 & 5 \\ -2 & 5 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{65}$$

With this expression $-2x_1 = x_2$, we can find the two eigenvectors associated with matrix A.

$$v_1 = \begin{pmatrix} 1 \\ -2 \end{pmatrix} \text{ and } v_2 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}. \tag{66}$$

Once this point has been reached, if the quadratic form is rewritten, the reader can understand how simple it is and, consequently, its resolution or programming will also be more straightforward.

$$P(y) = \lambda_1 y_1^2 + \lambda_2 y_2^2. \tag{67}$$

Let us recall $Q(x) = 2x_1^2 - 4x_1x_2 + 5x_2^2$, and find the matrix P.

$$P = \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}. \tag{68}$$

If the matrix P is normalized, the following expression is reached,

$$P = \frac{1}{\text{dist}} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}. \tag{69}$$

With dist $=\sqrt{1^2 + (-2)^2}$ as the distance.

$$P = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}. \tag{70}$$

Retrieving the expression, $A = PDP^T$ takes us to $D = P^T AP$, where D is the following matrix:

$$D = \begin{bmatrix} 6 & 0 \\ 0 & 1 \end{bmatrix}. \tag{71}$$

These variable changes help simplify the objective function by undoing the crossed variables.

Before:
Chapter 5: Introduction Quantum Mechanics *Quantum mechanics* [32] is a theory that describes the physical properties of nature on an atomic scale.

The first revolution[18] of quantum mechanics is the basis of several advances to our modern society. Almost all modern electronics in the last 50 years have been based on the properties of quantum mechanics. Semiconductors such as diodes, transistors, integrated circuits, etc., have led to the considerable growth of electronics today.

Quantum mechanics, in addition to studying the motion of particles, also allows us to understand the properties of materials and their features to manufacture transistors. These are the basis of all modern electronics and the control system of millions of devices that we use today. However, in this thesis work, we focus on the second revolution of quantum mechanics, that is, in using the properties of quantum mechanics to empower computing. For this, we need to know how quantum information science is structured (4).

The *Quantum information science* also known as QIS, is the area of information science that depends on the effects of quantum mechanics. Figure (4) breaks down the subtasks of quantum information science.

During the last decades, the scientific community has dedicated a lot of time and has provided considerable resources to QIS [42]. As a result of this delivery, improvements have been achieved in the scientific advances that we see reflected in publications, conferences, and concrete solutions such as D-Wave, IBMQ, Xanadu, etc. Quantum computing, in particular, and quantum information science is a hot topic because of its novelty and the promising developments it predicts.

In this thesis work, all the postulates of quantum mechanics on which we rely are referenced by [24].

0.1 Moore Law

Another aspect to consider understanding the importance of the properties of quantum mechanics and thus empower computing is *Moore's law*, which states that the number of transistors that can be integrated into a single chip doubles every 18 months. This process Figure (14) leads to a doubling of the memory and a doubling of the calculation speed. Therefore, it is expected that the size of the characteristic of the wafer (thin plate of semiconductor material) will be less than 10nm during this year (2020). At this point, the individual properties of atoms and electrons would begin to dominate, so Moore's law would no longer be valid. Therefore, the demands of the miniaturization of electronics will eventually bring us to the point where quantum effects become important[42].

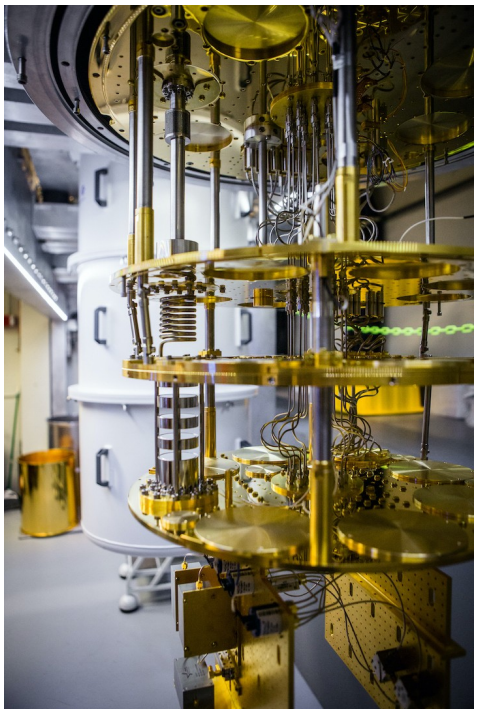

Figure 3: TBluefors dilution refrigerators used in the MIT Engineering Quantum Systems group to operate superconducting qubits at near-zero temperatures [39]

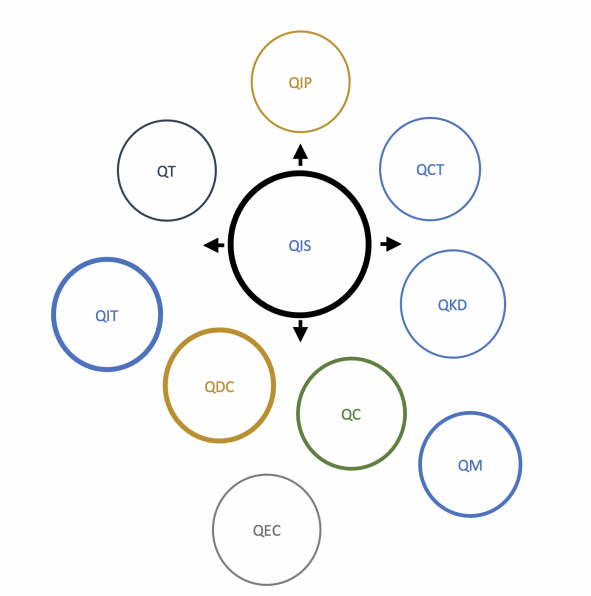

Figure 4: The areas of quantum information science (QIS)

Because Moore's law will stop working today, there are even more reasons for the scientific community to resort to QIP much sooner than it seems [42][17]. On the other hand, multi-core architecture

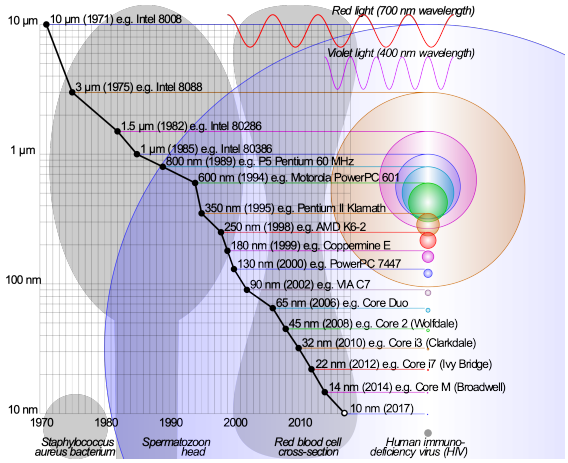

Figure 5: Moore law Roadmap: Quantum Computing Stack Exchange [29]

is becoming a practical approach; computational speed improvement can be achieved even without reducing the size of the feature by parallelization.

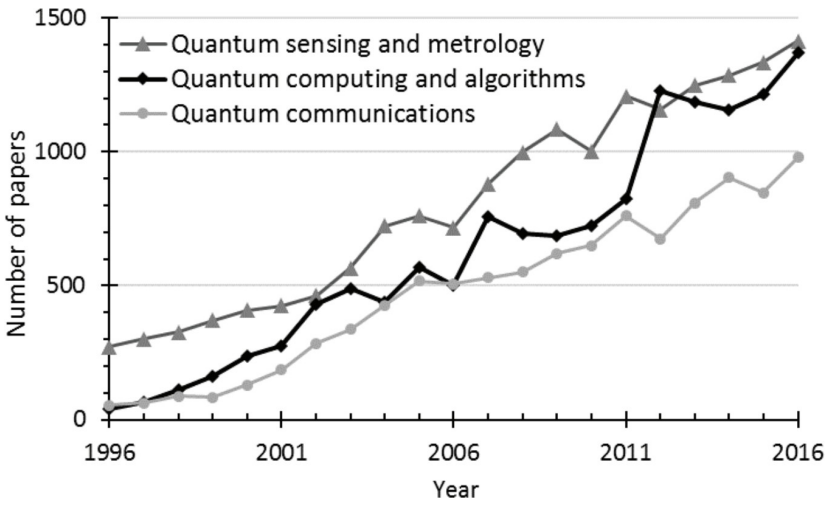

Figure 6: The number of research papers published per year in quantum computing and technologies [35]

0.1.1 State of the Quantum Technologies

Another point to highlight is the fact that, despite the intensive development of quantum algorithms, the number of available quantum algorithms is still small (Fig. (15)) compared to that of classical algorithms basically because the current quantum gates are only several tens of quantum bits (qubits), which is relatively low for any significant quantum computing operation[30].

This delay was partial until very recently, and it was believed that quantum computing would never or seldom come true. However, the latest advances in the different techniques (D-Wave, IBMQ, Xanadu, ...) of quantum gate implementations, as well as the proof of the precision threshold theorem [21], give rise to optimism (Figures (16) and (17)) that quantum computers (13) to large-scale could

become a reality quite soon [30]. We can also appreciate (Figures (18) and (19)) the metrics and milestones to help monitor the development of quantum computing and the companies and startups involved in the 2018 quantum computing ecosystem.

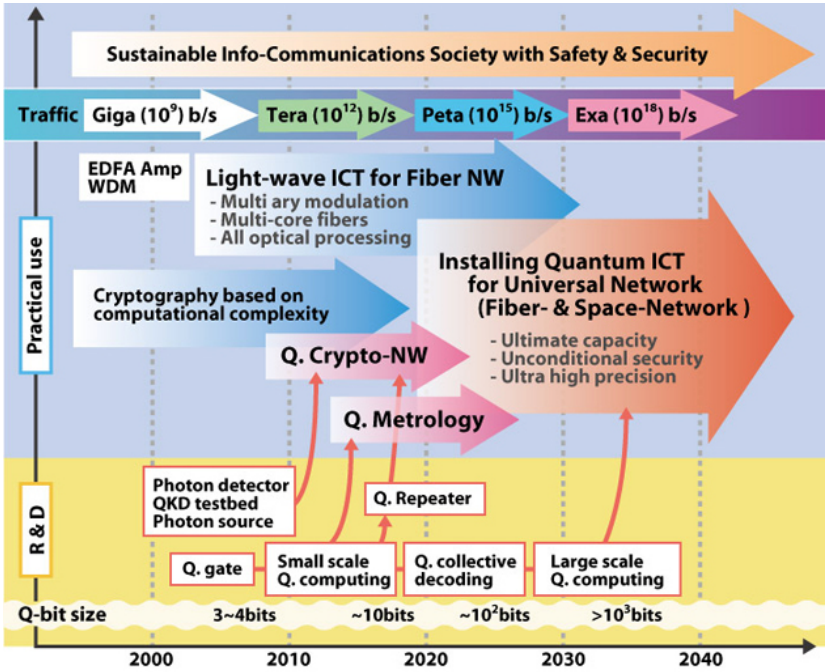

Figure 7: Quantum Computing is becoming the talk of the town [1]

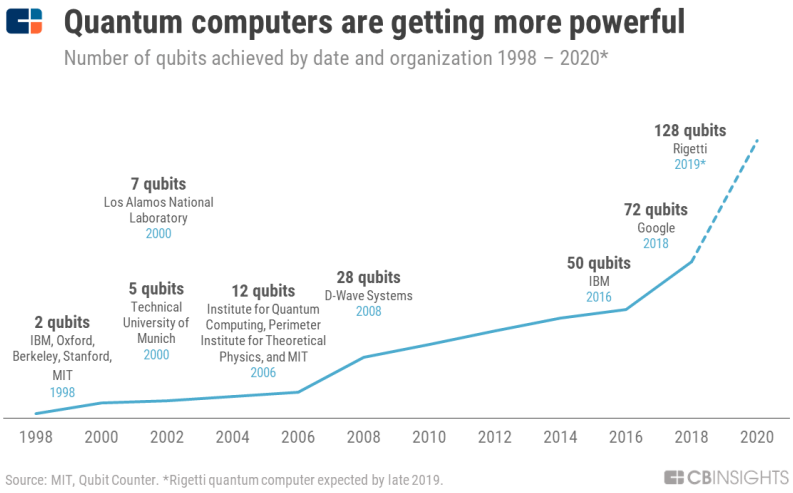

Figure 8: The number of qubits achieved by date and organization. Roadmap by MIT [20]

One of the most significant problems that QIS faces is the physical deployment issues. There are many potential technologies, such as nuclear magnetic resonance (NMR), ion traps, quantum cavity electrodynamics, photonics, quantum dots, and superconducting technologies, to name just a few. However, it is not clear which technology will prevail. For example, Xanadu (photonics) technology seems to be most likely for quantum teleportation[19][4].

Right now, there is a big battle going on between the significant manufacturers of quantum computers to achieve the highest number of qubits and 'impose' their scalability plan. In knowing who will be able to define the standard and, above all, get the quantum supremacy [3].

0.2 Noisy Intermediate-Scale Quantum

The *Noisy Intermediate-Scale Quantum* era known as (NISQ) era [30], is defined *as the era leading quantum processors to contain about 50 to a few hundred qubits. Still, it is not advanced enough to reach fault tolerance nor large enough to profit sustainably from quantum supremacy. It is used to describe the current state of the art in the fabrication of quantum processors.*

The real problem of this era is related to *decoherence* [8]. *Decoherence* is associated with the interaction of qubits with environments that blur the fragile states of overlap (entanglement). This results in the introduction of random errors due to the environment. However, there are quantum error correction techniques known as the *Quantum Error Correction Concept* (QECC)[32][9]. One of the powerful applications of quantum error correction is based on the protection of quantum information, as it is dynamically subjected to quantum computing. Imperfect quantum gates affect quantum computing by introducing errors into the computed data. Also, imperfect control gates add errors into the processed sequences as incorrect operations can be applied. However, this imperfection gives rise to exciting computing techniques and algorithms based on variational calculations. This opens up a world of possibility to the era of *Quantum Machine Learning* (QML) [5][28][34]. The objective of QECC is to deal with errors introduced by quantum channels and those presented by (imperfect) quantum gates during the encoding and decoding process. Because of this, the reliability of the data processed by quantum computers depends on the probability of error per gate being below a certain threshold known as the precision threshold theorem. This is what NISQ defines as. *'Noisy'* because we don't have enough qubits leftover for error correction, so we'll have to use the imperfect qubits directly on the physical layer and *'Intermediate-Scale'* due to its reduced qubit (but not too small).
To understand quantum mechanics, we have to appreciate its postulates. These postulates provide a connection between the physical world and the mathematical formalism of quantum mechanics. It is important to emphasize that it is unnecessary to understand quantum mechanics in detail to know how to make a program on a quantum computer. But if we want to make intelligent and efficient algorithms, it is more than recommended to understand the fundamentals of quantum mechanics. The analogy to understand what we mean is the following: To program we can do it in *PhP*, and *python*, high-level languages, but we can also program in *C* or in *assembler* (machine language). If we want to be experts or make efficient algorithms, it would be useful to know the machine's architecture and to program in the machine language.

0.3 Postulate 1

The *postulate 1* is defined as *associated with any isolated physical system is a complex vector space with an internal product (Hilbert space) known as the state space of the system. The system is fully described by its state vector, which is a unit vector in the state space of the system.*

This postulate explains the space of the quantum state and describes the area where quantum mechanics takes place. This area is nothing more than linear algebra in Hilbert vector space [41]. It

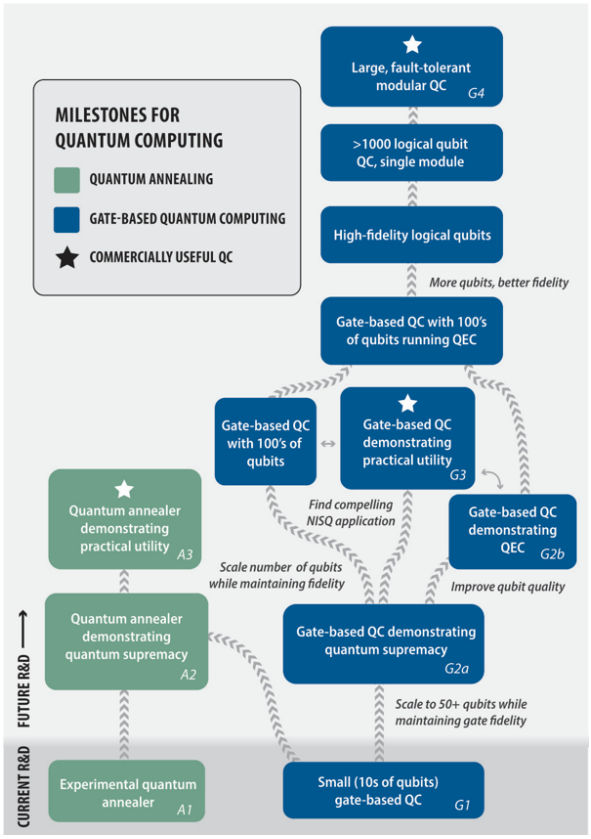

Figure 9: Metrics and milestones to help monitor the development of quantum computing. Roadmap by MIT [35]

is essential to know that, given a physical system, quantum mechanics does not tell us what the state space of that system is, nor can it tell us what the system's state vector is. Therefore, it is imperative to have this clear postulate. In other term, what we mean is that it is challenging to know the state of a quantum system at all times.

Let's consider that the simplest quantum mechanical system is the qubit. A qubit has a two-dimensional state space $|0\rangle$ and $|1\rangle$ that form an orthonormal basis for that state space. Then you can write an arbitrary state vector in the state space.

$$|\psi\rangle = a|0\rangle + b|1\rangle. \tag{72}$$

Where a and b are complex numbers. The condition that $|\psi\rangle$ is a unit vector is given by $\langle\psi|\psi\rangle = 1$, is therefore equivalent to $|a|^2 + |b|^2 = 1$. The term $\langle\psi|\psi\rangle = 1$ is known as the normalization condition for state vectors.

The way a qubit differs from a classic bit is that there are overlaps of these two states, in the form $a|0\rangle + b|1\rangle$, where it is not possible to say that the qubit is definitely in the state $|0\rangle$, or definitely in the state $|1\rangle$. In other words, what we mean is that the quantum state is a linear combination of the components a and b.

If we had a system of more than one qubit, the expression of the quantum state would be of the form $\sum_i a_i|\psi_i\rangle$, and we would have a system with the superposition of the states $|\psi_i\rangle$ and of amplitude a_i for the state $|\psi_i\rangle$.

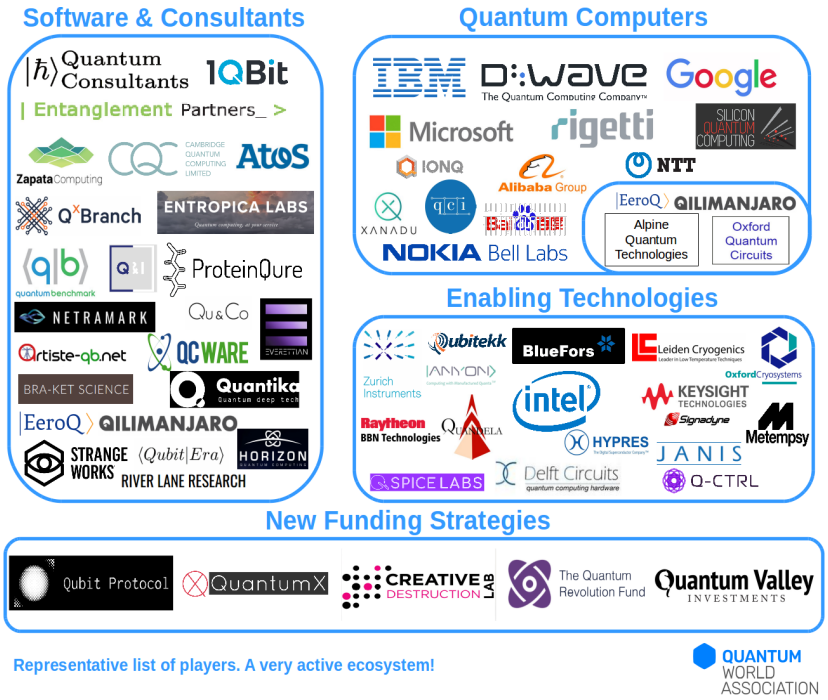

Figure 10: Companies and startups involved in the 2018 quantum computing ecosystem. Roadmap by Quantum World Association

0.4 Postulate 2

The *postulate 2* is defined as *a unitary transformation describes the evolution of a closed quantum system. That is, the state* $|\psi\rangle$ *of the system at the time* t_1 *is related to the state* $|\psi^{'}\rangle$ *of the system at the time* t_2 *by a unit operator* U *that depends only on times* t_1 *and* t_2, $|\psi^{'}\rangle = U|\psi\rangle$. *This postulate gives a standard for describing quantum state changes over time.*

From Ref. [25] we know that quantum mechanics does not tell us the state space or quantum state of a particular quantum system; it also does not tell us which unit operators U describe real-world quantum dynamics. On the other hand, quantum mechanics assures us that the evolution of any closed quantum system can be described in this way.

$$|\psi^{'}\rangle = U|\psi\rangle. \tag{73}$$

In a way, we are saying that if we want to describe an n qubit quantum system subject to time evolution, we must calculate its unit operators U. The challenge would be to find such unit operators. Quantum gates are somehow the operators that act on quantum states. This postulate is very interesting and requires that the quantum system be closed [32][31]. Moreover, various derivatives emerge from this postulate.

0.4.1 Postulate 2'

The *postulate 2'* is defined as *the time evolution of the state of a closed quantum system is described by the Schrödinger equation* (105).

$$i\hbar\frac{\delta|\psi\rangle}{\delta t} = H|\psi\rangle. \tag{74}$$

Where $\hbar$ is Planck's constant and H is a fixed hermitian operator known as the Hamiltonian of the closed system [32].

In some way, we can say that if we know the Hamiltonian of a system, then we understand its dynamics completely. This concept is precious for modelling the system, and we will use it a lot throughout our thesis.

During the 20th century, much of the scientific (physical) community has been dedicated to discovering the Hamiltonian of any quantum system. And the conclusion they reached is that, in general, finding out that the Hamiltonian necessary to describe a particular physical system is challenging.

The Hamiltonian is a Hermitian operator that allows us to make its spectral decomposition with eigenvalues of energy E and the normalized eigenvectors corresponding to energy E as eigenstates $|E\rangle$.

$$|H\rangle \ = \sum_{E} E|E\rangle\langle E|, \tag{75}$$

$$|E\rangle = exp(-i\frac{Et}{\hbar})|E\rangle. \tag{76}$$

The lowest energy is known as the ground state energy for the system, and the corresponding energy proper state (or adequate space or steady-state) is known as the ground state.

$$|\psi(t_2)\rangle = exp[\frac{-iH(t_1-t_2)}{\hbar}]|\psi(t_1)\rangle = U(t_1-t_2)|\psi(t_1)\rangle. \tag{77}$$

Where we define

$$U(t_1-t_2) \equiv exp[\frac{-iH(t_1-t_2)}{\hbar}]. \tag{78}$$

This interpretation is compelling and extremely useful since it is shown that any unitary operator U can be written in the form (110) tanking $\hbar = 1$ and $t_2 = 0$ the equation comes out to be (108)

$$U = exp(-iK). \tag{79}$$

With K, a Hermitian operator.

0.5 Postulate 3

The *postulate 3* is defined as *quantum measurements are described using a M_m collection of measurement operators. These are the operators that operate in the state space of the system being measured. The m index refers to the measurement results in the experiment. If the state of the quantum system is $|\psi\rangle$ immediately before the measurement, the probability that the result m will occur is given by the equation* (111).

$$p(m) = \langle\psi|M_m^T M_m|\psi\rangle. \tag{80}$$

The state of the system after the measurement is (112).

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|M_m^T M_m|\psi\rangle}}. \tag{81}$$

And, the measurement operator satisfies the completeness equation [32] that is given by the following equation (113) for all the values of the quantum state $|\psi\rangle$.

$$\sum_m M_m^T M_m = Ip(m) = \langle\psi|M_m^T M_m|\psi\rangle = 1. \tag{82}$$

The value of the measure is the probability described by $|a|^2 + |b|^2 = 1$.

If we want to make the different M_m observations, the operations we would be doing are the following:

$$M_0 = |0\rangle\langle 0| = \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}. \tag{83}$$

$$M_1 = |1\rangle\langle 1| = \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} = \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}. \tag{84}$$

With $\langle\psi|$ the conjugate of $|\psi\rangle$, represented by $|\psi\rangle = \langle\psi|^T$

$$M_0|0\rangle = |0\rangle\langle 0|0\rangle = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\0\end{bmatrix} = |0\rangle. \tag{85}$$

$$M_0|1\rangle = |0\rangle\langle 0|1\rangle = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix} = 0. \tag{86}$$

knowing that $|0\rangle\perp|1\rangle$, $\langle 0|1\rangle$ disappears; It is cancelled. If we project on any state, we will have:

$$M_0|\psi\rangle = |0\rangle\langle 0|\psi\rangle = |0\rangle a|0\rangle + b|1\rangle = a|0\rangle. \tag{87}$$

We can generalize (116): let M_0, let i be any qubit and let $|\psi\rangle$ be a multi-state of qubits, the measurement or the projection on the state $|0\rangle$ can be expressed as:

$$Tr\left[|\psi\rangle\langle\psi|M_0^i\right]. \tag{88}$$

If the qubit i is measured in the state $|0\rangle$, then the system will be in the state expressed by (120).

$$\frac{M_0^i|\psi\rangle}{\|M_0^i|\psi\rangle\|_2}. \tag{89}$$

Another way to get the result of the measurements is to remember that the measurement operator is Hermitian; this translates to $M_0^2 = M_0$ the same for $M_1^2 = M_1$. Also remembering that the relationship of completeness obeys the equation $I = M_0^T M_0 + M_1^T M_1 = M_0 + M_1$.

One of the crucial applications of (0.13) is to distinguish quantum states. We recall that since the quantum system must be closed (0.11)), getting to find out the quantum states represents a titanic and less intuitive task as in classical computing.

To clarify what we have just advanced, we will demonstrate the absurdity. We consider two non-orthogonal quantum states $|\psi_1\rangle$ and $|\psi_2\rangle$ and assume that the measurement is possible. If $|\psi_1\rangle$ and $|\psi_2\rangle$ are prepared, the measures (observations) will respond to the completeness (113) equations so that we can write:

$$\langle\psi_1|M_1|\psi_1\rangle = 1; \langle\psi_2|M_2|\psi_2\rangle = 1. \tag{90}$$

Knowing that $\sum_i M_i = I$ therefore $\langle\psi_1|M_1|\psi_1\rangle = 1$ and must $\langle\psi_1|M_2|\psi_1\rangle = 0$ and $\sqrt{M_2}|\psi\rangle = 0$. If we decompose $|\psi_2\rangle = \alpha|\psi_1\rangle + \beta|\varphi\rangle$ with $|\psi_1\rangle$ and $|\varphi\rangle$ they are orthonormal. This leads us to the fact that $|\alpha|^2 + |\beta|^2 = 1$ and that $|\beta| < 1$ while $|\psi_1\rangle$ and $|\psi_2\rangle$ are not orthonormal. With $\sqrt{M_2}|\psi\rangle = \beta\sqrt{M_2}|\varphi\rangle$. What contradicts completeness's equation (111).

$$\langle\psi_2|M_2|\psi_2\rangle = |\beta|^2<\varphi|M_2|\varphi\rangle \leq |\beta|^2 < 1. \tag{91}$$

Continuing with *postulate 3*, projective measurements form a particular case of it, being very useful and straightforward. Due to its simplicity, this measurement is the basis of many algorithms to know the observables.

A projective measurement is described by an observable, M, a Hermitian operator in the system's state space being observed. The observable has a spectral decomposition.

$$M = \sum_m mP_m. \tag{92}$$

where P_m is known as the projector in the proper space of M with the right value m. If we measure on the state $|\psi\rangle$, the probability of having the result m is

$$p(m) = \langle\psi|P_m|\psi\rangle. \tag{93}$$

so, the quantum state just after the measurement will be:

$$\frac{P_m|\psi\rangle}{\sqrt{\langle\psi|P_m|\psi\rangle}}. \tag{94}$$

Otherwise, what we are saying is that $\langle M\rangle = \langle\psi|M|\psi\rangle$. We can generalize this formula with the mean and variance:

$$[\Delta M]^2 = \langle(M - \langle M\rangle)^2\rangle = \langle M^2\rangle - \langle M\rangle^2 \Delta M = \sqrt{\langle M^2\rangle - \langle M\rangle^2}. \tag{62}$$

This formula (62) is the basis of Heisenberg's uncertainty principle [32]. The important thing about the Heisenberg principle is that we cannot simultaneously measure/know the position and velocity of the electron (a particle). Therefore, it is impossible to determine its trajectory. We are somehow telling ourselves that measurement is destructive (but this is not the basis of Heisenberg's principle) because the position and velocity of the particle are in overlap. Measuring one collapses the wave function and destroys the other component/s.

A mathematical explanation can be described as follows. Suppose A and B are two Hermitian operators, and $|\psi\rangle$ is a quantum state. Suppose that $\langle\psi|AB|\psi\rangle = x + iy$, where x and y are real. Applying the switches and anti-switches to the Hermitian operators (matrices) A and B, we arrive at $\langle\psi[A, B]\psi\rangle = 2iy$ and $\langle\psi|\{A, B\}|\psi\rangle = 2x$. This implies that:

$$|\langle\psi|[A, B]|\psi\rangle|^2 + \langle\psi|\ A, B|\psi\rangle|^2 = 4|\langle\psi|AB|\psi\rangle|^2\ \ . \tag{95}$$

For the Cauchy-Schwarz inequality

$$|\langle\psi|AB|\psi\rangle|^2 \leq \langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle. \tag{96}$$

underestimating the negative term, we arrive at:

$$|\langle\psi|[A, B]|\psi\rangle|^2 \leq 4\langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle. \tag{97}$$

if we now consider two observables M_1 and M_2, and substitute $A = M_1 - \langle M_1\rangle$ and $B = M_2 - \langle M_2\rangle$ in the last equation, we obtain the Heisenberg uncertainty principle from the equation (129).

$$\Delta M_1 \Delta M_2 \geq \frac{\langle\psi[M_1, M_2]\psi\rangle}{2}. \tag{98}$$

The correct interpretation of the uncertainty principle is that if we prepare a large number of quantum systems in identical states, $|\psi\rangle$, and then make measurements of M_1 in some of those systems, and of M_2 in others, then the standard deviation ΔM_1 of the results of M_1 multiplied by the standard deviation ΔM_2 of the results of M_2 will satisfy the inequality $\Delta M_1 \Delta M_2 \geq \frac{\langle\psi[M_1, M_2]\psi\rangle}{2}$.

In the commutation relationship for the observable X coordinates and moment P is, $[X, P] = j\hbar$. If we introduce it in the equation above, we get to (130):

$$\langle \Delta X \rangle^2 \langle \Delta P \rangle^2 = \frac{\hbar^2}{4}. \tag{99}$$

We make a parenthesis to explain the behaviour of the phase-in quantum mechanics. We already know that quantum mechanics is defined in the complex vector space (Hilbert space). We also know that a vector representation of a vector (wave) can be described with its argument and angle. Besides, the phase as an operator applied to a quantum state in quantum mechanics does not change the quantum state.

Now, let us consider that the state $e^{i\theta}|\psi\rangle$, where $|\psi\rangle$, is a state vector and θ is a real number. We say that the state $e^{i\theta}|\psi\rangle$, is equal to $|\psi\rangle$ where the factor $e^{i\theta}$ is known with the global phase of the system [32][17]. This property is fascinating and useful when writing a quantum algorithm. Saving this operation entails a gain in time and computational cost.

Suppose we want to make the measurements of the observables M_m on the quantum state $e^{i\theta}|\psi\rangle$, with $|\psi\rangle$ the state vector. Then, the respective measurements will be given by the following equations:

$$\langle \psi | M_m | \psi \rangle \langle \psi | e^{-i\theta} M_m^T M_m e^{i\theta} | \psi \rangle = \langle \psi | M_m^T M_m | \psi \rangle. \tag{100}$$

We see that the global phase does not affect measures, but another phase does. This phase is known as the relative phase [17]. We will use an example to explain it. Let's consider two quantum states:

$$|\psi_1\rangle = a|0\rangle + b|1\rangle \quad \text{and} \quad |\psi_2\rangle = a|0\rangle - b|1\rangle. \tag{101}$$

We see that the state amplitude $|1\rangle$ of the first quantum state $|\psi_1\rangle$ is $+b$ and a, the state amplitude $|0\rangle$ of the second quantum state $|\psi_2\rangle$ is $-b$. We see that the only difference is the sign, not the amplitude. If two quantum states have the same amplitudes and differ exclusively by the phase (sign), this phase is known by the relative phase of the system. And generically, we can write it as follows $a = exp(i\theta)b$. This concept is fascinating and is the basis of quantum gates that will allow quantum computing.

0.6 Postulate 4

The *postulate 4* is defined as *the state-space of a composite physical system is the tensor product of the state spaces of the components of physical systems. Furthermore, if we have systems numbered from 1 to n, and the number of system i is prepared in the state $|\psi_i\rangle$, then the joint state of the total system is $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$.*

This postulate is the basis for creating the complex system of more than two qubits or quantum states. This postulate also allows us to define one of the most exciting and puzzling ideas associated with composite quantum systems: entanglement. Consider the two-qubit states $|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$, this state has the remarkable property that there are no unique qubit states $|a\rangle$ and $|b\rangle$ such that $|\psi\rangle = |a\rangle|b\rangle$. In other words, we say that $|\psi\rangle \neq |a\rangle|b\rangle$. This property is one of the reasons for the empowerment of quantum computing.

0.7 Postulate 5 and 6

In this thesis work, we are based on the postulates listed in this reference [24] *Quantum Computation and Quantum Information*, where postulate 5 (The temporal evolution of a system) of quantum mechanics [10] is contemplated like our postulate 2' (0.12.1) and the postulate 6 (commutation rules) of quantum mechanics that define the positional and momentum operators that satisfy the following commutation rules, they are treated as operators not like postulate.

0.8 Summary

This section's right conclusion highlights that these four postulates of quantum mechanics define how we can conceptualize and face a problem about quantum mechanics and its computation. The first postulate establishes the space for quantum mechanics by specifying how the state of an isolated quantum system should be described. The second postulate illuminates us on the dynamics of the closed quantum systems and its description through the Schrödinger equation and using the unitary evolution. In the third postulate, we are explained how to make the measurement describing the importance of the characteristics (restrictions) when extracting information (measuring) from our quantum systems. And finally, the fourth postulate reveals how we can create composite systems. One of the most shocking and interesting ideas of quantum mechanics is that we cannot directly observe the state vector and that it is in charge of deciphering the behaviour of any quantum system. Let's imagine that we want to know what position the cat is in (20). In a classic system, thinking

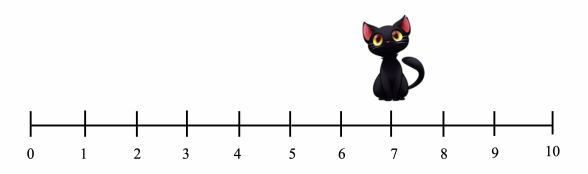

Figure 11: Observability of a classical system

about computing, the location (state vector) of the cat is given by the variable $x = 7$

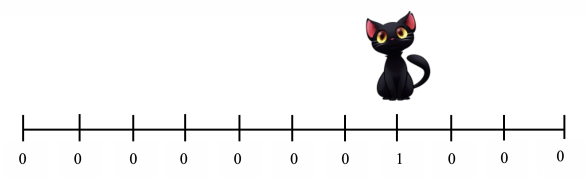

Figure 12: Observability of a quantum system

In a quantum system, the position (see figure (21)) of the cat is not so quickly known. In quantum, each element in the state vector contains the probability of finding the cat in a specific place. And it is represented by:

$$|x\rangle = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow \begin{array}{c} \text{Probability of} \\ \text{cat being at} \\ \text{position 7} \end{array}. \tag{102}$$

Classical physics, classical computation, and our intuition tell us that the fundamental properties of an object, such as energy, position, and velocity, are directly accessible to observation. However, these quantities no longer appear essential in quantum mechanics, depend on the state vector, and cannot be directly observed. Furthermore, merely observing a classical system does not necessarily

change the system's state; instead, for a quantum system, observation is an invasive procedure that generally changes the state of the system (the state vector).

After:

textbfChapter 5: Introduction Quantum Mechanics *Quantum mechanics* [32] is a theory that describes the physical properties of nature on an atomic scale.

This section will give a complete description of the basic postulates of quantum mechanics. These postulates are important to connect the physical world and the mathematical formalism of quantum mechanics. First of all, we will review the limitation faced by Moore's law. Then we will analyze the state of quantum technologies. Finally, and before focusing on the postulates of quantum mechanics, we will briefly introduce the era in which quantum computing finds itself.

The first revolution [18] of quantum mechanics is the basis of several advances to our modern society. Almost all modern electronics in the last 50 years have been based on the properties of quantum mechanics. Semiconductors such as diodes, transistors, integrated circuits, etc., have led to the considerable growth of electronics today.

Quantum mechanics, in addition to studying the motion of particles, also allows us to understand the properties of materials and their features to manufacture transistors. These are the basis of all modern electronics and the control system of millions of devices that we use today. However, in this thesis, we focus on the second revolution of quantum mechanics, that is, in using the properties of quantum mechanics to empower computing (13).

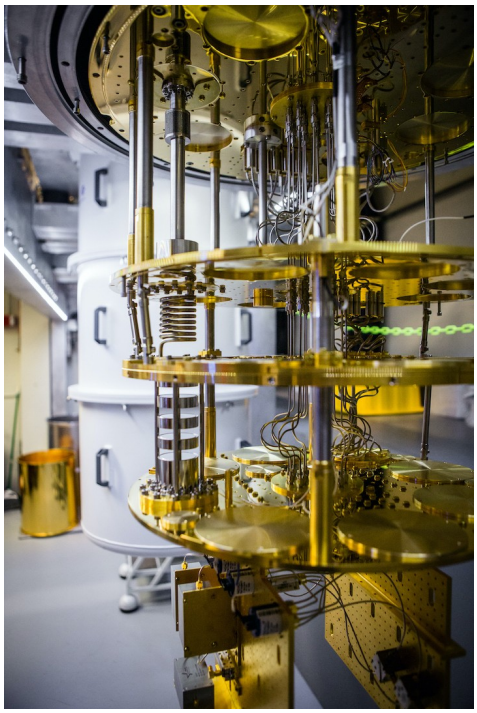

Figure 13: TBluefors dilution refrigerators used in the MIT Engineering Quantum Systems group to operate superconducting qubits at near-zero temperatures [39]

The *Quantum information science* also known as QIS, is the area of information science that depends on the effects of quantum mechanics. During the last decades, the scientific community has dedicated a lot of time and has provided considerable resources to QIS [42]. As a result of this delivery, improvements have been achieved in the scientific advances that we see reflected in publications,

conferences, and concrete solutions such as D-Wave, IBMQ, Xanadu, etc. Quantum computing, in particular, and quantum information science is a hot topic because of its novelty and the promising developments it predicts.

In this thesis work, all the postulates of quantum mechanics on which we rely are referenced by [24].

0.9 Moore Law

Another aspect to consider understanding the importance of the properties of quantum mechanics and thus empower computing is *Moore's law*, which states that the number of transistors that can be integrated into a single chip doubles every 18 months. This process Figure (14) leads to a doubling of the memory and a doubling of the calculation speed. Therefore, it is expected that the size of the characteristic of the wafer (thin plate of semiconductor material) will be less than 10nm during this year (2020). At this point, the individual properties of atoms and electrons would begin to dominate, so Moore's law would no longer be valid. Therefore, the demands of the miniaturisation of electronics will eventually bring us to the point where quantum effects become important [42].

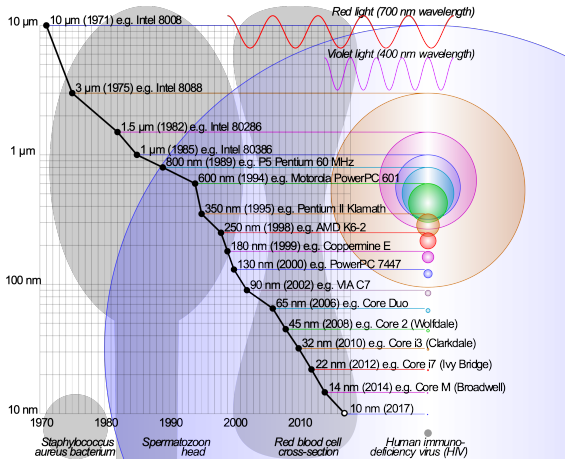

Figure 14: Moore law Roadmap: Quantum Computing Stack Exchange [29]

Because Moore's law will stop working today, there are even more reasons for the scientific community to resort to QIP much sooner than it seems [42, 17]. On the other hand, multi-core architecture is becoming a practical approach; computational speed improvement can be achieved even without reducing the size of the feature by parallelisation.

0.9.1 State of the Quantum Technologies

Another point to highlight is the fact that, despite the intensive development of quantum algorithms, the number of available quantum algorithms is still small (Fig. (15)) compared to that of classical algorithms basically because the current quantum gates are only several tens of quantum bits (qubits), which is relatively low for any significant quantum computing operation [30].

This delay was partial until very recently, and it was believed that quantum computing would never or seldom come true. However, the latest advances in the different techniques (D-Wave, IBMQ, Xanadu, ...) of quantum gate implementations, as well as the proof of the precision threshold theorem [21], give rise to optimism (Figures (16) and (17)) that quantum computers (13) to large-scale could

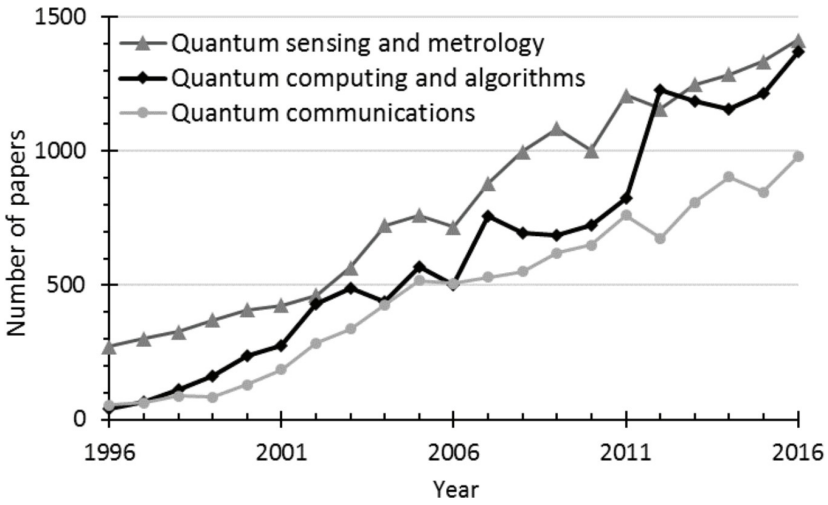

Figure 15: The number of research papers published per year in quantum computing and technologies [35]

become a reality quite soon [30]. We can also appreciate (Figures (18) and (19)) the metrics and milestones to help monitor the development of quantum computing and the companies and startups involved in the 2018 quantum computing ecosystem.

One of the most significant problems that QIS faces is the physical deployment issues. There are many potential technologies, such as nuclear magnetic resonance (NMR), ion traps, quantum cavity electrodynamics, photonics, quantum dots, and superconducting technologies, to name just a few.

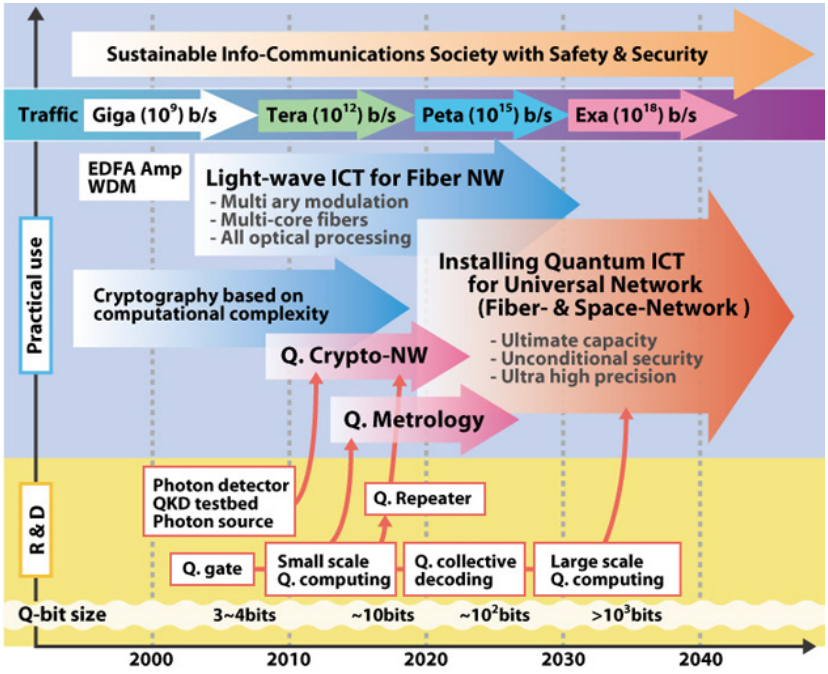

Figure 16: Quantum Computing is becoming the talk of the town [1]

However, it is not clear which technology will prevail. For example, Xanadu (photonics) technology seems to be most likely for quantum teleportation [**8715261**, 19].

Right now, there is a big battle going on between the significant manufacturers of quantum computers to achieve the highest number of qubits and 'impose' their scalability plan. In knowing who will be able to define the standard and, above all, get the quantum supremacy [3].

0.10 Noisy Intermediate-Scale Quantum

The *Noisy Intermediate-Scale Quantum* era known as (NISQ) era [30], is defined *as the era leading quantum processors to contain about 50 to a few hundred qubits. Still, it is not advanced enough to reach fault tolerance nor large enough to profit sustainably from quantum supremacy. It is used to describe the current state of the art in the fabrication of quantum processors.*

To summarise, the computers are challenging to achieve, and in the near term, there will NISQ computers with limited performance. To seize quantum computing during the NISQ era, algorithms with low resource demands and capable of returning approximate solutions are explored. In addition, quantum states cannot be indefinitely maintained over time, and the purely quantum properties are steadily lost during the execution of a quantum algorithm. Until the present time, the two greatest achievements are the double accomplishment of the so-called quantum supremacy, that is, using a quantum computer to solve a problem more efficiently and with better performance than any classical computer. This means that the devices in the NISQ era are not expected to be more powerful and change the world by themselves but rather to be an intermediate step towards a new generation of computers.

The real problem of this era is related to *decoherence* [8]. *Decoherence* is associated with the interaction of qubits with environments that blur the fragile states of overlap (entanglement). This results in the introduction of random errors due to the environment. However, there are quantum error correction techniques known as the *Quantum Error Correction Concept* (QECC) [32, 9]. One of the powerful applications of quantum error correction is based on the protection of quantum information, as it is dynamically subjected to quantum computing. Imperfect quantum gates affect quantum computing by introducing errors into the computed data. Also, imperfect control gates add errors into the processed sequences as incorrect operations can be applied. However, this imperfection gives

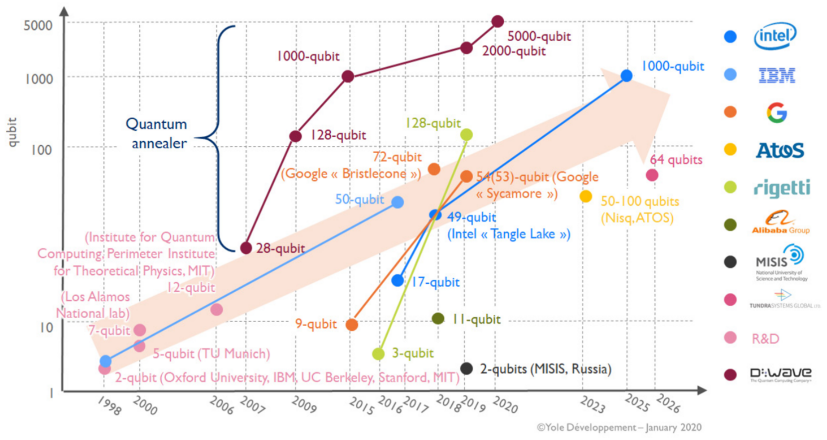

Figure 17: The number of qubits achieved by date and organisation. Roadmap by YOLE Development [**YOLED**]

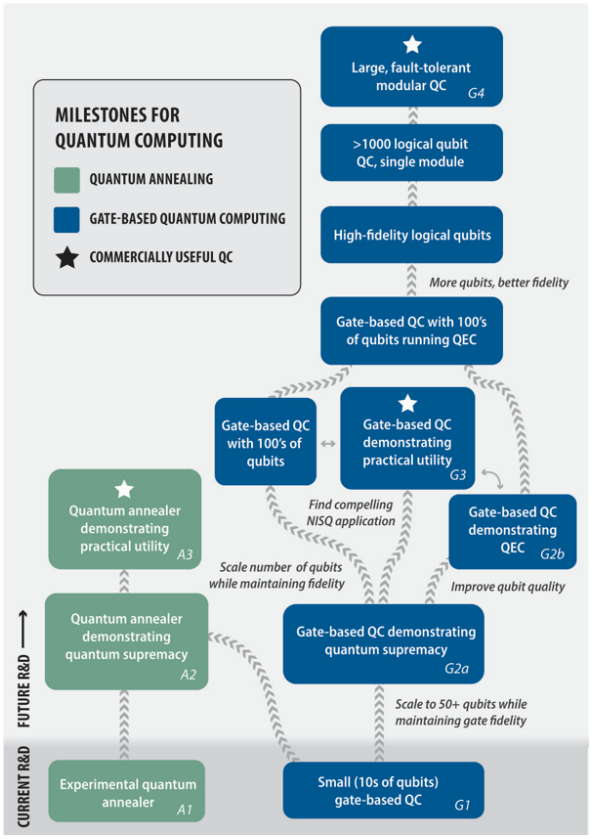

Figure 18: Metrics and milestones to help monitor the development of quantum computing. Roadmap by MIT [35]

rise to exciting computing techniques and algorithms based on variational calculations. This opens up a world of possibility to the era of *Quantum Machine Learning* (QML) [5, 28, 34]. The objective of QECC is to deal with errors introduced by quantum channels and those presented by (imperfect) quantum gates during the encoding and decoding process. Because of this, the reliability of the data processed by quantum computers depends on the probability of error per gate being below a certain threshold known as the precision threshold theorem. This is what NISQ defines as. *'Noisy'* because we don't have enough qubits leftover for error correction, so we'll have to use the imperfect qubits directly on the physical layer and *'Intermediate-Scale'* due to its reduced qubit (but not too small).

To understand quantum mechanics, we have to appreciate its postulates. These postulates provide a connection between the physical world and the mathematical formalism of quantum mechanics. It is important to emphasise that it is unnecessary to understand quantum mechanics in detail to know how to make a program on a quantum computer. But if we want to make intelligent and efficient algorithms, it is more than recommended to understand the fundamentals of quantum mechanics. The analogy to understand what we mean is the following: To program we can do it in *PhP*, and *python*, high-level languages, but we can also program in *C* or in *assembler* (machine language). If we want to be experts or make efficient algorithms, it would be useful to know the machine's architecture and to program in the machine language.

In the next section, we will present the postulates of quantum mechanics necessary to understand and, above all, delve into quantum computing. This thesis is based on the postulates listed in this reference [24] *Quantum Computation and Quantum Information*

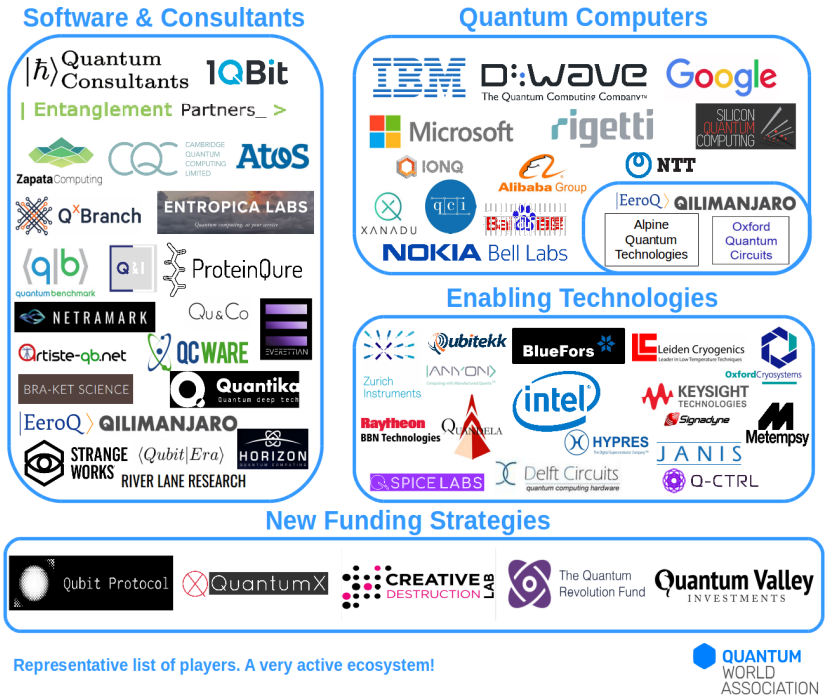

Figure 19: Companies and startups involved in the 2018 quantum computing ecosystem. Roadmap by Quantum World Association

0.11 Postulate 1

The *postulate 1* is defined as *associated with any isolated physical system is a complex vector space with an internal product (Hilbert space) known as the state space of the system. The system is fully described by its state vector, which is a unit vector in the state space of the system.*

This postulate explains the space of the quantum state and describes the area where quantum mechanics takes place. This area is nothing more than linear algebra in Hilbert vector space [41]. It is essential to know that, given a physical system, quantum mechanics does not tell us what the state space of that system is, nor can it tell us what the system's state vector is. Therefore, it is imperative to have this clear postulate. In other term, what we mean is that it is challenging to know the state of a quantum system at all times.

Let's consider that the simplest quantum mechanical system is the qubit. A qubit has a two-dimensional state space $|0\rangle$ and $|1\rangle$ that form an orthonormal basis for that state space. Then you can write an arbitrary state vector in the state space.

$$|\psi\rangle = a|0\rangle + b|1\rangle. \tag{103}$$

Where a and b are complex numbers. The condition that $|\psi\rangle$ is a unit vector is given by $\langle\psi|\psi\rangle = 1$, is therefore equivalent to $|a|^2 + |b|^2 = 1$. The term $\langle\psi|\psi\rangle = 1$ is known as the normalisation condition for state vectors.

The way a qubit differs from a classic bit is that there are overlaps of these two states, in the form $a|0\rangle + b|1\rangle$, where it is not possible to say that the qubit is definitely in the state $|0\rangle$, or definitely in the state $|1\rangle$. In other words, what we mean is that the quantum state is a linear combination of the components a and b.

If we had a system of more than one qubit, the expression of the quantum state would be of the form $\sum_i a_i|\psi_i\rangle$, and we would have a system with the superposition of the states $|\psi_i\rangle$ and of amplitude a_i for the state $|\psi_i\rangle$.

0.12 Postulate 2

The *postulate 2* is defined as *a unitary transformation describes the evolution of a closed quantum system. That is, the state $|\psi\rangle$ of the system at the time t_1 is related to the state $|\psi^{'}\rangle$ of the system at the time t_2 by a unit operator U that depends only on times t_1 and t_2, $|\psi^{'}\rangle = U|\psi\rangle$. This postulate gives a standard for describing quantum state changes over time.*

From Ref. [25] we know that quantum mechanics does not tell us the state space or quantum state of a particular quantum system; it also does not tell us which unit operators U describe real-world quantum dynamics. On the other hand, quantum mechanics assures us that the evolution of any closed quantum system can be described in this way.

$$|\psi^{'}\rangle = U|\psi\rangle. \tag{104}$$

In a way, we are saying that if we want to describe an n qubit quantum system subject to time evolution, we must calculate its unit operators U. The challenge would be to find such unit operators. Quantum gates are somehow the operators that act on quantum states. This postulate is very interesting and requires that the quantum system be closed [32][31]. Moreover, various derivatives emerge from this postulate.

0.12.1 Postulate 2'

The *postulate 2'* is defined as *the time evolution of the state of a closed quantum system is described by the Schrödinger equation* (105).

$$i\hbar\frac{\delta|\psi\rangle}{\delta t} = H|\psi\rangle. \tag{105}$$

Where $\hbar$ is Planck's constant and H is a fixed hermitian operator known as the Hamiltonian of the closed system [32].

In some way, we can say that if we know the Hamiltonian of a system, then we understand its dynamics completely. This concept is precious for modelling the system, and we will use it a lot throughout our thesis.

During the 20th century, much of the scientific (physical) community has been dedicated to discovering the Hamiltonian of any quantum system. And the conclusion they reached is that, in general, finding out that the Hamiltonian necessary to describe a particular physical system is challenging.

The Hamiltonian is static and a Hermitian operator that allows us to make its spectral decomposition with eigenvalues of energy E and the normalised eigenvectors corresponding to energy E as eigenstates $|E\rangle$.

$$|H\rangle \ = \sum_E E|E\rangle\langle E|, \tag{106}$$

$$|E\rangle = exp(-i\frac{Et}{\hbar})|E\rangle. \tag{107}$$

The equation (107) is valid only in the case of having a static Hamiltonian. The lowest energy is known as the ground state energy for the system, and the corresponding energy proper state (or adequate space or steady-state) is known as the ground state.

$$|\psi(t_2)\rangle = exp[\frac{-iH(t_1 - t_2)}{\hbar}]|\psi(t_1)\rangle = U(t_1 - t_2)|\psi(t_1)\rangle. \tag{108}$$

Where we define

$$U(t_1 - t_2) \equiv exp[\frac{-iH(t_1 - t_2)}{\hbar}]. \tag{109}$$

This interpretation is compelling and extremely useful since it is shown that any unitary operator U can be written in the form (110) tanking $\hbar = 1$ and $t_2 = 0$ the equation comes out to be (108)

$$U = exp(-iK). \tag{110}$$

With K, a Hermitian operator.

0.13 Postulate 3

The *postulate 3* is defined as *quantum measurements are described using a M_m collection of measurement operators. These are the operators that operate in the state space of the system being measured. The m index refers to the measurement results in the experiment. If the state of the quantum system is $|\psi\rangle$ immediately before the measurement, the probability that the result m will occur is given by the equation* (111).

$$p(m) = \langle\psi|M_m^T M_m|\psi\rangle. \tag{111}$$

The state of the system after the measurement is (112).

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|M_m^T M_m|\psi\rangle}}. \tag{112}$$

And, the measurement operator satisfies the completeness equation [32] that is given by the following equation (113) for all the values of the quantum state $|\psi\rangle$.

$$\sum_m M_m^T M_m = Ip(m) = \langle\psi|M_m^T M_m|\psi\rangle = 1. \tag{113}$$

The value of the measure is the probability described by $|a|^2 + |b|^2 = 1$.

If we want to make the different M_m observations, the operations we would be doing are the following:

$$M_0 = |0\rangle\langle 0| = \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}. \tag{114}$$

$$M_1 = |1\rangle\langle 1| = \begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix} = \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}. \tag{115}$$

With $\langle\psi|$ the conjugate of $|\psi\rangle$, represented by $|\psi\rangle = \langle\psi|^T$

$$M_0|0\rangle = |0\rangle\langle 0|0\rangle = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\0\end{bmatrix} = |0\rangle. \tag{116}$$

$$M_0|1\rangle = |0\rangle\langle 0|1\rangle = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix} = 0. \tag{117}$$

knowing that $|0\rangle\perp|1\rangle$, $\langle 0|1\rangle$ disappears; It is cancelled. If we project on any state, we will have:

$$M_0|\psi\rangle = |0\rangle\langle 0|\psi\rangle = |0\rangle a|0\rangle + b|1\rangle = a|0\rangle. \tag{118}$$

We can generalise (116): let M_0, let i be any qubit and let $|\psi\rangle$ be a multi-state of qubits, the measurement or the projection on the state $|0\rangle$ can be expressed as:

$$Tr\left[|\psi\rangle\langle\psi|M_0^i\right]. \tag{119}$$

If the qubit i is measured in the state $|0\rangle$, then the system will be in the state expressed by (120).

$$\frac{M_0^i|\psi\rangle}{\|M_0^i|\psi\rangle\|_2}. \tag{120}$$

Another way to get the result of the measurements is to remember that the measurement operator is Hermitian; this translates to $M_0^2 = M_0$ the same for $M_1^2 = M_1$. Also remembering that the relationship of completeness obeys the equation $I = M_0^T M_0 + M_1^T M_1 = M_0 + M_1$.

One of the crucial applications of (0.13) is to distinguish quantum states. We recall that since the quantum system must be closed (0.11)), getting to find out the quantum states represents a titanic and less intuitive task as in classical computing.

To clarify what we have just advanced, we will demonstrate the absurdity. We consider two non-orthogonal quantum states $|\psi_1\rangle$ and $|\psi_2\rangle$ and assume that the measurement is possible. If $|\psi_1\rangle$ and $|\psi_2\rangle$ are prepared, the measures (observations) will respond to the completeness (113). Defining $E_i \equiv\sum_{j:f(j)=i} M_j^\dagger M_j$, where the probability of measuring j such that $f(j) = 1$ and $f(j) = 2$ must be 1. These observations E_i may be written as:

$$\langle\psi_1|E_1|\psi_1\rangle = 1; \quad \langle\psi_2|E_2|\psi_2\rangle = 1. \tag{121}$$

Knowing that $\sum_i E_i = I$ therefore $\langle\psi_1|E_1|\psi_1\rangle = 1$ and must $\langle\psi_1|E_2|\psi_1\rangle = 0$, and$\sqrt{E_2}|\psi\rangle = 0$. If we decompose $|\psi_2\rangle = \alpha|\psi_1\rangle + \beta|\varphi\rangle$ with $|\psi_1\rangle$ and $|\varphi\rangle$ they are orthonormal. This leads us to the fact that $|\alpha|^2+|\beta|^2 = 1$ and that $|\beta| < 1$ while $|\psi_1\rangle$ and $|\psi_2\rangle$ are not orthonormal. With$\sqrt{E_2}|\psi\rangle = \beta\sqrt{E_2}|\varphi\rangle$. What contradicts completeness's equation (111).

$$\langle\psi_2|E_2|\psi_2\rangle = |\beta|^2\langle\varphi|E_2|\varphi\rangle \leq |\beta|^2 < 1. \tag{122}$$

Continuing with *postulate 3*, projective measurements form a particular case of it, being very useful and straightforward. Due to its simplicity, this measurement is the basis of many algorithms to know the observables.

A projective measurement is described by an observable, M, a Hermitian operator in the system's state space being observed. The observable has a spectral decomposition.

$$M = \sum_m mP_m. \tag{123}$$

where P_m is known as the projector in the proper space of M with the right value m. If we measure on the state $|\psi\rangle$, the probability of having the result m is

$$p(m) = \langle\psi|P_m|\psi\rangle. \tag{124}$$

so, the quantum state just after the measurement will be:

$$\frac{P_m|\psi\rangle}{\sqrt{\langle\psi|P_m|\psi\rangle}}. \tag{125}$$

Otherwise, what we are saying is that $\langle M\rangle = \langle\psi|M|\psi\rangle$. We can generalise this formula with the mean and variance:

$$[\Delta M]^2 = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2 \Delta M = \sqrt{\langle M^2 \rangle - \langle M \rangle^2}. \tag{62}$$

One of the differences to highlight is differentiating *measurement operations (M)* from *projectors (P)*, since $P^2 = P$, but $M^2! = M$.

This formula (62) is the basis of Heisenberg's uncertainty principle [32]. The important thing about the Heisenberg principle is that we cannot simultaneously measure/know the position and velocity of the electron (a particle). Therefore, it is impossible to determine its trajectory. We are somehow telling ourselves that measurement is destructive (but this is not the basis of Heisenberg's principle) because the position and velocity of the particle are in overlap. Measuring one collapses the wave function and destroys the other component/s.

A mathematical explanation can be described as follows. Suppose A and B are two Hermitian operators, and $|\psi\rangle$ is a quantum state. Suppose that $\langle \psi | AB | \psi \rangle = x + iy$, where x and y are real. Applying the switches and anti-switches to the Hermitian operators (matrices) A and B, we arrive at $\langle \psi [A, B] \psi \rangle = 2iy$ and $\langle \psi | \{A, B\} | \psi \rangle \ = 2x$. This implies that:

$$|\langle \psi | [A, B] | \psi \rangle|^2 + \langle \psi | \ A, B | \psi \rangle|^2 = 4 |\langle \psi | AB | \psi \rangle|^2 \ \ . \tag{126}$$

For the Cauchy-Schwarz inequality

$$|\langle \psi | AB | \psi \rangle|^2 \leq \langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle. \tag{127}$$

underestimating the negative term, we arrive at:

$$|\langle \psi | [A, B] | \psi \rangle|^2 \leq 4 \langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle. \tag{128}$$

if we now consider two observables M_1 and M_2, and substitute $A = M_1 - \langle M_1 \rangle$ and $B = M_2 - \langle M_2 \rangle$ in the last equation, we obtain the Heisenberg uncertainty principle from the equation (129).

$$\Delta M_1 \Delta M_2 \geq \frac{\langle \psi [M_1, M_2] \psi \rangle}{2}. \tag{129}$$

The correct interpretation of the uncertainty principle is that if we prepare a large number of quantum systems in identical states, $|\psi\rangle$, and then make measurements of M_1 in some of those systems, and of M_2 in others, then the standard deviation ΔM_1 of the results of M_1 multiplied by the standard deviation ΔM_2 of the results of M_2 will satisfy the inequality $\Delta M_1 \Delta M_2 \geq \frac{\langle \psi [M_1, M_2] \psi \rangle}{2}$.

In the commutation relationship for the observable X coordinates and moment P is, $[X, P] = j\hbar$. If we introduce it in the equation above, we get to (130):

$$\langle \Delta X \rangle^2 \langle \Delta P \rangle^2 = \frac{\hbar^2}{4}. \tag{130}$$

We make a parenthesis to explain the behaviour of the phase-in quantum mechanics. We already know that quantum mechanics is defined in the complex vector space (Hilbert space). We also know that a vector representation of a vector (wave) can be described with its argument and angle. Besides, the phase as an operator applied to a quantum state in quantum mechanics does not change the quantum state.

Now, let us consider that the state $e^{i\theta}|\psi\rangle$, where $|\psi\rangle$, is a state vector and θ is a real number. We say that the state $e^{i\theta}|\psi\rangle$, is equal to $|\psi\rangle$ where the factor $e^{i\theta}$ is known with the global phase of the system [32, 17]. This property is fascinating and useful when writing a quantum algorithm. Saving this operation entails a gain in time and computational cost.

Suppose we want to make the measurements of the observables M_m on the quantum state $e^{i\theta}|\psi\rangle$, with $|\psi\rangle$ the state vector. Then, the respective measurements will be given by the following equations:

$$\langle \psi | M_m | \psi \rangle \langle \psi | e^{-i\theta} M_m^T M_m e^{i\theta} | \psi \rangle = \langle \psi | M_m^T M_m | \psi \rangle. \tag{131}$$

We see that the global phase does not affect measures, but another phase does. This phase is known as the relative phase [17]. We will use an example to explain it. Let's consider two quantum states:

$$|\psi_1\rangle = a|0\rangle + b|1\rangle \quad \text{and} \quad |\psi_2\rangle = a|0\rangle - b|1\rangle. \tag{132}$$

We see that the state amplitude $|1\rangle$ of the first quantum state $|\psi_1\rangle$ is $+b$ and a, the state amplitude $|0\rangle$ of the second quantum state $|\psi_2\rangle$ is $-b$. We see that the only difference is the sign, not the amplitude. If two quantum states have the same amplitudes and differ exclusively by the phase (sign), this phase is known by the relative phase of the system. And generically, we can write it as follows $a = exp(i\theta)b$. This concept is fascinating and is the basis of quantum gates that will allow quantum computing.

0.14 Postulate 4

The *postulate 4* is defined as *the state-space of a composite physical system is the tensor product of the state spaces of the components of physical systems. Furthermore, if we have systems numbered from 1 to n, and the number of system i is prepared in the state* $|\psi_i\rangle$*, then the joint state of the total system is* $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle$.

This postulate is the basis for creating the complex system of more than two qubits or quantum states. This postulate also allows us to define one of the most exciting and puzzling ideas associated with composite quantum systems: entanglement. Consider the two-qubit states $|\psi\rangle = \frac{|00\rangle+|11\rangle}{\sqrt{2}}$, this state has the remarkable property that there are no unique qubit states $|a\rangle$ and $|b\rangle$ such that $|\psi\rangle = |a\rangle|b\rangle$. In other words, we say that $|\psi\rangle \neq |a\rangle|b\rangle$. This property is one of the reasons for the empowerment of quantum computing.

0.15 Summary

This section's right conclusion highlights that these four postulates of quantum mechanics define how we can conceptualise and face a problem about quantum mechanics and its computation. The first postulate establishes the space for quantum mechanics by specifying how the state of an isolated quantum system should be described. The second postulate illuminates us on the dynamics of the closed quantum systems and its description through the Schrödinger equation and using the unitary evolution. In the third postulate, we are explained how to make the measurement describing the importance of the characteristics (restrictions) when extracting information (measuring) from our quantum systems. And finally, the fourth postulate reveals how we can create composite systems. One of the most shocking and interesting ideas of quantum mechanics is that we cannot directly observe the state vector and that it is in charge of deciphering the behaviour of any quantum system. Let's imagine that we want to know what position the cat is in (20). In a classic system, thinking

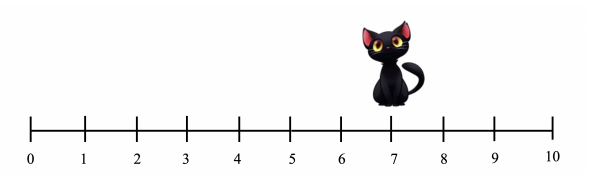

Figure 20: Observability of a classical system

about computing, the location (state vector) of the cat is given by the variable $x = 7$

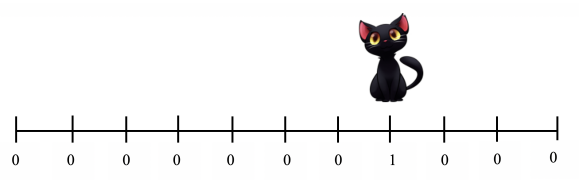

Figure 21: Observability of a quantum system

In a quantum system, the position (see figure (21)) of the cat is not so quickly known. In quantum, each element in the state vector contains the probability of finding the cat in a specific place. And it is represented by:

$$|x\rangle = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow \begin{array}{c}\text{Probability of} \\ \text{cat being at} \\ \text{position 7}\end{array}. \tag{133}$$

Classical physics, classical computation, and our intuition tell us that the fundamental properties of an object, such as energy, position, and velocity, are directly accessible to observation. However, these quantities no longer appear essential in quantum mechanics, depend on the state vector, and cannot be directly observed. Furthermore, merely observing a classical system does not necessarily change the system's state; instead, for a quantum system, observation is an invasive procedure that generally changes the state of the system (the state vector).

Before:
Section 7.8: The Pauli Operators The Pauli operators X, Y, Z (also known as $\sigma_x, \sigma_y, \sigma_z$) correspond to the measurement of the turn along the x^-, y^- and z^- axes respectively. Its actions in the base states are given by where it is clear that the base states are elements of Z:

$$X|0\rangle = |1\rangle, X|1\rangle = |0\rangle, Y|0\rangle = -j|1\rangle, Y|1\rangle = j|0\rangle, Z|0\rangle = |1\rangle, Z|1\rangle = -|1\rangle. \tag{134}$$

After:We have left a space between each equality to make it easier to read.
Section 7.8: The Pauli Operators
The Pauli operators $X, Y$and$Z$ (also known as $\sigma_x, \sigma_y, \sigma_z$) correspond to the measurement of the turn along the x^-, y^- and z^- axes respectively. Its actions in the base states are given by where it is clear that the base states are elements of Z:

$$X|0\rangle = |1\rangle, \quad X|1\rangle = |0\rangle, \quad Y|0\rangle = -j|1\rangle, \quad Y|1\rangle = j|0\rangle, \quad Z|0\rangle = |1\rangle, \quad Z|1\rangle = -|1\rangle. \tag{135}$$

Before:
Section 7.9: Hadamard Gate
With

$$R_z(\varphi) = \begin{bmatrix} e^{-i\varphi/2} & 0 \\ 0 & e^{i\varphi/2} \end{bmatrix} = \cos\left(\frac{\varphi}{2}\right) I_2 - isin\left(\frac{\varphi}{2}\right) Z = e^{-\frac{i\varphi}{2}Z}. \tag{136}$$

$$R_y(\theta) = \begin{bmatrix} cos\left(\frac{\theta}{2}\right) & -sin\left(\frac{\theta}{2}\right) \\ sin\left(\frac{\theta}{2}\right) & cos\left(\frac{\theta}{2}\right) \end{bmatrix} = \cos\left(\frac{\theta}{2}\right) I_2 - isin\left(\frac{\theta}{2}\right) Z = e^{-\frac{i\theta}{2}Y}. \tag{137}$$

$$R_x(\psi) = \begin{bmatrix} cos\left(\frac{\psi}{2}\right) & -sin\left(\frac{\psi}{2}\right) \\ sin\left(\frac{\psi}{2}\right) & cos\left(\frac{\psi}{2}\right) \end{bmatrix} = \cos\left(\frac{\psi}{2}\right) I_2 - isin\left(\frac{\psi}{2}\right) Z = e^{-\frac{i\psi}{2}X}. \tag{138}$$

After: We have corrected some typos that we have seen in the equations of rotations.
Section 7.9: Hadamard Gate
With

$$R_z(\varphi) = \begin{bmatrix} e^{-i\varphi/2} & 0 \\ 0 & e^{i\varphi/2} \end{bmatrix} = \cos\left(\frac{\varphi}{2}\right) I_2 - isin\left(\frac{\varphi}{2}\right) Z = e^{-\frac{i\varphi}{2}Z}. \tag{139}$$

$$R_y(\theta) = \begin{bmatrix} cos\left(\frac{\theta}{2}\right) & -sin\left(\frac{\theta}{2}\right) \\ sin\left(\frac{\theta}{2}\right) & cos\left(\frac{\theta}{2}\right) \end{bmatrix} = \cos\left(\frac{\theta}{2}\right) I_2 - isin\left(\frac{\theta}{2}\right) Y = e^{-\frac{i\theta}{2}Y}. \tag{140}$$

$$R_x(\psi) = \begin{bmatrix} cos\left(\frac{\psi}{2}\right) & -isin\left(\frac{\psi}{2}\right) \\ -isin\left(\frac{\psi}{2}\right) & cos\left(\frac{\psi}{2}\right) \end{bmatrix} = \cos\left(\frac{\psi}{2}\right) I_2 - isin\left(\frac{\psi}{2}\right) X = e^{-\frac{i\psi}{2}X}. \tag{141}$$

The rotation operators are generated by exponentiation of the Pauli matrices according to:

$$exp(iAx) = cos(x)I + isin(x)A, \tag{142}$$

where A is one of the three Pauli Matrices.

Before:
Section 7.10: Gate R_ϕ

$$U_3(\theta,\phi,\lambda) = \begin{bmatrix} cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}sin(\frac{\theta}{2}) & e^{i\lambda+i\phi}cos(\frac{\theta}{2}) \end{bmatrix}. \tag{143}$$

After: We have put the variables i in common factors to make the equation easier to read.
Section 7.10: Gate R_ϕ

$$U_3(\theta,\phi,\lambda) = \begin{bmatrix} cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}sin(\frac{\theta}{2}) & e^{i(\lambda+\phi)}cos(\frac{\theta}{2}) \end{bmatrix}. \tag{144}$$

Before:
Section 9.1.1: Quadratic Unconstrained Binary Optimization Problems

$$H(x)_{\text{QUBO}} = \sum_{i}^{N} \sum_{j<i} Q_{ij} x_i x_j + \sum_{i}^{N} Q_i x_i. \tag{145}$$

$$H(a_i, b_{ij}; q_i)_{\text{QUBO}} = \sum_{i}^{N} \sum_{j<i} b_{ij} q_i q_j + \sum_{i}^{N} a_i q_i. \tag{146}$$

This form can be easily found in the D-Wave formulation. The transformation between Ising and QUBO is $s = 2x - 1$. Let demonstrate that QUBO and the Ising of the Hamiltonian are similar. This means that we will have the algorithm in Ising form by writing an algorithm for QUBO with a single variable change. That is very useful to have the algorithm for various platforms based on quantum gates or quantum annealing.

$$H(s) = \sum_{i}^{N} \sum_{j<i} J_{ij} s_i s_j + \sum_{i}^{N} h_i s_i. \tag{147}$$

With s_i and $s_j \in \{-1, 1\}$. For the translation in QUBO formulation, let's consider x_i and $x_j \in \{0, 1\}$ and using the spin relation $s = 2x - 1$, we can remap the Hamiltonian as follow:

$$\begin{aligned} H(s) &= \sum_{i}^{N} \sum_{j<i} J_{ij}(2x_i - 1)(2x_j - 1) + \sum_{i}^{N} h_i(2x_i - 1) \\ &= \sum_{i}^{N} \sum_{j<i} J_{ij}(4x_i x_j - 2x_i - 2x_j + 1) + \sum_{i}^{N} (2h_i x_i - h_i). \end{aligned} \tag{148}$$

Regrouping all the constants into C_0 we have the following expression:

$$H\left(s\right) = \sum_{i}^{N} \sum_{j<i} 4J_{ij} x_i x_j - \sum_{i}^{N} x_i \sum_{j<i} 2J_{ij} - \sum_{i}^{N} \sum_{j<i} 2J_{ij} x_j + \sum_{i}^{N} 2h_i x_i - C_0. \tag{149}$$

By grouping x_i terms together, we can write, $a_i = \sum_{j<i}^{N} 2J_{ij} + 2h_i$, so:

$$H\left(s\right) = \sum_{i}^{N} \sum_{j<i} 4J_{ij} x_i x_j - \sum_{i}^{N} a_i x_i - 2 \sum_{i}^{N} \sum_{j<i} J_{ij} x_j + C_0. \tag{150}$$

Let us develop the term $\sum_{i}^{N} \sum_{j<i} J_{ij} x_j$ in term of x_i.

$$\begin{aligned} \sum_{i}^{N} \sum_{j<i} J_{ij} x_j &= J_{10} x_0 + J_{20} x_0 + J_{21} x_1 + J_{30} x_0 + J_{31} x_1 + J_{32} x_2 + \dots \\ &+ J_{N0} x_0 + J_{N1} x_1 + J_{N2} x_2 + J_{N2} x_3 + J_{N,N-1} x_{N-1}. \end{aligned} \tag{151}$$

We can observe that each column has a term:

$$\left(J_{10} + J_{20} + J_{30} + \ldots + J_{N0}\right) x_0 + \left(J_{21} + J_{31} + \ldots + J_{N1}\right) x_1 + \ldots + \left(J_{N,N-1}\right) x_{N-1}. \tag{152}$$

Let's cast the J_{ij} as some constants b_i, so:

Terms				
Problem Expression	Linear Coefficient	Quadratic Coefficient	Variable	States
QUBO (scalar)	a_i	$a_{i,j}$	q_i	$\{0,1\}$
QUBO (matrix)	$Q_{i,j}$	$Q_{i,j}$	x_i	$\{0,1\}$
Ising	h_i	$J_{i,j}$	s_i	$\{-1,1\}$

Table 1: Comparation between Ising and QUBO representation and related terminology.

$$b_0x_0 + b_1x_1 + b_2x_2 + \ldots + b_{N-1}x_{N-1}. \tag{153}$$

Since there is no x_N in the original sum, so $b_N = 0$. So we can write that:

$$\sum_{i}^{N}\sum_{j<i} J_{ij}x_j = \sum_{i}^{N} b_i x_i. \tag{154}$$

So, our Hamiltonian can be written as:

$$H\left(s\right) = \sum_{i}^{N}\sum_{j<i} 4J_{ij}x_ix_j - \sum_{i}^{N} a_ix_i - 2\sum_{i}^{N} b_ix_i + C_0. \tag{155}$$

Let $J_{ij}^{'} = 4J_{ij}$ and $h_i^{'} = a_i - 2b_i$, therefore,

$$H\left(s\right) = \sum_{i}^{N}\sum_{j<i} J_{ij}^{'}x_ix_j - \sum_{i}^{N} h_i^{'}x_i + C_0 H\left(s\right) = H\left(x\right) + C_0. \tag{156}$$

Where we can experiment that Ising $H(s)$ and QUBO $H(x)$ are similar in form and relations; they are isomorphic.

To convert the coefficients from QUBO to Ising:

$$\begin{aligned} J_{ij} &= \frac{1}{4}Q_{ij} \\ h_i &= \frac{1}{2}Q_{ii} + \frac{1}{4}\sum_{i<j} Q_{ij}. \end{aligned} \tag{157}$$

Or from Ising to QUBO:

$$\begin{aligned} Q_{ij} &= 4J_{ij} \\ Q_{ii} &= 2h_i - \frac{1}{2}\sum_{i<j} Q_{ij}. \end{aligned} \tag{158}$$

After: We have set all limits of the sum to N instead of having some at n.
Section 9.1.1: Quadratic Unconstrained Binary Optimization Problems

$$f(x)_{\text{QUBO}} = \sum_{i}^{N}\sum_{j<i}^{N} Q_{ij}x_ix_j + \sum_{i}^{N} Q_ix_i. \tag{159}$$

$$H(a_i, b_{ij}; q_i)_{\text{QUBO}} = \sum_{i}^{N}\sum_{j<i}^{N} b_{ij}q_iq_j + \sum_{i}^{N} a_iq_i. \tag{160}$$

This form can be easily found in the D-Wave formulation. The transformation between Ising and QUBO is $s = 2x - 1$. Let demonstrate that QUBO and the Ising of the Hamiltonian are similar. This means that we will have the algorithm in Ising form by writing an algorithm for QUBO with a single variable change. That is very useful to have the algorithm for various platforms based on quantum gates or quantum annealing.

$$H(s) = \sum_{i}^{N} \sum_{j<i}^{N} J_{ij} s_i s_j + \sum_{i}^{N} h_i s_i. \tag{161}$$

With s_i and $s_j \in \{-1, 1\}$. For the translation in QUBO formulation, let's consider x_i and $x_j \in \{0, 1\}$ and using the spin relation $s = 2x - 1$, we can remap the Hamiltonian as follow:

$$\begin{aligned} H(s) &= \sum_{i}^{N} \sum_{j<i}^{N} J_{ij}(2x_i - 1)(2x_j - 1) + \sum_{i}^{N} h_i(2x_i - 1) \\ &= \sum_{i}^{N} \sum_{j<i}^{N} J_{ij}(4x_i x_j - 2x_i - 2x_j + 1) + \sum_{i}^{N}(2h_i x_i - h_i). \end{aligned} \tag{162}$$

Regrouping all the constants into C_0 we have the following expression:

$$H\left(s\right) = \sum_{i}^{N} \sum_{j<i}^{N} 4J_{ij} x_i x_j - \sum_{i}^{N} x_i \sum_{j<i}^{N} 2J_{ij} - \sum_{i}^{N} \sum_{j<i}^{N} 2J_{ij} x_j + \sum_{i}^{N} 2h_i x_i - C_0. \tag{163}$$

By grouping x_i terms together, we can write, $a_i = \sum_{j<i}^{N} 2J_{ij} + 2h_i$, so:

$$H\left(s\right) = \sum_{i}^{N} \sum_{j<i}^{N} 4J_{ij} x_i x_j - \sum_{i}^{N} a_i x_i - 2 \sum_{i}^{N} \sum_{j<i}^{N} J_{ij} x_j + C_0. \tag{164}$$

Let us develop the term $\sum_{i}^{N} \sum_{j<i}^{N} J_{ij} x_j$ in term of x_i.

$$\begin{aligned} \sum_{i}^{N} \sum_{j<i}^{N} J_{ij} x_j &= J_{10} x_0 + J_{20} x_0 + J_{21} x_1 + J_{30} x_0 + J_{31} x_1 + J_{32} x_2 + \dots \\ &+ J_{N0} x_0 + J_{N1} x_1 + J_{N2} x_2 + J_{N2} x_3 + J_{N,N-1} x_{N-1}. \end{aligned} \tag{165}$$

We can observe that each column has a term:

$$\left(J_{10} + J_{20} + J_{30} + \ldots + J_{N0}\right) x_0 + \left(J_{21} + J_{31} + \ldots + J_{N1}\right) x_1 + \ldots + \left(J_{N,N-1}\right) x_{N-1}. \tag{166}$$

Let's cast the J_{ij} as some constants b_i, so:

$$b_0 x_0 + b_1 x_1 + b_2 x_2 + \ldots + b_{N-1} x_{N-1}. \tag{167}$$

Since there is no x_N in the original sum, so $b_N = 0$. So we can write that:

$$\sum_{i}^{N} \sum_{j<i}^{N} J_{ij} x_j = \sum_{i}^{N} b_i x_i. \tag{168}$$

So, our Hamiltonian can be written as:

$$H\left(s\right) = \sum_{i}^{N} \sum_{j<i}^{N} 4J_{ij} x_i x_j - \sum_{i}^{N} a_i x_i - 2 \sum_{i}^{N} b_i x_i + C_0. \tag{169}$$

Terms				
Problem Expression	Linear Coefficient	Quadratic Coefficient	Variable	States
QUBO (scalar)	a_i	$a_{i,j}$	q_i	$\{0,1\}$
QUBO (matrix)	$Q_{i,j}$	$Q_{i,j}$	x_i	$\{0,1\}$
Ising	h_i	$J_{i,j}$	s_i	$\{-1,1\}$

Table 2: Comparation between Ising and QUBO representation and related terminology.

Let $J_{ij}^{'} = 4J_{ij}$ and $h_i^{'} = a_i - 2b_i$, therefore,

$$H\left(s\right) = \sum_{i}^{N}\sum_{j<i}^{N} J_{ij}^{'} x_i x_j - \sum_{i}^{N} h_i^{'} x_i + C_0 H\left(s\right) = H\left(x\right) + C_0. \tag{170}$$

Where we can experiment that Ising $H(s)$ and QUBO $H(x)$ are similar in form and relations; they are isomorphic.

To convert the coefficients from QUBO to Ising:

$$\begin{aligned} J_{ij} &= \frac{1}{4} Q_{ij} \\ h_i &= \frac{1}{2} Q_{ii} + \frac{1}{4} \sum_{i<j}^{N} Q_{ij}. \end{aligned} \tag{171}$$

Or from Ising to QUBO:

$$\begin{aligned} Q_{ij} &= 4J_{ij} \\ Q_{ii} &= 2h_i - \frac{1}{2} \sum_{i<j}^{N} Q_{ij}. \end{aligned} \tag{172}$$

Before:

Section 9.2.3: Quantum approximate optimization algorithm

$$e^{-i\left(\sum_j H_j\right)t} = \lim_{N\to\infty} \left(e^{-iH_0 \frac{t}{N} - iH_1 \frac{t}{N}} * \ldots^{-iH_{m-1} \frac{t}{N}}\right)^N. \tag{173}$$

Since the limit of this series is infinite, when we implement this in quantum computing, we must truncate the function by introducing a quantifiable bounded error ε refers to $\|e^{-iHt} - U\| \leq \varepsilon$.

After: We add the description of N

Section 9.2.3: Quantum approximate optimization algorithm

$$e^{-i\left(\sum_j H_j\right)t} = \lim_{N\to\infty} \left(e^{-iH_0 \frac{t}{N} - iH_1 \frac{t}{N}} * \ldots^{-iH_{m-1} \frac{t}{N}}\right)^N. \tag{174}$$

Since the limit of this series is infinite with $N \in Z^+$, when we implement this in quantum computing, we must truncate the function by introducing a quantifiable bounded error ε refers to $\|e^{-iHt} - U\| \leq \varepsilon$.

Before:
Section 11.2.1: Social Workers' Problem based on new VRP formulation

In this proposal, we take advantage of the formulation of the VRP to establish our proposal. We pursue to avoid using the inequality constraints and use the least number of qubits. We have very few real qubits with the real environments we are using. But to do some comparative studies, we would rather use simulators with a greater number of qubits than the quantum computer. To be able to test our algorithm. Therefore, we will base our algorithm on techniques (VRP, TSP) already consolidated to achieve efficiency in many qubits. We use VRP's universal formulation to model the main part of the proposed algorithm.

Let $G = (V, E, c)$ be a complete graph directed with $V = \{0, 1, 2, .., n\}$, as the set of nodes and $E = \{(i, j) : i, j \in V, i \neq j\}$ as the set of arcs, where node 0 represents the central, for a team of k social workers with the same capacity ρ and n remaining nodes that represent geographically dispersed patients.

Each patient $i \in V$–$\{0\}$ has a specific demand for visits $d_i \leq \rho$. The non-negative travel cost W_{ij} is associated with each arc $(i, j) \in E$. To simplify, we consider that the distances are symmetrical. Where x_{ij} are the decision variables of the paths between two patients. The minimum number of social workers needed to care for all patients is $\frac{\sum_{i=1}^{n} d_i}{Q}$.

Minimize:

$$\sum_{k=1}^{m} \sum_{i=1}^{l} \sum_{j=1, i \neq j}^{n} W_{ij} x_{ijk,}. \tag{175}$$

Subject to:

$$\sum_{k=1}^{m} \sum_{j=1}^{n} x_{ijk} = 1 \quad \forall i \in 1, \ldots, n, \tag{176}$$

$$\sum_{k=1}^{m} \sum_{i=1}^{n} x_{jik} = 1 \quad \forall j \in 1, \ldots, n, \tag{177}$$

$$\sum_{i=1}^{l} di \sum_{j=1}^{n} x_{ijk} \leq q \quad \forall k \in 1, \ldots, m, \tag{178}$$

$$\sum_{j=1}^{n} x_{0jk} \ = K \quad \forall k \in 1, \ldots, m, \tag{179}$$

$$\sum_{j=1}^{n} x_{j0k} \ = K, \quad \forall k \in 1, \ldots, m, \tag{180}$$

$$\sum_{i=1}^{n} x_{ihk} - \sum_{j}^{n} x_{hjk} = 0 \quad \forall h \in 1, \ldots, n \quad \text{and} \quad \forall k \in 1, \ldots, m, \tag{181}$$

$$x_{ijk} \in 0, 1, \quad \forall i, j \in 0, \ldots, n, i \neq j \quad \forall k \in 1, \ldots, m. \tag{182}$$

In this formulation, the objective function equation (186) minimizes total travel savings taking into account the new cost function with the time window. The restrictions equations (187) and (188) impose that exactly the arcs k leave the plant; (190) and (191) are the restrictions on the degree of entry and exit of the social worker from the central office. The constraints (192) are the route of continuity and the elimination of sub-courses, which ensure that the solution does not contain a

sub-route disconnected from the exchange. Restrictions (193) are mandatory. The restriction (189) is the demand of the social workers.

Up to this point, the mathematical formulation of equations (186) to (193) represents a conventional CVRP. To solve a scheduling problem, we need a time variable. The introduction of time (schedule) in the original QAOA and QUBO formulations of the CVRP is a significant obstacle to formulating several important VRP restrictions associated with the VRPTW time window.

Our CVRP QAOA formulation proposal incorporates the schedule (calendar) of table (**??**). This new formulation describes the temporal evolution of each social worker equivalent to the VRPTW. Our proposal is expressed by equations (194) and (195).

$$W_{ij} = d_{ij} + f\left(t_{ij}\right). \tag{183}$$

$$f\left(t_{ij}\right) = \gamma \frac{\left(\tau_{i-}\tau_j\right)^2}{d_{\max} - d_{\min}}. \tag{184}$$

Where W_{ij} is our cost/weight and time window function, d_{ij} is the distance between the patient i and j and $f(t_{ij})$ is our time window's function. $f(t_{ij})$ is a growing function, and we model it by a quadratic function to weigh short distances concerning large ones. We are taking into account that the first weight function $W_{ij} = d_{ij}$ is a distance function, we want to make $f(t_{ij})$ behave like d_{ij}, and thus, be able to take full advantage of the behaviour of the primary objective function. $\gamma > 0$ is a weighted degree parameter of our time window function; τ_i is the start time of a time slot for patient i and τ_j for the patient j. where $d_{\max}$ represents the maximum distance between all patients and, $d_{\min}$ is the minimum distance between the gaps of all patients. The term $T_{ij} = (\tau_{i-}\tau_j) > 0$ is the time window.

The simplified Hamiltonian resulting from the schedule optimization problem is as follows:

$$\begin{aligned} H = &\sum_{ij\in E} W_{ij}x_{i,j} + A\sum_{i=1}^{n}(1 - \sum_{j\in\delta(i)^+}^{N} x_{i,j})^2 + A\sum_{i=1}^{n}(1 - \sum_{j\in\delta(i)^-}^{N} x_{ji})^2 + A(k - \sum_{i\in\delta(0)^+}^{N} x_{0,i})^2 + \\ &A(k - \sum_{j\in\delta(0)^+}^{N} x_{j,0})^2. \end{aligned} \tag{185}$$

After: We have simplified the definition as we have it implemented. We have unified the limits of the sums.

Section 11.2.1: Social Workers' Problem based on new VRP formulation

In this proposal, we take advantage of the formulation of the CVRP to establish our proof of the concept. It is worth saying that we pursue to avoid using the inequality constraints and use the least number of qubits according to this NISQ era. Nevertheless, to do some comparative studies, we would rather use simulators with more qubits than quantum computers to test our algorithm. Therefore, we will base our algorithm on techniques (VRP, TSP) already consolidated to achieve efficiency in many qubits. We use VRP's universal formulation to model the routing part of the proposed VRPTW.

Let $G = (V, E)$ be a complete graph directed with $V = \{0, 1, 2, .., n\}$, as the set of nodes and $E = \{(i, j) : i, j \in V, i \neq j\}$ as the set of arcs, where node 0 represents the central, for a team of K

social workers with the same capacity q and n remaining nodes that represent geographically dispersed patients.

The non-negative travel cost W_{ij} is associated with each arc $(i, j) \in E$. Let d_{ij} be our distance matrix and to simplify, we consider that the distances are symmetrical. Where x_{ij} are the decision variables of the paths between the patient i and j.

Minimize:

$$\sum_{i=1}^{n} \sum_{j=1, i \neq j}^{n} W_{ij} x_{ij,}. \tag{186}$$

Subject to:

$$\sum_{j=1}^{n} x_{ij} = 1 \quad \forall i \in 1, \ldots, n, \tag{187}$$

$$\sum_{i=1}^{n} x_{ji} = 1 \quad \forall j \in 1, \ldots, n, \tag{188}$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} x_{ij} d_{ij} \leq q, \tag{189}$$

$$\sum_{j=1}^{n} x_{0j} = K \quad \forall i \in 1, \ldots, n, \tag{190}$$

$$\sum_{j=1}^{n} x_{j0} = K, \quad \forall i \in 1, \ldots, n, \tag{191}$$

$$u_i - u_j + n x_{i,j} \leq n - 1 \quad 1 \leq i \neq j \leq n. \tag{192}$$

$$x_{ij} \in \{0, 1\}, \quad \forall i, j \in 0, \ldots, n, i \neq j. \tag{193}$$

In this formulation, the objective function equation (186) minimizes the new cost function with the time window (194). The restrictions equations (187) and (188) declare that each social worker can only be one node at any time (that means we will only visit once the patient). The restriction (189) establishes that any social worker can travel more distance than allowed. In the case of wanting to measure the time, here, what we would do is change the matrix d_{ij} for a matrix of the maximum contract time. The constraint (190) establishes that all the social workers start from Depot and (191) establishes that all the social workers end at the Depot. The constraints (192) are the route of continuity and the elimination of sub-courses, which ensure that the solution does not contain a sub-route disconnected from the exchange. Restrictions (193) describes that x_{ij}, are binary variables.

Up to this point, the mathematical formulation of equations (186) to (193) represents a conventional CVRP. To solve a scheduling problem, we need a time variable. The introduction of time (schedule) into the QUBO formulations of the CVRP is a significant obstacle to formulating several important VRP restrictions associated with the VRPTW time window [27].

Our CVRP formulation proposal must incorporate the schedule (calendar) of table (**??**).

During the state of the art of these formulations carried out, we have found several articles [27, 12, 16] that solve the TSP and VRP for annealing computers [7, 6, 11]. However, the number of variables is still intractable for the current size of quantum computers. The **number of qubits** of the TSPTW[27], is proportional to $N^3 + N^2 \log_2 N$, and for this VRPTW[16], is N^4. For this reason, we propose a new VRPTW formulation ((186) and (195)) with a heuristic function executed by an classical algorithm that generates a description of a quantum circuit as advocate the following

reference [13]. With this strategy, we aim to reduce the number of the qubits from N^4 to $N2$ for our proposed VRPTW for solving our SWP.

For example, a possible formulation of the VRP uses N^4 variables where N is the number of cities, thus with only 5 towns, we would go to 625 necessary variables. In quantum computing, each of these variables can be represented with a qubit, and that is why computers possessing 625 qubits would be needed to carry out these tasks. In the case of N^4, the number of the qubits 625 is more than the most powerful quantum computer based on the gate model has to date. The gate-based computers have around 100 qubits making this task intractable today. The number of qubits is higher for computers based on quantum annealing, reaching 2000 qubits like the D-Wave computer. However, the correspondence between variables and qubits will not be one-to-one due to the architecture of these computers, so that we will have a smaller number of useful qubits. The following reference [14] deals with the topology and graph problem mapping on the D-Wave 2000Q QPU computer in detail.

The new time window formulation of our VRPTW is expressed by the equations (194) and (195).

$$W_{ij} = d_{ij} + f\left(t_{ij}\right). \tag{194}$$

$$f\left(t_{ij}\right) = \gamma \frac{\left(\tau_{i-}\tau_j\right)^2}{d_{\max} - d_{\min}}. \tag{195}$$

Where W_{ij} is our cost/weight and time window function, d_{ij} is the distance between the patient i and j and $f(t_{ij})$ is our time window's function. $f(t_{ij})$ is a growing function, and we model it by a quadratic function to weigh short distances concerning large ones. We are taking into account that the first weight function $W_{ij} = d_{ij}$ is a distance function, we want to make $f(t_{ij})$ behave like d_{ij}, and thus, be able to take full advantage of the behaviour of the primary objective function. $\gamma > 0$ is a weighted degree parameter of our time window function; τ_i is the start time of a time slot for patient i and τ_j for the patient j. where $d_{\max}$ represents the maximum distance between all patients and, $d_{\min}$ is the minimum distance between the gaps of all patients. The term $T_{ij} = (\tau_{i-}\tau_j) > 0$ is the time window.

The simplified Hamiltonian resulting from the schedule optimization problem is as follows:

$$\begin{aligned} H = &\sum_{ij\in E}^{n} W_{ij}x_{i,j} + A\sum_{i=1}^{n}(1 - \sum_{j\in\delta(i)^+}^{n} x_{i,j})^2 + A\sum_{i=1}^{n}(1 - \sum_{j\in\delta(i)^-}^{n} x_{ji})^2 + A(k - \sum_{i\in\delta(0)^+}^{n} x_{0,i})^2 + \\ &A(k - \sum_{j\in\delta(0)^+}^{n} x_{j,0})^2. \end{aligned} \tag{196}$$

The number of the qubits after applying our strategy will be:

$$\textbf{Num qubits}_{\text{SWP}} = \binom{n}{2} = \frac{n!}{2!(n-2)!} = \frac{n(n-1)}{2} + \epsilon. \tag{197}$$

Where the ϵ is the ancillary variables given by $\sum_{i=1}^{\lceil log_2 b\rceil} 2^i y_i$ according to the capacity restriction(189). In the case of removing the symmetry; the number of qubits will be $n(n-1) + \epsilon$.

Before:

Section 11.2.1: Social Workers' Problem based on a QUBO approach

Next, we calculate these variables. We start with J_{ij} as is summarized in table (**??**).

$$J_{ij} = \begin{cases} \frac{q_{i,j}+q_{i,j}}{4} & i < j \\ 0 & otherwise \end{cases} \tag{198}$$

After: We have removed italic from the equation.

Next, we calculate these variables. We start with J_{ij} as is summarized in table (**??**).

$$J_{ij} = \begin{cases} \frac{q_{i,j}+q_{i,j}}{4} & i < j \\ 0 & \text{otherwise} \end{cases} \tag{199}$$

Before:
Section 11.2.2: The algebraic approach of the Hamiltonian Formulation
We can simplify our objective function to be implemented in quantum.

After: We have introduced a definition and a demonstration so that the reader can see the correspondence between the two expressions.

Section 11.2.2: The algebraic approach of the Hamiltonian Formulation
We can simplify our objective function to be implemented in quantum. Let us demonstrate that the following expression holds.

$$\sum_{i=1}^{n}(\sum_{j=1}^{n} X_{ij} - 1)^2 = \sum_{i=1}^{n}(e_i \otimes 1_n^T Z - 1)^2. \tag{200}$$

Thus, we can say:

$$(e_i \otimes 1_n) = \sum_{j=1}^{n} X_{ij}. \tag{201}$$

Let us write down $e_i = (0 \dots 0 \dots 1 \dots 0 \dots 0)$, $1_n^T = (1 \dots 1)$, both have dimension n and $Z = (X_{11}X_{12}X_{13} \dots X_{1n}X_{21}X_{22} \dots X_{2n} \dots X_{nn})^T$ with n^2 dimensions.

We can reach the following expression: $e_i \otimes 1_n = (0 \cdot (1 \dots 1) \dots 1 \cdot (1 \dots 1) \dots 0 \cdot (1 \dots 1) \dots) = (0000 \dots 0000 \dots 1111 \dots 0000 \dots 0000)$.

As Z is defined, we can calculate the following expression as:

$(e_i \otimes 1_n) \cdot Z = 0 \cdot X_{11} + 0 \cdot X_{12} + \dots 0 \cdot X_{1n} \dots + \dots 1 \cdot X_{i1} + 0 \cdot X_{i2} + \dots + 1 \cdot X_{in} + 0 \cdot X_{in+1} + \dots = X_{i1} + + X_{in} = \sum_{j=1}^{n} X_{ij}$.

In the end, we see that we arrive at the expression we want (229). So now we only have to substitute it into our simplified SWP formulation (196).

Before:
Section 12.5: Variational Quantum Classifier

To date, two dominant categories allow designing quantum classifiers. Although almost all are inspired by the classical classifiers (kernel or neural networks) [2], there is a new category of classifiers that respond to the current era of quantum computing (NISQ); hybrid and variational classifiers.

After: We have introduced a definition and demonstration so that the reader can see where some expressions are coming from.

Section 12.5: Variational Quantum Classifier

To date, two dominant categories allow designing quantum classifiers. Although almost all are inspired by the classical classifiers (kernel or neural networks) [2], there is a new category of classifiers that respond to the current era of quantum computing (NISQ); hybrid and variational classifiers.

Let us find the operator that will help us to create our classifier.

- ◇ Let n be the number of qubits.
- ◇ Let $\vec{x}$ be a vector of dimension m.
- ◇ Let $\vec{\theta}$, a matrix of dimension $n(m+1)$.
- ◇ Given a row i, we will say that $\vec{\theta_i}: = \vec{\theta_i}^{(w)} + \theta_i^{(b)}$
  - where $\vec{\theta_i}^{(w)}$ has dimension m and $\theta_i^{(b)}$ dimension 1.
- ◇ Let us define generically $\vec{\theta_i} \cdot \vec{x}: = \vec{\theta_i}^{(w)} \cdot \vec{x} + \theta_i^{(b)}$.

Taking into account all, one way to define the model will be:

$$U(\vec{x}, \vec{\theta}) = \bigotimes_{i=0}^{n-1} U_i(\vec{x}, \vec{\theta_i}),$$

where: (for example)

$$U_i(\vec{x}, \vec{\theta_i}) = R_y(\vec{\theta_i}^{(b)}) R_z(\vec{\theta_i} \cdot \vec{x}).$$

- ◇ Let $|\psi(\vec{x})\rangle$ be a functional quantum state.
- ◇ Let $f_i : R^m \to C$ be complex function.

$$|\psi(\vec{x})\rangle = \sum_{i=0}^{2^n-1} f_i(\vec{x}) \, |i\rangle \, , \tag{202}$$

$$\sum_{i=0}^{2^n-1} |f_i(\vec{x})|^2 = 1. \tag{203}$$

The circuit $\mathcal{U}(\vec{x}, \vec{\theta})$ approximates the state as:

$$|\psi(\vec{x})\rangle \sim \mathcal{U}(\vec{x}, \vec{\theta}) \, |0\rangle^{\otimes n} \, , \qquad \text{with} \qquad \mathcal{U}(\vec{x}, \vec{\theta}) = \prod_{i=1}^{k} U(\vec{x}, \vec{\theta_i}), \tag{204}$$

with better results as the number of layers k increases and n the number of the classes.

- $\vec{\theta} = \{\vec{\theta_i}\}$ is found with classical optimization techniques.
- Cost function = Distance($|\psi(\vec{x})\rangle$,$\mathcal{U}(\vec{x}, \vec{\theta})\,|0\rangle^{\otimes n}$).

In the next section, we will dive deeply into the Ansatz analysis.

Before:

Section 11.2.2 The algebraic approach of the SWP formulation We are looking for a more compact Hamiltonian way to make it easier to codify in quantum. To do this, we vectorise the decision variables x_{ij}. We know that vectorization [26][36] of a matrix is a linear transformation that converts the matrix into a column vector. So, let $vec\,(X)$, the column vector $mn \times 1$ obtained by stacking the columns of the matrix X one on top of the other:

$$vec(X) = [x_{1,1}, \ldots, x_{1,m}, \ldots, x_{1,n}, \ldots, x_{m,n}]^T . \tag{205}$$

We also know that vectorisation is frequently used with the Kronecker product to express matrix multiplication as a linear transformation in matrices. In particular.

$$\begin{aligned} &vec(ABC) = (C^T \otimes A)vec(B)vec(ABC) = (I^T \otimes AB)vec(C) = \\ &(C^T B^T \otimes I)vec(A)vec(AB) = (I^T \otimes A)vec(B) = (B^T \otimes I)vec(A). \end{aligned} \tag{206}$$

If we apply vectorization as a linear sum, the matrix vectorization operation can be written in terms of a linear sum. Let e_i be the nth canonical base vector for n dimensional space, that is:

$$e_i = [0, \ldots, 0, \ldots, 0, \ldots, 1, \ldots, 0, \ldots, 0]^T . \tag{207}$$

Let B_i a block matrix $mn \times m$ defined as follows:

$$B_i = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ I_m \\ 0 \\ \vdots \\ 0 \end{bmatrix} = e_i \otimes I_m. \tag{208}$$

B_i consists of n block matrices of size $m \times m$, stacked in columns, and all these matrices are all zero except the ith, which is an identity matrix $m \times mI_m$.

Then the vectorized version of X can be expressed as follows:

$$vec(X) = \sum_{i=1}^{n} B_i X e_i. \tag{209}$$

The multiplication of X by e_i extracts the ith column, while the multiplication by B_i places it in the desired position in the final vector. Alternatively, the linear sum can be expressed using the Kronecker product:

$$vec(X) = \sum_{i=1}^{n} (e_i \otimes I_m) X e_i = \sum_{i=1}^{n} (e_i \otimes I_m) X^T. \tag{210}$$

With $Xe_i = X^T$. Where $^{\mathrm{T}}$ is the transpose.

We can simplify our objective function to be implemented in quantum.

0.15.1 Vectorization form of our formulation

The formulation of quantum annealing has been described in countless articles[22] [40][37] as one of the combinatorial optimisation algorithms solving approaches. Moreover, this formulation is the basis of the new techniques called to be the flagship of quantum computation. Our QAOA/VQE formulation takes after reference [38], showing the detailed development for our case. Let the vector Z of the decision variables x_{ij} with $Z \in 0, 1^N$ and $N = n(n+1)$:

$$Z = [x_{01}, x_{02}, x_{03}, \ldots, x_{10}, x_{12}, x_{13}, \ldots, x_{n(n-1)}]^T. \tag{211}$$

And applying equation (234) and (226) taking into account that the decision variable is now Z , we arrive at equation (237).

$$H = W^T Z + A\sum_{i=1}^{n}\left(1 - \left(e_{in}^T\right) Z\right)^2 + A\sum_{i=1}^{n}\left(1 - v_i^T Z\right)^2 + A\left(k - \left(e_{0n}\right)^T Z\right)^2 + A\left(k - v_0^T Z\right)^2. \tag{212}$$

With:

$$W_{ij} = d_{ij} + \gamma\frac{\left(\tau_{i-}\tau_j\right)^2}{d_{\max} - d_{\min}}. \tag{213}$$

Now, let's develop the resultant equation.

$$\begin{aligned} H = {} & W^T Z + A\sum_{i=1}^{n}\left(\left(\left(e_{in}^T\right) Z\right)^2 - 2\left(e_{in}^T\right) z + 1\right) + A\sum_{i=1}\left(\left(v_i^T Z\right)^2 - 2v_i^T Z + 1\right) \\ & + A\left[\left(\left(e_{0n}\right)^T Z\right)^2 - 2k\left(e_{0n}\right)^T Z + k^2\right] + A\left[\left(v_0^T Z\right)^2 - 2k\left(v_0^T Z\right) + k^2\right], \end{aligned} \tag{214}$$

$$\begin{aligned} H = {} & W^T Z + A\sum_{i=1}^{n}\left[\left(e_{in}^T\right) Z\right]^2 + \left[v_i^T Z\right]^2 - 2A\left[\left(e_{in}^T\right) + v_i^T\right] Z + 2A + A[\left[\left(e_{0n}^T\right) + v_0^T\right]^2 Z \\ & - 2AKe_{0n}^T + v_0^T Z + 2Ak^2]. \end{aligned}$$

Regrouping the terms in the quadratic formulation $Z^T QZ + g^T Z \ + C$:

$$\begin{aligned} H = {} & A\sum_{i=1}^{n}\left[\left(e_i \otimes I_n\right)^2 Z^2 + \left[v_i^T\right]^2 Z^2\right] + w - 2A\sum_{i=1}^{n}\left[\left(e_i \otimes I_n^T\right) + v_i^T\right] \\ & - 2Ak\left[\left(e_0 \otimes 1_n\right)^T + v_0^T\right] + 2An + 2Ak^2. \end{aligned} \tag{215}$$

With the variables Q, g and C:

$$Q = \sum_{i=1}^{n}\left[\left(e_i \otimes I_n\right)^2 + \left[v_i^T\right]^2\right] = \sum_{i=1}^{n}[e_i \otimes I_n e_i \otimes I_n^T + [v_i v_i^T]]. \tag{216}$$

$$g = w - 2A\sum_{i=1}^{n}\left[\left(e_i \otimes I_n^T\right) + v_i^T\right] - 2Ak\left[\left(e_0 \otimes 1_n\right)^T + v_0^T\right]. \tag{217}$$

$$C = +2An + 2Ak^2. \tag{218}$$

After:

Section 11.2.2 The algebraic approach of the SWP formulation

We are looking for a more compact formulation to make it easier to codify in quantum, and to achieve this, we vectorise the decision variables x_{ij}. We know that vectorisation [26, 36] of a matrix is a linear transformation that converts the matrix into a column vector. So, let vec (X), the column vector $mn \times 1$ obtained by stacking the columns of the matrix X one on top of the other:

$$\text{vec}(X) = [x_{1,1}, \ldots, x_{1,m}, \ldots, x_{1,n}, \ldots, x_{m,n}]^T . \tag{219}$$

We also know that vectorisation is frequently used with the Kronecker product to express matrix multiplication as a linear transformation in matrices. In particular:

$$\text{vec}(ABC) = (C^T \otimes A)\text{vec}(B) = (I^T \otimes AB)\text{vec}(C). \tag{220}$$

$$\text{vec}(BC) = (I \otimes B)\text{vec}(C). \tag{221}$$

$$\text{vec}(CB) = (B^T \otimes I)\text{vec}(C). \tag{222}$$

If we apply vectorisation as a linear sum, the matrix vectorisation operation can be written in terms of a linear sum. Let e_i be the n^{th} canonical base vector for n dimensional space, that is:

$$e_i = [0, \ldots, 0, \ldots, 0, \ldots, 1, \ldots, 0, \ldots, 0]^T . \tag{223}$$

Let B_i a block matrix $nm \times m$ defined as follows:

$$B_i = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ I_m \\ 0 \\ \vdots \\ 0 \end{bmatrix} = e_i \otimes I_m. \tag{224}$$

B_i consists of n block matrices of size $m \times m$, stacked in columns, and all these matrices are all zero except the i^{th}, which is an identity matrix $m \times mI_m$.

Then the vectorised version of X can be expressed as follows:

$$\text{vec}(X) = \sum_{i=1}^{n} B_i X e_i. \tag{225}$$

The multiplication of X by e_i extracts the i^{th} column, while the multiplication by B_i places it in the desired position in the final vector. Alternatively, the linear sum can be expressed using the Kronecker product:

$$\text{vec}(X) = \sum_{i=1}^{n} (e_i \otimes I_m) X e_i = \sum_{i=1}^{n} (e_i \otimes I_m) X^T. \tag{226}$$

With $Xe_i = X^T$. Where $^{\text{T}}$ is the transpose.

Now, let us define Z with n^2 dimensions as follows:

$$Z = (X_{11}X_{12}X_{13} \ldots X_{1n}X_{21}X_{22} \ldots X_{2n} \ldots X_{nn})^T. \tag{227}$$

We can simplify our objective function to be implemented in quantum algebraically. Let us demonstrate that the following expression holds:

$$\sum_{i=1}^{n}(\sum_{j=1}^{n} X_{ij} - 1)^2 = \sum_{i=1}^{n}(e_i \otimes 1_n^T Z - 1)^2. \tag{228}$$

Thus, we can say:

$$(e_i \otimes 1_n^T)Z = \sum_{j=1}^{n} X_{ij}. \tag{229}$$

With

$$e_i = (0 \dots 0 \dots 1 \dots 0 \dots 0), \tag{230}$$

and

$$1_n^T = (1 \dots 1), \tag{231}$$

both have dimension n.

Let us write down $e_i \otimes 1_n^T$ taking in account all the definitions.

$$\begin{aligned} e_i \otimes 1_n^T &= (0 \cdot (1 \dots 1) \dots 1 \cdot (1 \dots 1) \dots 0 \cdot (1 \dots 1) \dots) \\ &= (0000 \dots 0000 \dots 1111 \dots 0000 \dots 0000), \end{aligned} \tag{232}$$

According to the equation (227), we can calculate the following expression as:

$$\begin{aligned} &(e_i \otimes 1_n^T) \cdot Z = 0 \cdot X_{11} + 0 \cdot X_{12} + \dots 0 \cdot X_{1n} \dots + \dots 1 \cdot X_{i1} + 0 \cdot X_{i2} + \dots + 1 \cdot X_{in} + 0 \cdot X_{in+1} + \dots \\ &= X_{i1} + + X_{in} = \sum_{j=1}^{n} X_{ij}. \end{aligned} \tag{233}$$

In the end, we see that we arrive at the expression (229) we want. So, now we only have to substitute it into our simplified SWP formulation (196).

0.15.2 Vectorisation form of our formulation

This section will develop the vectorisation form of the SWP. Let Z the vector of the decision variables X_{ij} with $Z \in \{0,1\}^N$ and $N = n(n-1)$:

$$Z = [X_{01}, X_{02}, X_{03}, \dots, X_{10}, X_{12}, X_{13}, \dots, X_{n(n-1)}]^T, \tag{234}$$

In addition, let us denote $v_i = (Z'_{i'j})_{i'j}$ with:

$$Z'_{i'j} = \begin{cases} 1 & \text{if} \quad j = i \quad \text{for any} \quad i' \\ 0 & \text{otherwise,} \end{cases} \tag{235}$$

and let us denote $v_0 = (Z''_{ij})$ with:

$$Z''_{ij} = \begin{cases} 1 & \text{if} \quad j = 0 \\ 0 & \text{otherwise.} \end{cases} \tag{236}$$

Now applying equations (234), (226), (235) and (235) into the simplified SWP formulation (196), we arrive at the next equation.

$$H = W^T Z + A\sum_{i=1}^{n}\left(1 - \left(e_i \otimes I_n^T\right) Z\right)^2 + A\sum_{i=1}^{n}\left(1 - v_i^T Z\right)^2 + A\left(k - (e_0 \otimes I_n)^T Z\right)^2 + A\left(k - v_0^T Z\right)^2. \tag{237}$$

With:

$$W_{ij} = d_{ij} + \gamma\frac{(\tau_{i-}\tau_j)^2}{d_{\max} - d_{\min}}. \tag{238}$$

Now, let's develop the resultant equation.

$$H = W^T Z + A\sum_{i=1}^{n}\left(\left(\left(e_i \otimes I_n^T\right) Z\right)^2 - 2\left(e_i \otimes I_n^T\right) Z + 1\right) + A\sum_{i=1}^{n}\left(\left(v_i^T Z\right)^2 - 2v_i^T Z + 1\right)$$
$$+ A\left[\left((e_0 \otimes I_n)^T Z\right)^2 - 2k\,(e_0 \otimes I_n)^T Z + k^2\right] + A\left[\left(v_0^T Z\right)^2 - 2k\left(v_0^T Z\right) + k^2\right],$$

$$H = W^T Z + A\sum_{i=1}^{n}\left[\left(e_i \otimes I_n^T\right) Z\right]^2 + \left[v_i^T Z\right]^2 - 2A\left[\left(e_i \times I_n^T\right) + v_i^T\right] Z + 2A + A[\left[\left(e_0 \otimes I_n^T\right) + v_0^T\right]^2 Z$$
$$- 2AK(e_0 \otimes I_n^T) + v_0^T Z + 2Ak^2]. \tag{239}$$

Regrouping the terms in the quadratic formulation $Z^T QZ + g^T Z\ + C$:

$$H = A\sum_{i=1}^{n}\left[(e_i \otimes I_n)^2 Z^2 + \left[v_i^T\right]^2 Z^2\right] + w - 2A\sum_{i=1}^{n}\left[\left(e_i \otimes I_n^T\right) + v_i^T\right]$$
$$- 2Ak\left[(e_0 \otimes 1_n)^T + v_0^T\right] + 2An + 2Ak^2. \tag{240}$$

With the variables Q, g and C:

$$Q = \sum_{i=1}^{n}\left[(e_i \otimes I_n)^2 + \left[v_i^T\right]^2\right] = \sum_{i=1}^{n}[(e_i \otimes I_n)(e_i \otimes I_n^T) + [v_i v_i^T]]. \tag{241}$$

$$g = w - 2A\sum_{i=1}^{n}\left[\left(e_i \otimes I_n^T\right) + v_i^T\right] - 2Ak\left[(e_0 \otimes 1_n)^T + v_0^T\right]. \tag{242}$$

$$C = +2An + 2Ak^2. \tag{243}$$

From this point, we can use any solver based on annealing to solve we formulation. Then, if we want to translate it into the gate-based computer, we will only need to map it to the Ising model and select which solver could be adequate.

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