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Vladik Kreinovich The University of Texas at El Paso, vladik@utep.edu

Oscar Galindo *The University of Texas at El Paso*, ogalindomo@miners.utep.edu

Olga Kosheleva The University of Texas at El Paso, olgak@utep.edu

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# Review Many Known Quantum Algorithms Are Optimal: Symmetry-Based Proofs

Vladik Kreinovich<sup>®</sup>, Oscar Galindo, and Olga Kosheleva<sup>®</sup>

University of Texas at El Paso; vladik@utep.edu, ogalindomo@miners.utep.edu, olgak@utep.edu \* Correspondence: vladik@utep.edu (V.K.)

- Abstract: Many quantum algorithms have been proposed which are drastically more efficient that
- <sup>2</sup> the best of the non-quantum algorithms for solving the same problems. A natural question is: are
- these quantum algorithms already optimal in some reasonable sense or they can be further
- improved? In this paper, we review recent results showing that many known quantum algorithms
- 5 are actually optimal. Several of these results are based on appropriate invariances (symmetries).
- 6 Keywords: quantum computing; optimal algorithms; invariance; symmetry

# 7 1. Formulation of the Problem

8 1.1. Need for quantum computing

Modern computers are extremely fast, but still there are many practical problem that require even faster computations. For example, high-performance computers, after computing for several hours, help us come up with a reasonably accurate prediction of tomorrow's weather. It turns out that similar algorithms can help us predict where a tornado will turn in the next 15 minutes – but this computation also requires several hours on modern computers, too late for this prediction to be practically useful.

How can we make computer faster? There are many interesting engineering ideas how to do it, but there is also a fundamental limitation – that, according to relativity theory, nothing can travel faster than the speed of light c = 300000 km/sec; see, e.g., [9, 33]. For a usual laptop which is about 30 cm in size this means that it takes  $10^{-9}$  seconds – 1 nanosecond – for a signal to go from one side of the laptop to the other. During this time, a usual 4 GHz laptop already performs 4 operations. From this viewpoint, the only way to make computer substantially faster is to make them significantly smaller.

Already in modern computers, each memory cell is very small – up to 10 nanometers (nm), comparable with the nm size of a single molecule. As a result, each cell contains several thousand molecules. If we make cells even smaller, their size will be comparable with the size of a single molecule. At such sizes, we can no longer use Newtonian mechanics, we need to take into account that the micro-world is governed by different equations – the equations of quantum physics [9,33]. Computing on such a level is known as *quantum computing* 

# 1.2. Need for quantum algorithms

One of the important challenges of quantum computing is that in quantum physics – in contrast to Newtonian physics – the results are non-deterministic: we can only predict the probabilities of different outcomes. The classical example of such a probabilistic uncertainty is radioactivity, one of the first observed quantum phenomena: we can predict the probability that an atom will decay – and thus, accurately predict the amount of radiation – but we cannot predict at which moment of time each individual atom will decay.

Because of this probabilistic uncertainty, we cannot simply use the usual algorithms on the micro-level: we will then, in general, get different results with different probabili-

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- ties, while in computations, we usually want to come up with a single result. Thus, we need to develop new algorithms.
- 41 1.3. Quantum algorithms: successes
- Quantum algorithms have indeed been successfully developed for solving all fundamental aspects of computation needs; see, e.g., [26,35]. Not only the resulting algorithms
  produce deterministic (or almost deterministic) results, many of them compute these
  results even faster than the best non-quantum algorithms for solving the same problems.
- To briefly describe these successes, let us recall what are the fundamental computation needs. To enumerate these needs, let us recall what we humans want.
- We want to understand how the world works, to predict what will happen this is,
   crudely speaking, what science is about. For example, we want to predict where
   the tornado will turn.
- We also want to understand how can we improve the situation this is, crudely speaking, what engineering is about. For example, how can we make tornadoes
- change their course? How can we make houses less vulnerable to tornadoes?
- Finally, we want to communicate or not with others, so we need to develop techniques for communication only with the intended folks.
- Quantum algorithms are useful in solving all these main problems of science and engi neering:
- In the general prediction problem, we need to find a model that fits all the ob-. servations. In a usual engineering problem, we need to find a design and/or a 59 control that satisfies a given specification. In most of these problems, once we have 60 a model, a design, or a control, it is computationally feasible to check whether this 61 model, design, etc. satisfies the given specifications, it is searching for a satisfactory 62 model, design, etc. which is computationally intensive. There exists a quantum 63 algorithm that speeds us such a search. This algorithm – proposed by Lev Grover – finds an element in an unsorted list in time  $\sqrt{n}$ , which is much faster than n steps 65 needed in the non-quantum case [16,17,26,35]. Quantum algorithms are also useful in optimization. 67
- An additional way to speed up computations comes from the fact that in prediction problems such as predicting tomorrow's weather to be on the safe side, we take into account today's meteorological data in all nearby locations, even though most of this data is actually irrelevant. To speed up computations, it is desirable to decide which inputs and relevant and which are not. In this analysis, quantum computing also help namely, we can use Deutsch-Jozsa algorithm; see, e.g., [26,35].
- Finally, special algorithms have been developed for quantum communications –
   which is especially important since it is known that by using quantum computing,
- we can break the RSA encryption (and similar encryptions) and these encryptions
- are behind most of the current computer security techniques [26,29,30,35].

# 78 1.4. Quantum algorithm: remaining challenges and what we cover in this paper

As we have mentioned, the existing quantum algorithms work very well. However, a next natural question is: are these algorithms optimal – in some reasonable sense – or we can do better? In this paper, we overview several results that show that many quantum algorithms are indeed optimal. These proofs are based on the invariance (symmetry) techniques.

Of course, these results are just the beginning of the study. Quantum computing is a developing field, many new algorithm are being developed all the time, and, as quantum computers will become practical, this will definitely further boost the invention of new algorithms. We hope that the results reviewed in this paper will help researchers to analyze the optimality of other quantum algorithms as well. We start, in Section 2, with a brief reminder of the quantum basics – basics which are needed to understand the main ideas behind the existing quantum algorithms and behind the proofs of their optimality. In Section 3, we describe the relation between optimality – that we want to prove – and symmetries – i.e., invariance with respect to different transformations. After that, we present the proofs of optimality of different quantum algorithms for quantum data processing: Grover's algorithm in Section 4, parallel-related teleportation algorithm in Section 5, and an optimization-related quantum annealing algorithm in Section 6.

It should be mentioned that other quantum algorithms are also known to be optimal: optimality of Deutsch-Josza algorithm is proven in [20] Deutsch-Josza, and optimality of quantum communication algorithm in [15].

#### 101 2. Quantum basics

102 2.1. Quantum states

In "classical" (= non-quantum) physics, each object, each system can be in different states s, s', ... In quantum physics, such classical state are denoted by  $|s\rangle$ ,  $|s'\rangle$ , etc. An unusual feature of quantum physics is that, in addition to such states, we can also have *superpositions* of such states, i.e., states of the type

$$c \cdot |s\rangle + c' \cdot |s'\rangle + \dots, \tag{1}$$

where  $c, c', \ldots$  are complex numbers for which

$$|c|^2 + |c'|^2 + \ldots = 1,$$
(2)

where, as usual, for a complex number  $c = a + b \cdot i$ , its modulus |c| is defined as  $|c| = \sqrt{a^2 + b^2}$ . If the system is in the state (1), and we use a classical measurement instrument to measure the state, then:

• we will get state *s* with probability  $|c|^2$ ,

• we will get state s' with probability  $|c'|^2$ , etc.

<sup>108</sup> These probabilities should add up to 1, which explains the formula (2).

In particular, a quantum analogue of a *bit* (binary digit) – i.e., of a system that can be in two different states 0 and 1 – is a *quantum but* (*qubit*, for short) that can be in any state

$$c_0 \cdot |0\rangle + c_1 \cdot |1\rangle, \tag{3}$$

where  $c_0$  and  $c_1$  are complex numbers for which

$$|c_0|^2 + |c_1|^2 = 1. (4)$$

In the state (3), the probability that we will observe 0 is  $|c_0|^2$ , and the probability that we will observe 1 is equal to  $|c_1|^2$ .

Similarly, for a 2-bit system – which in classical physics, can be in 4 different states 00, 01, 10, and 11 – a general quantum state is equal to

$$c_{00} \cdot |00\rangle + c_{01} \cdot |01\rangle + c_{10} \cdot |10\rangle + c_{11} \cdot |11\rangle.$$
(5)

In principle, we can have general complex numbers. Interestingly, in most quantum algorithms, only real-valued coefficients  $c, c', \ldots$  are used. An explanation of this is provided, e.g., in [2].

#### 114 2.2. Quantum measurements

In general, if we have *n* classical states  $s_1, \ldots, s_n$ , and we want to detect, in a quantum state  $\sum \alpha_i \cdot s_i$ , which of these states we are in, we get each  $s_i$  with probability  $|\alpha_i|^2$  – and once the measurement process detects the state  $s_i$ , the actual state turns into  $s_i$ . Instead of the classical states  $s_1, \ldots$ , we can use any other sequence of states  $s'_i = \sum_j t_{ij} \cdot s_j$ , as long as they are *orthonormal* (= orthogonal and normal) in the sense that:

• for each *i*, we have  $||s'_i||^2 = 1$ , where  $||s'_i||^2 \stackrel{\text{def}}{=} \sum_i |t_{ij}|^2$  (normal), and

• for each *i* and *i'*, we have  $s'_i \perp s'_{i'}$ , i.e.,  $\langle s'_i | s'_{i'} \rangle = 0$ , where  $\langle s'_i | s'_{i'} \rangle \stackrel{\text{def}}{=} \sum_j t_{ij} \cdot t^*_{i'j}$ 

#### 122 (orthogonal).

In this case, if we have a state  $\sum \alpha'_i \cdot s'_i$ , then with probability  $|\alpha'_i|^2$ , the measurement result is  $s'_i$  and the state turns into  $s'_i$ .

In general, instead of a sequence of orthogonal vectors, we can have a sequence of orthogonal linear spaces  $L_1, L_2, \ldots$  where  $L_i \perp L_j$  means that  $s_i \in L_i$  and  $s_j \in L_j$ implies  $s_i \perp s_j$ . In this case, every state *s* can be represented as a sum  $s = \sum s_i$  of the vectors  $s_i \in L_i$ . As a result of the measurement, with probability  $||s_i||^2$ , we conclude that the state is in the space  $L_i$ , and the original state turns into a new state  $s_i / ||s_i||$ .

#### 130 2.3. Composite systems

A 2-bit system is the simplest example of a *composite system*, when we consider two independent subsystems as a single system. In classical physics, if the first system is in one of the states s, s', ..., and the second system is in one of the states t, t', ..., then the set of all possible states of the composite system is the set of all the pairs (s, t) – which is also known as a *Cartesian product*  $S \times T$  of the set  $S = \{s, s', ...\}$  of possible states of the first system and the set  $T = \{t, t', ...\}$  of possible states of the second system.

In quantum physics, if the first system was in the general quantum state (1) and the second system is in a similar quantum state

$$a \cdot |t\rangle + a' \cdot |t'\rangle + \dots,$$
 (6)

then the state of the composite system – known as the *tensor product* of the states (1) and (6):

$$(c \cdot |s\rangle + c' \cdot |s'\rangle + \ldots) \otimes (a \cdot |t\rangle + a' \cdot |t'\rangle + \ldots), \tag{7}$$

is equal to

$$c \cdot a \cdot |s, t\rangle + c \cdot a' \cdot |s, t'\rangle + \ldots + c' \cdot a \cdot |s', t\rangle + c' \cdot a' \cdot |s', t'\rangle + \ldots$$
(8)

In particular, for classical states, e.g., when c = a = 1 and  $c' = \ldots = a' = \ldots = 0$ , we get  $|s\rangle \otimes |t\rangle = |s, t\rangle$ .

*Comment.* It should be mentioned that the transformation of two states of subsystems into a single state of a composite system is linear in each of the values c, c', ..., and a, a',... This linearity comes from the need to make sure that for the independent subsystems, the probability of observing (s, t) is equal to the product of the probabilities of observing s and t. This is true for the formula (8), when this equality follows from the fact that for every two complex numbers c and a, we have  $|c \cdot a|^2 = |c|^2 \cdot |a|^2$ .

#### 145 2.4. How quantum states change

States may change with time. In quantum physics, all changes are linear – for the same reason why composition of two states is linear. In other words, each state

$$c_1 \cdot |s_1\rangle + \ldots + c_n \cdot |s_n\rangle \tag{9}$$

is transformed into the state

$$c_1' \cdot |s_1\rangle + \ldots + c_n' \cdot |s_n\rangle, \tag{10}$$

for which

$$c'_i = \sum_{j=1}^n T_{ij} \cdot c_j \tag{11}$$

for some coefficient  $T_{ij}$ . The matrix  $T = ||T_{ij}||$  is *unitary*:  $T^{\dagger}T = TT^{\dagger} = I$ , where I is the unit matrix, and  $T_{ij}^{\dagger} \stackrel{\text{def}}{=} T_{ji}^{*}$ , where  $c^{*}$  denotes *complex conjugate*:  $(a + b \cdot i)^{*} \stackrel{\text{def}}{=} a - b \cdot i$ .

Note that every such transformation is reversible: once we apply the transformation T, we can then apply the transformation  $T^{\dagger}$  and, due to the property  $T^{\dagger}T = I$ , get back the original state.

For 1-qubit systems, one of such transformation is *Hadamard transformation H* for which

$$H(|0\rangle) = |0'\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle; \quad H(|1\rangle) = |0'\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} \cdot |0\rangle - \frac{1}{\sqrt{2}} \cdot |1\rangle. \tag{11}$$

#### 151 2.5. How functions are represented in quantum algorithms

In this section, we will deal only with functions  $y = f(x_1, ..., x_n)$  of boolean (0-1) variables – since these are the basic functions implemented by different "gates", of which computers are built. We cannot simple represent these functions as transforming *n* boolean values  $x_i$  into a single boolean value *y*, since such transformation is, in general, irreversible. For example, for the "and"-function  $y = f(x_1, x_2) = x_1 \& x_2$ , if we know that y = 0, we cannot uniquely reconstruct the original pair  $(x_1, x_2)$ :

- we could have  $(x_1, x_2) = (0, 0)$ ,
- we could have  $(x_1, x_2) = (0, 1)$ , or
- we could have  $(x_1, x_2) = (1, 0)$ .

To make the corresponding transformation reversible, a function  $y = f(x_1, ..., x_n)$  is represented as

$$T_f(x_1, \dots, x_n, y) = (x_1, \dots, x_n, y \oplus f(x_1, \dots, x_n)),$$
(12)

where  $a \oplus b$  is exclusive "or" – or, what is the same, addition modulo 2, an operation for which  $0 \oplus 0 = 1 \oplus 1 = 0$  and  $0 \oplus 1 = 1 \oplus 0 = 1$ . One can check that thus defined transformation is reversible: namely, if we apply the transformation  $T_f$  twice, we get back the original state  $(x_1, ..., x_n, y)$  – simply because  $a \oplus a = 0$  for all a.

Comment. While this is the prevailing representation of functions in quantum computing,
 it should be mentioned in some cases, a different representation is preferable; see,
 e.g., [11].

## **3. Relation Between Optimality and Invariance (Symmetry)**

#### 169 3.1. What is invariance (symmetry)

In many cases, there are some natural transformations that does not change the 170 system. This "not changing" is called *invariance*. For example, suppose that we have 171 an unsorted list, and we are looking for an element with a ceratin property in this list. 172 For convenience, we can denote one of the list's elements by  $s_1$ , another one by  $s_2$ , 173 etc., but in this problem, it does not matter which element is called  $s_1$ , which  $s_2$ , etc. – 1 74 any permutation  $\pi: \{1, \ldots, n\} \to \{1, \ldots, n\}$  would retain the problem. Thus, in this 175 problems, permutations are invariances. In other problems, we will have other natural 176 invariances. 177

In physics, invariance is called *symmetry* – since it naturally generalizes geometric invariances (symmetries); see, e.g., [33?].

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#### 180 4. What does "optimal" mean

Usually, when we talk about "optimal", we mean that on the set of all alternatives  $A, A', \ldots$ , there is an *objective function* describing the quality of different alternatives, and we are looking for the alternative A with the largest (or sometimes the smallest) value of this objective function. For example, when we select between different quantum – i.e., in general, probabilistic – algorithms for solving a given problem, we may want to maximize that probability f(A) that the algorithm A will lead to the desired solution.

However, this is a somewhat simplified description of what we usually mean by 187 optimality. Often, there are several alternatives  $A_1$ ,  $A_2$ , etc., with the exact same largest 1 88 value  $f(A_1) = f(A_2) = \dots$  of the objective function. In this case, we can use this 189 non-uniqueness to optimize something else. For example, in the above case, we can 190 minimize the average time needed for the algorithm to finish. This means, in effect, that 1 91 the original optimality criterion is not final, we can modify it and come up with a new, 1 92 more complex criterion according to which an alternative A is better than the alternative 193 A' – we will denote it by A < A'– if: 1 94

• either f(A') < f(A)

• or we have f(A) = f(A') and also g(A') < g(A) for the additional objective function g(A).

If this still leads to several equally optimal alternatives, we can use this non-uniqueness
to optimize something else – until we get to the *final* optimality criterion, for which there
is exactly one optimal alternative.

To simplify the analysis, it is useful to ignore all these objective functions f(A), g(A), etc., and to only consider what really matters: for each pair (A, A'), according to this criterion:

- when we have A' better than A (A < A'),
- when we have A better than A'(A' < A), and
- when A and A' are equally good; we will denote it by  $A \sim A'$ .

In precise terms, by an *optimality criterion* that the set A of all alternatives, we mean a pair of relations < and  $\sim$  with the following natural properties:

- if A < A' and A' < A'', then A < A'';
- if A < A' and  $A' \sim A''$ , then A < A'';
- if  $A \sim A'$  and A' < A'', then A < A'';
- if  $A \sim A'$  and  $A' \sim A''$ , then  $A \sim A''$ ;
- if  $A \sim A'$ , then  $A' \sim A$ ; and
- if A < A', then we cannot have  $A \sim A'$ .

This pair of relations is known as a *pre-order*: it is similar to order, with the main difference that we can have  $A \sim A'$  without having A = A'.

An alternative  $A_{opt}$  is called *optimal* if for every other alternative A, we have  $A < A_{opt}$  or  $A \sim A_{opt}$ . An optimality criterion is called *final* if there is exactly one alternative which is optimal with respect to this criterion.

4.1. For invariant criteria, optimal alternative is also invariant

In many cases, there exists a reversible transformation  $T : A \to A - e.g.$ , permutation – which does not change the situation. In this case, it makes sense to require that this transformation will not change which alternative is better. In precise terms, we say that an optimality criterion is *T-invariant* if the following conditions are satisfied:

• if A < A', then T(A) < T(A');

• if  $A \sim A'$  then  $T(A) \sim T(A')$ .

<sup>227</sup> Many results from this paper used the following lemma (see, e.g., [25]):

**Lemma.** For every final *T*-invariant optimality criterion, its optimal alternative  $A_{opt}$  is also *T*-invariant, i.e.,  $T(A_{opt}) = A_{opt}$ . **Proof.** The fact that  $A_{opt}$  means that for every  $A \in A$ , we have either  $A < A_{opt}$ or  $A \sim A_{opt}$ . In particular, this is true for  $T^{-1}(A)$ , i.e., either  $T^{-1}(A) < A_{opt}$  or  $T^{-1}(A) \sim A_{opt}$ . Due to *T*-invariance, we can conclude that either  $A < T(A_{opt})$  or  $A \sim T(A_{opt})$ . This is true for every alternative *A*, which means that the alternative  $T(A_{opt})$  is also optimal. However, the optimality criterion is final, which means that there is only one optimal criterion. Thus, indeed,  $T(A_{opt}) = A_{opt}$ . The lemma is proven.

<sup>237</sup> Due to this lemma, if the optimality criterion is *T*-invariant, then to find optimal <sup>238</sup> alternative, it is sufficient to find *T*-invariant alternatives. Let us start checking optimality <sup>239</sup> with Grover's algorithm.

#### 240 5. Grover's Algorithm Is Optimal

241 5.1. Formulation of the problem

We are solving the following problem. We have a list of elements  $e_1, \ldots, e_n$ . We have an algorithm f(i) that, given an element  $e_i$  – i.e., in effect, the index i – checks whether this element has the desired property. We want to find an element that has this property. For simplicity, we will consider the case when there is exactly one such element  $i_0$ .

Let us describe this problem is quantum computing-related terms. What we want is an index  $i_0$  of the desired element. In quantum computing terms, this means that we want to end up in a state  $|i_0\rangle$ . As we have mentioned, in general, quantum processes are probabilistic, so instead of the exact state  $|i_0\rangle$ , we may end up in a superposition state:

$$c_{1} \cdot |1\rangle + \ldots + c_{i_{0}-1} \cdot |i_{0}-1\rangle + c_{i_{0}} \cdot |i_{0}\rangle + c_{i_{0}+1} \cdot |i_{0}+1\rangle + \ldots + c_{n} \cdot |n\rangle.$$
(13)

In quantum terms, the algorithm that checks whether a given element has the desired property has the form  $T_f(|i, y\rangle) = |i, y \oplus f(x)\rangle$ , i.e.:

• for  $i \neq i_0$ , we have  $T_f(|i,0\rangle) = |i,0\rangle$  and  $T_f(|i,1\rangle) = |i,1\rangle$ , while

• for  $i = i_0$ , we have  $T_f(|i_0, 0\rangle) = |i_0, 1\rangle$  and  $T_f(|i_0, 1\rangle) = |i_0, 0\rangle$ .

In terms of the Hadamard states  $|0'\rangle$  and  $|1'\rangle$ , we get the following:

- for  $|0'\rangle$ , for all *i*, we have  $T_f(|i\rangle \otimes |0'\rangle) = |i\rangle \otimes |0'\rangle$ ;
- for  $|1'\rangle$ , for all  $i \neq i_0$ , we have  $T_f(|i\rangle \otimes |1'\rangle) = |i\rangle \otimes |1'\rangle$ , while for  $i = i_0$ , we have  $T_f(|i_0\rangle \otimes |1'\rangle) = -|i_0\rangle \otimes |1'\rangle$ .

So, for  $|0'\rangle$ , nothing changes, and for  $|1'\rangle$ , the additional bit  $|1'\rangle$  remains the same, but the previous state (13) changes to:

$$c_{1} \cdot |1\rangle + \ldots + c_{i_{0}-1} \cdot |i_{0}-1\rangle - c_{i_{0}} \cdot |i_{0}\rangle + c_{i_{0}+1} \cdot |i_{0}+1\rangle + \ldots + c_{n} \cdot |n\rangle.$$
(14)

Let us denote this transformation from (13) to (14) by U.

Our goal is to start with some state, and, by applying this transformation U and some other transformation(s) S, eventually come up with the desired element  $i_0$ .

#### 257 5.2. Invariance (symmetry): reminder

As we have mentioned earlier, in this problem, the natural invariances (symmetries) are invariances with respect to all possible permutations  $\pi : \{1, ..., n\} \rightarrow \{1, ..., n\}$ . It is therefore reasonable to require that our optimality criterion is invariant with respect to all permutations. Due to the above Lemma, this implies that the optimal algorithm should also be permutation-invariant, in particular:

- that the initial state should be permutation-invariant, and
- that all transformations *S* should be permutation-invariant.

265 5.3. Towards the optimal algorithm: which transformations are permutation-invariant?

The fact that the initial state is permutation-invariant means that  $c_i = c_{i'}$  for all *i* and i' – since every two indices *i* and *i'* can be obtained from each other by an appropriate permutation. Thus, the initial state must have the form

$$c_1 \cdot |1\rangle + \ldots + c_1 \cdot |n\rangle, \tag{14}$$

for some  $c_1$ . Due to the normalization requirement (2), we have  $|c_1| = 1/\sqrt{n}$ . In quantum mechanics, states differing by a constant are considered the same state, so we can simply take  $c_1 = 1/\sqrt{n}$ . Then the initial state takes the form:

$$\frac{1}{\sqrt{n}} \cdot |1\rangle + \ldots + \frac{1}{\sqrt{n}} \cdot |n\rangle.$$
(15)

<sup>266</sup> This is exactly the initial state of Grover's algorithm.

A general transformation is describes by a matrix  $S_{ij}$ . For this matrix, permutation invariance means that all the elements  $S_{ii}$  are equal to each other – similar argument as before. Let us denote this common value by *a*. Similarly, all the elements  $S_{ij}$  with  $i \neq j$  should also be equal to each other. Let us denote this common value by *b*. In these terms, the corresponding linear transformation transforms the vector  $c_i$  into a new vector

$$c'_i = a \cdot c_i + b \cdot \sum_{j \neq i} c_j. \tag{16}$$

This expression can be equivalently described as

$$c'_{i} = (a - b) \cdot c_{i} + b \cdot C, \text{ where } C \stackrel{\text{def}}{=} \sum_{j=1}^{n} c_{j}.$$
(17)

We want to make sure that this transformation preserved the fact that the probabilities add up to 1, i.e., that

$$\sum_{i=1}^{n} |c_j'|^2 = 1.$$
(18)

As we have mentioned earlier, it is sufficient to consider situations in which all the coefficients  $c'_i$  are real numbers. In this case,  $|c'_j|^2 = (c'_j)^2$ , and, due to (17), the condition (18) takes the form

$$(a-b)^{2} \cdot \left(\sum_{i=1}^{n} c_{i}^{2}\right) + 2 \cdot (a-b) \cdot b \cdot C^{2} + n \cdot b^{2} \cdot C^{2} = 1,$$
(19)

i.e., due to the fact that  $\sum_{i=1}^{n} c_i^2 = 1$ , that

$$(a-b)^{2} + (2 \cdot (a-b) \cdot b + n \cdot b^{2}) \cdot C^{2} = 1.$$
 (20)

This equality has to hold for all *C*, so we must have

$$2 \cdot (a-b) \cdot b + n \cdot b^2 = (2 \cdot (a-b) + n \cdot b) \cdot b = 0.$$
(21)

If b = 0, then  $a = \pm 1$ , so the transformation *S* either leaves the state unchanged or multiplies all the coefficient  $c_i$  by -1-i.e., in effect, also leaves the state unchanged. So, to get a non-trivial transformation, we need to take  $b \neq 0$ . In this case,  $2 \cdot (a - b) + n \cdot b = 0$ ;

since, without losing generality, we can take a - b = 1, we get b = -2/n. Thus, a = (a - b) + b = 1 - 2/n, and this transformation takes the form

$$c'_{i} = \left(1 - \frac{2}{n}\right) \cdot c_{i} - \frac{2}{n} \cdot \sum_{j \neq i} c_{j}.$$
(21)

<sup>267</sup> This is also exactly the transformation used in Grover's algorithm!

In what order shall we apply the algorithms U and S? If we apply U twice or Stwice, we get back the same state. Thus, it makes sense to apply these two algorithms interchangingly. The first application should be of U, since if we apply S to the initial state, we get the same state multiplied by a constant. Thus, we arrive at the following algorithm:

- we start with the initial state (15);
- then, we apply the transformation *U*;
- after that, we apply the transformation *S*;
- then, again we apply U; etc.

This is exactly Grover's algorithm. Thus, the Grover's algorithm is the only permutationinvariant one. And since the optimal algorithm must be permutation-invariant, we therefore conclude that Grover's algorithm is optimal.

#### <sup>280</sup> 6. Parallelization: Teleportation Algorithm Is Optimal

## 281 6.1. Need for parallelization

From the theoretical viewpoint, the fact that, e.g., Grover's algorithm is optimal is interesting. However, from the practical viewpoint, the fact that we cannot improve this algorithm constitutes a limitation on how fast we can compute – even if we use quantum computing. In problems in which the Grover's speed up is not sufficient, we need to use other ideas to achieve a further speedup.

To further speed up computations, a natural idea is to have several quantum computers working in parallel, so that each of them solves a part of the problem. This idea is similar to how we humans solve complex problems: if a task is too difficult for one person to solve – be it building a big house or proving a complex theorem – several people team up and together solve the task.

#### 292 6.2. Need for teleportation

To successfully collaborate, quantum computers need to exchange intermediate states of their computations. Here lies a problem: for complex problems, we would like to use computers located in different geographic areas, but a quantum state gets changed when it is sent far away.

Researchers have come up with a way to avoid this sending, called *teleportation*.
There exists a scheme for teleportation [3,26,27].

#### 299 6.3. What we do in this section

A priori, it is not clear how good is the current teleportation scheme: maybe there are other schemes which are faster (or better in some other sense)? In this section, we show that the existing teleportation scheme is, in some reasonable sense, unique – and, in this sense, is the best. This result first appeared in [12].

304 6.4. Standard quantum teleportation algorithm: reminder

305 6.4.1. Need for communication

At one location, we have a particle in a certain state; we want to send this state to some other location.

<sup>308</sup> Usually, the sender is denoted by *A* and the receiver by *B*. In communications, it is <sup>309</sup> common to call the sender Alice, and to call the receiver Bob. States corresponding to Alice are usually described by using a subscript *A*, and states corresponding to Bob are usually described by using a subscript *B*.

6.4.2. Communication is straightforward in classical physics but a challenge in quantumphysics

In classical (pre-quantum) physics, the communication problem has a straightforward solution: if we want to communicate a state, we measure all possible characteristics of this state, send these values to Bob, and let Bob reproduce the object with these characteristics. This is how, e.g., 3D printing works. This solution is based on the fact that in classical (non-quantum) physics we can, in principle, measure all characteristic of a system without changing it.

The problem is that in quantum physics, such a straightforward approach is not possible: as we have mentioned, in quantum physics, every measurement changes the state – and moreover, irreversibly deletes some information about the state. For example, if we start with a state  $\alpha_0 \cdot |0\rangle + \alpha_1 \cdot |1\rangle$ , all we get after the measurement is either 0 or 1, with no way to reconstruct the values  $\alpha_0$  and  $\alpha_1$  that characterize the original state. Since we cannot use the usual straightforward approach for communicating a state, we need to use an indirect approach. This approach is known as *teleportation*.

327 6.4.3. What we consider in this section

In this section, we consider the simplest possible quantum state – namely, the 328 quantum analogue of the simplest possible non-quantum state. In the non-quantum 329 case, a system can be in several different states. The state passing problem makes sense 330 only when the system can be in at least two different states – otherwise, if we know 331 beforehand what state we want to send, there is no need to send any information, Bob can 332 simply reproduce the known state. The simplest case when communication is needed is 333 when the number of possible states is as small as possible but still larger than 1 - i.e., the 334 case when the system can be in two different states. In the computer, such situation can 335 be naturally described if we associate these two possible states with 0 and 1. 336

In these terms, the problem is as follows:

Alice has a state

$$\alpha_0 \cdot |0\rangle + \alpha_1 \cdot |1\rangle \tag{22}$$

that she wants to communicate to Bob – a person at a different location.

• As a result of this process, Bob should have the same state.

340 6.4.4. Notations

Let us indicate states corresponding to Alice with a subscript *A*, and states corresponding to Bob with a subscript *B*. The state (22) is not exclusively Alice's and it is not exclusively Bob's, so to describe this state, we will use the next letter – letter *C*. In these terms, Alice has a state

$$\alpha_0 \cdot |0\rangle_C + \alpha_1 \cdot |1\rangle_C \tag{23}$$

that she wants to communicate to Bob.

<sup>342</sup> 6.4.5. Preparing for teleportation: an entangled state

To make teleportation possible, Alice and Bob prepare a special entangled state:

$$\frac{1}{\sqrt{2}} \cdot |0_A 1_B\rangle + \frac{1}{\sqrt{2}} \cdot |1_A 0_B\rangle. \tag{24}$$

<sup>343</sup> This state is a superposition of two classical states:

- the state  $0_A 1_B$  in which A is in state 0 and B is in state 1, and
- the state  $1_A 0_B$  in which A is in state 1 and B is in state 0.

6.4.6. What is the joint state of A, B, and C at the beginning of the procedure

In the beginning, the state *C* is independent of *A* and *B*. So, the joint state is a tensor product of the *AB*-state (24) and the *C*-state (23):

$$\frac{\alpha_0}{\sqrt{2}} \cdot |0_A \mathbf{1}_B \mathbf{0}_C\rangle + \frac{\alpha_1}{\sqrt{2}} \cdot |0_A \mathbf{1}_B \mathbf{1}_C\rangle + \frac{\alpha_0}{\sqrt{2}} \cdot |\mathbf{1}_A \mathbf{0}_B \mathbf{0}_C\rangle + \frac{\alpha_1}{\sqrt{2}} \cdot |\mathbf{1}_A \mathbf{0}_B \mathbf{1}_C\rangle.$$
(25)

#### 347 6.4.7. First stage: measurement

In the first stage of the standard teleportation algorithm, Alice performs a measurement procedure on the parts A and C which are available to her. In general, to describe the possible results of measuring a state s with respect to linear spaces  $L_i$ , we need to represent s as the sum

$$s = \sum s_i, \tag{26}$$

with  $s_i \in L_i$ .

In the standard teleportation algorithm, we perform the measurement with respect to the following four linear spaces  $L_i = L_B \otimes t_i$ , where  $L_B$  is the set of all possible linear combinations of  $|0\rangle_B$  and  $|1\rangle_B$ , and the states  $t_i$  have the following form:

$$t_{1} = \frac{1}{\sqrt{2}} \cdot |0_{A}0_{C}\rangle + \frac{1}{\sqrt{2}} \cdot |1_{A}1_{C}\rangle; \quad t_{2} = \frac{1}{\sqrt{2}} \cdot |0_{A}0_{C}\rangle - \frac{1}{\sqrt{2}} \cdot |1_{A}1_{C}\rangle;$$
  
$$t_{3} = \frac{1}{\sqrt{2}} \cdot |0_{A}1_{C}\rangle + \frac{1}{\sqrt{2}} \cdot |1_{A}0_{C}\rangle; \quad t_{4} = \frac{1}{\sqrt{2}} \cdot |0_{A}1_{C}\rangle - \frac{1}{\sqrt{2}} \cdot |1_{A}0_{C}\rangle.$$
(27)

One can easily check that the states  $t_i$  are orthonormal, hence the spaces  $L_i$  are orthogonal. To describe the result of measuring the state (25) with respect to these linear spaces, we must first represent the state (25) in the form  $s = \sum s_i$ , with  $s_i \in L_i$ . For this purpose, we can use the fact that, due to the formulas (27), we have

$$|0_{A}0_{C}\rangle = \frac{1}{\sqrt{2}} \cdot t_{1} + \frac{1}{\sqrt{2}} \cdot t_{2}; \quad |1_{A}1_{C}\rangle = \frac{1}{\sqrt{2}} \cdot t_{1} - \frac{1}{\sqrt{2}} \cdot t_{2};$$
$$|0_{A}1_{C}\rangle = \frac{1}{\sqrt{2}} \cdot t_{3} + \frac{1}{\sqrt{2}} \cdot t_{4}; \quad |1_{A}0_{C}\rangle = \frac{1}{\sqrt{2}} \cdot t_{3} - \frac{1}{\sqrt{2}} \cdot t_{4}.$$
 (28)

Substituting the expressions (28) into the formula (25), we get

$$\begin{split} \frac{\alpha_0}{\sqrt{2}} \cdot |1\rangle_B \otimes \left(\frac{1}{\sqrt{2}} \cdot t_1 + \frac{1}{\sqrt{2}} \cdot t_2\right) + \frac{\alpha_1}{\sqrt{2}} \cdot |1\rangle_B \otimes \left(\frac{1}{\sqrt{2}} \cdot t_3 + \frac{1}{\sqrt{2}} \cdot t_4\right) + \\ \frac{\alpha_0}{\sqrt{2}} \cdot |0\rangle_B \otimes \left(\frac{1}{\sqrt{2}} \cdot t_3 - \frac{1}{\sqrt{2}} \cdot t_4\right) + \frac{\alpha_1}{\sqrt{2}} \cdot |0\rangle_B \otimes \left(\frac{1}{\sqrt{2}} \cdot t_1 - \frac{1}{\sqrt{2}} \cdot t_2\right), \\ \left(\frac{\alpha_0}{2}|1_B\rangle + \frac{\alpha_1}{2}|0_B\rangle\right) \otimes t_1 + \left(\frac{\alpha_0}{2}|1_B\rangle - \frac{\alpha_1}{2}|0_B\rangle\right) \otimes t_2 + \\ \left(\frac{\alpha_1}{2}|1_B\rangle + \frac{\alpha_0}{2}|0_B\rangle\right) \otimes t_3 + \left(\frac{\alpha_1}{2}|1_B\rangle - \frac{\alpha_0}{2}|0_B\rangle\right) \otimes t_4. \end{split}$$

So, we get a representation of the type (26), with

$$s_{1} = \left(\frac{\alpha_{0}}{2} \cdot |1_{B}\rangle + \frac{\alpha_{1}}{2}|0_{B}\rangle\right) \otimes t_{1}, \quad s_{2} = \left(\frac{\alpha_{0}}{2} \cdot |1_{B}\rangle - \frac{\alpha_{1}}{2} \cdot |0_{B}\rangle\right) \otimes t_{2},$$
$$s_{3} = \left(\frac{\alpha_{1}}{2} \cdot |1_{B}\rangle + \frac{\alpha_{0}}{2} \cdot |0_{B}\rangle\right) \otimes t_{3}, \quad s_{4} = \left(\frac{\alpha_{1}}{2} \cdot |1_{B}\rangle - \frac{\alpha_{0}}{2} \cdot |0_{B}\rangle\right) \otimes t_{4}.$$

Here, for each *i*, we have

thus

$$||s_i||^2 = \left|\frac{\alpha_0}{2}\right|^2 + \left|\frac{\alpha_1}{2}\right|^2 = \frac{1}{4} \cdot (|\alpha_0|^2 + |\alpha_1|^2) = \frac{1}{4},$$

350 thus  $||s_i|| = \frac{1}{2}$ .

So, with equal probability of  $\frac{1}{4}$ , we get one of the following four states – and Alice knows which one it is:

$$(\alpha_{0} \cdot |\mathbf{1}_{B}\rangle + \alpha_{1} \cdot |\mathbf{0}_{B}\rangle) \otimes t_{1}; \ (\alpha_{0} \cdot |\mathbf{1}_{B}\rangle - \alpha_{1} \cdot |\mathbf{0}_{B}\rangle) \otimes t_{2}; (\alpha_{1} \cdot |\mathbf{1}_{B}\rangle + \alpha_{0} \cdot |\mathbf{0}_{B}\rangle) \otimes t_{3}; \ (\alpha_{1} \cdot |\mathbf{1}_{B}\rangle - \alpha_{0} \cdot |\mathbf{0}_{B}\rangle) \otimes t_{4}.$$

$$(29)$$

351 6.4.8. Second stage: communication

On the second stage, Alice sends to Bob the measurement result. As a result, Bob knows in which the four states (29) the system is.

- 6.4.9. Final stage: Bob "rotates" his state and thus, get the original state teleported to him
- On the final stage, Bob performs an appropriate transformation of his state *B*.
- In the first case, he uses a unitary transformation that swaps  $|0\rangle_B$  and  $|1\rangle_B$ , for which  $t_{01} = t_{10} = 1$  and  $t_{00} = t_{11} = 0$ .
- In the second case, he uses a unitary transformation for which  $t_{01} = 1$ ,  $t_{10} = -1$ and  $t_{00} = t_{11} = 0$ .
- In the third case, he already has the desired state.
- In the fourth case, he uses a unitary transformation for which  $t_{00} = -1$ ,  $t_{11} = 1$ , and  $t_{01} = t_{10} = 0$ .
- As a result, in all fours cases, he gets the original state  $\alpha_0 \cdot |0\rangle_B + \alpha_1 \cdot |1\rangle_B$ .

6.5. The main result of this section: the standard quantum teleportation algorithm is, in some
 reasonable sense, unique

366 6.5.1. Formulation of the problem

Teleportation is possible because we have prepared an *entangled* state (24), i.e., a state  $s_{AB}$  in which the states of Alice and Bob are not independent, i.e., a state that does not have a form  $s_A \otimes s_B$ . However, (24) is not the only possible entangled state. Let us consider, instead, a general joint state of two qubits:

$$a_{00} \cdot |0_A 0_B\rangle + a_{01} \cdot |0_A 1_B\rangle + a_{10} \cdot |1_A 0_B\rangle + a_{11} \cdot |1_A 1_B\rangle.$$
(3a)

What will happen if we use this more general entangled state instead of the one that isused in the known teleportation algorithm?

369 6.5.2. Analysis of the problem

For the state (24a), the joint state of all three subsystems has the form

$$\begin{aligned} &\alpha_{0} \cdot a_{00} \cdot |0_{A}0_{B}0_{C}\rangle + \alpha_{1} \cdot a_{00} \cdot |0_{A}0_{B}1_{C}\rangle + \\ &\alpha_{0} \cdot a_{01} \cdot |0_{A}1_{B}0_{C}\rangle + \alpha_{1} \cdot a_{01} \cdot |0_{A}1_{B}1_{C}\rangle + \\ &\alpha_{0} \cdot a_{10} \cdot |1_{A}0_{B}0_{C}\rangle + \alpha_{1} \cdot a_{10} \cdot |1_{A}0_{B}1_{C}\rangle + \\ &\alpha_{0} \cdot a_{11} \cdot |1_{A}1_{B}0_{C}\rangle + \alpha_{1} \cdot a_{11} \cdot |1_{A}1_{B}1_{C}\rangle. \end{aligned}$$
(25a)

Substituting expressions (28) into this formula, we get

$$\begin{aligned} \frac{\alpha_0}{\sqrt{2}} \cdot a_{00} \cdot |0\rangle_B \otimes (t_1 + t_2) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{00} \cdot |0\rangle_B \otimes (t_3 + t_4) + \\ \frac{\alpha_0}{\sqrt{2}} \cdot a_{01} \cdot |1\rangle_B \otimes (t_1 + t_2) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{01} \cdot |1\rangle_B \otimes (t_3 + t_4) + \\ \frac{\alpha_0}{\sqrt{2}} \cdot a_{10} \cdot |0\rangle_B \otimes (t_3 - t_4) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{10} \cdot |0\rangle_B \otimes (t_1 - t_2) + \end{aligned}$$

$$\frac{\alpha_0}{\sqrt{2}} \cdot a_{11} \cdot |1\rangle_B \otimes (t_3 - t_4) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{11} \cdot |1\rangle_B \otimes (t_1 - t_2),$$

thus  $s = S_1 \otimes t_1 + S_2 \otimes t_2 + \ldots$ , where

$$S_{1} = \left(\frac{\alpha_{0} \cdot a_{00}}{\sqrt{2}} + \frac{\alpha_{1} \cdot a_{10}}{\sqrt{2}}\right) \cdot |0\rangle_{B} + \left(\frac{\alpha_{0} \cdot a_{01}}{\sqrt{2}} + \frac{\alpha_{1} \cdot a_{11}}{\sqrt{2}}\right) \cdot |1\rangle_{B}$$

and  $S_2$ , ... are described by similar expressions.

This means that after the measurement, Bob will have the normalized state  $S_1 / ||S_1||$ . To perform teleportation, we need to transform this state into the original state  $\alpha_0 \cdot |0\rangle_B + \alpha_1 \cdot |1\rangle_B$ . Thus, the transformation from the resulting state  $S_1 / ||S_1||$  to the original state must be unitary. It is known that the inverse transformation to a unitary one is also unitary. In general, a unitary transformation transforms orthonormal states into orthonormal ones.

377 So, the inverse transformation that:

- maps the state  $|0\rangle_B$  (corresponding to  $\alpha_0 = 1$  and  $\alpha_1 = 0$ ) into a new state  $|1'\rangle_B \stackrel{\text{def}}{=}$ <sup>379</sup> const  $\cdot (a_{00} \cdot |0\rangle_B + a_{01} \cdot |1\rangle_B)$ , and
- maps the state  $|1\rangle_B$  (corresponding to  $\alpha_0 = 0$  and  $\alpha_1 = 1$ ) into a new state  $|0'\rangle_B \stackrel{\text{def}}{=}$ set const  $\cdot (a_{10} \cdot |0\rangle_B + a_{11} \cdot |1\rangle_B)$ ,
- transforms two original orthonormal vectors  $|0\rangle_B$  and  $|1\rangle_B$  into two new orthonormal ones  $|0'\rangle_B$  and  $|1'\rangle_B$ .

In terms of these new states, the entangled state (24a) takes the form

const 
$$\cdot (|0\rangle_A \otimes |1'\rangle_B + |1\rangle_B \otimes |0'\rangle_B).$$

From the requirement that the sum of the squares of absolute values of all the coefficients add up to 1, we conclude that  $2 \cdot \text{const}^2 = 1$ . Then  $\text{const} = \frac{1}{\sqrt{2}}$  and the entangled state takes the familiar form

$$\frac{1}{\sqrt{2}} \cdot (|0\rangle_A \otimes |1'\rangle_B + |1\rangle_B \otimes |0'\rangle_B).$$
(24)

This is exactly the entangled state used in the standard teleportation algorithm. So, we can make the following conclusion.

6.5.3. Conclusion of this section

From the technical viewpoint, the only entangled state that leads to a successful teleportation is the state (24) corresponding to the standard quantum teleportation algorithm – for some orthornomal states  $|0'\rangle_B$  and  $|1'\rangle_B$ .

Thus, we have shown that, indeed, the existing quantum teleportation algorithm is unique – so we should not waste our time and effort looking for more efficient alternative quantum teleportation algorithms.

#### <sup>393</sup> 7. Optimization: Quantum Annealing Schedules Are Optimal

*7.1. Quantum annealing: ideas, successes, and challenges* 

One of the important practical problems is optimization. An important challenge 395 is that often, the existing optimization techniques lead to a local optimum. One way to 396 avoid local optima is *annealing*: whenever we find ourselves in a possibly local optimum, 397 we jump out with some probability and continue search for the true optimum. Since 398 quantum processes are probabilistic, a natural way to organize such a probabilistic 399 perturbation of the deterministic optimization is to use quantum effects, i.e., to perform 4 0 0 quantum annealing. This idea was first proposed in [10,19] and has been used successfully 4 01 since then. 4 0 2

- <sup>403</sup> It turns out that often, quantum annealing works much better than non-quantum
- one; see, e.g., see, e.g., [4–6,8,18,21,22,24,28,31,32,34]. Quantum annealing is the main
- technique behind the only commercially available computational devices that use quantum effects D-Wave computers; see, e.g., [4,21,32].
- The efficiency of quantum annealing depends on the proper selection of the annealing schedule, i.e., schedule that describes how the perturbations decrease with time. Empirically, it has been found that two schedules work best: power law and exponential ones. In this section, following [14], we prove that these two schedules are indeed optimal (in some reasonable sense).

#### 412 7.2. Formulation of the problem

In general, the state of a quantum system is described by a complex-valued function  $\psi(t)$  (known as the *wave function*), and the dynamics of a quantum system is described by Schroedinger's equations

$$\mathbf{i} \cdot \boldsymbol{\hbar} \cdot \frac{\partial \boldsymbol{\psi}}{\partial t} = H \boldsymbol{\psi},\tag{30}$$

where, as before, i  $\stackrel{\text{def}}{=} \sqrt{-1}$  and *H* is a corresponding linear operator. In these terms, annealing-type modification means adding additional terms – decreasing with time – to the operator *H*, i.e., replacing the original equation (30) with the modified equation

$$\mathbf{i} \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = H\psi + \gamma(t) \cdot H_0 \psi, \tag{31}$$

- where  $H_0$  describes the deviation, and  $\gamma(t)$  monotonically tends to 0 as t increases.
- The efficiency of quantum annealing strongly depends on the proper selection of the annealing schedule, i.e., the dependence of  $\gamma(t)$  on time *t*. Empirically, depending on the specific optimization problem, two scheduled work the best:
- the power law annealing schedule  $\gamma(t) = A \cdot t^a$ , for some A and a < 0; see, e.g., • [22,23]; and
- the exponential annealing schedule  $\gamma(t) = A \cdot \exp(a \cdot t)$  for some *A* and *a* < 0; see, e.g., [7,23].
- <sup>421</sup> In this section, we provide a theoretical proof that these schedules are indeed optimal.

#### 422 7.3. Physical meaning of annealing

The general idea of using simulating physical phenomena in optimization is that a physical systems tends to end up in a state with the smallest possible energy. For example, in a gravitational field, this means getting to as low a position as possible. In principle, we can place a ball on top of the mountain – which will constitute a local minimum of energy. However, if a strong wind blows and disturbs the ball, it will start falling down. It may reach a few local minima along the way, but eventually it will reach the lowest possible position at the foot of the mountain.

So, a natural way to use simulated physical phenomena for optimization is to
simulate a system for which, for all the values of the parameters, its energy is equal to
the value of minimized objective function. In general, in Schroedinger equations, energy
is represented by the operator *H*, so for quantum annealing, this operator must represent
the desired objective function.

#### 7.4. Need to select a family of schedules

The original optimization problem is usually not formulated in terms of energy. So, how we transform it into energy depends in our choice of units. We will get completely different results if we use a typical macro-world unit like Joule or a typical micro-world unit like MeV. If we select a different unit, this means that in original unit, instead of *H*, we will have  $C \cdot H$ , where *C* is the ratio of the units. If for the original operator *H* the best schedule was  $\gamma(t)$ , then for the new operator  $C \cdot H$ , the best schedule is  $C \cdot \gamma(t)$ , since the corresponding equation

$$\mathbf{i} \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = C \cdot H \psi + C \cdot \gamma(t) \cdot H_0 \psi \tag{32}$$

is equivalent to the original equation (31) if we re-scale the time, i.e., consider t/C instead of the original time t.

Since, as we have mentioned, the choice of the energy unit is rather arbitrary, this means that we cannot select a single annealing schedule  $\gamma(t)$ : with each such optimal schedule, in different energy units, a schedule  $C \cdot \gamma(t)$  is optimal. Thus, we can only select a *family*  $\{C \cdot \gamma(t)\}_{C>0}$  of annealing functions, in which a function  $\gamma(t)$  is fixed, and the parameter *C* can take any positive value.

#### 448 7.5. Need for re-scaling time and the resulting invariances (symmetries)

We are looking for the dependence of  $\gamma(t)$  on time, but the numerical value of time also depends on the choice if the measuring unit. If we replace the original unit of time by a  $\lambda$  times smaller unit, then, for each moment of time, the original numerical value *t* is replaced by a new value  $\lambda \cdot t$ . For example, if we replace minutes by seconds, then 2 minutes becomes  $60 \cdot 2 = 120$  seconds.

It is reasonable to requires that the relative quality of a family not change if we simply change the unit for time: e.g., if

$$\{C \cdot \gamma_1(t)\}_{C>0} < \{C \cdot \gamma_2(t)\}_{C>0},$$

then we should have

$$\{C \cdot \gamma_1(\lambda \cdot t)\}_{C>0} < \{C \cdot \gamma_2(\lambda \cdot t)\}_{C>0}.$$

The numerical value of time also depends on the choice of the starting point. If we replace the original starting point with the one which is  $t_0$  units earlier, then all numerical values t are replaced with shifted values  $t + t_0$ . It also makes sense to require that the relative quality of two families not depend on the choice of the starting point, i.e., that if

$$\{C \cdot \gamma_1(t)\}_{C>0} < \{C \cdot \gamma_2(t)\}_{C>0},$$

then we should have

$$\{C \cdot \gamma_1(t+t_0)\}_{C>0} < \{C \cdot \gamma_2(t+t_0)\}_{C>0}.$$

#### 54 7.6. Resulting proof

According to our Lemma, once we assumed that the optimality criterion is invariant, then the optimal family must be invariant.

For invariance with respect to changing the unit of time, this means that

$$\{C \cdot \gamma(\lambda \cdot t)\}_{C>0} = \{C \cdot \gamma(t)\}_{C>0}.$$

This inequality means, in particular, that the function  $\gamma(\lambda \cdot t)$  from the first family belongs to the second family, i.e., that for every t and  $\lambda$ , we have  $\gamma(\lambda \cdot t) = C(\lambda) \cdot \gamma(t)$ for some C depending on  $\lambda$ . It is known (see, e.g., [1]) that the only monotonic solutions to this functional equation are power laws  $\gamma(t) = A \cdot t^a$ .

Similarly, for invariance with respect to a starting point, invariance means that  $\{C \cdot \gamma(t+t_0)\}_{C>0} = \{C \cdot \gamma(t)\}_{C>0}$ . This inequality means, for every *t* and *t*<sub>0</sub>, we have  $\gamma(t+t_0) = C(t_0) \cdot \gamma(t)$  for some *C* depending on *t*<sub>0</sub>. It is known (see, e.g., [1]) that the only monotonic solutions to this functional equation are exponential laws  $\gamma(t) = A \cdot \exp(a \cdot t)$ .

- Thus, the power law and the exponential law are indeed the only invariant functions - and thus, the optimal law must be either a power law or an exponential law.
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#### References

- 1. Aczél, J.; Dhombres, J. Functional Equations in Several Variables; Cambridge University Press, 2008.
- Bautista, I.; Kreinovich, V.; Kosheleva, O.; Nguyen, H.P. Why it is sufficient to have real-valued amplitudes in quantum computing, In: *Soft Computing: Biomedical and Related Applications*, Nguyen Hoang Phuong; Kreinovich, V., Eds.; Springer: Cham, Switzerland, 2021; pp. 131–136.
- 3. Bennett, C.H.; Brassard, G.; Crépeau, C.; Jozsa, R.; Peres, A.; Wootters, W.K. Teleporting an unknown quantum state via dual classical and Einstein-Podolsky–Rosen channels. *Physical Review Letters* **1993**, *70*, 1895–1899.
- 4. Boixo, S.; Ronnow, T.F.; Isakov, S.V.; Wang, Z.; Wecker, D.; Lidar, D.A.; Martinis, J.M.; Troyer, M. Evidence for quantum annealing with more than one hundred qubits, *Nature Physics* **2014**, *10*, 218–224.
- 5. Brooke, J.; Bitko, D.; Rosenbaum, T.F.; Aeppli, G. Quantum annealing of a disordered magnet, *Science* 1999, 284, 779–781.
- 6. Crosson, E.; Farhi, E.; Lin, C.Y.-Y.; Lin, H.-H.; Shor, P. Different Strategies for Optimization Using the Quantum Adiabatic Algorithm, 2014, arXiv:1401.7320.
- Das, A.; Chakrabarti, B.K.; Stinhcombe, R.B. Quantum annealing in a kinetically constrained system, *Physical Review Letters* 2005, 72, Paper 026701.
- 8. Farhi, E.; Goldstone, J.; Gutmann, S.; Lapan, J.; Ludgren, A.; Preda, D. A quantum adiabatic evolution algorithm applied to random instances of an NP-complete problem, *Science* **2001**, *292*, 472–475.
- 9. Feynman, R.; Leighton, R.; Sands, M. The Feynman Lectures on Physics; Addison Wesley: Boston, Massachusetts, 2005.
- 10. Finnila, A.B.; Gomez, M.A.; Sebenik, C.; Stenson, C.; Doll, J.D. Quantum annealing: A new method for minimizing multidimensional functions", *Chemical Physics Letters* **1994**, 219(5–6), 343–348.
- 11. Galindo, O.; Bokati, L.; Kreinovich, V. Towards a more efficient representation of functions in quantum and reversible computing, Proceedings of the Joint 11th Conference of the European Society for Fuzzy Logic and Technology EUSFLAT'2019 and International Quantum Systems Association (IQSA) Workshop on Quantum Structures, Prague, Czech Republic, September 9–13, 2019.
- Galindo, O.; Kosheleva, O.; Kreinovich, V. Towards parallel quantum computing: standard quantum teleportation algorithm is, in some reasonable sense, unique, In: Seki, H.; Nguyen, C.H.; Huynh, V.-N.; Inuiguchi, M., Eds., USB Proceedings of the 7th International Symposium on Integrated Uncertainty in Knowledge Modelling and Decision Making IUKM'2019, Nara, Japan, March 27–29, 2019, pp. 23–34.
- 13. Galindo, O.; Kosheleva, O.; Kreinovich, V. How to efficiently store intermediate results in quantum computing: theoretical explanation of the current algorithm; In: *Credible Asset Allocation, Optimal Transport Methods, and Related Topics*; Sriboonchitta, S.; Kreinovich, V.; Yamaka, W., Eds.; Springer: Cham, Switzerland, 2022, to appear.
- 14. Galindo, O; Kreinovich, V. What is the optimal annealing schedule in quantum annealing, Proceedings of the IEEE Series of Symposia on Computational Intelligence SSCI'2020, Canberra, Australia, December 1–4, 2020.
- 15. Galindo, O.; Kreinovich, V.; Kosheleva, O. Current quantum cryptography algorithm is optimal: a proof, Proceedings of the IEEE Symposium on Computational Intelligence for Engineering Solutions CIES'2018, Bengaluru, India, November 18–21, 2018.
- 16. Grover, L.K. A fast quantum mechanical algorithm for database search", Proceedings of the 28th ACM Symposium on Theory of Computing, 1996, pp. 212–219.
- 17. Grover, L.K. Quantum mechanics helps in searching for a needle in a haystack, *Physical Reviews Letters* 1997, 79(2), 325–328.
- 18. Heim, B.; Ronnow, T.F.; Isakov, S.V.; Troyer, M. Quantum versus classical annealing of Ising spin glasses, *Science* **2015**, *348*, 215–217.
- 19. Kadowaki, T.; Nishimori, H. Quantum annealing in the transverse Ising model, *Physical Reviews E* 1998, 58, Paper 5355.
- 20. Kreinovich, V.; Ceberio, M.; Alvarez, R.; How to use quantum computing to check which inputs are relevant: a proof that Deutsch-Jozsa algorithm is, in effect, the only possibility, Proceedings of the 2019 IEEE Symposium Series on Computational Intelligence SSCI'2019, Xiamen, China, December 6–9, 2019; pp. 828–832.

- Lanting, T.; Przybysz, A.J.; Smirnov, A.Yu.; Spedalieri, F.M.; Amin, M.H.; Berkley, A.J.; Harris, R.; Altomare, F.; Boixo, S.; Bunyk, P.; Dickson, N.; Enderud, C.; Hilton, J.P.; Hoskinson, E.; Johnson, M.W.; Ladizinsky, E.; Ladizinsky, N.; Neufeld, R.; Oh, T.; Perminov, I.; Rich, C.; Thom, M.C.; Tolkacheva, E.; Uchaikin, S.; Wilson, S.B.; Rose, G. Entanglement in a quantum annealing processor, *Physical Review X* 2014, 4(2), Paper 021041.
- 22. Morita, S.; Nishimori, H. Mathematical foundation of quantum annealing, Journal of Mathematical Physics 2008, 49, Paper 125210.
- 23. Mukherjee S.; Chakrabarti, B.K. Multivariable optimization: Quantum annealing and computation", *The European Physical Journal Special Topics* **2015**, 224, 17–24.
- 24. Muthukrishnan, D.; Albash, T.; Lidar, D.A. When Diabatic Trumps Adiabatic in Quantum Optimization, 2015, arXiv:1505.01249.
- 25. Nguyen, H.T.; Kreinovich, V. Applications of Continuous Mathematics to Computer Science; Kluwer: Dordrecht, 1997.
- Nielsen, M.A.; Chuang, I.L. *Quantum Computation and Quantum Information*; Cambridge University Press: Cambridge, U.K., 2000.
   Pirandola, S.; Eisert, J.; Weedbrook, C.; Furusawa, A.; Braunstein, S.L. Advances in quantum teleportation, *Nature Photonics* 2015,
- 9(10), 641–652.
  28. Santoro, G.E.; Tosatti, E. Optimization using quantum mechanics: quantum annealing through adiabatic evolution, *Journal of Physics A* 2006, 39, Paper R393.
- 29. Shor, P. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. Proceedings of the 35th Annual Symposium on Foundations of Computer Science, Santa Fe, New Mexico, November 20–22, 1994.
- 30. Shor, P. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer; *SIAM Journal on Computing* **1997**, *26*, 1484–1509.
- 31. Smelyanskiy, V.N.; Rieffel, E.G.; Knysh, S.I.; Williams, C.P.; Johnson, M.W.; Thom, M.C.; Macready, W.G.; Pudenz, K.L. A Near-Term Quantum Computing Approach for Hard Computational Problems in Space Exploration, 2012, arXiv:1204.2821.
- Steiger, S.; Heim, B.; Ronnow, T.; Troyer, M. Performance of quantum annealing hardware", In: *Electro-Optical and Infrared Systems: Technology and Applications XII; and Quantum Information Science and Technology*, Huckridge, D.A.; Ebert, R.; Gruneisen, M.T.; Dusek, M.; Rarity J.G., Eds., SPIE Proceedings, 2015, Vol. 9648, Paper 964816.
- 33. Thorne, K.S.; Blandford, R.D. Modern Classical Physics: Optics, Fluids, Plasmas, Elasticity, Relativity, and Statistical Physics; Princeton University Press: Princeton, New Jersey, 2017.
- 34. Venegas-Andraca, S.E.; Cruz-Santos, W.; McGeoch, C.; Lanzagorta, M. A cross-disciplinary introduction to quantum annealingbased algorithms, *Contemporary Physics* 2018, 59(2), 174–196.
- 35. Williams, C.P.; Clearwater, S.H. Ultimate Zero and One; Copernicus: New York, 2000.