

# Many Known Quantum Algorithms Are Optimal: Proofs

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**Abstract:** Many quantum algorithms have been proposed which are drastically more efficient than 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 are actually optimal. Several of these results are based on appropriate invariances.

**Keywords:** quantum computing; optimal algorithms; invariance

## 1. Formulation of the Problem

### 1.1. Need for quantum computing

Modern computers are extremely fast, but still there are many practical problems 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  $c = 300,000$  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 probabilities, while in computations, we usually want to come up with a single result. Thus, we need to develop new algorithms.

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### 41 1.3. Quantum algorithms: successes

42 Quantum algorithms have indeed been successfully developed for solving all funda-  
43 mental aspects of computation needs; see, e.g., [26,35]. Not only the resulting algorithms  
44 produce deterministic (or almost deterministic) results, many of them compute these  
45 results even faster than the best non-quantum algorithms for solving the same problems.

46 To briefly describe these successes, let us recall what are the fundamental computa-  
47 tion needs. To enumerate these needs, let us recall what we humans want.

- 48 • We want to understand how the world works, to predict what will happen – this is,  
49 crudely speaking, what science is about. For example, we want to predict where  
50 the tornado will turn.
- 51 • We also want to understand how can we improve the situation – this is, crudely  
52 speaking, what engineering is about. For example, how can we make tornadoes  
53 change their course? How can we make houses less vulnerable to tornadoes?
- 54 • Finally, we want to communicate – or not – with others, so we need to develop  
55 techniques for communication only with the intended folks.

56 Quantum algorithms are useful in solving all these main problems of science and engi-  
57 neering:

- 58 • In the general prediction problem, we need to find a model that fits all the ob-  
59 servations. In a usual engineering problem, we need to find a design and/or a  
60 control that satisfies a given specification. In most of these problems, once we have  
61 a model, a design, or a control, it is computationally feasible to check whether this  
62 model, design, etc. satisfies the given specifications, it is searching for a satisfactory  
63 model, design, etc. which is computationally intensive. There exists a quantum  
64 algorithm that speeds us such a search. This algorithm – proposed by Lev Grover –  
65 finds an element in an unsorted list in time  $\sqrt{n}$ , which is much faster than  $n$  steps  
66 needed in the non-quantum case [16,17,26,35]. Quantum algorithms are also useful  
67 in optimization.
- 68 • An additional way to speed up computations comes from the fact that in prediction  
69 problems – such as predicting tomorrow’s weather – to be on the safe side, we take  
70 into account today’s meteorological data in all nearby locations, even though most  
71 of this data is actually irrelevant. To speed up computations, it is desirable to decide  
72 which inputs are relevant and which are not. In this analysis, quantum computing  
73 also helps – namely, we can use Deutsch-Jozsa algorithm; see, e.g., [26,35].
- 74 • Finally, special algorithms have been developed for quantum communications –  
75 which is especially important since it is known that by using quantum computing,  
76 we can break the RSA encryption (and similar encryptions) – and these encryptions  
77 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

79 As we have mentioned, the existing quantum algorithms work very well. However,  
80 a next natural question is: are these algorithms optimal – in some reasonable sense –  
81 or we can do better? In this paper, we overview several results that show that many  
82 quantum algorithms are indeed optimal.

83 Of course, these results are just the beginning of the study. Quantum computing  
84 is a developing field, many new algorithms are being developed all the time, and, as  
85 quantum computers will become practical, this will definitely further boost the invention  
86 of new algorithms. We hope that the results reviewed in this paper will help researchers  
87 to analyze the optimality of other quantum algorithms as well.

### 88 1.5. Structure of this paper

89 We start, in Section 2, with a brief reminder of the quantum basics – basics which  
90 are needed to understand the main ideas behind the existing quantum algorithms and  
91 behind the proofs of their optimality. In Section 3, we describe the relation between

92 optimality – that we want to prove – and invariance with respect to different transforma-  
 93 tions. After that, we present the proofs of optimality of different quantum algorithms for  
 94 quantum data processing: Grover’s algorithm in Section 4, parallel-related teleportation  
 95 algorithm in Section 5, and an optimization-related quantum annealing algorithm in  
 96 Section 6.

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

## 100 2. Quantum basics

### 101 2.1. Quantum states

In “classical” (= non-quantum) physics, each object, each system can be in different states  $s, s', \dots$ . 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

$$c \cdot |s\rangle + c' \cdot |s'\rangle + \dots, \quad (1)$$

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

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

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

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

107 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 bit* (*qubit*, for short) that can be in any state

$$c_0 \cdot |0\rangle + c_1 \cdot |1\rangle, \quad (3)$$

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

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

108 In the state (3), the probability that we will observe 0 is  $|c_0|^2$ , and the probability that we  
 109 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

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

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

### 113 2.2. Quantum measurements

114 In general, if we have  $n$  classical states  $s_1, \dots, s_n$ , and we want to detect, in a  
 115 quantum state  $\sum \alpha_i \cdot s_i$ , which of these states we are in, we get each  $s_i$  with probability  
 116  $|\alpha_i|^2$  – and once the measurement process detects the state  $s_i$ , the actual state turns into  $s_i$ .

117 Instead of the classical states  $s_1, \dots$ , we can use any other sequence of states  $s'_i =$   
 118  $\sum_j t_{ij} \cdot s_j$ , as long as they are *orthonormal* (= orthogonal and normal) in the sense that:

- 119 • for each  $i$ , we have  $\|s'_i\|^2 = 1$ , where  $\|s'_i\|^2 \stackrel{\text{def}}{=} \sum_j |t_{ij}|^2$  (*normal*), and
- 120 • for each  $i$  and  $i'$ , we have  $s'_i \perp s'_{i'}$ , i.e.,  $\langle s'_i | s'_{i'} \rangle = 0$ , where  $\langle s'_i | s'_{i'} \rangle \stackrel{\text{def}}{=} \sum_j t_{ij} \cdot t_{i'j}^*$
- 121 (*orthogonal*).

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

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

### 129 2.3. Composite systems

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

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

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

$$(c \cdot |s\rangle + c' \cdot |s'\rangle + \dots) \otimes (a \cdot |t\rangle + a' \cdot |t'\rangle + \dots), \quad (7)$$

is equal to

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

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

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

### 144 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

$$c_1 \cdot |s_1\rangle + \dots + c_n \cdot |s_n\rangle \quad (9)$$

is transformed into the state

$$c'_1 \cdot |s_1\rangle + \dots + c'_n \cdot |s_n\rangle, \quad (10)$$

for which

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

for some coefficient  $T_{ij}$ . The matrix  $T = \|T_{ij}\|$  is *unitary*:  $T^\dagger T = T T^\dagger = I$ , 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

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

## 2.5. How functions are represented in quantum algorithms

In this section, we will deal only with functions  $y = f(x_1, \dots, x_n)$  of boolean (0-1) variables – since these are the basic functions implemented by different “gates”, of which computers are built. We cannot simply 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  $y = f(x_1, \dots, x_n)$  is represented as

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

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  $(x_1, \dots, x_n, y)$  – 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

### 3.1. What is invariance

In many cases, there are some natural transformations that does not change the system. This “not changing” is called *invariance*. For example, suppose that we have an unsorted list, and we are looking for an element with a certain property in this list. For convenience, we can denote one of the list’s elements by  $s_1$ , another one by  $s_2$ , etc., but in this problem, it does not matter which element is called  $s_1$ , which  $s_2$ , etc. – any permutation  $\pi : \{1, \dots, n\} \rightarrow \{1, \dots, n\}$  would retain the problem. Thus, in this problems, permutations are invariances. In other problems, we will have other natural invariances.

## 4. What does “optimal” mean

Usually, when we talk about “optimal”, we mean that on the set of all alternatives  $A, A', \dots$ , 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 optimality. Often, there are several alternatives  $A_1, A_2$ , etc., with the exact same largest

value  $f(A_1) = f(A_2) = \dots$  of the objective function. In this case, we can use this non-uniqueness to optimize something else. For example, in the above case, we can minimize the average time needed for the algorithm to finish. This means, in effect, that the original optimality criterion is not final, we can modify it and come up with a new, more complex criterion according to which an alternative  $A$  is better than the alternative  $A'$  – we will denote it by  $A < A'$  – if:

- 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  $\mathcal{A}$  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  $A_{\text{opt}}$  is called *optimal* if for every other alternative  $A$ , we have  $A < A_{\text{opt}}$  or  $A \sim A_{\text{opt}}$ . 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  $T : \mathcal{A} \rightarrow \mathcal{A}$  – 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  $T(A) \sim T(A')$ .

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

**Lemma.** For every final *T*-invariant optimality criterion, its optimal alternative  $A_{\text{opt}}$  is also *T*-invariant, i.e.,  $T(A_{\text{opt}}) = A_{\text{opt}}$ .

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

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

## 237 5. Grover's Algorithm Is Optimal

### 238 5.1. Formulation of the problem

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

Let us describe this problem in 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:

$$c_1 \cdot |1\rangle + \dots + c_{i_0-1} \cdot |i_0 - 1\rangle + c_{i_0} \cdot |i_0\rangle + c_{i_0+1} \cdot |i_0 + 1\rangle + \dots + c_n \cdot |n\rangle. \quad (13)$$

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

- 245 • 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
- 246 • for  $i = i_0$ , we have  $T_f(|i_0, 0\rangle) = |i_0, 1\rangle$  and  $T_f(|i_0, 1\rangle) = |i_0, 0\rangle$ .

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

- 248 • for  $|0'\rangle$ , for all  $i$ , we have  $T_f(|i\rangle \otimes |0'\rangle) = |i\rangle \otimes |0'\rangle$ ;
- 249 • 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  
 250  $T_f(|i_0\rangle \otimes |1'\rangle) = -|i_0\rangle \otimes |1'\rangle$ .

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:

$$c_1 \cdot |1\rangle + \dots + c_{i_0-1} \cdot |i_0 - 1\rangle - c_{i_0} \cdot |i_0\rangle + c_{i_0+1} \cdot |i_0 + 1\rangle + \dots + c_n \cdot |n\rangle. \quad (14)$$

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

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

### 254 5.2. Invariance: reminder

255 As we have mentioned earlier, in this problem, the natural invariances are invari-  
 256 ances with respect to all possible permutations  $\pi : \{1, \dots, n\} \rightarrow \{1, \dots, n\}$ . It is therefore  
 257 reasonable to require that our optimality criterion is invariant with respect to all permu-  
 258 tations. Due to the above Lemma, this implies that the optimal algorithm should also be  
 259 permutation-invariant, in particular:

- 260 • that the initial state should be permutation-invariant, and
- 261 • that all transformations  $S$  should be permutation-invariant.

### 262 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

$$c_1 \cdot |1\rangle + \dots + c_1 \cdot |n\rangle, \quad (14)$$

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:

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

263 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

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

This expression can be equivalently described as

$$c'_i = (a - b) \cdot c_i + b \cdot C, \text{ where } C \stackrel{\text{def}}{=} \sum_{j=1}^n c_j. \quad (17)$$

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

$$\sum_{j=1}^n |c'_j|^2 = 1. \quad (18)$$

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

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

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

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

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

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

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

$$c'_i = \left( 1 - \frac{2}{n} \right) \cdot c_i - \frac{2}{n} \cdot \sum_{j \neq i} c_j. \quad (21)$$

264 This is also exactly the transformation used in Grover's algorithm!

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

- 270 • we start with the initial state (15);
- 271 • then, we apply the transformation  $U$ ;
- 272 • after that, we apply the transformation  $S$ ;
- 273 • then, again we apply  $U$ ; etc.

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

## 277 **6. Parallelization: Teleportation Algorithm Is Optimal**

### 278 *6.1. Need for parallelization*

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

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

### 289 *6.2. Need for teleportation*

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

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

### 296 *6.3. What we do in this section*

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

### 301 *6.4. Standard quantum teleportation algorithm: reminder*

#### 302 *6.4.1. Need for communication*

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

305 Usually, the sender is denoted by  $A$  and the receiver by  $B$ . In communications, it is  
 306 common to call the sender Alice, and to call the receiver Bob. States corresponding to  
 307 Alice are usually described by using a subscript  $A$ , and states corresponding to Bob are  
 308 usually described by using a subscript  $B$ .

#### 309 *6.4.2. Communication is straightforward in classical physics but a challenge in quantum physics*

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

317 The problem is that in quantum physics, such a straightforward approach is not  
 318 possible: as we have mentioned, in quantum physics, every measurement changes the  
 319 state – and moreover, irreversibly deletes some information about the state. For example,  
 320 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  
 321 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*.

#### 6.4.3. What we consider in this section

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

In these terms, the problem is as follows:

- Alice has a state

$$\alpha_0 \cdot |0\rangle + \alpha_1 \cdot |1\rangle \quad (22)$$

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.

#### 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

$$\alpha_0 \cdot |0\rangle_C + \alpha_1 \cdot |1\rangle_C \quad (23)$$

that she wants to communicate to Bob.

#### 6.4.5. Preparing for teleportation: an entangled state

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

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

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):

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

#### 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

$$s = \sum s_i, \quad (26)$$

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:

$$\begin{aligned} t_1 &= \frac{1}{\sqrt{2}} \cdot |0_A 0_C\rangle + \frac{1}{\sqrt{2}} \cdot |1_A 1_C\rangle; & t_2 &= \frac{1}{\sqrt{2}} \cdot |0_A 0_C\rangle - \frac{1}{\sqrt{2}} \cdot |1_A 1_C\rangle; \\ t_3 &= \frac{1}{\sqrt{2}} \cdot |0_A 1_C\rangle + \frac{1}{\sqrt{2}} \cdot |1_A 0_C\rangle; & t_4 &= \frac{1}{\sqrt{2}} \cdot |0_A 1_C\rangle - \frac{1}{\sqrt{2}} \cdot |1_A 0_C\rangle. \end{aligned} \quad (27)$$

346 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

$$\begin{aligned} |0_A 0_C\rangle &= \frac{1}{\sqrt{2}} \cdot t_1 + \frac{1}{\sqrt{2}} \cdot t_2; & |1_A 1_C\rangle &= \frac{1}{\sqrt{2}} \cdot t_1 - \frac{1}{\sqrt{2}} \cdot t_2; \\ |0_A 1_C\rangle &= \frac{1}{\sqrt{2}} \cdot t_3 + \frac{1}{\sqrt{2}} \cdot t_4; & |1_A 0_C\rangle &= \frac{1}{\sqrt{2}} \cdot t_3 - \frac{1}{\sqrt{2}} \cdot t_4. \end{aligned} \quad (28)$$

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

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

thus

$$\begin{aligned} &\left( \frac{\alpha_0}{2} |1_B\rangle + \frac{\alpha_1}{2} |0_B\rangle \right) \otimes t_1 + \left( \frac{\alpha_0}{2} |1_B\rangle - \frac{\alpha_1}{2} |0_B\rangle \right) \otimes t_2 + \\ &\left( \frac{\alpha_1}{2} |1_B\rangle + \frac{\alpha_0}{2} |0_B\rangle \right) \otimes t_3 + \left( \frac{\alpha_1}{2} |1_B\rangle - \frac{\alpha_0}{2} |0_B\rangle \right) \otimes t_4. \end{aligned}$$

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

$$\begin{aligned} s_1 &= \left( \frac{\alpha_0}{2} \cdot |1_B\rangle + \frac{\alpha_1}{2} |0_B\rangle \right) \otimes t_1, & s_2 &= \left( \frac{\alpha_0}{2} \cdot |1_B\rangle - \frac{\alpha_1}{2} \cdot |0_B\rangle \right) \otimes t_2, \\ s_3 &= \left( \frac{\alpha_1}{2} \cdot |1_B\rangle + \frac{\alpha_0}{2} \cdot |0_B\rangle \right) \otimes t_3, & s_4 &= \left( \frac{\alpha_1}{2} \cdot |1_B\rangle - \frac{\alpha_0}{2} \cdot |0_B\rangle \right) \otimes t_4. \end{aligned}$$

Here, for each  $i$ , we have

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

347 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:

$$\begin{aligned} &(\alpha_0 \cdot |1_B\rangle + \alpha_1 \cdot |0_B\rangle) \otimes t_1; & (\alpha_0 \cdot |1_B\rangle - \alpha_1 \cdot |0_B\rangle) \otimes t_2; \\ &(\alpha_1 \cdot |1_B\rangle + \alpha_0 \cdot |0_B\rangle) \otimes t_3; & (\alpha_1 \cdot |1_B\rangle - \alpha_0 \cdot |0_B\rangle) \otimes t_4. \end{aligned} \quad (29)$$

348 6.4.8. Second stage: communication

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

- 351 6.4.9. Final stage: Bob “rotates” his state and thus, get the original state teleported to him  
 352 On the final stage, Bob performs an appropriate transformation of his state  $B$ .  
 353 • In the first case, he uses a unitary transformation that swaps  $|0\rangle_B$  and  $|1\rangle_B$ , for which  
 354  $t_{01} = t_{10} = 1$  and  $t_{00} = t_{11} = 0$ .  
 355 • In the second case, he uses a unitary transformation for which  $t_{01} = 1$ ,  $t_{10} = -1$   
 356 and  $t_{00} = t_{11} = 0$ .  
 357 • In the third case, he already has the desired state.  
 358 • In the fourth case, he uses a unitary transformation for which  $t_{00} = -1$ ,  $t_{11} = 1$ ,  
 359 and  $t_{01} = t_{10} = 0$ .  
 360 As a result, in all four cases, he gets the original state  $\alpha_0 \cdot |0\rangle_B + \alpha_1 \cdot |1\rangle_B$ .

361 6.5. The main result of this section: the standard quantum teleportation algorithm is, in some  
 362 reasonable sense, unique

### 363 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:

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

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

### 366 6.5.2. Analysis of the problem

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

$$\begin{aligned} & \alpha_0 \cdot a_{00} \cdot |0_A 0_B 0_C\rangle + \alpha_1 \cdot a_{00} \cdot |0_A 0_B 1_C\rangle + \\ & \alpha_0 \cdot a_{01} \cdot |0_A 1_B 0_C\rangle + \alpha_1 \cdot a_{01} \cdot |0_A 1_B 1_C\rangle + \\ & \alpha_0 \cdot a_{10} \cdot |1_A 0_B 0_C\rangle + \alpha_1 \cdot a_{10} \cdot |1_A 0_B 1_C\rangle + \\ & \alpha_0 \cdot a_{11} \cdot |1_A 1_B 0_C\rangle + \alpha_1 \cdot a_{11} \cdot |1_A 1_B 1_C\rangle. \end{aligned} \quad (25a)$$

Substituting expressions (28) into this formula, we get

$$\begin{aligned} & \frac{\alpha_0}{\sqrt{2}} \cdot a_{00} \cdot |0\rangle_B \otimes (t_1 + t_2) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{00} \cdot |0\rangle_B \otimes (t_3 + t_4) + \\ & \frac{\alpha_0}{\sqrt{2}} \cdot a_{01} \cdot |1\rangle_B \otimes (t_1 + t_2) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{01} \cdot |1\rangle_B \otimes (t_3 + t_4) + \\ & \frac{\alpha_0}{\sqrt{2}} \cdot a_{10} \cdot |0\rangle_B \otimes (t_3 - t_4) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{10} \cdot |0\rangle_B \otimes (t_1 - t_2) + \\ & \frac{\alpha_0}{\sqrt{2}} \cdot a_{11} \cdot |1\rangle_B \otimes (t_3 - t_4) + \frac{\alpha_1}{\sqrt{2}} \cdot a_{11} \cdot |1\rangle_B \otimes (t_1 - t_2), \end{aligned}$$

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

$$S_1 = \left( \frac{\alpha_0 \cdot a_{00}}{\sqrt{2}} + \frac{\alpha_1 \cdot a_{10}}{\sqrt{2}} \right) \cdot |0\rangle_B + \left( \frac{\alpha_0 \cdot a_{01}}{\sqrt{2}} + \frac{\alpha_1 \cdot a_{11}}{\sqrt{2}} \right) \cdot |1\rangle_B,$$

367 and  $S_2, \dots$  are described by similar expressions.

368 This means that after the measurement, Bob will have the normalized state  $S_1 / \|S_1\|$ .  
 369 To perform teleportation, we need to transform this state into the original state  $\alpha_0 \cdot$   
 370  $|0\rangle_B + \alpha_1 \cdot |1\rangle_B$ . Thus, the transformation from the resulting state  $S_1 / \|S_1\|$  to the original  
 371 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.

So, the inverse transformation that:

- maps the state  $|0\rangle_B$  (corresponding to  $\alpha_0 = 1$  and  $\alpha_1 = 0$ ) into a new state  $|1'\rangle_B \stackrel{\text{def}}{=} \text{const} \cdot (a_{00} \cdot |0\rangle_B + a_{01} \cdot |1\rangle_B)$ , and
  - maps the state  $|1\rangle_B$  (corresponding to  $\alpha_0 = 0$  and  $\alpha_1 = 1$ ) into a new state  $|0'\rangle_B \stackrel{\text{def}}{=} \text{const} \cdot (a_{10} \cdot |0\rangle_B + a_{11} \cdot |1\rangle_B)$ ,
- 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

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

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

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

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 orthonormal 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.

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

It turns out that often, quantum annealing works much better than non-quantum one; 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).

## 409 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

$$i \cdot \hbar \cdot \frac{\partial \psi}{\partial t} = H\psi, \quad (30)$$

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

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

410 where  $H_0$  describes the deviation, and  $\gamma(t)$  monotonically tends to 0 as  $t$  increases.

411 The efficiency of quantum annealing strongly depends on the proper selection of  
412 the annealing schedule, i.e., the dependence of  $\gamma(t)$  on time  $t$ . Empirically, depending  
413 on the specific optimization problem, two scheduled work the best:

- 414 • the power law annealing schedule  $\gamma(t) = A \cdot t^a$ , for some  $A$  and  $a < 0$ ; see, e.g.,  
415 [22,23]; and
- 416 • the exponential annealing schedule  $\gamma(t) = A \cdot \exp(a \cdot t)$  for some  $A$  and  $a < 0$ ; see,  
417 e.g., [7,23].

418 In this section, we provide a theoretical proof that these schedules are indeed optimal.

## 419 7.3. Physical meaning of annealing

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

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

## 432 7.4. Need to select a family of schedules

433 The original optimization problem is usually not formulated in terms of energy. So,  
434 how we transform it into energy depends in our choice of units. We will get completely  
435 different results if we use a typical macro-world unit like Joule or a typical micro-world  
436 unit like MeV. If we select a different unit, this means that in original unit, instead of  $H$ ,  
437 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

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

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

440 Since, as we have mentioned, the choice of the energy unit is rather arbitrary, this  
441 means that we cannot select a single annealing schedule  $\gamma(t)$ : with each such optimal  
442 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.

#### 7.5. Need for re-scaling time and the resulting invariances

We are looking for the dependence of  $\gamma(t)$  on time, but the numerical value of time also depends on the choice of 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 require 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

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

#### 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  $t_0$ , we have  $\gamma(t + t_0) = C(t_0) \cdot \gamma(t)$  for some  $C$  depending on  $t_0$ . 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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