

# Quantum Adiabatic Computation and the Travelling Salesman Problem

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The NP-complete problem of the travelling salesman (TSP) is considered in the framework of quantum adiabatic computation (QAC). We first derive a remarkable lower bound for the computation time for adiabatic algorithms in general as a function of the energy involved in the computation. Energy, and not just time and space, must thus be considered in the evaluation of algorithm complexity, in perfect accordance with the understanding that all computation is physical. We then propose, with oracular Hamiltonians, new quantum adiabatic algorithms of which not only the lower bound in time but also the energy requirement do not increase exponentially in the size of the input. Such an improvement in both time and energy complexity, as compared to all other existing algorithms for TSP, is apparently due to quantum entanglement. We also appeal to the general theory of Diophantine equations in a speculation on physical implementation of those oracular Hamiltonians.

## A lower bound on the adiabatic computation time

Right from the earlier days of quantum computation, NP-complete problems have been the subject of investigation within standard quantum mechanics [1] as well as in non-standard theory [2]. Then, with the advent of QAC [3] they are further pursued in the form of satisfiability problems [4, 5, 6] mostly with inconclusive results [7, 8] (see also [9, 10]). QAC has also been applied to the search of an unstructured database with the same time complexity as with Grover's [11, 12], or with a much shorter time but at a more substantial cost for the energy involved [13, 14, 15].

QAC starts with the readily constructible ground state  $|g_I\rangle$  of an initial Hamiltonian  $H_I$  which is then *adiabatically* extrapolated to the final Hamiltonian  $H_P$  so that the ground state  $|g\rangle$  of the latter which contains the information of the solution of the problem we want to solve could be obtained with reasonably high probability. The interpolation between  $H_I$  and  $H_P$  is facilitated by a time-dependent Hamiltonian in the time interval  $0 \leq t \leq T$ ,

$$\mathcal{H}(t) = f(t)H_I + g(t)H_P, \quad (1)$$

either in a temporally linear manner (in which case,  $f(t) = (1 - \frac{t}{T})$  and  $g(t) = \frac{t}{T}$ ), or otherwise (but with  $f(0) = 1 = g(T)$  and  $f(T) = 0 = g(0)$ ), and with or without the condition  $f(t) + g(t) = 1$  for all  $t$ . Such a time evolution is captured by the Schrödinger equation

$$\begin{aligned} i\partial_t |\psi(t)\rangle &= \mathcal{H}(t) |\psi(t)\rangle, \\ |\psi(0)\rangle &= |g_I\rangle. \end{aligned} \quad (2)$$

We next consider another state  $|\phi(t)\rangle$  which satisfies a closely related Schrödinger equation

$$\begin{aligned} i\partial_t |\phi(t)\rangle &= (f(t)H_I + \beta g(t)\mathbf{1}) |\phi(t)\rangle, \\ |\phi(0)\rangle &= |g_I\rangle, \end{aligned} \quad (3)$$

with arbitrary  $\beta$ , resulting in a phase ambiguity. Clearly up to a phase,

$$|\phi(t)\rangle = e^{i\xi(t)} |g_I\rangle. \quad (4)$$

From the difference between Eqs. (2) and (3),

$$\partial_t (|\psi(t)\rangle - |\phi(t)\rangle) = -i\mathcal{H}(t) (|\psi(t)\rangle - |\phi(t)\rangle) + ig(t)(H_P - \beta)|\phi(t)\rangle, \quad (5)$$

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we have

$$\begin{aligned}
\partial_t \|\psi(t) - \phi(t)\|^2 &= -2\Re(\langle \psi(t) | - \langle \phi(t) |) \partial_t (|\psi(t)\rangle - |\phi(t)\rangle), \\
&= 2g(t)\Im(\langle \psi(t) | - \langle \phi(t) |) (H_P - \beta)|\phi(t)\rangle), \\
&\leq 2g(t)\|(H_P - \beta)|\phi(t)\rangle\| \times \|\psi(t) - \phi(t)\|, \\
\partial_t \|\psi(t) - \phi(t)\| &\leq g(t)\|(H_P - \beta)|g_I\rangle\|,
\end{aligned} \tag{6}$$

where the first inequality is a result of the Schwarz inequality; and the second inequality from (4). Integrating the time variable on both sides of the last expression from 0 to  $T$  yields

$$\frac{\|\psi(T) - \phi(T)\|}{\|(H_P - \beta)|g_I\rangle\|} \leq \int_0^T g(\tau) d\tau. \tag{7}$$

The numerator of the left hand side is the distance between the final state of  $|\psi(T)\rangle$  and essentially its initial state at  $t = 0$ ,

$$\|\psi(T) - \phi(T)\| \leq 2. \tag{8}$$

Now, with the help of the following result

$$\begin{aligned}
\|(H_P - \beta)|g_I\rangle\| &= \sqrt{\langle g_I | (H_P - \beta)^2 | g_I \rangle}, \\
&= \sqrt{\langle g_I | H_P^2 | g_I \rangle - 2\beta \langle g_I | H_P | g_I \rangle + \beta^2}, \\
&= \sqrt{(\langle g_I | H_P^2 | g_I \rangle - \langle g_I | H_P | g_I \rangle^2) + (\beta - \langle g_I | H_P | g_I \rangle)^2}, \\
&\geq \sqrt{\langle g_I | H_P^2 | g_I \rangle - \langle g_I | H_P | g_I \rangle^2} \equiv \Delta_I E,
\end{aligned} \tag{9}$$

we have also

$$\frac{\|\psi(T) - \phi(T)\|}{\|(H_P - \beta)|g_I\rangle\|} \leq \frac{2}{\min_\beta \|(H_P - \beta)|g_I\rangle\|} \leq \frac{2}{\Delta_I E}. \tag{10}$$

This represents an upper bound whereby there is no restriction on how large the distance from the final state,  $|\psi(T)\rangle$ , to the initial state,  $|\phi(T)\rangle = e^{i\xi(T)}|g_I\rangle$ , must be.

Now, as the right hand side of (7) is a monotonically increasing function of  $T$  (thanks to the positivity of  $g(\tau)$ ), we can *choose* a minimum time  $T_{\min}$  in such a way that this right hand side is larger than the right hand side of (10), which is independent of  $T$ ,

$$\frac{2}{\Delta_I E} \leq \int_0^{T_{\min}} g(\tau) d\tau. \tag{11}$$

The meaning of this time  $T_{\min}$  must then be derived from the meaning of the right hand side of (10). Since this latter quantity represents an *unhindered* and *maximally allowable* exploration by the state vector  $|\psi(T)\rangle$  of the *whole* Hilbert space, we thus see that  $T_{\min}$  is accordingly the minimum time for such an unhindered exploration, in order to realise in general the full potential of the adiabatic computation. That is,  $T_{\min}$  is a lower bound on the evolution time whereby the whole Hilbert space can be explored unhindered, so that the final ground state, in particular, may be obtained with some high probability.

Of course, the computation could be run for a time  $T$  less than this  $T_{\min}$ , but then sufficient computation time has not in general been given for a *full* exploration of the underlying Hilbert space. For any run time less than  $T_{\min}$ , the state  $|\psi(T)\rangle$  can explore only some *smaller* portion of the Hilbert space. (As can be seen from (10), this portion is defined by a restrictive constraint on the distance from the state at time  $T$ ,  $|\psi(T)\rangle$ , to its initial state,  $|g_I\rangle = e^{-i\xi(T)}|\phi(T)\rangle$ .)

The last inequality (11) could also be expressed in the form of a time-energy relation,

$$2 \leq g(\theta) T_{\min} \Delta_I E, \tag{12}$$

with some  $\theta$  in the range  $0 < \theta < T_{\min}$ , thanks to the mean value theorem. This is our first main result [26].

This lower bound on the computation time incorporates the initial ground state  $|g_I\rangle$  and the spectrum of the final Hamiltonian together in  $\Delta_I E$ , which is defined in (9) as the energy spread of the initial state in terms of the final energy. The manner of the time extrapolation is further reflected in  $g(\theta)$ . The condition (12) states that the more the spread of the initial state in energy with respect to the final Hamiltonian, the less the lower bound on the running time.

It thus also emphasises the fact that energy must be considered in the running of QAC, and perhaps in all physical computation if they are indeed all physical in the end. It is interesting to further note that recent results obtained in [9] reflect well in the condition above.

This condition (12) must also contain in it the information about the energy gap between the instantaneous ground state and the first excited state, which in turn determines a lower bound on the computation time as indicated by the quantum adiabatic theorem. The dependence on the gap is not manifest but once again hidden in  $\Delta_I E$ , the energy spread of the initial ground state in terms of the energy eigenstates of the final Hamiltonian. This is not so surprising because (12) is derived directly from the Schrödinger equation, which is also the starting point for the derivation of any version of the quantum adiabatic theorem. We will see in the quantum adiabatic algorithms of the next Section that such an implicit gap dependence is born out in the perfect agreement of the lower bound (12) with all other lower bounds obtained directly from the energy gaps, if and when such gaps can be obtained.

### Energy in the consideration of algorithm complexity

We now apply our lower bound to various quantum adiabatic algorithms in the literature.

In order to find the item labeled by  $|m\rangle$  in an unstructured database with  $N$  items, one method [12] is to employ the initial Hamiltonian  $H_I = 1 - |g_I\rangle\langle g_I|$ , with the initial ground state  $|g_I\rangle$  that has equally distributed probability amplitudes among the  $N$  items,  $|g_I\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^N |i\rangle$ , together with the final Hamiltonian  $H_P = 1 - |m\rangle\langle m|$ , which admits  $|m\rangle$  as the non-degenerate ground state. In this case,  $\Delta_I E = \sqrt{N-1}/N$ .

With linear time extrapolation [5] also employed in the adiabatic computation (1), we substitute  $g(\tau) = \frac{\tau}{T}$  into (12) to obtain

$$O(\sqrt{N}) \leq T_{\min} \quad (13)$$

This lower bound can indeed be attained in a *local* adiabatic search [12]. Its time complexity, even though better than a straightforward classical search, is the same as Grover's quantum search.

Alternatively, for example, the same Hamiltonians but with different extrapolation as proposed in [14, 15],

$$g(\tau) = \frac{\tau}{T} + \sqrt{N} \frac{\tau}{T} \left(1 - \frac{\tau}{T}\right) \Rightarrow \int_0^T g(\tau) d\tau \sim T \times O(\sqrt{N}), \quad (14)$$

would lead to

$$O(1) \leq T_{\min}, \quad (15)$$

that is, a *constant* lower bound on the computation time, irrespective of the database size! This, however, could only be obtained at the expense of the energy being scaled as  $O(\sqrt{N})$  (contained in the term  $g(t)$  hidden in (14)), even if only for the intermediate time.

Even though being known previously [13, 14, 15], we want to reiterate here that energy consideration emerges naturally from QAC, as predominantly displayed in the relation (12), and wish to re-emphasise here the inevitable fact that, because all computation is physical, energy must be an independent dimension, besides those of time and space, in the evaluation of algorithm complexity.

### An adiabatic algorithm for TSP with non-polynomial energy resources

We will deal with the version of TSP [16] with  $M$  cities to be visited as a search problem for the shortest tour among  $M!$  possible tours, each of which connects all the cities and visits each

city once only. The distances between pairs of cities can be presented in a distance matrix, which may or may not be symmetrical, having elements  $d_{ij}$  being the (oriented) distance from the  $i$ -th city to the  $j$ -th city, and having vanishing diagonal elements,  $d_{ii} = 0$ .

A tour is labeled by an integer  $k$ ,  $k = 1, \dots, M!$ , which is the rank of a permutation of  $\langle 1, \dots, M \rangle$ . The length of a tour is labeled by  $l_k$ , which is the sum of appropriate  $d_{ij}$ . We also denote by  $l_{\max}$  a constant (not much) greater than the maximum tour length.

We state here an assumption (needed for this Section only) about the variance  $\Sigma_M$  in  $l_k$ ,

$$\Sigma_M \equiv \sqrt{\frac{1}{M!} \sum_{k=1}^{M!} (l_k - \bar{l})^2} \text{ decreases, if at all, less than exponentially in } M, \quad (16)$$

for asymptotically large  $M$ . That is, we expect that when we add one more city to the list to be visited, even though the number of possibilities now shoots up to  $(M+1)!$ , the difference/spread between the longest and the shortest tour lengths should not decrease exponentially. Indeed, with randomly distributed  $d_{ij}$  we can, thanks to the central limit theorem, show that  $\Sigma_M \sim O(\sqrt{M})$  for  $M \rightarrow \infty$ , namely, as  $\Sigma_M$  does increase, the assumption (16) is satisfied. We suspect that the assumption can be proven in the Euclidean version of the TSP, which is also an NP-complete problem [17]. In fact, it would be sufficient for our purpose if the TSP with the condition (16) is provably NP-complete still.

To employ QAC, we introduce an oracular Hamiltonian  $H_O$ , of infinite dimensions if necessary, which is diagonalised in the number states  $|n\rangle$ ,

$$\langle n|H_O|n\rangle = \begin{cases} l_{n+1}, & \text{for } 0 \leq n \leq M! - 1, \\ l_{\max}, & \text{for } M! \leq n. \end{cases} \quad (17)$$

Possible physical implementation of this oracular/hypothetical Hamiltonian will be discussed later.

We now need to find the ground state  $|n_0\rangle$  of  $H_O$  in order to obtain the tour information from  $n_0$  and the least tour length from the ground state energy, assuming no degeneracy. Following a quantum adiabatic algorithm introduced for Hilbert's tenth problem [18, 19, 20, 21, 22], we employ a linear time interpolation from the following initial Hamiltonian, with annihilation (creation) operators  $a$  ( $a^\dagger$ ),

$$H_I = (a^\dagger - \alpha^*)(a - \alpha), \quad (18)$$

which admits as the ground state the coherent state  $|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$ . The choice of the complex number  $\alpha$  will be crucial for the complexity of our algorithm.

The initial ground state  $|\alpha\rangle$  has a Poissonian probability distribution among the number states  $|n\rangle$ , with equal average occupation number and variance,  $\bar{n} = \sigma^2 = |\alpha|^2$ . As the oracular Hamiltonian  $H_O$  (17) is only non-constant for  $n \leq M! - 1$ , the choice

$$|\alpha|^2 = O(M!) \quad (19)$$

would yield, in the initial state, a variance  $\sigma^2$  in  $n$  that covers all the  $M!$  possibilities, and thus would lead to  $\Delta_I E$  in the inequality (12) taking the same magnitude as the measure  $\Sigma_M$  of the spread in the tour lengths among the  $M!$  tours,

$$\Delta_I E \sim O(\Sigma_M). \quad (20)$$

By the assumption (16) and according to (12), we now have a lower bound for the computation time which is now of the same order as the inverse of  $\Sigma_M$  and thus cannot grow exponentially in  $M$ . That is, we would gain in the computation time complexity if such a lower bound in time could be achieved for the QAC.

However, the price we must pay for such a sub-exponential, or even constant, growth is the exponential cost of the energy that must be supplied, as reflected in the choice (19),  $|\alpha|^2 = O(M!)$ , for the initial Hamiltonian (18). For much larger values of  $|\alpha|^2$ , the variance  $\sigma^2$  would be concentrating in large values of  $n$ , and accordingly  $\Delta_I E$  would be vanishingly small as is evident from the constant eigenvalues of  $H_O$  in (17) for  $M! < n$ . For much smaller value of  $|\alpha|^2$ , the variance  $\Delta_I E$  could be concentrating in an inappropriate domain of  $l_n$  which in general cannot lead to a sub-exponential or polynomial lower bound for the time complexity.

The situation is then similar to other algorithms of a previous Section which gain in the time complexity at the expense of the energy complexity. Fortunately, we could improve upon the situation to reduce the energy consumption.

### Another algorithm for TSP with polynomial energy resources

Instead of encoding a tour by a single number  $k$ , we now employ the  $M$ -tuple  $\langle m_1, \dots, m_M \rangle$ . Each  $m_i$  is a natural number and its first  $M$  values (for  $i$  ranges from 0 to  $M-1$ ) represent the  $M$  cities. For these, there are  $M^M$  tuples, including those with  $m_i = m_j$ , which do not correspond to a TSP tour. In order to put those that are not a TSP tour out of reach, we introduce a counterpart  $\tilde{l}_s$  of the tour length

$$\tilde{l}_s = \begin{cases} \text{tour length } l_s, & \text{if } s \text{ corresponds to a TSP tour,} \\ d^2 + l_{\max}, & \text{otherwise,} \end{cases} \quad (21)$$

where we could use, for example, the following correspondence between  $s$  and the  $M$ -tuples

$$s = 1 + m_1 + m_2 M + m_3 M^2 + \dots + m_M M^{(M-1)}. \quad (22)$$

In (21),  $d$  is a random number drawn from some arbitrarily chosen distribution that has a finite variance *independent* of  $M$ ,  $\sigma_d = C$ , so that for those  $s$  that are not a TSP tour,  $\tilde{l}_s \geq l_{\max}$ . Alternatively, one could obtain the same result by choosing  $d^2 = 0$  for even  $s$ , and  $d^2 = 2l_{\max}$  for odd  $s$  (that is,  $d^2 = (1 - (-1)^s)l_{\max}$ ).

We now start our QAC with the initial coherent state  $|\psi(0)\rangle = \otimes_{i=1}^M |\alpha_i\rangle$ , which is the ground state of the initial Hamiltonian

$$\tilde{H}_I = \sum_{i=1}^M (a_i^\dagger - \alpha_i^*) (a_i - \alpha_i), \quad (23)$$

which is in turn extrapolated linearly in time to an oracular Hamiltonian that is diagonalised in the number states  $|m_1 \dots m_M\rangle$  according to

$$\langle m_1 \dots m_M | \tilde{H}_O | m_1 \dots m_M \rangle = \begin{cases} \tilde{l}_s, & \text{for } 1 \leq s \leq M^M, \\ l_{\max}, & \text{for } M^M < s. \end{cases} \quad (24)$$

The aim of our computation is once again to find the ground state of  $\tilde{H}_O$ , with the ground state energy being the shortest tour length.

If we choose all the complex numbers  $\alpha_i$ 's such that

$$|\alpha_i|^2 = O(M), \quad (25)$$

then the energy requirement for (23) is only of  $O(M^2)$ , which is significantly lower than that of  $O(M!)$  of the last Section. Furthermore, with this choice, the variance/spread in  $s$  in the initial state, as can be computed easily from (22), will be of  $O(M^M)$ . And with this spread the energy variance (9) of the initial state in terms of the energy of (24) will also be of the same magnitude as the variance in the "tour lengths"  $\tilde{l}_s$ . That is, for large  $M$ ,  $\Delta_I E \rightarrow O(\sigma_d)$ , which is a predetermined constant independent of  $M$ , in an exponentially manner because of the exponential decrease in the proportion of TSP tours,  $(M!/M^M) \xrightarrow{M \rightarrow \infty} e^{-M}/\sqrt{M}$ .

Applying our inequality (12) here once again, we are led a lower bound in computation time approaching a constant value *independent* of the number of cities  $M$ . But this time the energy cost is only quadratic in  $M$ . This is our second main result.

Classical simulations of this QAC is rather expensive because of the  $M^M$  possibilities, instead of  $M!$  as in the usual formulation of TSP. Hence, the extraordinary gain above would only be possible with quantum computation. We suspect that quantum entanglement, which has not been fully exploited in QAC up until now, is responsible for this remarkable improvement.

The above algorithm can also be captured in the following QAC in a finite-dimensional Hilbert space with linear time interpolation between

$$H_I = 1 - |g_I\rangle\langle g_I|, \text{ and } H_P = \sum_{m_1=0}^{M-1} \dots \sum_{m_M=0}^{M-1} \tilde{l}_s |m_1 \dots m_M\rangle\langle m_1 \dots m_M|, \quad (26)$$

where  $|\psi(0)\rangle = |g_I\rangle = \bigotimes_{i=1}^M \left( \frac{1}{\sqrt{M}} \sum_{m_i=0}^{M-1} |m_i\rangle \right)$ .

Note that similar kind of oracular Hamiltonians is already employed in Grover's search [12] and involves some kind of non-local interactions, which may make their implementation more difficult than that of quantum circuits (which only require local interactions) but not impossible. However, the infinite-dimension formulation above (in (23) and (24)) could exhibit explicitly the requirement of energy through the  $\alpha_i$ 's in (23), and may be implemented physically with quantum optical means, among others.

### Physical Hamiltonians from the oracular Hamiltonians via Diophantine equations

For completeness, we outline here some ways forward, in principle, to a physical implementation of the oracular/hypothetical Hamiltonians (17, 24). The oracular Hamiltonian (17), for example, can be regarded as a computer program, with  $n$  being an input upon which  $y_n = \langle n|H_O|n \rangle$  is the output (without loss of generality, we choose  $y$  also to be natural numbers). According to the general theory of Diophantine equations [23, 24], corresponding to such a computer program (Turing machine) there is a Diophantine equation which only has integral solution in  $(x_1, \dots, x_K)$ ,

$$D(n, y_n; x_1, \dots, x_K) = 0, \quad (27)$$

for some  $K$ , if and only if  $y_n$  is indeed the output for the input  $n$ . This is a manifestation of the computational universality of Diophantine equations.

Following [18, 19, 20, 21, 22], we could then try to implement the physical Hamiltonian

$$H_P = l_{\max} \left( D \left( a_n^\dagger a_n, a_y^\dagger a_y; a_1^\dagger a_1, \dots, a_K^\dagger a_K \right) \right)^2 + a_y^\dagger a_y. \quad (28)$$

Thanks to the fact that Diophantine polynomials have only integral values, it can be shown that the ground state energy of this Hamiltonian is the shortest tour length we are after. This is the most general but certainly not the most efficient way to consider physical implementation of the oracular Hamiltonians. The appearance of extra  $K$  modes in (28) would require further consideration to ensure that we still have non-exponential complexity in both time and energy. These are outside the scope of the present paper.

### Summary and concluding remarks

We derived a remarkable lower bound on the computation time for QAC in general as a function of the energy necessary for the computation. Energy, being a physical quantity and an inseparable component of any physical process, emerges naturally in QAC, as predominantly displayed in the relation (12), and is thus an inevitable and a natural dimension in the complexity evaluation of an algorithm, in accordance with the view that all computation is physical. We then proposed some new quantum adiabatic algorithms, with oracular Hamiltonians, for the NP-complete TSP. Both the lower bound of the computation time and the energy required of our proposal do not scale exponentially with the number of cities involved. Enlisting the help of general theory of Diophantine equations, we speculated on a general way in principle to physically implement the oracular Hamiltonians of the algorithms. This, however, and whether such a favourable lower bound in the computation time could be achieved would require further detailed investigations elsewhere.

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- [26] Similar results can also be derived for a generalised QAC [6, 15, 25], where an extra term of the form  $h(t)H_E$  (with  $h(0) = h(T) = 0$ ) is added to (1) to represent some further freedom in the adiabatic paths.