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LETTER TO THE EDITOR

Adiabatic quantum gates and Boolean functions

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Abstract
We discuss the logical implementation of quantum gates and Boolean functions in the framework of quantum adiabatic method, which uses the language of ground states, spectral gaps and Hamiltonians instead of the standard unitary transformation language.

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1. Introduction

Recently, a newer subfield emerged by new works addressing the idea of developing quantum algorithms based on adiabatic evolution [1–3]. In the adiabatic quantum computation model, a computational procedure is described by the continuous time evolution of a time-dependent Hamiltonian. Here, we discuss the logical implementation of quantum gates and Boolean functions in the framework of adiabatic quantum method, which uses the language of ground states, spectral gaps and Hamiltonians instead of the standard unitary transformation language. This approach is legitimate because a quantum gate represents a device which performs a unitary transformation on selected qubits in a fixed period of time, using limited energetic resources, and this aspect is often neglected in the standard unitary gate language [4].

2. The adiabatic theorem

Consider a quantum system in a state $|\psi(t)\rangle$, which evolves according to the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \widehat{H}(t)|\psi(t)\rangle \tag{1}$$

where $\widehat{H}(t)$ is the Hamiltonian of the system (we let $\hbar = 1$). To state the adiabatic theorem, it is convenient and traditional to work with a re-scaled time $s = t/T$ where T is the total time

(or *delay schedule*). The Schrödinger equation restated in terms of the re-scaled time s then reads

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}|\psi(s)\rangle = T\widehat{H}(s)|\psi(s)\rangle. \tag{2}$$

The adiabatic theorem refers to a property of the states of the energy spectrum of $\widehat{H}(s)$ [5, 6]. For the sake of simplicity we shall suppose the spectrum of $\widehat{H}(s)$ to be entirely discrete. Also, we assume that the quantum system corresponds to a set of n qubits. In addition we suppose that

1. the eigenvalues $E_j(s)$ and the associated eigenstates $|\xi_j(s)\rangle$, $j = 0, \ldots, 2^n - 1$, of $\widehat{H}(s)$ are continuous and derivable functions of $s \in (0, 1)$;
2. the eigenvalues of $\widehat{H}(s)$ remains distinct throughout the transition period $s \in (0, 1)$: $E_j(s) \neq E_k(s), \forall j \neq k$.

The second condition is equivalent to the ordering condition: $E_0(s) < E_1(s) < \cdots < E_N(s)$. We say that $|\xi_0(s)\rangle$ is the groundstate, $|\xi_1(s)\rangle$ is the first excited state and $|\xi_N(s)\rangle$ is the Nth excited state of the system.

The Hamiltonian of the system is therefore given by

$$\widehat{H}(s) = \sum_{j=0}^{N} E_j(s)\widehat{P}_j(s) \tag{3}$$

where $N = 2^n - 1$, and $\widehat{P}_j(s) = |\xi_j(s)\rangle\langle\xi_j(s)|$ is the projector onto the subspace of $E_j(s)$. The Hamiltonian evolution from $\widehat{H}(0)$ to $\widehat{H}(1)$ induces the unitary transformation $\widehat{U}_T$ (the evolution operator). The evolution operator $\widehat{U}_T(s)$ satisfies the equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\widehat{U}_T(s) = T\widehat{H}(s)\widehat{U}_T(s). \tag{4}$$

The adiabatic theorem states that $\widehat{U}_T(s)$ has the following asymptotic property:

$$\lim_{T\to\infty} \widehat{U}_T(s)\widehat{P}_j(0) = \widehat{P}_j(s) \lim_{T\to\infty} \widehat{U}_T(s) \qquad j = 0, \ldots, N. \tag{5}$$

Thus, if $|j\rangle = |\xi_j(0)\rangle$ is an eigenvector of $\widehat{H}(0)$ belonging to the eigenvalue $E_j(s)$, then the vector $\widehat{U}_T(s)\widehat{P}_j(0)|j\rangle = \widehat{U}_T(s)|j\rangle$ tends toward a vector of the subspace of $E_j(s)$ when $T \to \infty$.

It is useful to estimate the minimum delay schedule T that it takes for this evolution to be adiabatic [7]. The crucial quantities for this transformation to be adiabatic are the minimum gap between the eigenstates

$$\delta_{\min} = \min_{j\neq k} \min_{0\leqslant s\leqslant 1} [E_j(s) - E_k(s)] \tag{6}$$

and the maximum rate at which the Hamiltonian can be modified

$$\Delta_{\max} = \max_{s\in[0,1]} \left\| \frac{\mathrm{d}}{\mathrm{d}s}\widehat{H}(s) \right\|_2. \tag{7}$$

It can be shown that a minimum delay schedule T with

$$T = \frac{\Delta_{\max}}{\varepsilon\delta_{\min}^2} \tag{8}$$

where $0 < \varepsilon \ll 1$, is sufficiently slow for the adiabatic evolution from $\widehat{H}(0)$ to $\widehat{H}(1)$.

3. Adiabatic quantum gates

3.1. Hadamard gate

Let us consider the case of the Hadamard gate

$$W = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{9}$$

which acts on a single qubit as following:

$$W|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad W|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \tag{10}$$

Now, let us consider the following Hamiltonian:

$$\widehat{H}(s) = (1-s)\widehat{H}_0 + s\widehat{H}_1 \tag{11}$$

where

$$\widehat{H}_0 = -E|0\rangle\langle 0| + E|1\rangle\langle 1| \tag{12}$$

and

$$\widehat{H}_1 = -\frac{E}{2}(|0\rangle + |1\rangle)(\langle 0| + \langle 1|) + \frac{E}{2}(|0\rangle - |1\rangle)(\langle 0| - \langle 1|). \tag{13}$$

It is convenient to choose $E = 1$. The initial Hamiltonian $\widehat{H}_0$ has the ground state $|\xi_0(0)\rangle = |0\rangle$ with $E_0(0) = -1$, and the excited state $|\xi_1(0)\rangle = |1\rangle$ with $E_1(0) = 1$. The final Hamiltonian $\widehat{H}_1$ has the ground state $|\xi_0(1)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ with $E_0(1) = -1$, and the excited state $|\xi_1(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ with $E_1(1) = 1$. Thus, if the conditions from the adiabatic theorem are satisfied, one obtains the results corresponding to the Hadamard gate.

One can easily calculate the energy gap and the matrix element as functions of s:

$$\delta(s) = 2\sqrt{1 - 2s + 2s^2} \tag{14}$$

$$\Delta(s) = \left|\langle\xi_1(s)|\frac{\mathrm{d}\widehat{H}}{\mathrm{d}s}|\xi_0(s)\rangle\right| = \frac{2s}{\sqrt{\left[s^2 + \left(1 - s + \frac{1}{2}\delta(s)\right)^2\right]\left[s^2 + \left(1 - s - \frac{1}{2}\delta(s)\right)^2\right]}}. \tag{15}$$

The gap $\delta(s)$ and the matrix element $\Delta(s)$ are smooth functions for $s \in [0, 1]$. The extreme values are obtained for $s = 1/2$: $\delta_{\min} = \delta(1/2) = \sqrt{2}$, $\Delta_{\max} = \Delta(1/2) = \sqrt{2}$. Thus, the minimum delay schedule for the adiabatic Hadamard gate is $T = \frac{1}{\sqrt{2}}\varepsilon^{-1}$.

3.2. Controlled-NOT gate

The prototypical controlled operation is the controlled-NOT (CNOT). CNOT is a quantum gate with two input qubits, known as the *control qubit* $|c\rangle$ and target qubit $|t\rangle$, respectively. In terms of the computational basis, the action of the CNOT is given by

$$|c\rangle|t\rangle \to |c\rangle|c \oplus t\rangle \tag{16}$$

where $\oplus$ is the modulo 2 addition. That is if the control qubit is set to $|1\rangle$ then the target qubit is flipped, otherwise the target qubit is left alone.

We consider the following Hamiltonian:

$$\widehat{H}(s) = (1-s)\widehat{H}_0 + s\widehat{H}_1 + As(1-s)\widehat{H}_{01} \tag{17}$$

where A is a constant

$$\widehat{H}_0 = E_3|00\rangle\langle 00| + E_2|01\rangle\langle 01| + E_1|10\rangle\langle 10| + E_0|11\rangle\langle 11| \tag{18}$$

$$\widehat{H}_1 = E_3|00\rangle\langle 00| + E_2|01\rangle\langle 01| + E_1\,|11\rangle\,\langle 11| + E_0|10\rangle\langle 10| \tag{19}$$

and

$$\widehat{H}_{01} = (E_1 - E_0)\,(|10\rangle\langle 11| + |11\rangle\langle 10|)\,. \tag{20}$$

The extra piece of the Hamiltonian, $\widehat{H}_{01}$, is turned off at the beginning and end of the evolution. In order to simplify the description we choose $E_k = k$, where $k = 0, 1, 2, 3$.

The first two eigenvalues of the Hamiltonian are

$$E_{0,1}(s) = \tfrac{1}{2}\big(1 \mp \sqrt{1 - 4s + 4(1 + A^2)s^2 - 8A^2s^3 + 4A^2s^4}\big). \tag{21}$$

If $A = 0$ then $E_0(s) = s$ and $E_1(s) = (1 - s)$ and the gap is $\delta_{01}(s) = (1 - 2s)$. Therefore, the adiabaticity condition cannot be satisfied because $\delta_{\min} = \delta_{01}(1/2) = 0$. Thus, we must have $A \neq 0$. It is convenient to choose $A = 1$. In this case, the eigenvalues are $E_0(s) = s(1 - s)$, $E_1(s) = [1 - s(1 - s)]$, $E_2 = 2$, $E_3 = 3$. The minimum gap is $\delta_{\min} = \delta_{01}(1/2) = 1/2$. It is easy to show that the matrix elements are constant: $\Delta_{01} = 1$ and $\Delta_{jk} = 0$, $(j, k) \neq (0, 1)$. Thus, the minimum delay schedule for the adiabatic CNOT gate is $T = 4\varepsilon^{-1}$.

3.3. Toffoli gate

The Toffoli gate has three input qubits. The first two qubits are control qubits, and they are unaffected by the action of the Toffoli gate. The third qubit is the target qubit that is flipped if both control qubits are set to $|1\rangle$. So, the effect of the Toffoli gate is described by

$$|c_1\rangle|c_2\rangle|t\rangle \rightarrow |c_1\rangle|c_2\rangle|c_1c_2 \oplus t\rangle. \tag{22}$$

The Hamiltonian is similar to that we used for the CNOT gate (19) with $A = 1$. Here we have

$$\begin{aligned}\widehat{H}_0 = {} & E_7|000\rangle\langle 000| + E_6|001\rangle\langle 001| + E_5|010\rangle\langle 010| + E_4|011\rangle\langle 011| \\ & + E_3|100\rangle\langle 100| + E_2|101\rangle\langle 101| + E_1|110\rangle\langle 110| + E_0|111\rangle\langle 111|\end{aligned} \tag{23}$$

$$\begin{aligned}\widehat{H}_1 = {} & E_7|000\rangle\langle 000| + E_6|001\rangle\langle 001| + E_5|010\rangle\langle 010| + E_4|011\rangle\langle 011| \\ & + E_3|100\rangle\langle 100| + E_2|101\rangle\langle 101| + E_1|111\rangle\langle 111| + E_0|110\rangle\langle 110|\end{aligned} \tag{24}$$

and

$$\widehat{H}_{01} = (E_1 - E_0)(|110\rangle\langle 111| + |111\rangle\langle 110|). \tag{25}$$

We assume that $E_k = k$, where $k = 0, \ldots, 7$. In this case, the eigenvalues are: $E_0(s) = s(1 - s)$, $E_1(s) = 1 - s(1 - s)$, $E_j = j$, $j = 2, \ldots, 7$. The minimum gap is $\delta_{\min} = \delta_{01}(1/2) = 1/2$. Also, it is easy to show that the matrix elements are constant: $\Delta_{01} = 1$ and $\Delta_{jk} = 0$, $(j, k) \neq (0, 1)$. Thus, the minimum delay schedule for the adiabatic Toffoli gate is also $T = 4\varepsilon^{-1}$.

4. Boolean functions

4.1. One-bit Boolean functions

Let us consider a one-bit Boolean function

$$f(x) : \{0, 1\} \to \{0, 1\}. \tag{26}$$

A convenient way of computing this function in the standard approach is to consider a two qubit computer which starts in the state $|x, y\rangle$. With an appropriate sequence of logic gates it is possible to transform this state into $|x, y \oplus f(x)\rangle$, where $\oplus$ indicates addition modulo 2. The first register is called the 'data' register, and the second register the 'target' register. If $y = 0$, then the final state of the second qubit is just the value $f(x)$. In general, it can be shown that given a classical circuit for computing f there is a quantum circuit of comparable efficiency which computes the unitary transformation:

$$|x, y\rangle \xrightarrow{U_f} |x, y \oplus f(x)\rangle \tag{27}$$

on a quantum computer. However, for computational purposes it is considered a 'black box'.

Here we show how the one-bit Boolean function (the 'black box') can be implemented using the adiabatic approach to quantum computation. We consider the following Hamiltonian:

$$\widehat{H}(s) = (1 - s)\widehat{H}_0 + s\widehat{H}_1 + s(1 - s)\widehat{H}_{01}. \tag{28}$$

The initial Hamiltonian is given by

$$\widehat{H}_0 = E_0^0|00\rangle\langle 00| + E_0^1|01\rangle\langle 01| + E_1^0|10\rangle\langle 10| + E_1^1|11\rangle\langle 11|. \tag{29}$$

The final and intermediate Hamiltonians take into account the values of the Boolean function

$$\begin{aligned}\widehat{H}_1 = {} & \left[(1 - f(0))E_0^0 + f(0)E_0^1\right]|00\rangle\langle 00| + \left[f(0)E_0^0 + (1 - f(0))\,E_0^1\right]|01\rangle\langle 01| \\ & + \left[(1 - f(1))E_1^0 + f(1)E_1^1\right]|10\rangle\langle 10| + \left[f(1)E_1^0 + (1 - f(1))E_1^1\right]|11\rangle\langle 11|\end{aligned} \tag{30}$$

$$\widehat{H}_{01} = f(0)\left(E_0^1 - E_0^0\right)(|00\rangle\langle 01| + |01\rangle\langle 00|) + f(1)\left(E_1^1 - E_1^0\right)(|10\rangle\langle 11| + |11\rangle\langle 10|). \tag{31}$$

For example, let us consider the function

$$\overline{x} = \begin{cases} 1, & x = 0 \\ 0, & x = 1 \end{cases} \tag{32}$$

which is equivalent to

$$|x, y\rangle \xrightarrow{\overline{x}} |x, y \oplus \overline{x}\rangle\,. \tag{33}$$

The final and intermediate Hamiltonians are

$$\widehat{H}_1 = E_0^0|01\rangle\langle 01| + E_0^1|00\rangle\langle 00| + E_1^0|10\rangle\langle 10| + E_1^1|11\rangle\langle 11| \tag{34}$$

$$\widehat{H}_{01} = \left(E_0^1 - E_0^0\right)(|00\rangle\langle 01| + |01\rangle\langle 00|). \tag{35}$$

One can see that the computation is achieved by switching the eigenstates $|00\rangle$ and $|01\rangle$ corresponding to the eigenvlalues E_0^0 and E_0^1, respectively. The intermediate Hamiltonian $\widehat{H}_{01}$ makes sure that this switching is done without crossing the eigenvalues during the adiabatic evolution.

Now, let us return to the general case. It is convenient to choose $E_k = k$, where $k = 0, \ldots, 3$. In this case, the eigenvalues are

$$\begin{aligned} E_0^{0,1}(s) &= \tfrac{1}{2}\left[1 \mp \sqrt{1 - 4f(0)s + 4f(0)s^2(1 - 2s + s^2)}\right] \\ E_1^{0,1}(s) &= \tfrac{1}{2}\left[5 \mp \sqrt{1 - 4f(1)s + 4f(1)s^2(1 - 2s + s^2)}\right]. \end{aligned} \tag{36}$$

The minimum gaps are

$$\delta_0^{0,1}(1/2) = \sqrt{1 - \tfrac{3}{4}f(0)} \qquad \delta_1^{0,1}(1/2) = \sqrt{1 - \tfrac{3}{4}f(1)}. \tag{37}$$

For $f(0) = f(1) = 1$ we obtain $\delta_{\min} = 1/2$. Also, it is easy to show that the matrix elements are constant

$$\Delta_{x,y}^{i,j} = \begin{cases} 1, & x = y, i \neq j \\ 0, & x \neq y \end{cases} \tag{38}$$

where $x, y \in \{0, 1\}$ and $i, j \in \{0, 1\}$. Thus, the minimum delay schedule for the adiabatic computation of the one-bit Boolean function is $T = 4\varepsilon^{-1}$.

4.2. n-bit Boolean functions

Let us consider a more general, n-bit Boolean function

$$f(x) : \{0, 1\}^n \to \{0, 1\}. \tag{39}$$

This function can be computed with the Hamiltonian (28) where

$$\widehat{H}_0 = \sum_{x=0}^{2^n-1} \left[E_x^0 |x, 0\rangle\langle x, 0| + E_x^1 |x, 1\rangle\langle x, 1|\right] \tag{40}$$

$$\begin{aligned} \widehat{H}_1 = \sum_{x=0}^{2^n-1} \Big\{ &\left[(1 - f(x))E_x^0 + f(x)E_x^1\right] |x, 0\rangle\langle x, 0| \\ &+ \left[f(x)E_x^0 + (1 - f(x))\, E_x^1\right] |x, 1\rangle\langle x, 1| \Big\} \end{aligned} \tag{41}$$

$$\widehat{H}_{01} = \sum_{x=0}^{2^n-1} f(x) \left(E_x^1 - E_x^0\right) (|x, 0\rangle\langle x, 1| + |x, 1\rangle\langle x, 0|). \tag{42}$$

Assuming that $E_0^0 = 0$, $E_0^1 = 1$, $E_1^0 = 2, \ldots, E_{2^n-1}^0 = 2^{n+1} - 2$, $E_{2^n-1}^1 = 2^{n+1} - 1$, we obtain the following eigenvalues:

$$E_x^{0,1}(s) = \frac{E_x^0 + E_x^1}{2} \mp \frac{1}{2}\sqrt{1 - 4f(x)s + 4f(x)s^2(1 - 2s + s^2)}. \tag{43}$$

The minimum gaps are

$$\delta_x^{0,1}(1/2) = \left|E_x^0(1/2) - E_x^1(1/2)\right| = \sqrt{1 - \tfrac{3}{4}f(x)}. \tag{44}$$

For $f(x) = 1$ we have $\delta_{\min} = 1/2$. It can be easily shown that the matrix elements are

$$\Delta_{x,y}^{i,j} = \begin{cases} 1, & x = y, i \neq j \\ 0, & x \neq y \end{cases} \tag{45}$$

where $x, y \in \{0, 1, \ldots, 2^n - 1\}$ and $i, j \in \{0, 1\}$. Thus, the minimum delay schedule for the adiabatic computation of the n-bit Boolean function is also $T = 4\varepsilon^{-1}$.

The computation is performed by switching between the eigenstates $|x, 0\rangle$ and $|x, 1\rangle$ corresponding to the eigenvlalues E_x^0 and E_x^1, respectively. The switching depends on the values of the Boolean function f. The intermediate Hamiltonian $\widehat{H}_{01}$ makes sure that this switching is done without crossing the eigenvalues during the adiabatic evolution.

5. Conclusions

It is well known that the Hadamard and Toffoli gates represent the simplest universal set of gates [8, 9]. The Toffoli gate can perform exactly all classical reversible computation. The Hadamard gate is all that one needs to add to classical computations in order to achieve the full quantum computation power, since the Hadamard gate is the Fourier transform over the group Z_2. From a conceptual point of view, this is the simplest and most natural universal set of gates that one can hope for. Here, we have discussed the logical implementation of quantum gates and Boolean functions in the framework of quantum adiabatic method, which uses the language of ground states, spectral gaps and Hamiltonians instead of the standard unitary transformation language. We have shown that the unitary quantum gates and Boolean functions can be easily implemented using simple adiabatic Hamiltonians.

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