ON MOLECULAR BONDING LOGIC AND MATRIX REPRESENTATION OF CONSTANT AND BALANCED BOOLEAN FUNCTIONS

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Representing a bonding manifold of a molecule or molecular cluster by a graph given by a set of vertices associated with atoms and a set of edges imitating bonds, the bonding edge encoding formalism is defined on n-tuples qubits in terms of the NOT logic gate acting on the "non-bonded" string. This formalism is illustrated by the simplest diatomic and triatomic molecules whose adjacency matrices generate different quadratic Boolean functions, among which the balanced function appears. In this regard, we review the Deutsch–Jozsa quantum algorithm, well-known in quantum computing, that discriminates between the balanced and constant Boolean functions. A novel matrix representation of the constant-balanced quantum oracle within this algorithm is elaborated. The proposed approach is generalized to distinguish between constant and evenly balanced Boolean functions.

1. Introduction

Quantum computation [1, 2] is based on a number of queries to a black-box quantum device that is usually referred to as a quantum oracle. Let f_n be a Boolean function of n variables, i.e., $f_n : Z_2^n \to Z_2$, where $Z_2 = \{0, 1\}$ is a bit. The set of all n-tuples $\mathbf{x} := (x_1, x_2, ..., x_n) \in Z_2^n$ on which $f_n(\mathbf{x}) = 1$ defines the support, 1_{f_n}, of f_n. $0_{f_n} = Z_2^n \setminus 1_{f_n}$ is then the subset of Z_2^n, where $f_n(\mathbf{x}) = 0$. The Hamming weight of f_n is $w(f_n) := |1_{f_n}|$. Obviously, $w(f_n) = \Sigma_{\mathbf{x}\in Z_2^n} f_n(\mathbf{x})$. An arbitrary Boolean function is identified by its truth table defined by $f_n(\mathbf{x}) = 0$ and $f_n(\mathbf{x}) = 1$.

A quantum n-qubit oracle [1, 2] is generated by f_n and operates on the Hilbert space $C^{2\,\otimes(n+1)}$ as the unitary operator $\hat{U}_{f_n}$ (the so-called oracle call) that maps an input state $|\mathbf{x}\rangle \otimes |y\rangle$; $(y \in Z_2)$ to the output state $|\mathbf{x}\rangle \otimes |y \oplus f_n(\mathbf{x})\rangle$,

$$\hat{U}_{f_n}|\mathbf{x}\rangle \otimes |y\rangle := |\mathbf{x}\rangle \otimes |y \oplus f_n(\mathbf{x})\rangle\,, \qquad (1)$$

where $\oplus$ denotes addition modulo 2. Relation (1) implies that this quantum oracle can be accessed via U_{f_n}: it marks an n-qubit string $|\mathbf{x}\rangle \in C^{2\,\otimes n}$ by means of its unitary oracle gate (1) and thus answers whether a given f_n possesses a certain property or not. $|\mathbf{x}\rangle := \otimes_i^n |x_i\rangle$ is defined as a work n-qubit string (control register) belonging to the $w$ork Hilbert space $C_w^{2\,\otimes n}$ of f_n and $|y\rangle$ is a $t$arget (or oracle, ancillary) qubit from C_t^2. The evaluation of given properties of f_n by a quantum oracle is performed by the corresponding quantum algorithm. Many quantum algorithms are implemented at the molecular level (see [3–9] and references therein) associated with a two-state representative or qubit [10], such as, e.g., a spin-1/2 electron. Among them is the Deutsch–Jozsa quantum algorithm that discriminates between a constant and a balanced Boolean function [1, 2].

The goal of the present work is twofold: first, to define the mapping of the manifold of various chemical bonds onto Z_2^n that implies a novel molecular domain of implementation of quantum algorithms and, second, to propose an approach to resolve the Deutsch–Jozsa quantum algorithm based on the trace of the unitary operators involved in the oracle query and suggested to be rather efficient while implemented on the bonding manifold.

2. Z_2^n Patterning of Molecular Bonding Manifold

Let $\mathcal{M}$ be a stable ground-state neutral molecule that is composed of a finite set $\mathrm{V}_{\mathcal{M}}$ of atoms $\{\mathcal{A}_\alpha\}_\alpha$ such that $\mathcal{M} = \bigcup_{\alpha=1}^{\mathrm{M}} \mathcal{A}_\alpha$, where $|\mathrm{V}_{\mathcal{M}}| = \mathrm{M}$. A bonding manifold $\mathcal{B}(\mathcal{M})$ of a given molecule $\mathcal{M}$ is, by definition, a set of chemical bonds which connect, in a pairwise manner, atoms of $\mathcal{M}$ to one another. In this sense, a molecule $\mathcal{M}$ is a finite, indirect, simple (non-weighted), and loop-free graph $\mathrm{G}(\mathcal{M}|\mathrm{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$ (see, e.g., [11]) given by a finite set $\mathrm{V}_{\mathcal{M}}$ of M vertices $v_1, \ldots, v_{\mathrm{M}}$, associated with atoms, and by a finite set $\mathrm{E}_{\mathcal{M}}$ of edges or bonds.

By definition, $\partial(i)$ maps an each edge $i \in \mathrm{E}_{\mathcal{M}}$ to a pair of vertices: $\partial(i) := (v, v')$ which it connects, i.e., in a sense, $\mathrm{E}_{\mathcal{M}} \subseteq \mathrm{V}_{\mathcal{M}} \otimes \mathrm{V}_{\mathcal{M}}$. Equivalently, two vertices $v, v' \in \mathrm{V}_{\mathcal{M}}$ of this graph are connected or adjacent by edge $i \equiv (v, v') \in \mathrm{E}_{\mathcal{M}}$ or, symbolically, $v \sim v'$, iff $v \in \partial(i)$ and $v' \in \partial(i)$. Any pair of vertices $v, v' \in \mathrm{V}_{\mathcal{M}}$ of a graph $\mathrm{G}(\mathcal{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$ that corresponds to a stable molecule $\mathcal{M}$, i.e., the so-called molecular graph, are connected or not. The star $S(v) \subseteq \mathrm{E}$ of the vertex $v \in \mathrm{V}$ is the set of the edges incident with v. The degree, $\deg(v)$, of the vertex v is defined as $\deg(v) := |S(v)|$. Given $v \in \mathrm{V}$, the neighborhood of $v, N(v) \subseteq \mathrm{V}$, is the set of vertices adjacent to v. If the graphs whose two vertices are connected by more than one edge are excluded, it is evident that $\deg(v) = |N(v)|$. It is obvious that, for any molecular graph $\mathrm{G}(\mathcal{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$ and for each $v \in \mathrm{V}_{\mathcal{M}}$, $\deg(v) \geq 1$.

Let us prepare a logic or "cluster" state of $\mathcal{M}$ on the corresponding molecular graph $\mathrm{G}(\mathcal{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$. For this reason, we define the **Bonding Edge Encoding** (**BEE** in short):

Definition 1: One bit is encoded into each bond (edge) in such a manner that a given edge (v, v') is in the logic state "0" if it does not exist in E (that is, this edge is empty) and in "1" otherwise (that is, there does exist this edge).

Actually, **Edge Bonding Encoding** is the mapping from the molecular bonding manifolds $\{\mathrm{E}_{\mathcal{M}}\}$ to Z_2^n. Hence, we have

Definition 2: A logic state $\mathcal{S}$ of $\mathcal{M} \equiv \mathrm{G}(\mathcal{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$ is $\mathbf{BEE}(\mathrm{E}_{\mathcal{M}}) \subseteq Z_2^n$ where $n = \binom{\mathrm{M}}{2}$.

Definition 2 assumes the existence of some orderings of vertices of $\mathrm{G}(\mathcal{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$ on $\mathrm{V}_{\mathcal{M}}$ and their pairs on $\mathrm{V}_{\mathcal{M}} \otimes \mathrm{V}_{\mathcal{M}}$. The corresponding logic state $\mathcal{S}_{\mathcal{M}}$ is an n-tuple or string (so-called "bonded" string) $\mathcal{S}_{\mathcal{M}} = (\ldots, 0_{k-1}, 1_k, 0_{k+1}, \ldots) \in Z_2^n$ implying that the k-th pair of vertices of G is interconnected by a bond. It is also assumed the existence of the 'non-bonded' string $\mathbf{0} \equiv (0_1, \ldots, 0_k, \ldots, 0_n)$. Within the BEE formalism, a bonding is then interpreted as a logical network determined by a sequence $\mathcal{R}$ of logic gates $\mathcal{R} = \prod_{k=1}^{n} \mathcal{R}_k$, which are successively applied to a "non-bonded" string or input register $\mathbf{0}$ to yield the output-register string $(\ldots, 0_{k-1}, 1_k, 0_{k+1}, \ldots)$. The k-th logic gate $\mathcal{R}_k$ acts on the k-th pair of vertices of $\mathbf{0}$ as the "bonding" operator that creates a bond or edge within this pair, thus producing the "bonding" string $\mathbf{d}_k = (0_1, \ldots, 0_{k-1}, 1_k, 0_{k+1}, \cdots, 0_n)$. It is clear that $\mathcal{R}_k$ is the $\mathrm{NOT}^{[k]}$ gate, a NOT logic gate determined by the Pauli operator $\hat{\sigma}_x$ [1] that acts on the k-th component of the $\mathbf{0}$ string.

Above, the adjacency of a pair of vertices of a graph $\mathrm{G}(\mathcal{M})$ has been defined. The associated adjacency matrix $\mathbf{\Gamma}$ is the $n \times n$ matrix with the matrix elements $\mathbf{\Gamma}_{vv'} = 1$ if $v \sim v'$ and $\mathbf{\Gamma}_{vv'} = 0$ otherwise. The adjacency matrix of any molecular graph is real and symmetric with a zero diagonal. $\mathbf{\Gamma}$ naturally determines the quadratic Boolean function $f_n : Z_2^n \to Z_2$ defined as [12]

$$f_n(\mathbf{x}) := \sum_{i<j}^{\oplus} \mathbf{\Gamma}_{ij} x_i x_j. \tag{2}$$

In other words, the term $x_i x_j$ occurs in the Boolean function $f_n(\mathbf{x})$ related to the graph $\mathrm{G}(\mathcal{M}) = (\mathrm{V}_{\mathcal{M}}, \mathrm{E}_{\mathcal{M}})$ iff $(i,j) \in \mathrm{E}_{\mathcal{M}}$. Let us consider, for illustration, the cluster states of a diatomic molecule $\mathcal{M} = \mathrm{AB}$ and triatomic molecules ABC linear, I, and triangular, II. Their graphs are, respectively, referred to as G(AB|2), G(ABC-I|3), and G(ABC-II|3). The adjacency matrices of these graphs are the following:

$$\mathbf{\Gamma}_{\mathrm{AB}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{\Gamma}_{\text{ABC-I}} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\mathbf{\Gamma}_{\text{ABC-II}} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{3}$$

By virtue of Eq. (2), $\mathbf{\Gamma}_{\mathrm{AB}}, \mathbf{\Gamma}_{\text{ABC-I}}$, and $\mathbf{\Gamma}_{\text{ABC-II}}$ generate, respectively, the 2- and 3-variable quadratic Boolean functions

$$f_{\mathrm{AB}}(\mathbf{x}) = x_1 x_2, \quad f_{\text{ABC-I}}(\mathbf{x}) = x_1 x_2 \oplus x_2 x_3,$$

$$f_{\text{ABC-II}}(\mathbf{x}) = x_1 x_2 \oplus x_1 x_3 \oplus x_2 x_3. \tag{4}$$

Evidently, $1_{f_{\mathrm{AB}}} = \{(1,1)\}$, $1_{f_{\text{ABC-I}}} = \{(1,1,0), (0,1,1)\}$, and $1_{f_{\text{ABC-II}}} = \{(1,1,0), (1,0,1), (0,1,1), (1,1,1)\}$. The truth tables of these Boolean functions can be readily obtained, and they are presented in Tables 1 and 2. Obviously, the truth table of f_{AB} corresponds to the AND logic operation [1]. The truth table of $f_{\text{ABC-I}}$ represents the carry out bit $c' := ab \oplus ac \oplus bc$ (or Maj(a,b,c), the "majority" function) in the classical full adder operating on the input triple (a,b,c) [13]. $f_{\text{ABC-II}}$ is a balanced Boolean function that is the function with $w(f_{\text{ABC-II}}) = 2^2$, i.e. $f_{\text{ABC-II}}$ takes an equal number of 0's and 1's. In contrast, the former two functions are not balanced. To distinguish the balanced functions from the others, the Deutsch–Jozsa algorithm was designed, in particular. Its quantum analogue is treated in the next two Sections.

T a b l e 1. Truth table of the Boolean function f_{AB} defined by Eq. (4)

x_1	x_2	f_{AB}
0	0	0
1	0	0
0	1	0
1	1	1

3. Deutsch–Jozsa Quantum Algorithm

The entire class of 2^{2^n} Boolean functions $f_n : Z_2^n \to Z_2$ is filtered by the Deutsch–Jozsa quantum algorithm [14–16] into the constant and balanced subclasses. A Boolean function f_n is constant if it takes a constant value, either 0 (i.e., $w(f_n) = 0$) or 1 ($w(f_n) = 2^n$) or balanced if $w(f_n) = 2^{n-1}$. Notice that the Hamming weight of constant Boolean functions of n variables is always even and that of the balanced ones is odd or even depending on $n = 1$ and $n > 1$, respectively. For any n, there are only two constant and $b_n = (2^n)!/[(2^{n-1})!]^2$ balanced Boolean functions (e.g., $b_3 = 70$) [17].

The Deutsch–Jozsa quantum algorithm operates only on these two subclasses and distinguishes between them, implying that a balanced Boolean function is the negation of the constant one: simply, "balance $\equiv \neg$ constant and vice versa". If $n = 1$, there exist only $2^{2^1} = 4$ Boolean functions $\{f_1\}$: two constant, $f_1^{[1]}$ and $f_1^{[2]}$, and two balanced, $f_1^{[3]}$ and $f_1^{[4]}$, shown in Table 3. The number of Boolean functions $\{f_2\}$ defined on Z_2^2 is $2^{2^2} = 16$. Their truth table is Table 4. Among them, there are 2 constant functions, $f_2^{[1]}$ and $f_2^{[2]}$, and 6 balanced, $f_1^{[i]}, I = 3 - 8$. The rest 6 functions are neither constant nor balanced. If $n > 1$, the latter functions are $2^{2^n} - (2 + b_n)$. About them, the Deutsch–Jozsa quantum algorithm is unable to deduce anything worth [16]. It must, therefore, be a promise that a given Boolean function is either constant or balanced [18], or, equivalently, some restrictions on the class of Boolean functions should be imposed *a* priori, while the Deutsch–Jozsa quantum algorithm is applied [14].

Let us briefly recapitulate a one-qubit implementation of the Deutsch–Jozsa quantum algorithm [14–16]. We suggest that given qubits $|x\rangle$ and $|y\rangle$ are pure quantum states, say, $|0\rangle$ and $|1\rangle$, and let f_1 be a Boolean function that defines the oracle gate $\hat{U}_{f_1}$ via (1) [19]. We define the gate $\hat{V}[f_1] := \hat{H}^w \hat{U}_{f_1} \hat{H}^t \hat{H}^w \hat{U}^t_{\mathrm{NOT}}$, where $\hat{H}$ and $\hat{U}_{\mathrm{NOT}}$ are the Hadamard and NOT gates, respectively. Applying $\hat{V}[f_1]$ to $|0\rangle \otimes |0\rangle$ yields

$$\hat{V}[f_1]|0\rangle \otimes |0\rangle =$$

$$= \begin{cases} (-1)^{f_1(0)}|0\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle), & f_1 = f_1^{[k]}, \quad k = 1, 2 \\ (-1)^{f_1(0)}|1\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle), & f_1 = f_1^{[k]}, \quad k = 3, 4, \end{cases} \tag{5}$$

and, therefore, if $\hat{V}[f_1]$ maps the input work qubit $|0\rangle$ to $\pm|0\rangle$, f_1 is constant, and if it maps $|0\rangle$ to $\pm|1\rangle$, f_1 is balanced. In other words, if the measurement of the output work qubit yields $\pm|0\rangle$, f_1 is constant, and if the measurement does not yield $\pm|0\rangle$, f_1 is balanced. Let us assume that the ancillary state $|y\rangle$ in Eq. (1) lies in the subspace spanned by the superposed state $(|0\rangle - |1\rangle)/\sqrt{2}$, and the work input state $|x\rangle$ is $|0\rangle$ or $|1\rangle$. As a consequence of Eq. (5), multiplying (1) by $\langle y|$ and taking a partial trace over C_t^2, one may redefine the action of $\hat{U}_{f_1}$ without ancillary qubits (see, e.g., [14, 16, 19–23])

$$\hat{U}_{f_1}|x\rangle := (-1)^{f_1(x)}|x\rangle. \tag{6}$$

4. Matrix Representation of Constant-Balanced Oracle

Consider the matrix representation of the unitary gate $\hat{U}_{f_1}$ in the work-target orthonormal basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ of $C_w^2 \otimes C_t^2$. $f_1^{[1]}$ is then represented by the matrix $|0\rangle\hat{I}_2\langle 0| + |1\rangle\hat{I}_2\langle 1|$, $f_1^{[2]}$ by $|0\rangle\hat{\sigma}_x\langle 0| + |1\rangle\hat{\sigma}_x\langle 1|$, $f_1^{[3]}$ by $|0\rangle\hat{I}_2\langle 0| + |1\rangle\hat{\sigma}_x\langle 1|$, and $f_1^{[4]}$ by $|0\rangle\hat{\sigma}_x\langle 0| + |1\rangle\hat{I}_2\langle 1|$, where the 2×2 identity operator $\hat{I}_2$ and $\hat{\sigma}_x$, the Pauli operator, are defined on C_t^2. These matrices demonstrate that, for $|y\rangle \in \{(|0\rangle + |1\rangle)\sqrt{2}\} \subset C_t^2$, $\hat{U}_{f_1}|x\rangle = |x\rangle$ and, for $|y\rangle \in \{(|0\rangle - |1\rangle)\sqrt{2}\}$,

$$\hat{U}_{f_1^{[k]}} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{(-1)^{k-1}}{\sqrt{2}}(|0\rangle + (-1)^{w(f_1^{[k]})}|1\rangle). \tag{7}$$

The traces of the matrices of $\hat{U}_{f_1^{[k]}}$ ($1 \le k \le 4$), defined as

$$\mathrm{Tr}[\hat{U}_{f_1^{[k]}}] := \Sigma_{x \in Z_2, y \in Z_2} \mathrm{Tr}[|x\rangle|y\rangle\langle y \oplus f_1^{[k]}(x)|\langle x|], \tag{8}$$

Table 2. Truth tables of the Boolean functions $f_{\mathrm{ABC\text{-}I}}$ and $f_{\mathrm{ABC\text{-}II}}$ defined by Eq. (4)

x_1	x_2	x_3	$f_{\mathrm{ABC\text{-}I}}$	$f_{\mathrm{ABC\text{-}II}}$
0	0	0	0	0
1	0	0	0	0
0	1	0	0	0
0	0	1	0	0
1	1	0	1	1
1	0	1	0	1
0	1	1	1	1
1	1	1	0	1

Table 3. Boolean functions defined on Z_2 and treated as the output columns of the truth table

x_1	$f_1^{[1]}$	$f_1^{[2]}$	$f_1^{[3]}$	$f_1^{[4]}$
0	0	1	0	1
1	0	1	1	0

Table 4. 16 two-variable Boolean functions

x_1	x_2	$f_1^{[1]}$	$f_1^{[2]}$	$f_1^{[3]}$	$f_1^{[4]}$	$f_1^{[5]}$	$f_1^{[6]}$	$f_1^{[7]}$	$f_1^{[8]}$	$f_1^{[9]}$	$f_1^{[10]}$	$f_1^{[11]}$	$f_1^{[12]}$	$f_1^{[13]}$	$f_1^{[14]}$	$f_1^{[15]}$	$f_1^{[16]}$
0	0	0	1	0	0	0	1	1	1	1	0	0	1	0	1	1	0
0	1	0	1	0	1	1	1	0	0	0	1	0	1	0	1	0	1
1	0	0	1	1	0	1	0	1	0	0	0	1	1	0	0	1	1
1	1	0	1	1	1	0	0	0	1	0	0	0	0	1	1	1	1

are, respectively, equal to $2^2, 0, 2,$ and 2. The generalization of this result to constant and balanced Boolean functions $\{f_n\}$ of n variables is straightforward: the matrix of $\hat{U}_{f_n}$ in the standard work-target orthonormal basis $\{|\mathbf{0}\rangle \otimes |0\rangle, ..., |\mathbf{1}\rangle \otimes |1\rangle\}$ of $C_w^{2\ \otimes n} \otimes C_t^2$ is equal to

$$\Sigma_{\mathbf{x}\in 0_{f_n}} |\mathbf{x}\rangle \hat{I}_2 \langle \mathbf{x}| + \Sigma_{\mathbf{x}\in 1_{f_n}} |\mathbf{x}\rangle \hat{\sigma}_x \langle \mathbf{x}|. \tag{9}$$

This proves

Proposal 1: The constant functions $f_n^{[1]}(\mathbf{x}) := 0$ and $f_n^{[2]}(\mathbf{x}) := 1, \forall\ \mathbf{x} \in Z_2^n$ generate the unitary gates on $C_w^{2\ \otimes n} \otimes C_t^2$ whose traces,

$$\mathrm{Tr}[\hat{U}_{f_n^{[k]}}] = \Sigma_{\mathbf{x}\in Z_2^n, y\in Z_2} \mathrm{Tr}[|\mathbf{x}\rangle |y\rangle \langle y \oplus f_n^{[k]}(\mathbf{x})| \langle \mathbf{x}|],$$

$$k = 1, 2, \tag{10}$$

are, respectively, equal to 2^{n+1} and 0. An arbitrary balanced Boolean function f_n is characterized by $\mathrm{Tr}[\hat{U}_{f_n}] = 2^n$.

With regard to the Deutsch–Jozsa quantum algorithm, Proposal 1 determines that a given Boolean function f_n of n variables is either $f_n^{[1]}$ or $f_n^{[2]}$, or an arbitrary balanced function iff $\mathrm{Tr}[\hat{U}_{f_n}] = 2^{n+1}$, or 0, or 2^n, respectively. This allows us to suggest another implementation of the Deutsch–Jozsa algorithm on the subclasses of constant and balanced Boolean functions of n variables. Let $|\mathbf{0}\rangle \otimes |0\rangle \in C_w^{2\ \otimes n} \otimes C_t^2$. $\hat{H}_w^{\otimes n}$ transforms $|\mathbf{0}\rangle \otimes |0\rangle$ to

$$\frac{1}{\sqrt{2^n}} \Sigma_{\mathbf{x}\in Z_2^n} |\mathbf{x}\rangle \otimes |0\rangle. \tag{11}$$

Applying further $\hat{U}_{f_n}$ to (11) gives

$$\hat{U}_{f_n} \hat{H}_w^{\otimes n} |\mathbf{0}\rangle \otimes |0\rangle =$$

$$= \frac{1}{\sqrt{2^n}} [\Sigma_{\mathbf{x}\in 1_{f_n}} |\mathbf{x}\rangle \otimes |1\rangle + \Sigma_{\mathbf{x}\in 0_{f_n}} |\mathbf{x}\rangle \otimes |0\rangle]. \tag{12}$$

Equation (12) results in

$$\langle 0| \otimes \langle \mathbf{0}| \hat{H}_w^{\otimes n} \hat{U}_{f_n} \hat{H}_w^{\otimes n} |\mathbf{0}\rangle \otimes |0\rangle = \begin{cases} 1, & f_n = f_n^{[1]}, \\ 0, & f_n = f_n^{[2]}, \\ \frac{1}{2}, & \forall \text{ balanced } f_n, \end{cases} \tag{13}$$

i.e., if the measurement of $\hat{H}_w^{\otimes n} \hat{U}_{f_n} \hat{H}_w^{\otimes n}$ in the $(n+1)$-qubit state $|\mathbf{0}\rangle \otimes |0\rangle$ or defined by the projection $|\mathbf{0}\rangle \otimes |0\rangle\langle 0| \otimes \langle \mathbf{0}|$ (measurement operator), yields the expectation value equal to 1 (0) if f_n coincides with $f_n^{[1]}$ ($f_n^{[2]}$) and equal to 1/2 if f_n is balanced, though, rigorously speaking, it suffices to obtain either 1 and 0 or something else, due to the aforementioned negation between the constant and balanced Boolean functions and the ignorance of the rest ones. Note that (13) also discriminates between the two constant functions. One suggests that this approach can be useful for the n-qubit NMR realization of the Deutsch–Jozsa algorithm [7, 24, 25] and, for arbitrary mixed quantum states, usually probed in the conventional NMR quantum computing (see [26] and references therein). It is also worth mentioning a link of the above implementation with the ensemble of quantum algorithms [19, 27] based on measuring the expectation value $\langle \hat{\sigma}_z \rangle_t$ for the target qubit.

To this end, consider a subclass of the so-called "biased" Boolean functions which are neither constant nor balanced [28, 29]. This class is not empty for $n \geq 2$. As follows from Eq. (9), for a given Boolean function f_n, $\mathbf{x} \in 1_{f_n}$ generates the traceless $\hat{\sigma}_x$ gate $|\mathbf{x}\rangle \hat{U}_{f_n} \langle \mathbf{x}|$. This leads to

Proposal 2: An arbitrary Boolean function f_n that takes N_1 values of 0 ($|0_{f_n}| = N_1$) and N_2 values of 1 ($w(f_n) = N_2$ and $N_1 + N_2 = 2^n$) implements the unitary gate $\hat{U}_{f_n}$ on $C_w^{2\ \otimes n} \otimes C_t^2$ with $\mathrm{Tr}[\hat{U}_{f_n}] = 2^{N_1+1}$; and to

Corollary: For a given Boolean function f_n, the corresponding unitary map $\hat{U}_{f_n}$ with $\log_2(\mathrm{Tr}[\hat{U}_{f_n}]) = N_1 + 1$ determines whether $w(f_n) = \Sigma_{\mathbf{x}} f_n(\mathbf{x})$ is even or odd. It is even if $2|N_2 = 2^n - N_1$ and odd otherwise. Equivalently, if $\log_2(\mathrm{Tr}[\hat{U}_{f_n}])$ is odd, $\Sigma_{\mathbf{x}} f_n(\mathbf{x})$ is even, and if $\log_2(\mathrm{Tr}[\hat{U}_{f_n}])$ is even, $\Sigma_{\mathbf{x}} f_n(\mathbf{x})$ is odd.

5. Summary

Concluding, we have defined the logic, cluster states of molecular bonding patterns by mapping them to the corresponding graphs and encoding these graphs in terms of bits. We have proposed the Bonding Edge Encoding formalism to implement logic gates on the cluster states and to invoke the concept of the adjacency matrix to construct quadratic Boolean functions associated with bonding manifolds. Simple illustrations of this approach have particularly resulted in some balanced Boolean function that lies in the core of the Deutsch–Jozsa quantum algorithm. Second, it has been demonstrated for the first time that the constant and balanced Boolean functions are distinguished from one another by entirely different traces of their corresponding unitary operators that are experimentally accessible. This feature, as believed, can be used as another way to analyze the Deutsch–Jozsa quantum algorithm (see, in this regard, [7, 19, 30]). On the other hand, Proposal 2 can be treated as another approach to discriminate between constant and evenly balanced Boolean functions in the generalized Deutsch–Jozsa algorithm [21, 31]. Corollary definitely shows that this approach is useful to resolve the parity problem [32] that consists in whether the Hamming weight of f_n is even or odd [33].

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ПРО МОЛЕКУЛЯРНО-КЛАСТЕРНІ ЛОГІЧНІ СТАНИ І МАТРИЧНІ ПРЕДСТАВЛЕННЯ СТАЛИХ І БАЛАНСНИХ БУЛЕВИХ ФУНКЦІЙ

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Р е з ю м е

Подаючи різноманітні зв'язки молекули чи молекулярного кластера графом, заданим безліччю вершин, асоційованих з атомами, і чисельністю ребер, що імітують зв'язки, визначено формалізм координування останніх на множині n-кратних кубіт у термінах логічної операції NOT. Запропонований формалізм проілюстровано прикладами найпростіших дво- і триатомних молекул, матриці суміжності, яких породжують різні квадратичні булеві функції, також і балансні. У зв'язку з цим розглянуто відомий квантовий алгоритм Дойча–Джоша, що відрізняє балансні і сталі булеві функції. Подано нове матричне представлення стало–балансного "квантового оракула", що дозволяє розрізняти сталі і двічі балансні булеві функції.