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

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S u m m a r y

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.