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Quantum entanglement in the NMR implementation of the Deutsch–Jozsa algorithm

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Abstract. A scheme to execute an n-bit Deutsch–Jozsa (DJ) algorithm using n qubits has been implemented for up to three qubits on an NMR quantum computer. For the one- and the two-bit Deutsch problem, the qubits do not get entangled, and the NMR implementation is achieved without using spin–spin interactions. It is for the three-bit case, that the manipulation of entangled states becomes essential. The interactions through scalar J-couplings in NMR spin systems have been exploited to implement entangling transformations required for the three bit DJ algorithm.

Keywords. Quantum computation; entanglement; nuclear magnetic resonance; DJ-algorithm.

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The utilization of the intrinsically quantum mechanical nature of the physical world to widen the scope of computational algorithms is one of the important discoveries of this decade [1–3]. It was shown recently that quantum computers can perform certain computational tasks nontrivially faster than classical computers [4–6]. NMR has been the most successful technique to implement quantum algorithms till date [7,8], even though the debate continues about its implications [9].

The Cleve version of the DJ algorithm [10], which requires $n+1$ qubits to solve the n-bit Deutsch problem, has been implemented by several research groups using NMR [11–14]. It has been shown recently that the n-bit Deutsch problem can be solved using n qubits alone [15].

In this paper, we experimentally demonstrate that the n-bit DJ algorithm does not require $n + 1$ qubits for its implementation. By doing away with the extra qubit, the algorithm can be more easily accessed for a greater number of qubits. Furthermore, the one-bit and two-bit implementations of the modified version do not involve quantum entanglement [15,16]. In these cases, only the concept of coherent superposition is exploited, to prepare 'in parallel' an input state which is a superposition of all possible classical inputs, and the experiment has been performed without using spin–spin interactions. It is in the implementation for three or more qubits that quantum entanglement plays a vital role. It hence emerges from our results that the DJ problem for one and two input qubits is not

in essence a quantum problem. The non-trivial quantum features in the algorithm show up only in the implementation for three or more qubits. The NMR implementation of the modified DJ algorithm for one and two qubits uses selective pulses that achieve rotations in the subspaces of individual spins. The non-trivial phase shifts essential for the three-bit problem have been implemented using composite z-pulses. A judicious combination of selective rf pulses and free evolution intervals (under the interaction Hamiltonian), has been employed to construct the required entangling transformations.

Consider an n-bit binary string x; a function f can be defined on this n-bit domain space to a 1-bit range space, with the restriction that either the output is the same for all inputs (the function is 'constant') or the output is 0 for half the inputs and 1 for the other half (the function is 'balanced'). All the 2^n possible input strings are valid inputs for the function ($f(x) = \{0, 1\}$). In quantum computation, these n-bit logical strings are in one-to-one correspondence with the eigenstates of n-qubits, and one can hence label the logical string x by the eigenstate $|x\rangle$. Classically, for an n-bit domain space, one needs to compute the function at least $2^{n-1} + 1$ times in order to determine whether it is constant or balanced. The DJ algorithm achieves this on a quantum computer using only a single function call [4,10].

The usual implementation of the DJ algorithm for n bits requires $n + 1$ qubits, the function f being encoded through an f-dependent unitary transformation

$$|x\rangle_{n\text{-bit}}|y\rangle_{1\text{-bit}} \xrightarrow{U_f} |x\rangle_{n\text{-bit}}|y \oplus f(x)\rangle_{1\text{-bit}}, \tag{1}$$

where $\oplus$ denotes addition modulo 2. The implementation of the unitary transformation U_f, along with the Hadamard transformation, then suffices to distinguish the function as constant or balanced [4,10]. A Hadamard transformation on one qubit mixes the eigenstates maximally,

$$\begin{array}{l} |0\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |1\rangle \xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{array} ; \; H = H^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{2}$$

The Hadamard transformation for n-qubits is the tensor product of the one-qubit transformation ($H^n = H \otimes H \otimes H \otimes \cdots \otimes H$), its action on the n-qubit eigenstates being

$$H^n|x\rangle = \frac{1}{2^{n/2}} \sum_{y=0}^{2^n-1} (-1)^{\oplus \sum_j x_j y_j} |y\rangle, \tag{3}$$

where x_j and y_j are the jth entries of the n-bit strings x and y.

A modified scheme can be designed to solve the n-bit Deutsch problem, using n qubits alone [15]. Here, for every function f a unitary transformation is constructed, such that its action on the eigenstates of n-qubits is

$$|x\rangle_{n\text{-bit}} \xrightarrow{U_f} (-1)^{f(x)}|x\rangle_{n\text{-bit}}. \tag{4}$$

It is instructive to explore the relationship between eqs (1) and (4) and to see how exactly we are able to get rid of the extra qubit for the function call required in the older scheme. The original motivation behind including the extra qubit for the function call in eq. (1) was to construct a reversible(unitary) way of implementing otherwise irreversible function f.

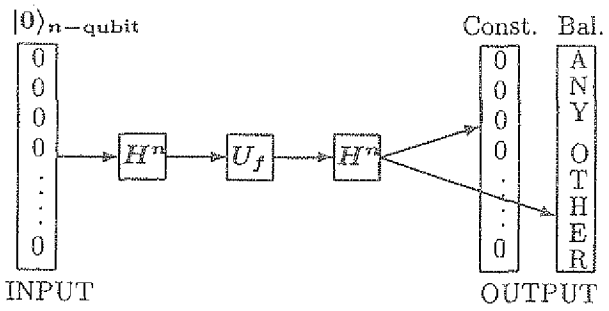

Figure 1. The block diagram for the modified DJ algorithm.

However, it turns out that we can unitarily implement f without this extra qubit. The way the function is being implemented in eq. (4) is through phase shifts which is a purely quantum mechanical concept and has no classical analogue. On the other hand, eq. (1) has a classical motivation and it indeed reduces to a classical implementation if applied to just the eigenstates of the qubits involved. This brings out the interesting fact that one should not always use classical ways of implementing logic even on eigenstates, and it might be useful to directly implement quantum schemes without bothering about corresponding classical analogues.

Consider n qubits, all in the state $|0\rangle$; a Hadamard transformation H^n converts this state to a linear superposition of all 2^n eigenstates with equal amplitudes and no phase differences. The unitary transformation U_f (defined in eq. (4)) acting on this state, introduces an f-dependent phase factor in each eigenstate in the superposition. At this juncture, all information about f is encoded in the quantum state of the n qubits. A Hadamard transformation H^n is once again applied in order to extract the function's constant or balanced nature:

$$|0\rangle \xrightarrow{H^n} \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle \xrightarrow{U_f} \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} (-1)^{f(x)}|x\rangle \xrightarrow{H^n}$$
$$\frac{1}{2^n} \sum_{x=0}^{2^n-1} \sum_{y=0}^{2^n-1} (-1)^{f(x)} (-1)^{\oplus \sum_i x_j y_j} |y\rangle. \tag{5}$$

The final expression for the output state in eq. (5) has an amplitude 1 for the state $|0\rangle_{n\text{-bit}}$ for a constant function and an amplitude 0 for a balanced function.

The categorization of the function as constant or balanced through a single function call using n qubits, is shown pictorially in figure 1.

The number of functions for the n-bit Deutsch problem is ${}^N C_{N/2} + 2$ (where $N = 2^n$). The experimental implementation of the modified DJ algorithm for n bits requires the realization of the unitary transformation corresponding to each of these functions, alongwith the n-bit Hadamard transformation, on a physical system. We now proceed towards the NMR implementation of the modified DJ algorithm for one, two and three qubits, where the number of functions are 4, 8, and 72 respectively.

The pseudo-Hadamard transformation [17] (practically equivalent to the Hadamard operator described in eq. (2)) achieved by a $(90^\circ)_y$ pulse on a spin, has been utilized in our

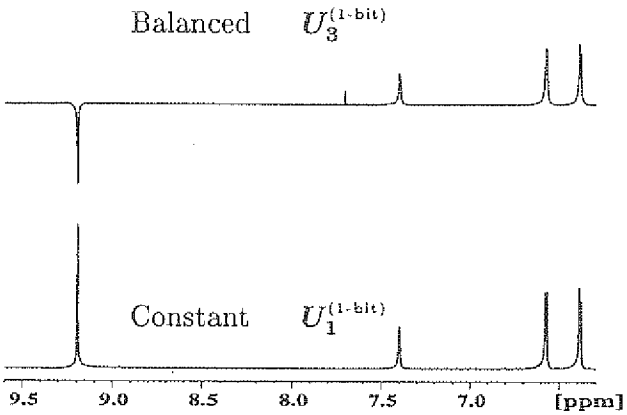

Figure 2. The modified DJ algorithm for one qubit implemented on 5-nitro-2-furaldehyde, the proton resonating at 9.2 ppm being chosen as the computation qubit.

experiments. For the case of two and three qubits, the same has been achieved by a $(90^\circ)_y$ pulse applied non-selectively on all the spins.

The n-bit unitary transformations U_f corresponding to the functions f, are diagonal in the eigenbasis and find a natural description in terms of the single-spin operators,

$$I^{(j)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ; \quad \sigma_z^{(j)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{6}$$

where j labels the qubit involved. The action of U_f on an eigenstate (as described in eq. (4)), has been used to calculate the explicit matrix forms of U_f, for every function f.

The operator representations of the four unitary transformations for the one-bit modified DJ algorithm are

$$\begin{aligned} U_1^{(1\text{-bit})} &= I^{(1)} \quad \text{(const.)}, \\ U_2^{(1\text{-bit})} &= -I^{(1)} \quad \text{(const.)}, \\ U_3^{(1\text{-bit})} &= \sigma_z^{(1)} \quad \text{(bal.)}, \\ U_4^{(1\text{-bit})} &= -\sigma_z^{(1)} \quad \text{(bal.)}. \end{aligned} \tag{7}$$

A pseudo-Hadamard operation achieved by a $(90^\circ)_y$ pulse is applied on a thermal initial state, in order to create a coherent superposition prior to applying the desired unitary transformations U_f. The constant functions correspond to a 'do-nothing' operation, while the balanced functions are achieved by a rotation by the angle π about the z-axis of the spin, up to a global phase factor. These z-rotations have been implemented using composite-z pulses, whereby a rotation by an arbitrary angle θ about the z-axis, can be decomposed as a set of rotations about the x and y axes [18]:

$$(\theta)_z \equiv (\pi/2)_x (\theta)_y (\pi/2)_{-x}. \tag{8}$$

Global phase changes are not detectable in NMR and are hence ignored. The spectrum reflects the constant or balanced nature of the function implemented (figure 2). After the

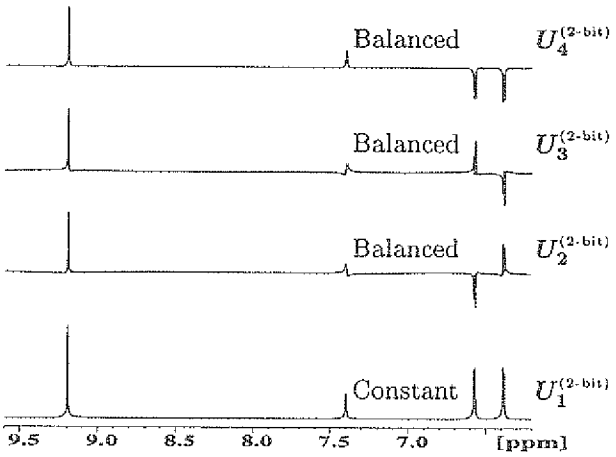

Figure 3. The modified DJ algorithm for two qubits, implemented on 5-nitro-2-furaldehyde with the two qubits resonating at 6.47 ppm and 6.29 ppm respectively.

implementation of a balanced function, the qubit is in a state out-of-phase with the rest of the spectrum. The modified DJ algorithm for one qubit demonstrates the power inherent in even a single bit of quantum information.

All the 8 unitary transformations corresponding to the functions for the two-qubit case are given in terms of $I^{(j)}$ and $\sigma_z^{(j)}$ as

$$\begin{aligned}
U_1^{(2\text{-bit})} &= I^{(1)} \otimes I^{(2)} && \text{(const.)}, \\
U_2^{(2\text{-bit})} &= \sigma_z^{(1)} \otimes I^{(2)} && \text{(bal.)}, \\
U_3^{(2\text{-bit})} &= I^{(1)} \otimes \sigma_z^{(2)} && \text{(bal.)}, \\
U_4^{(2\text{-bit})} &= \sigma_z^{(1)} \otimes \sigma_z^{(2)} && \text{(bal.)}, \\
U_i^{(2\text{-bit})} &= -U_{i-4} \ (i = 5, 6, 7, 8) \ . &&
\end{aligned} \tag{9}$$

All these operators are direct products of single spin operators. They are thus incapable of generating entangled states and can be implemented by operations on individual spins. A pseudo-Hadamard transformation was performed on all the spins (initially in thermal equilibrium) prior to the execution of the desired U_i transformations. The two constant functions correspond to the 'do-nothing' operation, experimentally. The NMR implementation of the balanced functions $U_2^{(2\text{-bit})}$ and $U_3^{(2\text{-bit})}$ involves rotations by π about the z-axis in the single-spin subspaces of spins 1 and 2 respectively, and have been achieved using composite-z pulses (eq. (8)). The $U_4^{(2\text{-bit})}$ transformation too, does not require the scalar J spin interaction and is implemented as successive π rotations about the z-axes of spins 1 and 2 respectively. The balanced functions are distinguished by one (or both) the spins being out-of-phase with the rest of the NMR spectrum (figure 3). Only half the total number of functions have been shown in the one and two-qubit cases, as the others are merely negatives of these, and lead to the same spectral patterns (spectra not shown).

The three-qubit DJ algorithm affords the simplest example where quantum entanglement plays a definitive role in the computation. We reiterate here, that a computation is truly

quantum in character only when entanglement is present. The task here is to implement 72 unitary transformations, the explicit operator forms for 9 of which are

$$\begin{aligned}
U_1^{(3\text{-bit})} &= I^{(1)} \otimes I^{(2)} \otimes I^{(3)} \quad \text{(const.)},\\
U_2^{(3\text{-bit})} &= \sigma_z^{(1)} \otimes I^{(2)} \otimes I^{(3)} \quad \text{(bal.)},\\
U_3^{(3\text{-bit})} &= I^{(1)} \otimes I^{(2)} \otimes \sigma_z^{(3)} \quad \text{(bal.)},\\
U_4^{(3\text{-bit})} &= \sigma_z^{(1)} \otimes \sigma_z^{(2)} \otimes I^{(3)} \quad \text{(bal.)},\\
U_5^{(3\text{-bit})} &= \sigma_z^{(1)} \otimes \sigma_z^{(2)} \otimes \sigma_z^{(3)} \quad \text{(bal.)},\\
U_6^{(3\text{-bit})} &= \tfrac{1}{2}\sigma_z^{(1)} \otimes (I^{(2)} \otimes I^{(3)} + \sigma_z^{(2)} \otimes I^{(3)}\\
&\qquad + I^{(2)} \otimes \sigma_z^{(3)} - \sigma_z^{(2)} \otimes \sigma_z^{(3)}) \quad \text{(bal.)},\\
U_7^{(3\text{-bit})} &= \tfrac{1}{2}\sigma_z^{(2)} \otimes (I^{(1)} \otimes I^{(3)} + \sigma_z^{(1)} \otimes I^{(3)}\\
&\qquad + I^{(1)} \otimes \sigma_z^{(3)} - \sigma_z^{(1)} \otimes \sigma_z^{(3)}) \quad \text{(bal.)},\\
U_8^{(3\text{-bit})} &= \tfrac{1}{2}\sigma_z^{(3)} \otimes (I^{(1)} \otimes I^{(2)} + \sigma_z^{(1)} \otimes I^{(2)}\\
&\qquad + I^{(1)} \otimes \sigma_z^{(2)} - \sigma_z^{(1)} \otimes \sigma_z^{(2)}) \quad \text{(bal.)},\\
U_9^{(3\text{-bit})} &= \tfrac{1}{2}(\sigma_z^{(1)} \otimes I^{(2)} \otimes I^{(3)} + I^{(1)} \otimes I^{(2)} \otimes \sigma_z^{(3)}\\
&\qquad - \sigma_z^{(1)} \otimes \sigma_z^{(2)} \otimes I^{(3)} + I^{(1)} \otimes \sigma_z^{(2)} \otimes \sigma_z^{(3)}) \text{ (bal.)}.
\end{aligned} \tag{10}$$

The operators $U_1^{(3\text{-bit})}$– $U_5^{(3\text{-bit})}$ can be decomposed as direct products of single-spin operators and are tshus non-entangling transformations. The operators $U_6^{(3\text{-bit})}$–$U_9^{(3\text{-bit})}$ cannot be decomposed as direct products of single-spin operators and are hence capable of generating entangled states from non-entangled ones. The operators $U_6^{(3\text{-bit})}$, $U_7^{(3\text{-bit})}$, and $U_8^{(3\text{-bit})}$, are entangling in different two-spin subspaces and can be factored as direct products of a single-spin operator and a two-particle entangling transformation. They can thus generate states in which two qubits are entangled, with the third qubit remaining non-entangled with either of them. On the other hand, the transformation $U_9^{(3\text{-bit})}$ does not allow any such simplifications. It is maximally entangling and leads to states that are three-qubit entangled. These 9 functions are thus divided into three categories namely, non-entangling, two-qubit entangling, and maximally (three-qubit) entangling. The remaining functions are similar in form, and can be classed into one or the other of these categories.

The result of experimentally applying the non-entangling transformations $U_1^{(3\text{-bit})}$–$U_5^{(3\text{-bit})}$, after a pseudo-Hadamard transformation on a thermal equilibrium state, is shown in figure 4. The constant function $U_1^{(3\text{-bit})}$ is the unit operator, and corresponds to the 'no pulse' or the 'do-nothing' operation. The balanced functions $U_2^{(3\text{-bit})}$ and $U_3^{(3\text{-bit})}$ correspond to a rotation by the angle π about the z-axis of the first and the third spins respectively, without perturbing the other spins. This has been achieved by a spin-selective $[\pi]_z$ pulse in each case, using composite z-pulses (eq. (8)). The spectrum is categorized by the spin in question being out-of-phase with the rest of the spectrum. The transformation $U_4^{(3\text{-bit})}$ has been implemented by two spin-selective $[\pi]_z$ pulses applied consecutively on the first and the second spins respectively, and leads to a spectrum with both these spins being out-of-phase with the third. The non-entangling balanced function $U_5^{(3\text{-bit})}$, has been implemented by successive spin-selective $[\pi]_x$ pulses on all the three spins.

The two-qubit entangling transformation $U_6^{(3\text{-bit})}$, is achieved by the pulse sequence

$$[\pi/2]_z^2 \;\; [\pi/2]_z^3 \;\; \overset{(\tau_{23}/2)}{\text{———}} \;\; [\pi]_x^2 \;\; [\pi]_x^3 \;\; \overset{(\tau_{23}/2)}{\text{———}} \;\; [\pi]_x^1 \,,$$

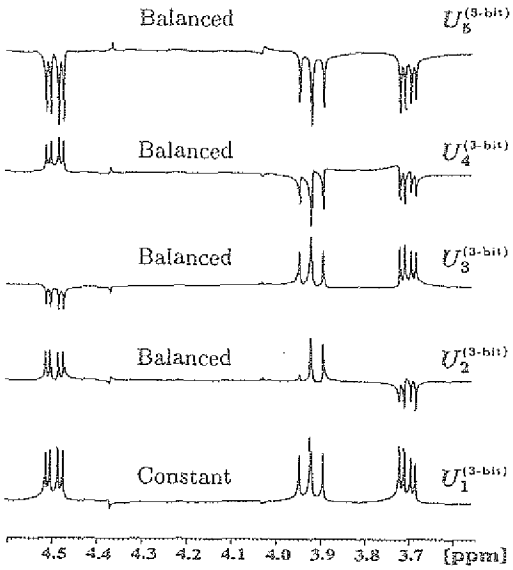

Figure 4. The refined DJ algorithm for three qubits, implemented on 2,3-dibromopropionic acid. The functions shown are all non-entangling in nature.

where $\tau_{23} = 1/J_{23}$ and 1, 2 and 3 are qubit labels. The operators $U_7^{(3\text{-bit})}$ and $U_8^{(3\text{-bit})}$ correspond to cyclic permutations of the qubits. The spin-selective π pulses in the middle of the free evolution period τ_{23} refocus the chemical shift evolution. The pulse sequence (applied after a pseudo-Hadamard transformation on all three qubits in a thermal initial state) results in a density matrix with the product operator form $-I_x^1 + 2I_x^2 I_z^3 + 2I_z^2 I_x^3$, leading to a spectrum with the multiplet of the first qubit inverted, and an antiphase doublet of doublet pattern for the other two qubits (figure 5). The three-qubit entangling function $U_9^{(3\text{-bit})}$ is implemented by the pulse sequence

$$[\pi/2]_z^1\,[\pi/2]_z^3 \xrightarrow{(\tau_{12}/2)} [\pi]_x^1\,[\pi]_x^2 \xrightarrow{(\tau_{12}+\tau_{23})/2} [\pi]_x^2\,[\pi]_x^3 \xrightarrow{(\tau_{23}/2)}$$

leading to an antiphase spectral pattern for all three qubits, corresponding to the product operators $2I_x^1 I_z^2 + 2I_z^2 I_x^3 + 4I_z^1 I_x^2 I_z^3$ (figure 5). The spectra in figure 5 suffer from phase distortions arising from the inaccurate refocusing of the chemical shifts during the τ periods, and J-evolution during long spin-selective composite-z pulses ($[\pi]_z^i \equiv [\pi/2]_x^i [\pi]_y^i [\pi/2]_{-x}^i =$ 42 msec).

This implementation of the DJ algorithm does not require the initial preparation of the spins in a pseudo-pure state, since the thermal equilibrium state serves equally well as a good initial state. The observable spectral result is the same in both cases, though beginning with a pseudo-pure state creates some (undetectable) multiple-quantum coherences. Further, it is interesting to note that the application of an entangling transformation to an unentangled state does not always lead to an entangled state. In particular, for the three-bit DJ algorithm implemented on thermal initial states, the final output state (carrying information about the function's constant or balanced nature), is unentangled, even though some of the unitary transformations required are entangling in nature.

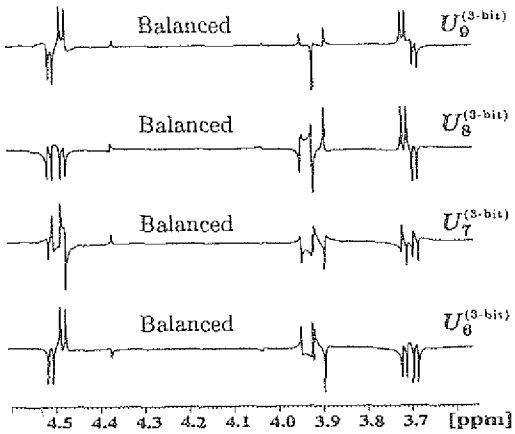

Figure 5. Entangling balanced functions implemented on the three-qubit system of 2,3-dibromopropionic acid.

The final pseudo-Hadamard transformation to extract the constant or balanced nature of the function (figure 1) is cancelled by the $(90)^\circ$ read-out pulse usually used in NMR experiments, and the computation essentially culminates in the application of the desired U_f function after the first pseudo-Hadamard transformation.

A modification to the usual DJ algorithm enabled an n-bit implementation using n qubits. The required unitary transformations were tailored to eliminate the need for the extra qubit, and the modified DJ algorithm was tested experimentally for one, two and three qubits. While the one and two qubit cases use non-entangling unitary transformations, it was noted that for three (or more) qubits, multi-particle entangling transformations are essential. The NMR implementation of such entangling transformations requires the presence and manipulation of spin–spin interactions [19].

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