Quantum coherence and entanglement in the avian compass

James A. Pauls,[1] Yiteng Zhang,[2] Gennady P. Berman,[3] and Sabre Kais[4,5,*]

[1]*Goshen College, Goshen, Indiana 46526, USA*
[2]*Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA*
[3]*Theoretical Division, T-4, MS B-213, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[4]*Department of Chemistry, Department of Physics, and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA*
[5]*Qatar Environment and Energy Research Institute, Qatar Foundation, Doha, Qatar*

The radical-pair mechanism is one of two distinct mechanisms used to explain the navigation of birds in geomagnetic fields, however little research has been done to explore the role of quantum entanglement in this mechanism. In this paper we study the lifetime of radical-pair entanglement corresponding to the magnitude and direction of magnetic fields to show that the entanglement lasts long enough in birds to be used for navigation. We also find that the birds appear to not be able to orient themselves directly based on radical-pair entanglement due to a lack of orientation sensitivity of the entanglement in the geomagnetic field. To explore the entanglement mechanism further, we propose a model in which the hyperfine interactions are replaced by local magnetic fields of similar strength. The entanglement of the radical pair in this model lasts longer and displays an angular sensitivity in weak magnetic fields, both of which are not present in previous models.

I. INTRODUCTION

The ability of many animal species such as birds, insects, and mammals to sense the geomagnetic field for orientation and navigation has led to great interest in the field of biophysics [1,2]. There are currently two leading hypotheses to explain this remarkable ability: the magnetite-based mechanism and the radical-pair mechanism [3–7]. The latter mechanism has been supported by results in the field of spin chemistry [8,9] and by biological experiments [10]. Recently several authors have raised the intriguing possibility that living systems may use nontrivial quantum effects to optimize their orientation behavior [3,4,11,12]. Much effort has been made to demonstrate the radical-pair mechanism and improve the models. Ritz *et al.* [13] proposed a basic model and a physical metric $s'(\theta)$ as a vision-based signal. Based on the previous work, Lau *et al.* [14] claimed the photoselection effects from the directionality of the light entering a bird's eye, rather than the intrinsic ordering of their molecular precursors, could help the radical pairs generate the anisotropic distributions, which in principle has basically the same function as $s'(\theta)$. Furthermore, Hogben *et al.* [15] demonstrated that entangled initial states are not necessary in terms of compass sensitivity. However, even if the initial spin state is neither entangled nor coherent, coherences can also arise during the spin evolution as a result of the differential reactivity of the singlet and triplet states [15]. Therefore, the entanglement and coherence may still have an effect on the bird's sense of the magnetic field. As long as we can confirm the positive role of the entanglement in the radical-pair mechanism for the chemical compass, we can connect the chemical compass model with quantum information, so we can propose some quantum control protocols to realize the relevant experiments to improve the navigation system.

Cai *et al.* [5] suggested that entanglement, rather than mere quantum coherence, is the contributing factor that allows the avian compass to achieve its high level of sensitivity. Recently, Kominis [16] also argued that spin-selective radical-ion-pair reactions are able to offer an exquisite magnetic sensitivity. If this is so, does the duration of the entanglement last long enough to impact biological processes and is the duration of entanglement sensitive to the inclination of the radical pair with respect to the earth's magnetic field? To answer these questions, we revisit the radical-pair mechanism with the candidate chemical reaction [4]. First, we recheck the triplet yields with respect to several typical assumed decay rates. Second, we examine the lifetime of radical-pair entanglement corresponding to various external magnetic-field strengths to see if it lasts long enough to allow the biological system to use the results. Third, we attempt to use the entanglements, instead of the vision-based signal $s'(\theta)$, as a signal of direction and we explore the angular dependence of the radical-pair entanglement with respect to the geomagnetic-field direction. Finally, based on our results, we propose a different model to explore the underlying details. We find that the entanglement present in our proposed model displays both directional sensitivity and a sufficiently long duration of entanglement.

II. MODEL

Following Ritz *et al.* [13], we include only the Zeeman interaction and the hyperfine interaction in the Hamiltonian of the system

$$H = g\mu_B \sum_{i=1}^{2} \vec{S}_i \cdot (\vec{B} + \hat{A}_i \cdot \vec{I}_i), \qquad (1)$$

where the first term is the Zeeman interaction and the second term is the hyperfine interaction. (We assume that each electron is coupled to a single nucleus.) In addition, $\vec{I}_i$ is the nuclear spin operator; $\vec{S}_i$ is the electron spin operator, i.e., $\vec{S} = \vec{\sigma}/2$ with $\vec{\sigma}$ being the Pauli matrices; g is the g factor of the electron, which is chosen to be $g = 2$; μ_B is the Bohr magneton of the electron; and $\hat{A}_i$ is the hyperfine coupling tensor, a 3×3

*kais@purdue.edu

matrix. As proposed in Ref. [13], we model the radical-pair dynamics with a Liouville equation

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H,\rho(t)] - \frac{k_S}{2}\{Q^S,\rho(t)\}$$
$$- \frac{k_T}{2}\{Q^T,\rho(t)\}, \qquad (2)$$

where H is the Hamiltonian of the system; Q^S is the singlet projection operator, i.e., $Q^S = |S\rangle\langle S|$, and $Q^T = |T_+\rangle\langle T_+| + |T_0\rangle\langle T_0| + |T_-\rangle\langle T_-|$ is the triplet projection operator, where $|S\rangle$ is the singlet state and $(|T_+\rangle, |T_0\rangle, |T_-\rangle)$ are the triplet states [17]; $\rho(t)$ is the density matrix for the system; and k_S and k_T are the decay rates for the singlet state and triplet states, respectively.

III. CALCULATIONS AND RESULTS

For our calculations we assume that the initial state of the radical pair is a perfect singlet state $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. Therefore, the initial condition for the density matrix is $\rho(0) = \frac{1}{4}\hat{I}_N \otimes Q^S$, where the electron spins are in the singlet states and nuclear spins are in a completely mixed state, which is a 4×4 identity matrix. Assuming that the recombination rate is independent of spin, the decay rates for the singlet and triplet should be the same [13], $k_S = k_T = k$, i.e., k is the recombination rate for both the singlet and triplet states. The external weak magnetic field $\vec{B}$, representing the earth's magnetic field in Eq. (1), depends on the angles θ and φ with respect to the reference frame of the immobilized radical pair, i.e., $\vec{B} = B_0(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, where $B_0 = 0.5$ G is the magnitude of the local geomagnetic field. Without losing the essential physics, φ can be assumed to be 0.

Since the radical pair must be very sensitive to different alignments of the magnetic field, it is necessary to assume that the hyperfine coupling tensors in Eq. (1) are anisotropic. However, for the sake of simplicity, we employ the hyperfine coupling as anisotropic for one radical and as isotropic for the other [13], i.e.,

$$\hat{A}_1 = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{A}_2 = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

(in Gauss).

Using the parameters defined above, we calculate the influence of different decay rates on the triplet yield Φ_T, as the external magnetic field varies, to determine the values of the decay rates that are reasonable for biological systems. We define the triplet yield as [12,17] $\Phi_T = k \int_0^\infty \text{Tr}[Q^T\rho(t)]dt$, where $Q^T = |T\rangle\langle T|$ and $|T\rangle = |T_+\rangle + |T_0\rangle + |T_-\rangle$. From Fig. 1 we can tell that the effect of the radical-pair decay rates on the triplet yield has a twofold function [13]. For a very high decay rate, i.e., larger than 10 μs^{-1}, the rapid decay of the radical pair prevents efficient singlet-triplet mixing, as can be seen by the increase of the triplet yield in the weak magnetic field. Consequently, the weak magnetic field has very little effect on the triplet yields with rapid decay rates. However, for very slow decay rates, i.e., smaller than 0.1 μs^{-1}, the triplet yield increases up to its maximum almost immediately when the magnetic field increases from zero, but is essentially static
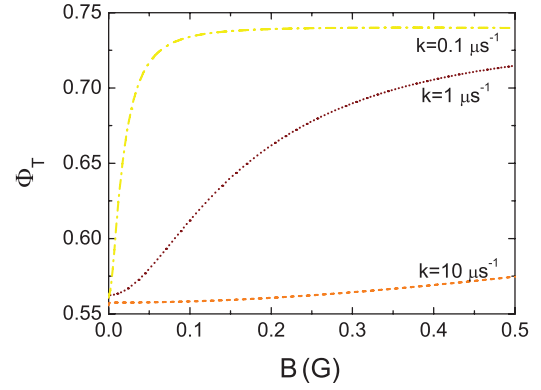

FIG. 1. (Color online) Triplet yields of three different decay rates as a function of the external magnetic-field magnitude. The black line, for which $k = 1$ μs^{-1}, seems to be a reasonable curve.

as the magnetic field continues to increase. In contrast, for $k = 1$ μs^{-1}, the quantity of $\frac{\partial\Phi_T}{\partial B}$ is relatively significant, which is essential to detect the weak magnetic field. Therefore, a decay rate on the order of 1 μs^{-1} seems to be optimum for the detection of a weak magnetic field. For all further calculations with this model we have assumed this value for our decay rate, i.e., $k = 1$ μs^{-1}, which is consistent with the results of Ref. [12], in which the authors claimed that the decay rate is on the order of μs^{-1}, even though Gauger and Benjamin [18] commented that the decay rate should be on the order of hundreds of microseconds, which can actually be seen as the limit for the radical-pair mechanism to function. Therefore, 1 μs^{-1} still works for us as the optimum.

Having fixed the decay rate to be 1 μs^{-1}, we study the radical-pair entanglement as a function of the magnitude of the geomagnetic field. The z axis of the radical pair is aligned at an angle of $68°$ with the magnetic-field vector, which is the angle at which an earth-strength magnetic field produces the largest triplet yield [13]. In this paper we use negativity as the metric of entanglement $N(\rho) = \frac{\|\rho^{T_A}\|_1 - 1}{2}$, where $\|\rho^{T_A}\|_1$ is the trace norm of the partial transpose of the system's density matrix [19,20]. The results are shown in Fig. 2. We can see that when the magnetic fields are weaker than the earth's magnetic field, or as strong as 1 G, the entanglement curves are almost
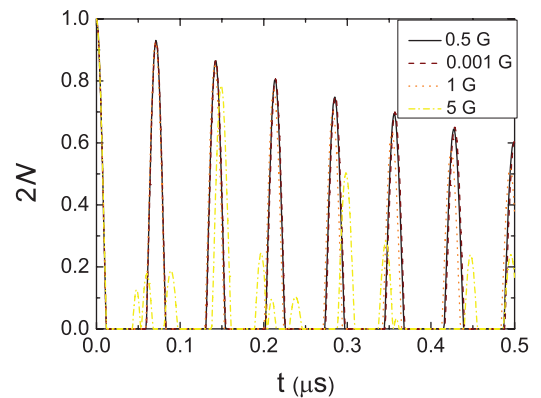

FIG. 2. (Color online) Entanglements (twice the negativity) for different magnitudes of the magnetic field for an angle of $68°$ between the z axis of the radical pair and the magnetic field.

identical. There does not appear to be any unique behavior that distinguishes a field in the neighborhood of 0.5 G. However, in the earth's magnetic field, the entanglement will be robust periodically, at least during the first 0.5 μs, which is longer than the suggested duration of radical-pair separation [4]. Actually, recent work has shown that the flavin-tryptophan radical pair in cryptochrome can last as long as 5 μs *in vitro* [21]. Gauger *et al.* [3] also obtained a similar inspiring result for entanglement and suggested that periodic disappearance caused by the entanglement alternated between the electron spins and the nuclear spins at each site and a stronger magnetic field (e.g., 5 G) will disturb this periodicity. Previous research on the magnetic-field sensitivity of the chemical compass has demonstrated that the entanglement is helpful only if nature allows birds to optimize their behavior [5]. On these grounds one can say that the entanglement lasts long enough to play a crucial role in the orientation of birds. So we can say that the entanglement could play a role in the orientation and navigation of birds.

In order for entanglement to also act as a signal of direction, the entanglement must be angle dependent. While the calculation gives us a surprising result, in Fig. 3, that is, the dynamics of entanglement does not change with angle, i.e., entanglement is not sensitive to the angle between the z axis of the radical pair and the earth's magnetic field. Therefore, it is reasonable to conclude that the entanglement of the radical pair cannot provide the same information as the vision-based signal $s'(\theta)$. In other words, using this model, the entanglement of the system does not directly affect the birds' ability to orient themselves. However, all of the curves provide us a robust entanglement during the simulated intervals (0.5 μs). Therefore, we can make a brave hypothesis that the entanglement is a necessary condition for the suggested chemical compass. Also, there might be indirect mechanisms for birds to utilize entanglement.

The above result (Fig. 3) shows that the dynamics of entanglement almost remain the same for different angles under the symmetric hyperfine tensors. This raises the following question. What will happen if there is an asymmetric hyperfine tensor? Although hyperfine tensors of organic radicals are usually symmetric, since there is no direct evidence of the candidate for the magnetoreceptors and based on the
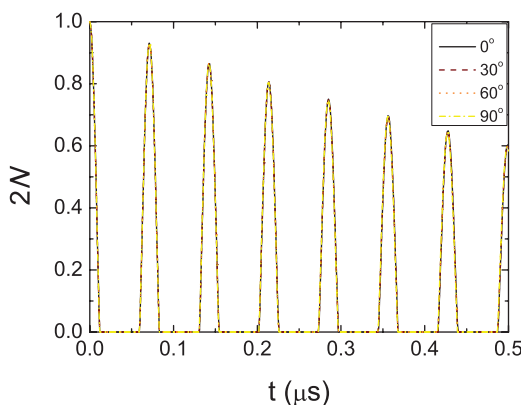

FIG. 3. (Color online) Entanglements for different angles. All curves are practically identical. In the geomagnetic field, entanglement does not change with orientation.
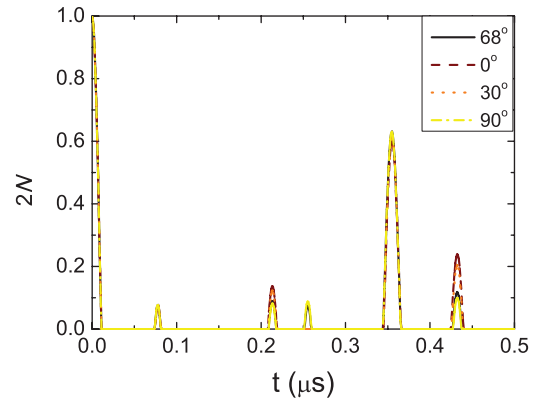

FIG. 4. (Color online) Entanglements for different angles under the hyperfine coupling tensors $\hat{A}_i^b$.

complicated biological environment, we can examine a few asymmetry cases to try to find the underlying effects of the hyperfine coupling. The asymmetric hyperfine tensor we examine are

$$\hat{A}_1^b = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \quad \hat{A}_2^b = \begin{pmatrix} 5 & 5 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

and

$$\hat{A}_1^c = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \quad \hat{A}_2^c = \begin{pmatrix} 0 & 5 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

From Figs. 4 and 5 we can easily see that the hyperfine coupling tensor pair of $\hat{A}_i^c$ gives an intriguing result: The dynamics of the entanglement is clearly dependent on the system's orientation. This result inspired us to develop an alternative model in which only the external magnetic fields are considered since in the case of $\hat{A}_i^c$ there are only two nonzero terms.

IV. ALTERNATIVE MODEL

Previously, we had assumed that one electron of the radical pair experiences an anisotropic hyperfine coupling, while the other experiences an isotropic one. However, this model cannot produce an angular-sensitive entanglement. In contrast, the hyperfine coupling tensors $\hat{A}_i^c$ led to an angular-sensitive result.
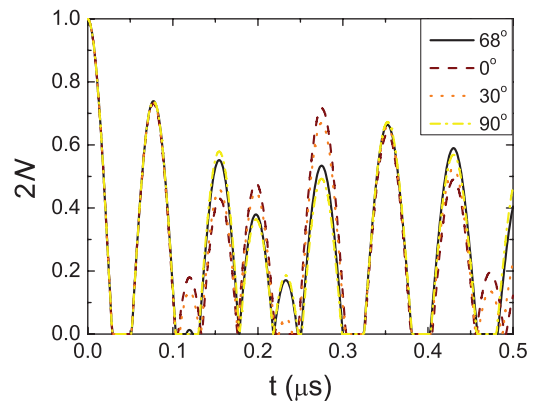

FIG. 5. (Color online) Entanglements for four angles under the hyperfine coupling tensors $\hat{A}_i^c$.

Inspired by this result, we propose that each electron interacts with additional local magnetic fields $\vec{B}_i$ rather than with the hyperfine interactions. The Hamiltonian for this model is given by Eq. (1), but with $\hat{A}_i \cdot \vec{I}_i$ replaced by $\vec{B}_i$, the local magnetic field for the ith electron spin. We take the local fields to be $\vec{B}_1 = (0,0,4)$ and $\vec{B}_2 = (0,5,0)$.

In this case, we use the violation of the Clauser-Home-Shimony-Holt (CHSH) inequality [22] as the metric of entanglement, a version of Bell's inequality [23]. The CSHS inequality is given by $|E| \leqslant 2\lambda_{\max}^2$, where $|E| = |E(0,0) + E(0,t) + E(t,0) - E(t,t)|$, $E(t_1,t_2) = \langle \phi_{t_1} | (\vec{\sigma}_1 \cdot \vec{a})(\vec{\sigma}_2 \cdot \vec{b}) | \phi_{t_2} \rangle$ is the two-time correlation function for a spin pair, and $\vec{a}$ and $\vec{b}$ are the unit direction vectors. The quantity $\lambda_{\max}$ is the maximum eigenvalue for the measurement operator $(\vec{\sigma}_1 \cdot \vec{a})(\vec{\sigma}_2 \cdot \vec{b})$, which for our specific operator is equal to 1. When $|E|$ exceeds $2\lambda_{\max}^2 = 2$, the correlation between the two spins can no longer be explained classically, so the system is entangled.

Figure 6 shows the CHSH inequality as a function of time for various orientations of the system in a magnetic field of 0.5 G. Because there are now two perpendicular fields acting on the system, it is necessary to consider azimuthal orientation in addition to polar orientation. As shown in Fig. 6, as θ increases from $0°$ to $180°$, the time for which the electron pair is entangled increases from roughly 60 ns to nearly 90 ns, while for ϕ from $0°$ to $150°$ the variation of time of entanglement is restricted to an interval of less than 10 ns. It is interesting to

note that this variation in time of entanglement occurs roughly on the same 100-ns time scale that the two electrons remain separated [4].

Changing the relative angles and strengths of the local magnetic fields has a dramatic impact on the angular sensitivity. A change in the field strength of the first electron from 4 to 5 G is enough to dramatically increase both the azimuthal and angular sensitivity of the entanglement.

If indeed a protein such as cryptochrome is in part responsible for magnetoreception, there must be some directional bias of the orientation of the protein so that there will be a strong net signal. It is possible that this directional dependence could be provided by embedding within the membrane layers of photoreceptor cells. This form of embedding leaves the protein free to rotate about one axis [24], but greatly restricts the rotation about its second axis [25]. For this reason it is necessary for the radical-pair compass to be sensitive to rotation about one axis, while being virtually unaffected by rotation about the second. If the radical-pair compass were to be sensitive to rotation in both θ and ϕ, the result of randomly oriented proteins about the θ axis would average out to create a background signal that could potentially reduce the contrast of the radical-pair compass.

At the present time little is known about how cryptochrome is situated within the retina, in particular how it embeds onto or within the cell membrane [25]. There is no reason to assume that the z axis of the radical-pair model coincides with the fixed rotational axis of the embedded protein. As such, a configuration such as $\vec{B}_1 = (0,0,5)$ and $\vec{B}_2 = (0,5,0)$ might still produce a strong directional response under a coordinate transformation to the axis of protein rotation.

It should be pointed out that the angular dependance of entanglement in this model is not invariant under a reversal of the external magnetic field. While this might seem to contradict an inclination-only compass model, it is reasonable to assume that cryptochrome is either bound to both sides of the cell membrane or embedded within the membrane in both up and down orientations so that the net signal cannot discern the polarity of the geomagnetic field.
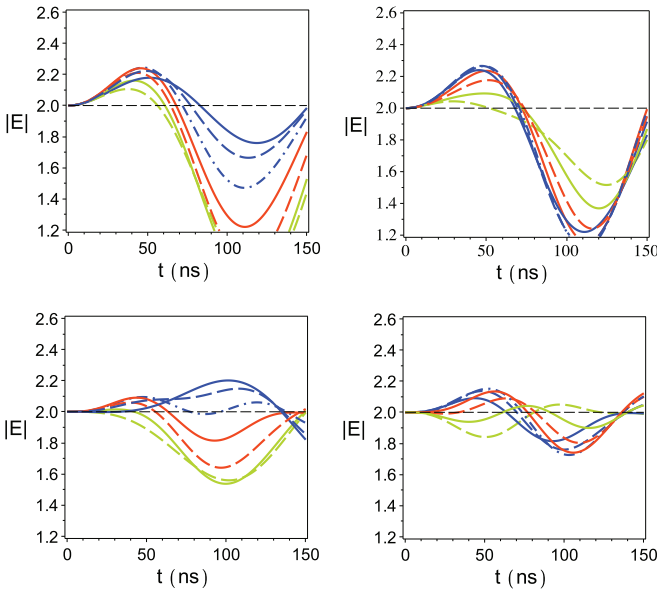

FIG. 6. (Color online) Polar and azimuthal dependences of the CHSH inequality. The dashed horizontal line represents the points above which the system is entangled. The various orientations are given by the lines: solid blue, $0°$; dashed blue, $30°$; dash-dotted blue, $60°$; solid red, $90°$; dashed red, $120°$; solid green, $150°$; and dashed green, $180°$. For the top two figures $\vec{B}_1 = (0,0,4)$ and $\vec{B}_2 = (0,5,0)$. The top left figure depicts the azimuthal dependence for fixed $\theta = 0°$, while the top right figure depicts the polar dependence for fixed $\varphi = 90°$. For the bottom two figures $\vec{B}_1 = (0,0,5)$ and $\vec{B}_2 = (0,5,0)$. The bottom left and bottom right figures similarly depict the azimuthal and polar dependences, respectively. For all four figures $k = 1 \ \mu s^{-1}$.

V. CONCLUSION

We have identified that the entanglement decay rate is one of the key factors in the radical-pair mechanism produced by the change of triplet yields (Fig. 1). Also, we confirmed that the entanglement endures long enough for living systems to conduct entanglement-based reactions. However, the dynamics of the entanglement is not sensitive to the change of angles between the z axis of the radical pair and the geomagnetic-field vector under the symmetric hyperfine tensor. For a certain asymmetric hyperfine tensor, the above situation is greatly improved. It appears that the anisotropic factors can play a very important role in the radical-pair mechanism and the chemical compass model. In contrast, as believed, the hyperfine tensor should be symmetric. Under this situation, if we still believe that entanglement plays a crucial role in the orientation of birds as demonstrated before, there must be an indirect mechanisms by which the entanglement can affect the birds' behavior.

In the future, the decay rates should be adjusted, for example, using different values for the decay rates of the singlet

state and the triplet state to improve our model. Actually, in this scenario, the unequal part of $k' = k_S - k_T$ can be seen as a noise. Also, the performance of the chemical compass can be very robust and even better under the correlated noise [5], therefore, we have reason to believe this will improve the results. The hidden bridge between the entanglement of the radical pair and the determination of orientation in a magnetic field should be sought.

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