Quaternionic particle in a relativistic box

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This study examines Quaternion Dirac solutions for an infinite square well. The quaternion result does not recover the complex result within a particular limit. This raises the possibility that quaternionic quantum mechanics may not be understood as a correction to complex quantum mechanics, but it may also be a structure that can be used to study phenomena that cannot be described through the framework of complex quantum mechanics.

PACS numbers:

I. INTRODUCTION

A physical theory may be better understood if it is generalized, for several reasons. Firstly, if a theory is understood as a particular case of a more general theory, then its limits are well established, and the variety of phenomena that may be described by this particular theory are also well defined. On the other hand, the general theory may have several theories at particular limits, and relations between particular cases of the general theory may be established. An example of this occurs in string theory, where different theories are connected by duality transformations (T-dualities).

However, this understanding may not easily be reached if the generalized theory introduces additional constraints. In this case, a solution of the generalized theory may not recover a well-known solution of the particular solution within a specific limit. As we know, the quaternion Dirac equation reduces to the complex Dirac equation if the quaternionic part of the potential goes to zero [1]. However, the quaternion case may have more constraints from boundary conditions. This may not be the case for the scattering of Dirac particles by a step potential [2], and the complex solution is recovered from the quaternion solution. On the other hand, as we shall see, the quaternion Dirac solution for the infinite square well does not recover the complex Dirac solution for the infinite square well. This means that the interpretation of the physical problem in the complex situation may not be analogous to the interpretation of the physical problem in the quaternionic situation.

In order to introduce our problem, we remember that a quaternion generalization of quantum mechanics is obtained by allowing the wave-function, which is evaluated over the complex number field, to be evaluated in the quaternion number field. Writing a quaternionic wave-function in the symplectic notation, we get

$$\Psi = U + jW,$$

so that $U$ and $W$ are functions evaluated over complex numbers and $j$ is one of the three quaternionic anti-commuting imaginary unities. The third imaginary unit is defined by $k = ij$, so that a general quaternion $Q$ is written with real coefficients such as $Q = A + Bi + Cj + Dk$. A quaternionic wave-function has more degrees of freedom than a complex wave-function, and it may have some probability density coming from the pure quaternionic term $jW$ of the wave-function [1].

Quaternionic generalization of quantum mechanics and of quantum field theory has been studied and collected by Adler [3]. However, Adler’s work is focused on formal aspects of quaternionic quantum mechanics, and specific examples are still required in order to determine whether there are measurable quaternionic effects. In the case of relativistic quantum mechanics, Davies [4] studied Lorentz invariant scalar potentials, and showed that this kind of potential may generate representation-dependent solutions. Another interesting result from Davies is the decoupling of the dynamics of the quaternionic part of the wave-function from the dynamics of the complex part of the wave-function. This raises the possibility that quaternionic effects may be impossible to be observed, and hence physically irrelevant. On the other hand, for a constant vector potential [1], the complex part is not decoupled from the quaternionic part, and then quaternionic effects may, in principle, be detected. This possibility may be observed based on several features of the solution. First of all, it has been ascertained that, in accordance with complex Dirac wave-functions, quaternionic Dirac wave-functions also have three energy regimes named the diffusion zone, the
evanescent zone and the Klein zone. A measurable quaternionic effect that may be observed is the energy range of the evanescent zone, which is sensitive to the value of the pure quaternionic part of the potential. Another interesting feature of this solution concerns the effect of the pure quaternionic term of the potential on the speed of the generated particles and anti-particles. The pure imaginary complex part of the potential has the effect of decelerating particles and generating anti-particles. In other words, we say that the usual barrier has a repulsive effect on particles and an attractive effect on anti-particles. We can suppose that this attractive character of the potential is responsible for accelerating anti-particles. In other words, we say that the usual barrier has a repulsive effect on particles and anti-particles. The pure imaginary complex part of the potential has the effect of decelerating particles and accelerating anti-particles. In other words, we say that the usual barrier has a repulsive effect on particles and anti-particles. The pure imaginary complex part of the potential has the effect of decelerating particles and accelerating anti-particles. The pure imaginary quaternion component of the potential has an attractive effect on anti-particles. We can suppose that this attractive character of the potential is responsible for generating Dirac anti-particles in the Klein zone. The pure imaginary quaternion component of the potential has an opposite effect, accelerating anti-particles and decelerating particles, and generating particles for energies belonging to the range of the Klein zone.

In this article we apply the solutions of the quaternion Dirac equation with a vector potential \[ \mathbf{A} \] to the infinite one-dimensional square well, a system that confirms that the quaternionic part of the potential generates measurable effects on wave-function. The relativistic infinite square well has already been studied for the complex case in various dimensions \[ \mathbb{R}^2, \mathbb{R}^3 \] and also for a finite square \[ \mathbb{R}^2, \mathbb{R}^3 \]. We extend it to the one-dimensional quaternion case. It must be said that many confining solutions for the complex Dirac equation have been developed, and some are already part of a textbook \[ \mathbb{R}^3, \mathbb{R}^3 \], and there are a variety of studies on different aspects of this subject, such as the boundary conditions \[ \mathbb{R}^3, \mathbb{R}^3 \] and confining solutions in scalar potentials \[ \mathbb{R}^2, \mathbb{R}^3 \]. None of these cases have been generalized for the quaternionic situation, accordingly this article is just a first step in understanding quantum relativistic confined solutions.

In Section II, we describe the quaternion Dirac equation and its solutions given from \[ \mathbb{R}^3, \mathbb{R}^3 \]. In Section III we describe the model and present our results. Section IV presents our conclusions and future perspectives.

II. THE QUATERNIONIC DIRAC SOLUTION FOR A STEP POTENTIAL

The anti-hermitian Dirac equation for an arbitrary quaternionic potential in the natural system of units \[ \mathbb{R}^3, \mathbb{R}^3 \] is

\[
\partial_t \Psi(r, t) = - \left[ \alpha \cdot \nabla + im \beta + \mathbf{h} \cdot \mathbf{V}(r) \right] \Psi(r, t). \tag{2}
\]

\( V_n(r) \) are the real components of \( \mathbf{V} \) for \( n = \{1, 2, 3\} \) and the complex units are contained in \( \mathbf{h} = (i, j, k) \). The 4 \( \times \) 4 matrices \( \mathbb{I}, \alpha_m, \beta \) satisfy the algebra

\[
\alpha_m = \alpha_m^\dagger, \quad \beta = \beta^\dagger, \quad \alpha^2 = \beta^2 = \mathbb{I}, \quad \{\beta, \alpha_m\} = 0 \quad \text{and} \quad \{\alpha_m, \alpha_n\} = 2\delta_{mn} \mathbb{I}, \tag{3}
\]

where \( \mathbb{I} \) is the 4 \( \times \) 4 unity matrix. The representation adopted for the calculations is

\[
\alpha_m = \begin{pmatrix} 0 & \sigma_m \\ \sigma_m & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}, \tag{4}
\]

where \( \mathbb{I}_2 \) represents a 2 \( \times \) 2 unity matrix and \( \sigma_m \) represents the 2 \( \times \) 2 Pauli matrices for \( m = \{1, 2, 3\} \). The most general potential for the Dirac equation may be written as \[ \mathbb{R}^3, \mathbb{R}^3 \]

\[
V = A_t(x) \mathbb{I} + A_t(x) \alpha + U(x) \beta + \Phi(x) \beta \gamma^5, \tag{5}
\]

where \( A_t \) and \( A_s \) are components of the four-potential and \( U \) and \( \Phi \) are real-valued functions. \( U \) generates the scalar term of the potential and \( \Phi \) generates the pseudo-scalar term. We consider a step potential

\[
\mathbf{V}(r, t) = \{ \mathbf{V} \text{ for } z > 0 \text{ and } 0 \text{ for } z < 0 \}. \tag{6}
\]

with \( \mathbf{V} = (V_1, V_2, V_3) \) a real constant vector. This potential can be identified with \( A_t \) of \[ \mathbb{R}^3, \mathbb{R}^3 \], and then represents a vector potential where the only non-zero component is the time component. The pure quaternionic term of the potential may be rewritten as \( V_1 = V_0 \) and \( W_0 = V_3 + iV_2 \), where, of course,

\[
W_0 = |W_0| e^{i\phi}, \quad \text{with} \quad |W_0| = \sqrt{V_2^2 + V_3^2} \quad \text{and} \quad \phi = \arctan \frac{V_2}{V_3}. \tag{7}
\]

The system is then composed of particles that move one-dimensionally and whose solution of the Dirac equation \[ \mathbb{R}^3, \mathbb{R}^3 \] is written in general as

\[
\Psi_{\pm} = (U + jW)e^{i(Q_\pm z - Et)} \tag{8}
\]
so that
\begin{equation}
Q_\pm^2 = q_\pm^2 + |W_0|^2 \pm 2\delta, \quad \text{where}
\end{equation}
\begin{equation}
q_\pm^2 = (E \pm V_0)^2 - m^2, \quad \delta = \sqrt{E^2V_0^2 + p^2|W_0|^2 - EV_0}, \quad \text{and} \quad p^2 = E^2 - m^2.
\end{equation}

The solution whose momentum is $Q_-$ is similar to the complex solution of the Dirac equation, where there are three characteristic energy zones, namely the diffusion zone, the evanescent zone and the Klein zone. One of the differences between the cases is that the range of the evanescent zone for the quaternion case is given by
\begin{equation}
\Delta E = \sqrt{|W_0|^2 + (m + V_0)^2} - \max[m, \sqrt{|W_0|^2 + (m - V_0)^2}].
\end{equation}
The energy range of the evanescent zone depends on the quaternionic term of the potential. On the other hand, the solution whose momentum is given by $Q_+$ has only the diffusion zone, and this energy zone is inhabited only by anti-particles. This is another difference in relation to the complex case, because the complex case presents a coexistence between particles and anti-particles with the same energy and different momenta. Finally, the wave-functions for the one-dimensional step are
\begin{equation}
\Psi_- = \left[ \begin{array}{c}
(1 - jW_0M_-)\chi \\
(A_- - jW_0N_-)\sigma_3\chi
\end{array} \right] e^{i(Q_-z - Et)} \quad \text{and} \quad \Psi_+ = \left[ \begin{array}{c}
(A_+ - jW_0N_+)\sigma_3\chi \\
(1 - jW_0M_+)\chi
\end{array} \right] e^{i(Q_+z - Et)}.
\end{equation}

This indicates that the quaternionic Dirac equation may have only the diffusion zone, and this energy zone is inhabited only by anti-particles. In this non-relativistic regime the parameters of the solutions are
\begin{equation}
A_\pm = \frac{Q_\pm}{E \mp V_0 + m \pm \frac{2}{E - m}}, \quad M_\pm = \frac{E \mp V_0 - m + Q_\pm A_\pm}{q_\pm^2 - Q_\pm^2}, \quad \text{and} \quad N_\pm = \frac{Q_\pm + A_\pm(E \mp V_0 + m)}{q_\pm^2 - Q_\pm^2}.
\end{equation}

III. THE QUATERNIONIC CONFINED DIRAC SOLUTIONS

The step solution presented in the former section has two possible momenta, and consequently we must consider two confined solutions, one for each momentum. However, in order to obtain a clearer understanding of the situation, we consider the non-relativistic limit which gives the usual quantum infinite square well

A. The non-relativistic limit

We consider the potential (14) as given by $V = (V_0, V_2, V_3)$, so that
\begin{equation}
V_0(r, t) = \begin{cases}
0 & \text{for } 0 < z < L \text{ and } \infty \text{ otherwise},
\end{cases}
\end{equation}

where $L$ is a real number that gives the width of the well. There is a constant and finite pure quaternionic potential inside the well, and in this situation the parameters of the solutions are
\begin{equation}
Q_\pm = p \pm |W_0|, \quad A_\pm = \frac{p}{E + m}, \quad M_\pm = \mp \frac{1}{|W_0|} \frac{p}{E + m}, \quad \text{and} \quad N_\pm = \mp \frac{1}{|W_0|}.
\end{equation}

We use $p > |W_0|$. For $|W_0| < p$ some signs must be flipped, but there is no change in the physical interpretation. In the non-relativistic limit, $Q_\pm \ll m$, and then $A_\pm, M_\pm \to 0$. The wave-functions (12) in this non-relativistic regime are
\begin{equation}
\Psi_+ = \left( \begin{array}{c}
je^{-i\phi}\sigma_3\chi \\
\chi
\end{array} \right) e^{i(Q_+z + Et)} \quad \text{and} \quad \Psi_- = \left( \begin{array}{c}
\chi \\
-je^{i\phi}\sigma_3\chi
\end{array} \right) e^{i(Q_-z + Et)}.
\end{equation}

The solution (10) describes free particles whose constant spinors depend neither on the energy nor on the potential, and hence cannot recover the complex result for $|W_0| = 0$. This indicates that the quaternionic Dirac equation may be fundamentally different from the complex Dirac equation, and that the complex limit only makes sense in specific cases. Using (10), wave-functions composed of particles in both directions for each momentum are
\begin{equation}
\Phi_\pm = A\Psi_\pm(Q_\pm) + B\Psi_\pm(-Q_\pm)
\end{equation}
where $A$ and $B$ are complex constants. Imposing the non-relativistic boundary conditions $\Phi_\pm(z = 0) = \Phi_\pm(z = L) = 0$, we obtain the quantized momenta

$$Q^{(n)}_\pm = \frac{n\pi}{L}. \quad (18)$$

This result does not necessarily imply that $|W_0| = 0$, because $\Phi_\pm$ and $\Phi_-$ were calculated independently, and we do not need to impose $Q_+ = Q_-$. The relation (18) in fact defines a constraint among the mass, the energy and the quaternionic potential parametrized by $|W_0|$ given by

$$E^{(n)}_\pm = (Q^{(n)}_\pm \mp |W_0|)^2 + m^2. \quad (19)$$

(19) may be understood as a relativistic conservation relation for the system, so that

$$Q_\pm = Q^{(n)}_\pm \mp |W_0| \quad (20)$$
defines an effective momentum. This result squares with the previous result where the velocity of the particle is influenced by the quaternionic potential [1], so that $|W_0|$ increases $Q_-$ and decreases $Q_+$. On the other hand, it is totally unexpected because we are in fact in the non-relativistic regime.

The effective momentum $Q_\pm$ has all the properties of the usual relativistic momentum, including a non-relativistic limit. On the other hand, correspondence between relativistic and non-relativistic quantities is still required, because better comprehension of the quaternion Schrödinger equation for confining potentials is needed. Although some progress had already been made [15, 16], more results are still needed in order to determine the cases in which the quaternionic quantum results may recover the complex results.

### B. The $Q_-$ solution

We consider the so-called “bag model” [17, 18], which has already been used [5] in studying the complex Dirac equation. Defining a space-dependent mass function $\mu(z)$, we get

$$\mu(z) = \{ m \text{ for } 0 < z < L \text{ and } M \text{ otherwise } \}. \quad (21)$$

In the limit $M \to \infty$, we have that $Q^2_\pm < 0$, and the wave-function becomes zero outside the well. Inside the square well, where $z \in (0, L)$, we have the time independent wave-function

$$\Psi_\mp = A \left[ \frac{1 - jW_0 M_\mp}{(A_\mp - jW_0 N_\mp)\sigma_3\chi} \right] e^{iqz} + B \left[ \frac{1 - jW_0 M_\mp}{(A_\mp + jW_0 N_\mp)\sigma_3\chi} \right] e^{-iqz} \quad (22)$$

$A$ and $B$ are complex constants. The second term corresponds to a particle moving from the right to the left, where the momentum is negative. Taking $Q_- \to -Q_-$ in $\Psi_\mp$ from (19), we get $A_\mp \to -A_\mp$, $M_- \to M_-$ and $N_- \to -N_-$, so that the second term of (22) is obtained. The model has boundary conditions so that

$$\Psi = \{ \beta\alpha\Psi_i \text{ at } z = 0 \text{ and } -\beta\alpha\Psi_i \text{ at } z = L \}. \quad (23)$$

These boundary conditions are such that the probability current flux is zero outside the well [5]. We might set $V_0 = 0$ and thus obtain a pure quaternion potential inside the square well, but we can perform the calculations for a general potential and take the limit of a pure quaternionic potential only at the end. Furthermore, we set the spin up solution using $\chi = (1, 0)^t$, so that $\sigma_3\chi = \chi$. Thus, from the boundary condition at $z = 0$ we get

$$\left[ \begin{array}{c} (A + B)(1 - jW_0 M_-)\chi \\
(A - B)(A_\mp - jW_0 N_-)\chi \end{array} \right] = i \left[ \begin{array}{c} (A - B)(A_\mp - jW_0 N_-)\chi \\
-(A + B)(1 - jW_0 M_-)\chi \end{array} \right]. \quad (24)$$

Hence,

$$\frac{B}{A} = \frac{iA_- - 1}{iA_\pm + 1} = \frac{iN_- + M_-}{iN_- - M_-}, \quad \text{and consequently}, \quad A_- = -\frac{N_-}{M_-}. \quad (25)$$

This result is absolutely general. However, we must consider the reality of the momentum of the particles. Real momenta determine that the particle belongs either to the diffusion energy zone or to the Klein energy zone. A pure imaginary momentum determines that the particle belongs to the evanescent energy zone. However, for the bag model
we are considering, \( M \to \infty \), then the wave-function is zero outside the square well and there is no physical mode on the evanescent zone. Real momenta implies that \( A_\pm \) is real from (13), and then we conclude that

\[
\frac{\mathcal{B}}{\mathcal{A}} = e^{i\theta} \quad \text{and} \quad \tan \theta = \frac{2A_-}{A_+ - 1}.
\]  

(26)

Where \( \theta \) is a phase difference between \( \mathcal{A} \) and \( \mathcal{B} \). Thus time-independent wave-function is

\[
\Psi_- = N_- \left[ \cos \left( Q_- z - \frac{\theta}{2} \right) - j W_0 \cos \left( Q_- z + \frac{\theta}{2} \right) \sin \left( Q_- z - \frac{\theta}{2} \right) + j W_0 \sin \left( Q_- z + \frac{\theta}{2} \right) \right],
\]  

(27)

where \( N_- \) is a normalization constant. The boundary condition at \( z = 0 \) for (27) gives that \( W_0 = A_- \), in accordance with (26). At \( z = L \), the boundary condition applied on (27) gives

\[
\cot \left( Q_- L - \frac{\theta}{2} \right) = -\cot \left( Q_- L + \frac{\theta}{2} \right) = A_-.
\]  

(28)

Consequently, the quantization obtained is

\[
\sin 2Q_- L = 0 \quad \text{so that} \quad Q_-^{(n)} = \frac{n\pi}{2L} \quad \text{for} \quad n \in \mathbb{N}.
\]  

(29)

Which obeys the relativistic constraint obtained on the non-relativistic case

\[
E_{\pm}^{(n)2} = (Q_{\pm}^{(n)} \mp |W_0|)^2 + m^2.
\]  

(30)

This result squares with the previous result [1], where the velocity of the particle is influenced by the quaternionic potential, so that \( |W_0| \) increases \( Q_- \) and decreases \( Q_+ \). Additionally, it recovers the non-relativistic limit [19], although the quantized momenta do not match.

In fact, the difference between the quantum results is not important, because the boundary conditions are different in each case, and so some difference would be expected. However, the result is astonishing because it differs significantly from the complex case. In (28) there are two conditions involved. The condition generated in the complex part of the wave-function has \( \theta/2 \) subtracted in the argument of the trigonometric function and the condition generated at the quaternion part of the wave-function has \( \theta/2 \) added to the trigonometric argument.

The additional quaternionic condition makes the quaternionic result very different from the complex result. In the complex solution the condition (28) is a transcendental equation, and the quantization is obtained numerically \( \mathbb{R} \). The quantization condition in the complex case is similar to the non-relativistic finite square well. On the other hand, in the quaternionic case, quantization is exact and given by a positive non-zero integer, similar to the non-relativistic infinite square well, although the difference between the quantized momenta in the quaternion case is half the difference in the energy on the non-relativistic square well.

From this result it may be interpreted that the principal difference between the quaternionic calculation and the complex calculation is related to its degrees of freedom. At the same time that the quaternion case has more terms to accommodate the probability density, it may generate more conditions and then constrain the system to a tighter condition compared to the complex case. We can speculate that the quaternionic potential may influence the result not necessarily as a physical field that can be varied to generate a physical effect, but it can alter the mathematical framework in a way that the quaternionic effect is not intended to correct the complex case, but to change the phenomenon that can be described.

### C. The \( Q_+ \) solution

We repeat the calculation for the Dirac solution with momentum \( Q_+ \), and the results are quite similar. The ansatz of the time independent wave-function is

\[
\Psi_+ = C \left[ (A_+ - j \frac{W_0}{W_0} N_+)\sigma_3 \chi \right] e^{iQ_+ z} + D \left[ (A_+ + j \frac{W_0}{W_0} N_+)\sigma_3 \chi \right] e^{-iQ_+ z},
\]  

(31)

with \( C \) and \( D \) complex constants. At, \( z = 0 \) the boundary condition (23) on a spin up wave-function gives

\[
\left[ (C - D)(A_+ - j \frac{W_0}{W_0} N_+) \chi \right] = \left[ (C + D)(1 - j \frac{W_0}{W_0} N_+) \chi \right] i.
\]  

(32)
\[
\frac{D}{C} = \frac{iA_+ + 1}{iA_+ - 1} = \frac{iN_+ - M_+}{iN_+ + M_+} \quad \text{Consequently,} \quad A_+ = -\frac{N_+}{M_+}, \quad \frac{D}{C} = e^{i\vartheta} \quad \text{and} \quad \tan \vartheta = -\frac{2A_+}{A_+^2 - 1}.
\]

Where \( \vartheta \) is the phase difference between \( C \) and \( D \). Thus time-independent wave-function is

\[
\Psi_+ = N_+ \left[ \frac{iA_+ \left[ \sin \left( Q_+ z - \frac{\vartheta}{2} \right) - jW_0 \sin \left( Q_+ z + \frac{\vartheta}{2} \right) \right]}{\cos \left( Q_+ z - \frac{\vartheta}{2} \right) - jW_0 \cos \left( Q_+ z + \frac{\vartheta}{2} \right)} \right],
\]

where \( N_+ \) is a normalization constant. The boundary condition at \( z = 0 \) for \( \Psi_+ \) gives that \( \cot \left( \frac{\vartheta}{2} \right) = -A_+ \), in accordance with (33). At \( z = L \), the boundary condition applied to \( \Psi_+ \) gives

\[
-cot \left( Q_+ L - \frac{\vartheta}{2} \right) = cot \left( Q_+ L + \frac{\vartheta}{2} \right) = A_+.
\]

Consequently, the quantization is obtained as

\[
\sin 2Q_+ L = 0 \quad \text{and consequently} \quad Q_+ = \frac{n\pi}{2L} \quad \text{for} \quad n \in \mathbb{N}.
\]

This result is absolutely similar to the \( Q_- \) case, the difference is that here there is only the diffusion energy zone.

**IV. CONCLUSION**

In this article we studied the quaternionic relativistic particle inside an infinite square well. The results show that the quantized momenta have a quantization condition similar to the energy quantization condition for the infinite square well. This is very different from the quantization of the complex Dirac square well, whose quantization of momentum is similar to the energy quantization of the energy of the finite square well.

We explain this difference as being due to the greater number of degrees of freedom and of constraints in the quaternionic case. The result discloses an interesting feature of quaternionic quantum mechanics. At the same time it has more degrees of freedom than complex quantum mechanics to accommodate at the probability density, the quaternionic wave-function duplicates the number of constraints. In the studied case, the new constraints come from the boundary conditions. The results permit us to state that quaternion quantum mechanics may be useful as a framework that permit us to study a physical system not as a correction of the complex case, but rather as a way of describing different phenomena. This can be concluded from the fact that the quaternion and the complex cases have quite different solutions for similar problems, and the complex solution cannot be recovered by simply setting a quaternionic parameter to zero.

The results raises the question about which kind of generalization is promoted by quaternion quantum mechanics. One can consider the quaternionic part of the wave-function as physically significant or as an additional degree of freedom which may generate a mathematical device to describe different phenomena which cannot be described by a complex wave-function. This question must be addressed using other constrained quantum systems, both relativistic and non-relativistic. The finite relativistic potential well seems probably the more obvious direction for a future research.

**ACKNOWLEDGEMENTS**

Sergio Giardino receives a financial grant from the CNPq for his research, and is grateful for the hospitality of Professor Paulo Vargas Moniz and the Centre for Mathematics and Applications at University of Beira Interior.

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