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UNITARY TRANSFORMATIONS, WEYL'S ASSOCIATION
AND THE ROLE OF CANONICAL TRANSFORMATIONS

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Abstract

Quantum mechanical operators can be associated with functions of p, q through the Weyl or Wigner transform. In this paper we develop alternative associations through the use of unitary transformations, and study the relation between unitary transformations and canonical transformations of the p, q labels.

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1. Introduction

One standard way of expressing quantum mechanics in a form similar to classical mechanics is through the use of Wigner's function¹⁾ which associates a c -number function $\rho(p, q)$ with the density operator $\hat{\rho}$ of a dynamical system. This type of association was first suggested (in a different context) by Weyl²⁾ for a general dynamical operator. According to this idea we associate with a quantum mechanical operator $\hat{A}(\hat{p}, \hat{q})$ a c -number function $A(p, q)$. The p 's and q 's are real parameters which in the classical limit become the classical momenta and coordinates, respectively. However, when \hbar is not small, the p, q space (W space for short) introduced through this association has a different structure³⁾ from the classical phase space. It is invariant only under linear inhomogeneous transformations rather than the full set of canonical transformations. This invariance property is the consequence of the rather unexpected mathematical fact that Wigner's function corresponding to a physically realizable state can only be a delta function if the singularity of the delta function lies on a straight line in the W space. This in turn arises because the Weyl association gives a special role to operators that are linear combinations of the \hat{p} and \hat{q} operators. However, quantum mechanics in general does not prefer these operator combinations since the whole theory is invariant under unitary transforms which can, for example, turn \hat{q} into $\hat{q} + \hat{p}^2$. Similarly, classical mechanics, being invariant under general canonical transformations, does not prefer straight lines in the phase space. Thus, this particular structure of the W space must arise purely from the way we have chosen to associate operators with functions of p and q , i.e. using Weyl's association to construct A_W . In this paper we will show that it is possible to develop alternative associations which single out different classes of operators and show more clearly the

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relation between unitary and canonical transformations, extending the discussion in ref. 3).

In the next section we set up the formalism and define the notation. In section 3 we study how the association changes under unitary transforms and present a method for obtaining new associations. Then in section 4 we look in some detail at the properties of one particular new association, while in section 5 we explore some of the consequences of having a plethora of alternative associations.

2. The formalism

We associate functions with operators through the trace

$$A(p,q) = \text{Tr}(\hat{A}(p,q)\hat{A}), \quad (1)$$

where \hat{A} is an arbitrary operator and the operator, $\hat{A}(p,q)$ is defined by

$$\hat{A}(p,q) = \frac{\hbar^3}{(2\pi)^3} \int d^3u d^3v \exp i[u \cdot (p-\hat{p}) + v \cdot (q-\hat{q})]. \quad (2)$$

In the x representation we have

$$\langle x' | \hat{A}(p,q) | x'' \rangle = \delta\left(\frac{x'+x''}{2} - q\right) \exp(i(x'-x'') \cdot \frac{p}{\hbar}), \quad (3)$$

Thus eq. (1) can be rewritten as

$$A(p,q) = \int d^3x d^3x' \delta\left(\frac{x'+x''}{2} - q\right) \exp(i(x'-x'') \cdot \frac{p}{\hbar}) \langle x'' | \hat{A} | x' \rangle \quad (4)$$

which is perhaps the more usual form¹⁾. Complementing eq. (1) we have the inverse relation

$$\hat{A} = \frac{1}{(2\pi\hbar)^3} \int \hat{A}(p,q) A(p,q) d^3p d^3q. \quad (5)$$

A final formula which we will be needing is the composition rule⁴⁾ (to associate functions with operator products)

$$\text{Tr}(\hat{A}(p,q)\hat{B}) = A(p,q) \exp \frac{i\hbar}{2} (\vec{v}_q \cdot \vec{v}_p - \vec{v}_p \cdot \vec{v}_q) B(p,q), \quad (6)$$

where the arrows indicate the direction the gradients act. If \hat{A} is the density operator $\hat{\rho}$, we call $\rho(p,q)$ Wigner's function.

This scheme is a special case of the following. We consider the dynamical operators as points in a linear vector space (because we can multiply operators with scalars and can add them together). In this vector space the operator set $\hat{A}(p,q)$ forms a basis and eq. (5) tells us how to expand an operator in this basis. The expansion coefficients are the c-number functions associated with the operator (in this basis). Equation (1) tells us how to construct the expansion coefficients. The labels p and q simply enumerate the basis. They serve as a label, similar to the 1,2,3 labels appearing on the orthogonal unit vectors which form the basis of Cartesian rectangulars in a Euclidean three space.

An alternate choice of basis is, for example,

$$\hat{A}_k(p,q) = \frac{\hbar^3}{(2\pi)^3} \int d^3u d^3v \exp(i u \cdot (p-\hat{p})) \exp(i v \cdot (q-\hat{q})). \quad (7)$$

In this case the inverse relation is

$$\hat{A} = \frac{1}{(2\pi\hbar)^3} \int \hat{A}_k(p,q) A_k(p,q) d^3p d^3q, \quad (8)$$

where $\hat{A}_k^\dagger(p,q)$ is the Hermitian conjugate of $\hat{A}_k(p,q)$. This basis is associated with standard ordering and the properties of the corresponding association are discussed by Mehta⁵⁾.

From these observations we extract the following general scheme. Let $\hat{B}(a,b)$ be a complete basis enumerated by the parameters a and b. Then the relevant expressions are

$$\hat{A} = \int da db \hat{B}(a,b) A_B(a,b) \\ A_B(a,b) = \text{Tr}(\hat{A}\hat{B}^{-1}(a,b))$$

where $\hat{B}^{-1}(a,b)$ is the inverse basis defined by

$$\text{Tr}(\hat{B}(a,b)\hat{B}^{-1}(a',b')) = \delta(a-a')\delta(b-b').$$

(For the previous association \hat{A}^{-1} is proportional to \hat{A} .) $A_g(a,b)$ is the c-number function associated with the operator A through the basis $B(a,b)$. [For details see ref. 6).]

If we have two different bases $\hat{g}(a,b)$, $\hat{g}'(a',b')$ there need not be a unitary transformation \hat{U} such that $\hat{U}\hat{g}\hat{U}^{-1} = \hat{g}'$ since, for example \hat{g} may be Hermitian, and \hat{g}' not. However, we may consider all such bases which are related to a particular basis through unitary transformations. In the next section we specify the problem more precisely considering as an example the class of bases which arise from $\hat{A}(p,q)$ through a one parameter set of unitary transformations.

3. Unitary transformation and the generation of new bases

In this section we discuss the properties of $\hat{A}(p,q)$ under unitary transformations. A similar analysis could be done for the $\hat{A}_k(p,q)$ of eq. (7) with similar results. We will consider only those unitary operators that can be generated by a succession of infinitesimal unitary operators. Thus we deal with unitary operators which can be written in the form

$$\hat{U}(t) = \exp it \hat{z}/\hbar, \quad (9)$$

where t is a real parameter (usually not time). More general transforms such as reflections can also be dealt with, but we restrict the present considerations to this class. The basic questions we raise, and answer are the following: (a) If we subject $\hat{A}(p,q)$ to the unitary transformation $\hat{U}(t)$, will it be useful to associate with this transformation a transformation of the labels p,q as well; (b) If so, what shall be a guiding principle in the choice of this transformation of the parameters p,q ?

Consider the transformed basis

$$\hat{A}(a,b,tz) = \hat{U}(t) \hat{A}(a,b) \hat{U}^{-1}(t), \quad (10)$$

where we have used a and b instead of p and q since as we shall see the a

and b are not the usual classical momenta and coordinates. The new basis we label $t\hat{z}$ to distinguish it from the old basis which would correspond to $t=0$. We can now set up a new association through

$$A_{tz}(a,b) = \text{Tr}(\hat{A}(a,b,t\hat{z})\hat{A}) \quad (11)$$

with the corresponding inverse relation. There is an alternative way of writing the new basis. We define two new operators

$$\hat{a}(t) = \hat{U}(t) \hat{p} \hat{U}^{-1}(t), \quad (12)$$

and

$$\hat{b}(t) = \hat{U}(t) \hat{q} \hat{U}^{-1}(t). \quad (13)$$

The new basis can now be written

$$\hat{A}(a,b,t\hat{z}) = \frac{\hbar^3}{(2\pi)^3} \int d^3u d^3v \exp i[u \cdot (a - \hat{a}(t)) + v \cdot (b - \hat{b}(t))]. \quad (14)$$

The new basis differs from the old basis only in that $\hat{a}(t)$ and $\hat{b}(t)$ are the preferred operators rather than \hat{p} and \hat{q} . For every relation in the old basis we have a corresponding one in the new basis. For example, the composition rule, eq. (6), remains the same only with a and b replacing p and q . To this extent the unitary transformation has had no effect.

However, the new labels a and b cannot in general be identified with p and q since they do not reduce to the classical momenta and coordinates in the classical limit. The question then arises as to how a and b can be related to p and q since what we want in the end are labels that resemble in some sense classical momenta and coordinates. (This then is our first guiding principle.) To answer this we let a and b be functions of t and consider how $A_{tz}(a(t), b(t))$ varies with t . Differentiating eq. (11) with respect to t we have

$$\begin{aligned} \frac{d}{dt} A_{tz}(a(t), b(t)) &= \frac{\partial}{\partial t} \text{Tr}(\hat{A}(a,b,tz)\hat{A}) + \frac{\partial a}{\partial t} \cdot \nabla_a A_{tz}(a,b) \\ &+ \frac{\partial b}{\partial t} \cdot \nabla_b A_{tz}(a,b) \end{aligned}$$

$$= z(a,b) \frac{2}{h} \sin \frac{\hbar}{2} (\vec{\nabla}_b \cdot \vec{\nabla}_a - \vec{\nabla}_a \cdot \vec{\nabla}_b) A_{tz}(a,b) + \frac{\partial a}{\partial t} \cdot \nabla_a A_{tz}(a,b) + \frac{\partial b}{\partial t} \cdot \nabla_b A_{tz}(a,b) \quad (15)$$

The first term on the right-hand side of eq. (15) has been rewritten as

$$\frac{\partial}{\partial t} \text{Tr}(\hat{A}(a,b,t\hat{z})\hat{A}) = \frac{1}{h} \text{Tr}([i\hat{A}(a,b,tz), \hat{z}]\hat{A}) \\ = z(a,b) \frac{2}{h} \sin \frac{\hbar}{2} (\vec{\nabla}_b \cdot \vec{\nabla}_a - \vec{\nabla}_a \cdot \vec{\nabla}_b) A_{tz}(a,b) \quad (16)$$

This last line follows from the composition rule, eq. (6), and the result

$$z(a,b) = \text{Tr}(\hat{A}(a,b,t\hat{z})\hat{z}) \equiv \text{Tr}(\hat{A}(a,b)\hat{z}) \quad (17)$$

There is no explicit t dependence in z(a,b), the function associated with the generator \hat{z} of the unitary transformation \hat{U} .

Equation (15) is the basic relation connecting the changes in $A_{tz}(a,b)$ and a,b. Notice its structure. The second and third terms depend only on the first derivatives $\nabla_a A_{tz}$ and $\nabla_b A_{tz}$, and express the change in A_{tz} due to the change in the parameters a and b. The first term contains higher derivatives as well, as shown in eq. (16) and expresses the change in A_{tz} due to the unitary transformation. These higher derivatives are all multiplied by ascending powers of \hbar . Consider now a change δA in a function $A_{tz}(a,b)$. If the change in this function can be thought of as arising entirely from a change in the parameters a,b, δA must be of the form $\delta a \cdot \nabla_a A + \delta b \cdot \nabla_b A$, i.e. must be linear in the first derivatives. Thus, eq. (15) describes a change in A which cannot be thought of as arising from a change of the labels a and b, independently of the function A where, in addition, this particular non-local feature of the change is linked to the presence of Planck's constant since the higher derivatives of A are multiplied by powers of \hbar .

We now sharpen our guiding principle and determine that transformation of the labels a and b which removes all those changes in $A_{tz}(a,b)$ which can be generated by a transformation of the labels a and b alone,

leaving behind the non-local changes which arise entirely through the presence of \hbar .

In eq. (15) let us then separate in the sine bracket the \hbar independent first term,

$$\nabla_b z(a,b) \cdot \nabla_a A_{tz}(a,b) - \nabla_a z(a,b) \cdot \nabla_b A_{tz}(a,b); \quad (18)$$

Putting, then, the coefficients of $\nabla_a A$ and $\nabla_b A$ equal to zero we find

$$\frac{\partial a}{\partial t} = -\nabla_b z \quad (18)$$

$$\frac{\partial b}{\partial t} = \nabla_a z \quad (19)$$

with

$$a(0) = p, \quad b(0) = q, \quad (20)$$

and z given by eq. (17). With a given z(a,b) these equations can be integrated to give a and b as functions of p, q and t. Note that a and b are obtained from p and q through the canonical transformation generated by z(p,q). If z(p,q) is no higher than quadratic in p and q, then the relabeling of the basis generated by eqs. (18-20) completely undoes the effects of the unitary transformation for all operators \hat{A} . In that case the unitary transformation merely shuffles the labels keeping the basis vectors unchanged. (In ordinary space it is similar to the rotations which rotate the x axis into the y axis, the y axis into the z axis, etc.) The general unitary transformation does more and its effect cannot be undone by a simple relabeling except, of course, in the classical limit. Our relabeling, i.e. eqs. (18-20), is in some sense that relabeling of the basis which minimizes the effect on the expansion coefficients of the unitary transformation applied to the basis.

With our present choice of a and b the right-hand side of eq. (15) will vanish if either z(a,b) or $A_{tz}(a,b)$ is no more than quadratic in a

and b. Other choices for the transformation of a and b are possible (we can label our basis vectors any way we like) but we believe our present one is a convenient one.

So far in our discussion we have talked as if \hat{p}, \hat{q} and $\hat{A}(p, q)$, the starting objects of the transformation, are somehow fundamental. We can equally well take the opposite point of view. Namely that \hat{a}, \hat{b} and $\hat{A}(a, b, t\hat{z})$ for t fixed are fundamental and that the usual p, q, etc. generated from them by the inverse transforms are less fundamental. The point being, of course, that none are any more fundamental than any other.

For later convenience we define

$$\hat{A}_t(p, q) \equiv \hat{A}[a(p, q, t), b(p, q, t), t\hat{z}] \quad (21)$$

As stressed previously if z is no more than quadratic in p and q, $A_t(p, q)$ will equal $A(p, q)$. This is just the well-known invariance³ of the usual Weyl association under linear inhomogeneous transformations (i.e. this class of z's generates linear inhomogeneous transformations). With all other choices of z we generate new, perfectly good, associations which endow the W space with different properties depending on t and z.

Due to the special properties of unitary and canonical transformations the new associations have many features in common with the original Weyl association. For example

$$\text{Tr}(\hat{A} \hat{\rho}) = \int d^3p d^3q A_t(p, q) \rho_t(p, q) \quad (22)$$

$$A_t(p, q) = \text{Tr}(\hat{A}_t(p, q) \hat{A}(p, q)) \quad (23)$$

where and similarly for $\rho_t(p, q)$. The composition rule, eq. (6), is unchanged when expressed in terms of $a(p, q, t)$ and $b(p, q, t)$, i.e.

$$\text{Tr}(\hat{A}(a, b, t\hat{z}) \hat{A}(b)) = A_{tz}(a, b) \exp \frac{i\hbar}{2} (\hat{V}_b \cdot \hat{V}_a - \hat{V}_a \cdot \hat{V}_b) B_{tz}(a, b) \quad (24)$$

Now, however, we may want to replace a and b with p and q using eqs. (18-20). This is, in general, quite complicated, but once z is given it can in principle be done. The first two terms in eq. (24) remain unchanged, i.e.

$$1 + \frac{i\hbar}{2} (\hat{V}_b \cdot \hat{V}_a - \hat{V}_a \cdot \hat{V}_b) = 1 + \frac{i\hbar}{2} (\hat{V}_q \cdot \hat{V}_p - \hat{V}_p \cdot \hat{V}_q) \quad (25)$$

since constants and Poisson brackets are invariant under canonical transformations. It thus follows that in the classical limit commutators still reduce to Poisson brackets; the quantum corrections will, in general, be different.

We now have a method for generating new associations at will.

A priori all these associations must be equally good since quantum mechanics is invariant under unitary transformations. The special structure in the W space, i.e. the preferential treatment of straight lines, arises because we have arbitrarily picked one \hat{A} out of this infinite set as being special. We could equally well have picked a \hat{A} which would have, for example, favoured a particular set of parabolae. This case will be discussed in the next section.

We are now in a position to see how unitary transformations generate canonical transformations. Consider the function

$$A(p, q, \hat{V}) = \text{Tr}(\hat{A}(p, q) \hat{V} \hat{A}^{-1}) \quad (26)$$

where \hat{V} is a unitary operator. It has been stressed^{3, 7} that $A(p, q, \hat{V})$ is not related to the $A(p, q)$ of eq. (1) by a canonical transformation on the p and q's. When we make the unitary transformation on \hat{A} , however, we are free to simultaneously change our basis. If for our new basis we take $\hat{A}_t(p, q)$ of eq. (21) with $\exp(itz/\hbar) = \hat{V}$, then the unitary transformation has just generated a canonical transformation, i.e.

$$\begin{aligned} \text{Tr}(\hat{\Delta}_t(p,q)\hat{V}\hat{A}^{-1}) &= \text{Tr} \hat{\Delta}(a(p,q),b(p,q))\hat{A} \\ &= A(a(p,q),b(p,q)) \end{aligned} \quad (27)$$

where a and b are related to p and q through the canonical transformation given by eqs. (18-20). Thus to have a unitary transformation generate canonical transformations we must do two things: first do the unitary transformation on the operator and second change the basis. Note that the new basis is related to the old by a unitary transformation and a change of labels.

The delta of eq. (7) is not related to the delta of eq. (2) by a unitary transformation. Hence applying unitary operators to it generates a whole new set of deltas.

4. An example

In this section we discuss an example to give a better understanding of the results of the previous section. Here we consider only a one dimensional problem and take the unitary operator to be
$$\hat{U} = \exp(it\hat{p}^3/3\hbar). \quad (28)$$
 The factor of 3 has been put in for later convenience. The parameter t has dimensions of (force \times mass) $^{-1}$. The $\hat{\alpha}$ and $\hat{\beta}$ operators of eqs. (12-13) are

$$\begin{aligned} \hat{\alpha}(t) &= \hat{p} \\ \hat{\beta}(t) &= \hat{q} + t\hat{p}^2, \end{aligned} \quad (29)$$

while a and b are given by

$$\begin{aligned} a(t) &= p \\ b(t) &= q + tp^2. \end{aligned} \quad (30)$$

The new delta from eqs. (14) and (21) is

$$\hat{\Delta}_t(p,q) = \frac{\hbar}{2\pi} \int du dv \exp i[u(p-\hat{p}) + v(q+tp^2 - \hat{q}-t\hat{p}^2)]. \quad (31)$$

This operator is easily expressed in the p representation [due to the special form of the unitary operator, eq. (28)] as

$$\begin{aligned} \langle p' | \hat{\Delta}_t(p,q) | p \rangle &= \delta\left(\frac{p'+tp''}{2} - p\right) \exp \frac{i}{\hbar} (p''-p')(qt+tp^2) \exp \frac{it(p'^3-p''^3)}{3\hbar} \\ &= \delta\left(\frac{p'+tp''}{2} - p\right) \exp \frac{i}{\hbar} (p''-p')q \exp \frac{it(p'-p'')^3}{12\hbar}, \end{aligned} \quad (32)$$

where in the last line we have made explicit use of the Dirac delta function factor. Fourier transforming to obtain the x representation, we have

$$\langle x' | \hat{\Delta}_t(p,q) | x \rangle = \left(\frac{4}{t\hbar^2}\right)^{1/3} \text{Ai} \left[-\left(\frac{4}{t\hbar^2}\right)^{1/3} \left(q - \frac{x'+x''}{2}\right) \right] \exp i(x'-x'')\frac{p}{\hbar}, \quad (33)$$

where Ai is the Airy function⁸. In the limit $t \rightarrow 0$ or $\hbar \rightarrow 0$ the Airy function reduces to a delta function and we recover eq. (3.).

Let us now consider the function associated with the projection operator $\delta(q'-q)$. We have

$$\text{Tr}(\hat{\Delta}_t(p,q) \delta(q'-q)) = \left(\frac{4}{t\hbar^2}\right)^{1/3} \text{Ai} \left[\left(\frac{4}{t\hbar^2}\right)^{1/3} (q'-q) \right]. \quad (34)$$

Thus, unlike the case of $\hat{\Delta}(p,q)$ we now have an Airy function instead of a delta function associated with the projection operator $\delta(q'-q)$.

Next, we consider the function associated with the projection operator of an energy eigenstate of a particle of mass m exposed to a constant force F . The wave function is

$$\psi(x) = \frac{1}{F^{1/2}} \left(\frac{2mF}{\hbar^2}\right)^{1/3} \text{Ai} \left[\frac{(x-E/F)}{\hbar^2} \left(\frac{2mF}{\hbar^2}\right)^{1/3} \right] \quad (35)$$

and the function associated with the density operator is

$$\rho_t(p,q) = \left| \frac{4}{F^3\hbar^2} \frac{1}{t-1/(2mF)} \right|^{1/3} \text{Ai} \left[\left(\frac{4}{F^3\hbar^2} \frac{1}{t-1/(2mF)}\right)^{1/3} \left(\frac{p^2}{2m} + Fq - E\right) \right]. \quad (36)$$

When $t = 1/(2mF)$ this reduces to a delta function. With this new association the delta functions are associated with parabola not straight lines. Now a physically realisable state can be described by a delta

function, if the latter is singular on the two-parameter family of parabolas

$$(q-q_0) + t(p-p_0)^2 = 0. \quad (37)$$

This happens because the present association is invariant under linear inhomogenous transformations in the new operators \hat{a} and \hat{b} .

The spatial density is no longer obtained by simply integrating over p but rather through

$$\begin{aligned} \rho(q') &= \text{Tr } \delta(q'-\hat{q}) \delta\left(F - F\hat{q} - \frac{\hat{q}^2}{2m}\right) \\ &= \int \frac{dp}{2\pi\hbar} \frac{dq}{\left(\frac{4}{\hbar^2}\right)^{1/3}} \text{Ai}\left[\frac{4}{\hbar^2}\right]^{1/3} (q'-q) \delta\left(E - Fq - \frac{p^2}{2m}\right). \end{aligned} \quad (38)$$

In this expression we used eq. (36) with $t = 4(2mF)$; thus $\rho_c(p,q)$ is the δ function factor while the Airy function factor is in turn the function associated with $\delta(q'-\hat{q})$. When compared to the normal Weyl association formula,

$$\rho(q') = \int \frac{dpdq}{2\pi\hbar} \delta(q-q') \left(\frac{8m}{F\hbar^2}\right)^{1/3} \text{Ai}\left[\frac{8m}{F\hbar^2}\right]^{1/2} \left(\frac{p^2}{2m} - Fq - E\right) \quad (39)$$

we see the following. In eq. (39) quantum effects arise through the finite width of the function associated with \hat{p} , the Airy function. In eq. (38) this function is a delta function, and the quantum effects arise due to the width in the function associated with the operator $\delta(q'-\hat{q})$ which is an Airy function. The spatial density is of course the same in both cases.

5. Conclusion

We have shown that it is possible to generate alternative associations to the Weyl association through unitary transformations giving rise to a whole equivalence class of Weyl's associations. These new associations are formally equally good since quantum mechanics does not, a priori, distinguish between operators related by unitary transformations.

These associations, however, give rise to functions with different properties in the (p,q) space. The choice of association in a particular problem is determined by convenience.

The existence of many different but equally good associations allows us to see how unitary transforms generate canonical transformations. A unitary transformation on an operator has only the effect of generating a canonical transformation in the p,q space if simultaneously with the unitary transformation we change the Weyl basis which gives rise to the p,q space. The new basis is related to old bases by a unitary transformation and a relabeling.

One of the most commonly encountered unitary transformations is the time evolution of the density matrix. If we choose the operator z generating the unitary transformation of our basis to be the Hamiltonian operator and take t to be the time, we can make the function associated with the density matrix evolve classically with time. The nonclassical part of the propagation will then be in the functions associated with other operators; a somewhat unusual interaction picture.

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