External breaking of ground-state symmetry

S. Malinowski

Department of Theoretical Physics, University of Łódź, PL-90-236 Łódź, ul. Pomorska 149/153, Poland (Received 19 August 1993)

Ground-state symmetry can be broken by an external field. The threshold value of the symmetrybreaking field may be roughly estimated by comparing experimentally the behavior of two identical physical quantities, as functions of the field, for the set of field directions equivalent, with respect to the action, to a group generator. The kinetic coefficients as the functions of magnetic induction B are used as an illustration.

I. INTRODUCTION

The breaking of the symmetry group of the medium by an external (scalar, vector, tensor, etc.) field consists in changing the translation symmetry and/or point symmetry of the medium. Any change of symmetry will be accompanied by a rapid variation of the coefficients appearing in the mathematical formulas describing a given physical phenomenon occurring in the crystal. If these coefficients are not of a scalar type, i.e., they are vectors or tensors, then, as a rule, with the change of the point symmetry, the character of the coefficients will also be changed. For example, the isotropic second-order tensor can take the form of the anisotropic one; the uniaxial crystal becomes biaxial, etc.

Unfortunately, the coefficients are some unknown functions of the field applied in order to break the crystal symmetry. For a given value of the nonscalar field, the coefficients acquire different (fortunately, very often significantly different^{1,2}) values for different directions of the field. An exception to this rule is provided by the socalled crystallographic equivalent directions for a given type of field. For each of these directions, the physical quantities describing the phenomena occurring in the crystal take the same value for the same value of the field. The equivalent directions are the ones which transform into each other under the action of the point-symmetry group of the crystal. For different groups we have (for a given field) the different sets of equivalent directions.

We see that the hypothesis concerning the external symmetry breaking of point symmetry by the nonscalar field is one of the simplest to be verified in an experimental way, because, in this case, apart from the changes of the values of coefficients, the set of equivalent directions changes, as well as the character of nonscalar coefficients. These latter features of symmetry breaking may be used to roughly estimate the threshold value of external field.

It is possible to establish the symmetry breaking for only one direction of the field provided we are able to detect the jump in the values of the coefficients. In an experiment performed with insufficient precision, the jump in the value of the coefficient may pass unnoticed if it is small and takes place in the narrow interval of the field and, in addition, the coefficient behaves, as the function of the field in the same way on both sides of the crossover region. In such a situation the measurement for other directions equivalent to the first one is indispensable. After crossing over some value of the field, called the threshold value, the previously equivalent physical phenomena wi11 no longer be equivalent. Namely, for equivalent directions, some of the identical curves representing a given coefficient as a function of the field will not coincide any longer above the threshold value. Owing to that, we are able to estimate the order of the threshold value. Carrying out more and more precise observations of the coefficient in the presumed interval of the threshold value of the field, we will finally notice the jump of the coefficient.

In Sec. II we restrict our considerations to the case when the symmetry of the ground state of the crystal is broken by an external magnetic induction B. In this case the measurement can be carried out by taking advantage of the relations between the kinetic coefficients of the transport phenomena. For the equivalent directions of the field B in a given crystal, we write the relations between the components of the conductivity tensor $\sigma_{ii}(\mathbf{B})$. The same relations hold true for the dielectric permittivity $\varepsilon_{ii}(\mathbf{B})$ and magnetic susceptibility $\chi_{ii}(\mathbf{B})$ tensors.^{3,4} So the relations written in Sec. II are sufficient to formulate the geometry of the experiment on the basis of the electric and heat conductivity, the magneto-optic effects, and the dynamic magnetic susceptibility. Some methods of measurement will be proposed in Sec. III.

II. RELATIONS FOR THE ELECTRIC CONDUCTIVITY TENSOR

The form of the material tensor and the pointsymmetry group of the crystal are mutually related. Of course, the interactions in the crystal determine its symmetry group. Fortunately, on our level of consideration, the notions of the symmetry of the physical phenomena (hence, the coefficients) and symmetry of the crystal can be used interchangeably.

The unitary generator g of the group G leads to the following relations between the components of the electric conductivity tensor:

$$
\sigma_{ij}(\mathbf{B}) = g_{il}g_{jk}\sigma_{lk}[\det(g_{il}^{-1})g^{-1}\mathbf{B}]
$$

= $g_{il}g_{jk}\sigma_{lk}(\mathbf{B}')$. (1)

This is the mathematical expression for the Neumann rule. In turn, for the antiunitary generator $g' = \theta g$, where θ is the time inversion operator, we have

 $\sigma_{ij}(\mathbf{B})=g_{il}g_{jk}\sigma_{kl}[-\det(g_{il}^{-1})g^{-1}\mathbf{B}]$

 $=g_{il}g_{jk}\sigma_{kl}(\mathbf{B}')$.

The above formula is the generalization^{5,6} to any antiuni tary generator of the point group of the Onsager rule,⁷

$$
\sigma_{ij}(\mathbf{B}) = \sigma_{ji}(-\mathbf{B})\,,\tag{3}
$$

originally formulated for the time inversion generator θ . In the above formulas g_{il} is the 3×3 matrix representa

 (2)

tion of the unitary part of the generator and $det(g_{il}^{-1})$ is the determinant of 3×3 matrix of the inverse element g^{-1} .

The characteristic features distinguishing the generator θ are as follows. The equivalent direction for the field **B** is the field $\mathbf{B}' = -\mathbf{B}$; the form of the tensor $\sigma_{ii}(\mathbf{B})$ is such that $\sigma_{ii}(\mathbf{B})/\sigma_{ii}(\mathbf{B}')=1$ (*i*, *j* = 1, 2, 3). The explicit form of the relations (1) and (2) for other group generators and the characteristic features of group generators are given in the Appendix. On this basis and, on the other hand, by knowing the set of generators for a given group, 8.9 we can write (Table I) the minimal but complete set of group characteristics (for example, for the electric conductivity tensor).

The set of directions equivalent to field $\mathbf{B} = [0,0,\mathbf{B}]$ (the star of magnetic induction 8) consists of, at most, two directions, $B, -B$. For this star, for all groups with the exception of the groups listed under position Nos. 32–34 in Table I, the tensor $\sigma_{ii}(\mathbf{B})$ takes the simplest form, for which the components σ_{i3} and σ_{3i} ($i = 1,2$) are identically equal to zero: $\sigma_{i3} = \sigma_{3i} = 0$. The final forms of the tensors σ_{ij} for other stars of field **B** can be also easily written. In many problems they are necessary but, fortunately, here they are not. In order to determine whether the symmetry has been broken (and if so, what group arises after the breaking symmetry) or not, it is sufficient to take into account only these relations between the components σ_{ij} , which are characteristic for a given generator.

$$
\sigma_{13}(\mathbf{B}) = -\sigma_{31}(\mathbf{B'}) \n= \sigma_{13}(\mathbf{B''}), \n\sigma_{31}(B) = \sigma_{13}(\mathbf{B''}), \n= \sigma_{31}(\mathbf{B''}), \n= \sigma_{31}(\mathbf{B''}), \n= -\sigma_{32}(\mathbf{B''}), \n= -\sigma_{32}(\mathbf{B''}), \n= -\sigma_{32}(\mathbf{B''}),
$$

where the field $\mathbf{B} = [B_x, B_y, B_z]$ is transformed to the direction $\mathbf{B}'=[B_x, B_y, -B_z]$ [Eqs. (4a) and (4a')] and direction $\mathbf{B}^{\prime\prime} = [-B_x, B_y, -B_z]$ [Eqs. 4(b) and 4(b')] under the action of the elements θC_{2z} and C_{2y} , respectively.

For the field $B=[0, B, 0]$ we have $B'=B''=B$, For the held $\mathbf{B} = [0, \mathbf{B}, 0]$ we have $\mathbf{B} = \mathbf{B} = \mathbf{E}$
 $\sigma_{12} = \sigma_{21} = \sigma_{23} = \sigma_{32} \equiv 0$, and $\sigma_{13} = -\sigma_{31}$. These relation cannot be broken by any reasonable value of B. If the field \bf{B} is antiparallel to the field \bf{M} of the sample, then with an increasing value of **B**, the value of $\sigma_{13}(\mathbf{B})$ will tend towards zero, and then, after changing the sign, its absolute value wi11 be systematically increasing. The state with reversed $M, M \rightarrow -M$, is also a stable state.

By applying the field $B = [0,0,B]$ ($B' = B'' = -B$), we can remagnetize our sample to the state with $\mathbf{M}||z$ axis. Then, the following groups are possible. $G = 2$ [case (i)], $G=2'2'2$ [case (ii)], $G=4$, 42'2', and so on [case (iii)]. The relations (4a), (4a'), (4b), and (4b') will be modified to the forms: $\sigma_{13} = \sigma_{31} = \sigma_{23} = \sigma_{32} = 0$; in addition, $\sigma_{12} \neq \sigma_{21}$ for $G = 2$; $\sigma_{12} = -\sigma_{21}$ for $G = 2'2'2, 4, 42'2'$, $\sigma_{11} = \sigma_{22}$ for $G = 4, 42'2'$ (compare with the conditions under No. 1, No. 33, No. 3, and No. 37 in Table I, respectively). It is not possible to distinguish the state of symmetry $G = 4$

III. BREAKING SYMMETRY AND MEASUREMENT

The problem of external symmetry breaking reduces to the problem of breaking at least one of the group generators. A generator of a given order can be broken as follows:

(i) To lower order. For example, the twofold axis may be broken to the onefold axis, i.e., to the identity element of a new group. In this case the forced symmetry group is the maximal subgroup of the ground-state symmetry group.

(ii) To the same order but of a different nature. For example, the twofold unitary axis may be broken to the twofold antiunitary axis or vice versa. To this case belongs, among other things, the rotations of the magnetic axes frame with respect to the crystallographic axes frame of the diamagnetic or paramagnetic phase of a sample.

(iii) To higher order. For example, the twofold axis may be broken to the fourfold axis. In this case the forced symmetry group is larger than the ground-state symmetry group.

Let us illustrate the above statements by the example of a ferromagnetic sample in the ground-state symmetry $G = 2'22'$ (case No. 34 in Table I) for which the magnetization vector M is parallel to the y axis. The characteristic relations for the θC_{2z} and C_{2y} generators are as follows:

$$
\sigma_{12}(\mathbf{B}) = \sigma_{21}(\mathbf{B'}) \tag{4a}
$$

$$
\sigma_{12}(\mathbf{B}) = \sigma_{21}(\mathbf{B}'),
$$
\n
$$
= -\sigma_{12}(\mathbf{B}'),
$$
\n
$$
\sigma_{21}(\mathbf{B}) = \sigma_{12}(\mathbf{B}')
$$
\n(4a')

$$
B = -\frac{\sigma_{12}(\mathbf{B'})}{\sigma_{21}(\mathbf{B''})},\tag{4b'}
$$

from that of symmetry $G = 42'2'$ by applying the field B $||z|$ axis. In such a case the history of a sample is decisive. Namely, the ferromagnetic ground state of symmetry $G = 2'22'$ is possible under the condition that above the Curie temperature, the sample had one of the following symmetries: $G = 2221'$, 4221', or 6221'; this is because only for those unbroken symmetries, the state below the Curie point with $M||z$ axis has the symmetries $G = 2'2'2$, 42'2', and 62'2', respectively. We see that the more information on the sample we have, the simpler the experiment will be to solve our problem.

By applying the field $B=[B, 0, 0]$ ($B'=-B''=B$) the ground state of symmetry $G = 2'22'$ can be transformed to the nonground state of symmetry $G = 22'2'$. This state will be realized because Eqs. (4b) and (4b') are modified to the form which implies the following relations between the components of σ_{ij} : $\sigma_{12} = \sigma_{21} = \sigma_{13} = \sigma_{31} = 0$ and $\sigma_{32} = -\sigma_{23}$, which are different from those for symmetry $G = 2'22'$. Similarly, above some value of the field $\mathbf{B}=[B_x, B_y, B_z], \mathbf{B}=[B_x, B_y, 0], \mathbf{B}=[B_x, 0, B_z], \text{ and}$ $\mathbf{B}=[0,B_{v},B_{v}]$, the ground state of symmetry $G=2'22'$ will be broken to the state of symmetry $G = 1$, $G = 2'$ (of generator θC_{2z}) (the full symbol of this group is $G = 112'$), $G = 2$ (of generator C_{2v}) (the full symbol $G = 121$), and $G = 2'$ (of generator $\theta C_{2x} = \theta C_{2z} \cdot C_{2y}$) (the full symbol $G = 2'11$), respectively.

In conclusion, the fields $\mathbf{B}=[0,0,B]$, $\mathbf{B}=[0,B_{v},B_{z}]$, and $\mathbf{B}=[B_x,B_y,B_z]$ can break the symmetry $G=2'22'$ to the symmetry $G = 2'2'2$ (or 42'2' or 62'2'), 2'11, 1, respectively. In such a case the relations (4a), (4a'), (4b), and (4b') are simultaneously modified. In turn, for the field $\mathbf{B} = [B_x, 0, B_z]$ the group $G = 121$ is possible provided the relations (4a) and (4a') are no longer valid. By applying the fields $\mathbf{B}=[B,0,0]$ and $\mathbf{B}=[B_{x},B_{y},0]$ we can obtain the symmetry $G = 22'2'$ and $G = 112'$, respectively, because the relations (4b} and (4b'} are no longer valid.

The measurement of the breaking field is reduced to finding the value of the field B above which one (no more!) of four characteristic relations, e.g.,

$$
\sigma_{13}(\mathbf{B}) = -\sigma_{31}(\mathbf{B'})
$$
 [cf. (4a)]

or

$$
\sigma_{23}(\mathbf{B}) = -\sigma_{23}(\mathbf{B''})
$$
 [cf. (4b)]

is no longer fulfilled. If we know the history of the sample we would know its broken symmetry groups. Then, the measurement of the value of the breaking field may be based on the knowledge of the broken symmetry group. Namely, by diminishing the value of the external field we expect the symmetry to be restored. Therefore, we could proceed in the reverse way to determine the point where the symmetry gets restored.

For some media, the measurement based on the magneto-optic phenomenon is the only one possible. It consists in the observation, as a function of field 8, the birefringence $\Delta n(\mathbf{B})$, polarizations of electromagnetic waves, and so on, for two of those equivalent directions in a group generator which will be broken. In order to avoid the differences in corrections originating from space dispersion of the electro-magnetic wave vector k, the measurement for the fields B and 8' must be carried out for the same propagation direction k.

IV. SUMMARY AND REMARKS

The space inversion operator i cannot be broken by applying an axial field B. However, it can be broken by an electric field E. In turn, the time inversion operator θ can be broken by field **B**, but not by field **E**. For some state of medium, it might appear technically impossible to obtain a sufficiently strong field B to break the group generator θ ; this is the case for the groups listed in position Nos. 16—31 of Table I. The electronic configuration of their ground state has an electric nature. Its response to the magnetic interaction is very weak. Then, the modification to a new electric configuration is possible but only by applying a very strong magnetic field. The induction of magnetic configuration (breaking the antiunitary generator θ) is possible theoretically but not technically, because here the extremely strong field is needed.

The theoretical idea presented here, of the rough estimate of the threshold value of field **B** may be essentially adopted to other (e.g., electric, pressure, etc.) fields. Recall that the measurement of breaking of one, two, \dots , group generators leads to the experimental observation of two, three, \dots , functions of field **B** along the equivalent directions in a group generator. We will be able to estimate the range of the threshold value of B by comparing the functions which are identical with respect to the action of the group generator. This will allow us to fit the experimental method more adequately to solve our problem. The more and more precise measurement in the interval of a previously estimated threshold value allows us to answer most questions concerning the physical mechanism of the external breaking of the ground state, the stability of ground state, 10 and other questions difficult to predict now.

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APPENDIX

Below, all the formulas are written in Cartesian coordinates. The generator C_{2z} (binary unitary rotation around the z axis) fixes the following equalities between the components of the tensors $\sigma_{ii}(\mathbf{B})$ and $\sigma_{ii}(\mathbf{B}')$, respectively,

$$
\begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix} = \begin{bmatrix} 11 & 12 & -13 \\ 21 & 22 & -23 \\ -31 & -32 & 33 \end{bmatrix};
$$
 (A1)

[31 32 33] $[-31 \ -32 \ 33 \]$
here the fields **B**=[B_x, B_y, B_z] and **B'**=[$-B_x, -B_y, B_z$] are equivalent. Four of these equalities are characteristi for the C_{2z} generator. These are $\sigma_{i3}(\mathbf{B})/\sigma_{i3}(\mathbf{B}')$ $=\sigma_{3i}(\mathbf{B})/\sigma_{3i}(\mathbf{B}')=-1$ ($i=1,2$) under the condition that **is not parallel to the** z **axis which, in turn, insures** that $\sigma_{i3} \neq 0$ and $\sigma_{3i} \neq 0$ (*i* = 1,2). In conclusion, the characteristic features of the C_{2z} generator are σ_{i3} $=\sigma_{3i} \equiv 0$ (i = 1,2) for **B**||z axis and $\sigma_{i3}(\mathbf{B})/\sigma_{i3}(\mathbf{B}')$ $(\overline{\sigma}_{31}(B)/\sigma_{3i}(B')=-1$ (i=1,2) for $B\neq z$ axis.

The characteristic features of other binary unitary or antiunitary rotations are of the same nature and can be easily read from the relation, given below, between the tensors for fields **B** and **B'**.

For brevity we will write below only the components of the $\sigma_{ii}(\mathbf{B}')$ tensor. For the generator θC_{2z} (binary antiunitary rotation around the z axis) we have

$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 11 & 21 & -31 \\ 12 & 22 & -32 \\ -13 & -23 & 33 \end{bmatrix}, \text{ for } \mathbf{B'} = [B_x, B_y, -B_z],
$$
\n(A2)

and for other generators,

 C_{2x} :

$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 11 & -12 & -13 \\ -21 & 22 & 23 \\ -31 & 32 & 33 \end{bmatrix}, \text{ for } \mathbf{B'} = [B_x, -B_y, -B_z],
$$
\n(A3)

(A4)

$$
\theta C_{2x}:
$$
\n
$$
\sigma_{ij}(\mathbf{B}') = \begin{bmatrix} 11 & -21 & -31 \\ -12 & 22 & 32 \\ -13 & 23 & 33 \end{bmatrix}, \text{ for } \mathbf{B}' = [-B_x, B_y, B_z],
$$

$$
C_{2y}:
$$
\n
$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 11 & -12 & 13 \\ -21 & 22 & -23 \\ 31 & -32 & 33 \end{bmatrix}, \text{ for } \mathbf{B'} = [-B_x, B_y, -B_z],
$$
\n(A5)

$$
C_{4z}:
$$
\n
$$
\sigma_{ij}(\mathbf{B}') = \begin{bmatrix} 22 & -21 & 23 \\ -12 & 11 & -13 \\ 32 & -31 & 33 \end{bmatrix}, \text{ for } \mathbf{B}' = [-B_y, B_x, B_z].
$$
\n(A6)

The xy plane of the cubic, hexagonal, tetragonal, and rhombohedral systems is the isotropic plane for kinetic phenomena. This property is preserved, in the form explained below, for the medium placed in an external magnetic field. The characteristi features of the C_{4z} generator are the following conditions, $\sigma_{11}(\mathbf{B})/\sigma_{22}(\mathbf{B}') = \sigma_{22}(B)/\sigma_{11}(\mathbf{B}') = 1$ and conditions, $\sigma_{11}(\mathbf{B})/\sigma_{22}(\mathbf{B'}) = \sigma_{22}(\mathbf{B})/\sigma_{11}(\mathbf{B'}) = 1$ and $\sigma_{12}(\mathbf{B})/\sigma_{21}(\mathbf{B'}) = \sigma_{21}(\mathbf{B})/\sigma_{12}(\mathbf{B'}) = -1$. In a similar way the characteristic features for the other threefold, fourfold, and sixfold (unitary and antiunitary) generators can be read from relations between the tensors for fields 8 and **B'**, given below. For θC_{4z} , we have

$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 22 & -12 & 23 \\ -21 & 11 & -13 \\ 23 & -13 & 33 \end{bmatrix},
$$

for $\mathbf{B'} = [B_y, -B_x, -B_z]$, (A7)

$$
S_{4z}\colon
$$

$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 22 & -21 & -23 \\ -12 & 11 & 13 \\ -32 & -31 & 33 \end{bmatrix}, \text{ for } \mathbf{B'} = [B_y, -B_x, B_z], \qquad C'_{21}:
$$
\n(A8)

Below, all the formulas concerning the rhombohedral and
hexagonal lattices are written in hexagonal coordinates in
which the x and y axes make an angle equal to
$$
2\pi/6
$$
.
For C_{3z} we obtain $\mathbf{B}' = [-B_y, B_x, -B_y, B_z]$,

 $\sigma_{ii}(\mathbf{B}') =$ $(11-12-21+22)$ $(11-21)$ $(23-13)$ $(11-12)$ 11 -13 $(32-31)$ -31 33

$$
(\mathbf{A}11)
$$

$$
S_{3z}: \mathbf{B'} = [B_y, -B_x + B_y, B_z],
$$

\n
$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} (11 - 12 - 21 + 22) & (11 - 21) & (13 - 23) \\ (11 - 12) & 11 & 13 \\ (31 - 32) & 31 & 33 \end{bmatrix},
$$

\n(A12)

$$
\theta S_{3z}: \mathbf{B'} = [-B_y, B_x - B_y, -B_z],
$$

\n
$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} (11 - 12 - 21 + 22) & (11 - 12) & (31 - 32) \\ (11 - 21) & 11 & 31 \\ (13 - 23) & 13 & 33 \end{bmatrix},
$$
\n(A13)

$$
C_{6z}: \mathbf{B'} = [B_x - B_y, B_x, B_z],
$$

\n
$$
\sigma_{ij} = (\mathbf{B'}) \begin{bmatrix} 22 & (21-22) & 23 \\ (12-22) & (11-12-21+22) & (13-23) \\ 32 & (31-32) & 33 \end{bmatrix},
$$

\n(A14)

$$
\theta C_{6z}: \mathbf{B'} = [-\mathbf{B}_x + B_y, -B_x, -B_z],
$$

\n
$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 22 & (12-22) & 32 \\ (21-22) & (11-12-21+22) & (31-32) \\ 23 & (13-23) & 33 \end{bmatrix},
$$

$$
(A15)
$$

$$
C'_{21}: \mathbf{B'} = [-B_y, -B_x, -B_z],
$$

\n
$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 22 & 21 & 23 \\ 12 & 11 & 13 \\ 32 & 31 & 33 \end{bmatrix},
$$
\n(A16)

$$
\theta C'_{21}: \mathbf{B'} = [B_y, B_x, B_z],
$$

\n
$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 22 & 12 & 32 \\ 21 & 11 & 31 \\ 23 & 13 & 33 \end{bmatrix},
$$
\n(A17)

$$
C_{21}'' : \mathbf{B}' = [B_y, B_x, -B_z],
$$

\n
$$
\sigma_{ij}(\mathbf{B}') = \begin{bmatrix} 22 & 21 & -23 \\ 12 & 11 & -13 \\ -32 & -31 & 33 \end{bmatrix}.
$$
 (A18)

 θS_{4z} :

$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 22 & -12 & -32 \\ -21 & 11 & 31 \\ -23 & -13 & 33 \end{bmatrix},
$$

for $\mathbf{B'} = [-B_y, B_x, -B_z]$, (A9)

 C_{31} :

$$
\sigma_{ij}(\mathbf{B'}) = \begin{bmatrix} 33 & 31 & 32 \\ 13 & 11 & 12 \\ 23 & 21 & 22 \end{bmatrix}, \text{ for } \mathbf{B'} = [B_y, B_x, B_z] .
$$
 (A10)

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