PHYSICAL REVIEW VOLUME 71, NUMBER 3 FEBRUARY 1, 1947

On a General Condition of Heisenberg for the S Matrix

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(Received October 18, 1946)

It is shown that the S matrix for an attractive exponential potential, which possesses redundant zeros, does not satisfy a general condition of Heisenberg. To insure the validity of Heisenberg's condition, we introduce the supplementary condition that the interaction potential should vanish for large distances from the scattering center. It is shown that the S matrices for the attractive exponential and the Coulomb potential cut off at a large distance R give correctly both the eigenvalues of energy and the asymptotic behavior of the wave functions for the s states in the limit $R\rightarrow\infty$.

1. INTRODUCTION

RECENTLY Heisenberg[1] has proposed a new formulation of the quantum theory which deals exclusively with such physical quantities as are directly observable, namely, the discrete energy values of stationary states of closed systems, and the asymptotic behavior of wave functions at infinity in collision processes. These physical quantities are determined by Heisenberg's S matrix, which plays the same fundamental role in Heisenberg's new scheme as the Hamiltonian and wave equation in the current scheme of quantum theory. It is possible to derive from the current scheme of quantum theory certain general properties of the S matrix, such as the unitary property[2] and the relativistic invariance,[3] which can be taken over into the new formulation of the quantum theory.

The determination of closed stationary states from the S matrix has been investigated by Heisenberg and Møller. For the following investigation it is sufficient to state Heisenberg's result for the s states of a particle under the action of a central force. Let $u_n(r)$ and $u_k(r)$ be, respectively, the radial wave functions of the discrete and the continuous energy states, normalized according to the equations

$$\int_0^\infty |u_n(r)|^2dr=1, \qquad \int_0^\infty u_k^*(r)u_{k'}(r)dr=\delta(k-k').$$

These wave functions satisfy the completeness relation

$$\sum\nolimits_n u_n^*(r)u_n(r')+\int_0^\infty u_k^*(r)u_k(r')dk=\delta(r-r'). \quad (1)$$

The asymptotic expressions of these wave functions for large distances are

$$u_n(r)\sim c_n(2\pi)^{-\frac{1}{2}}\exp(-|k_n|r), \quad (2)$$

$$u_k(r)\sim(2/\pi)^{\frac{1}{2}}\sin[kr+\delta(k)], \quad (3)$$

where c_n is a constant and $\delta(k)$ is the phase of u_k. Making use of the general relations

$$S(k)=\exp[2i\delta(k)] \quad (4)$$

and

$$S^*(k)S(k)=1, \quad (5)$$

Heisenberg obtained from (1)–(3) the following general relation for a large value of r:

$$\int_{-\infty}^\infty S(k)\exp(ikr)dk=\sum\nolimits_n|c_n|^2\exp(-|k_n|r). \quad (6)$$

The closed discrete states can be determined by analytic continuation from the real to the complex values of k. If $S(k)$ decreases sufficiently rapidly for large values of $|k|$, the left-hand side of (6) is equal to $2\pi i$ times the sum of the residues of $S(k)\exp(ikr)$ at the poles of $S(k)$ in the upper half of the complex plane. Identifying the discrete states with these poles, Heisenberg obtained

$$|c_n|^2=2\pi i[ResS(k)]_{k_n}. \quad (7)$$

For the S matrices such that the relation

$$S(k)S(-k)=1 \quad (8)$$

in the complex plane can be derived by analytic

[1] W. Heisenberg, Zeits. f. Physik **120**, 513 and 673 (1943) Heisenberg's third and fourth papers on the S matrix have not yet been published. I am indebted to Professor Pauli for communicating to me some results in the fourth paper.
[2] W. Pauli, *Meson Theory of Nuclear Forces* (Interscience Publishers, Inc., New York, 1946), p. 49.
[3] C. Møller, Danske Vid. Sels. Math.-fys. Medd. **23**, No. 1 (1945); **22**, No. 19 (1946).

continuation of the unitary condition (5) for real values of k, the poles of $S(k)$ in the upper half-plane have corresponding zeros in the lower half-plane. Hence, when the poles and zeros are on the imaginary axis,

$$|c_n|^2 = -2\pi[(dS/d|k|)_{-i|k_n|}]^{-1}. \quad (9)$$

This relation expressing the absolute magnitude of c_n in terms of $S(k)$ can also be directly derived by a method of Kramers[4] without using (6). We shall see below that there are cases in which (9) is satisfied but (6) is not satisfied.

2. REDUNDANT ZEROS

As recently reported,[5] the S matrix for an attractive exponential field presents a new feature in the eigenvalue problem. For the s states of a particle of mass m in the potential field

$$V(r) = -V_0 \exp(-r/a), \quad (10)$$

where V_0 and a are positive constants, the wave equation takes the form

$$-(\hbar^2/2m)(d^2u/dr^2 + k^2u) + V(r)u = 0. \quad (11)$$

The solutions of Eq. (11) for a positive value of energy are the Bessel functions

$$J_{\pm i\rho}[\alpha \exp(-r/2a)],$$

where

$$\rho = 2ak, \quad \alpha = 2a(2mV_0)^{\frac{1}{2}}/\hbar.$$

The wave function which vanishes at the origin is

$$u_k(r) = i(2\pi)^{-\frac{1}{2}}|\Gamma(i\rho+1)/J_{i\rho}(\alpha)| \times \{J_{-i\rho}(\alpha)J_{i\rho}[\alpha\exp(-r/2a)] - J_{i\rho}(\alpha)J_{-i\rho}[\alpha\exp(-r/2a)]\}, \quad (12)$$

the normalization constant being chosen such that the asymptotic expression of Eq. (12) for large r, namely,

$$u_k(r) \sim i(2\pi)^{-\frac{1}{2}}|\Gamma(i\rho+1)/J_{i\rho}(\alpha)| \times \left\{\frac{J_{-i\rho}(\alpha)(\alpha/2)^{i\rho}}{\Gamma(i\rho+1)}\exp(-ikr) - \frac{J_{i\rho}(\alpha)(\alpha/2)^{-i\rho}}{\Gamma(-i\rho+1)}\exp(ikr)\right\} \quad (13)$$

is of the form of Eq. (3). Comparing Eq. (12) with Eq. (3) and making use of Eq. (4), we see that

$$S(k) = \frac{J_{i\rho}(\alpha)\Gamma(i\rho+1)}{J_{-i\rho}(\alpha)\Gamma(-i\rho+1)}\left(\frac{\alpha}{2}\right)^{-2i\rho}. \quad (14)$$

$S(k)$ vanishes when $J_{i\rho}(\alpha)$ vanishes or $\Gamma(-i\rho+1)$ is infinitely large. Now $J_{i\rho}(\alpha)$ has no zeros in the lower half-plane of k except those on the imaginary axis.[6] Hence the first condition is equivalent to

$$J_{|\rho|}(\alpha) = 0. \quad (15)$$

The wave function corresponding to a zero k_n of Eq. (15) is[7]

$$u_n(r) = c_n(2\pi)^{-\frac{1}{2}}\Gamma(|\rho_n|+1)(2/\alpha)^{|\rho_n|} \times J_{|\rho_n|}[\alpha\exp(-r/2a)]. \quad (16)$$

The absolute magnitude of the constant c_n is given by Eq. (9) with S given by Eq. (14), as can be directly verified from the normalization condition.

The second condition

$$\Gamma(-ip\rho+1) = \infty \quad (17)$$

is satisfied by values of ρ such that

$$i\rho = |\rho| = 1, 2, 3\cdots. \quad (18)$$

The wave functions Eq. (12) corresponding to the eigenvalues of Eq. (18) vanish identically. The zeros given by Eq. (18) can be regarded as redundant. We shall denote in the following the values of ρ and k corresponding to the redundant zeros by ρ_r and k_r, respectively.

3. VALIDITY OF HEISENBERG'S GENERAL RELATION

Let us now study Heisenberg's general relation, Eq. (6), as it applies to the S matrix for the exponential potential. The integral

$$\int_{-\infty}^{\infty} S(k)\exp(ikr)dk$$

in (6) can be evaluated by contour integration.

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[4] H. A. Kramers, Hand- und Jahrbuch d. Chem. Physik 1, 312 (1938).

[5] S. T. Ma, Phys. Rev. 69, 668 (1946).

[6] Gray, Mathews and MacRobert, *Bessel Functions* (The Macmillan Company, New York, 1931), p. 88.

[7] H. Bethe and R. F. Bacher, Rev. Mod. Phys. 8, 111 (1936).

We have

$$\int_{-\infty}^{\infty} S(k)\exp(ikr)dk=\lim_{K\to\infty}\int_C S(k)\exp(ikr)dk +2\pi i\sum Res[S(k)\exp(ikr)], \quad (19)$$

where C denotes a semi-circle of radius K above the real axis, having its center at the origin, and the summation extends over all the poles in the upper half-plane. Equation (14) can be written in the form

$$S(k)=\Lambda_{i\rho}(\alpha)/\Lambda_{-i\rho}(\alpha)$$

if we put

$$J_p(\alpha)=(\alpha/2)^p\Lambda_p(\alpha)/\Gamma(p+1).$$

Now $\Lambda_p(\alpha)$ approaches the value 1 as p tends to infinity through a sequence of numbers not consisting of negative integers. Hence if K tends to infinity through a sequence such that $|\rho|$ is not integral

$$\lim_{K\to\infty}\int_C S(k)\exp(ikr)dk=\lim_{K\to\infty}\int_C \exp(ikr)dk =\int_{-\infty}^{\infty}\exp(ikr)dk=2\pi\delta(r)=0$$

since $r\neq 0$. Therefore

$$\int_{-\infty}^{\infty} S(k)\exp(ikr)dk=2\pi i\sum Res[S(k)\exp(ikr)] =\sum\nolimits_n|c_n|^2\exp(-|k_n|r) -2\pi\sum\nolimits_r\left(\frac{dS}{d|k|}\right)^{-1}_{-i|k_r|}\exp(-|k_r|r). \quad (20)$$

It can be easily shown from (14) that

$$(dS/d|k|)_{-i|k_r|}>0, \quad (21)$$

so that the second sum over the redundant eigenvalues is smaller than zero. Comparing Eq. (20) with Eq. (6) we see that Heisenberg's general condition is not satisfied by Eq. (14). It has recently been proposed by D. ter Haar[8] to make use of Eq. (21) for discarding the redundant zeros.

This example raises a question of the validity of Heisenberg's relation, Eq. (6). Heisenberg's derivation outlined in Section 1 holds good only if the difference between the exact wave function $u_k(r)$ and its asymptotic expression Eq. (3) is small in comparison with the wave function $u_n(r)$. This is not the case with the exponential potential, however, as can be seen from Eqs. (12), (3), and (2).

We can see how the difficulty of redundant eigenvalues arises from the approximate treatment by evaluating the integral

$$\int_0^{\infty} u_k^*(r)u_k(r')dk$$

for the exact wave function (12). From Eq. (12) we have

$$\int_0^{\infty} u_k^*(r)u_k(r')dk=\int_{-\infty}^{\infty} f(k;r,r')dk, \quad (22)$$

where

$$f(k;r,r')=(2\pi)^{-1}\{\Gamma(i\rho+1)\Gamma(-i\rho+1)/J_{i\rho}(\alpha)J_{-i\rho}(\alpha)\}\{J_{-i\rho}(\alpha)J_{i\rho}(\alpha)J_{i\rho}[\alpha\exp(-r/2a)] \times J_{-i\rho}[\alpha\exp(-r'/2a)]-J_{i\rho}(\alpha)^2J_{-i\rho}[\alpha\exp(-r/2a)]J_{-i\rho}[\alpha\exp(-r'/2a)]\}. \quad (23)$$

Now the integral of $f(k;r,r')$ taken round the semicircle C referred to above has the limit

$$\lim_{K\to\infty}\int_C f(k;r,r')dk=(2\pi)^{-1}\int_{-\infty}^{\infty}\{\exp[ik(r'-r)]-\exp[ik(r'+r)]\}dk =\delta(r'-r)-\delta(r'+r)=\delta(r'-r). \quad (24)$$

Hence

$$\int_{-\infty}^{\infty} f(k;r,r')dk=\delta(r'-r)+2\pi i\sum Res f(k;r,r'). \quad (25)$$

But at the poles where $\Gamma(i\rho+1)=\infty$ the residue vanishes. Hence

$$2\pi i\sum Res f(k;r,r')=-i\sum[Res J_{-i\rho}(\alpha)^{-1}]\Gamma(i\rho+1)\Gamma(-i\rho+1)J_{i\rho}(\alpha) \times J_{-i\rho}[\alpha\exp(-r/2a)]J_{-i\rho}[\alpha\exp(-r'/2a)] =-\sum\nolimits_n u_n^*(r)u_n(r')$$

[8] D. ter Haar, Physica, in the press.

so that

$$\int_0^\infty u_k^*(r)u_k(r')dk=\delta(r'-r)-\sum_n u_n^*(r)u_n(r'),$$

which is just Eq. (1). In spite of the factor $\Gamma(i\rho+1)$ in the integrand of Eq. (22) the summation in the final result extends only over the true eigenvalues. The above calculation may be taken to be a direct verification of the completeness relation. For large distances r and r', we have, by Eq. (2)

$$\int_0^\infty u_k^*(r)u_k(r')dk=\delta(r'-r)-(2\pi)^{-1}\sum_n|c_n|^2\exp[-|k_n|(r+r')]. \tag{26}$$

In the approximate treatment, however, we have

$$\begin{aligned}\int_0^\infty u_k^*(r)u_k(r')dk&=\delta(r'-r)-(2\pi)^{-1}\int_{-\infty}^{\infty}S(k)\exp[ik(r+r')]dk\\&=\delta(r'-r)-(2\pi)^{-1}\sum_n|c_n|^2\exp[-|k_n|(r+r')]\\&\qquad-i\sum_r Res\{S(k)\exp[ik(r+r')]\}_{i|k_r|},\end{aligned}$$

which has an additional term corresponding to the redundant zeros.

This discussion shows the necessity of introducing a supplementary condition for the validity of Heisenberg's general relation. We can take for the supplementary condition the condition that the potential $V(r)$ should vanish for large distances from the scattering center, because under such a condition the wave function $u_k(r)$ is equal exactly to the expression (3) for large distances and therefore Eq. (6) holds with certainty.

4. POTENTIALS CUT OFF AT A LARGE DISTANCE

Møller has investigated the exponential potential (10) cut off at a large distance R, i.e., the potential

$$\begin{aligned}V(r)&=-V_0\exp(-r/a)\quad(0<r<R)\\&=0\qquad\qquad\qquad(\quad r>R).\end{aligned} \tag{27}$$

The wave function $u_k(r)$ is now given exactly by (3) when $r>R$, and, except for a constant factor, given by (12) when $r<R$. The requirement of continuity of $u_k(r)$ and its derivative at $r=R$ gives

$$S(k)=-\exp(-2ikR)\frac{J_{-i\rho}(\alpha)J_{i\rho+1}[\alpha\exp(-R/2a)]+J_{i\rho}(\alpha)J_{-i\rho-1}[\alpha\exp(-R/2a)]}{J_{-i\rho}(\alpha)J_{i\rho-1}[\alpha\exp(-R/2a)]+J_{i\rho}(\alpha)J_{-i\rho+1}[\alpha\exp(-R/2a)]}. \tag{28}$$

For large values of $|k|$ in the upper half-plane of k such that $2a|k|$ is not an integer,

$$S(k)\exp(ikr)\sim-\exp[ik(r-2R)]\frac{J_{i\rho+1}[\alpha\exp(-R/2a)]}{J_{i\rho-1}[\alpha\exp(-R/2a)]}\sim-\frac{\Gamma(i\rho)}{\Gamma(i\rho+2)}\left(\frac{\alpha}{2}\right)^2\times\exp(-R/a)\exp[ik(r-2R)],$$

and so

$$\lim_{K\to\infty}\int_C S(k)\exp(ikr)dk$$

vanishes for $r>2R$.[9] In accordance with the general discussion of Section 1 the eigenvalues of k are the values of k in the lower half-plane satisfying the equation $S(k)=0$ or by Eq. (28)

$$J_{-i\rho}(\alpha)J_{i\rho+1}[\alpha\exp(-R/2a)]+J_{i\rho}(\alpha)J_{-i\rho-1}[\alpha\exp(-R/2a)]=0, \tag{29}$$

[9] Whittaker and Watson, *Modern Analysis* (Cambridge University Press, New York, 1927), p. 115.

an equation first obtained by ter Haar. Equation (29) reduces to Eq. (15) when $R\rightarrow\infty$. Thus the redundant zeros no longer appear if we cut off the potential at a large distance R and subsequently make R tend to infinity after the eigenvalues have been determined from the S matrix.

Though the potential (27) becomes the potential (10) when R becomes infinitely large, the expression (28) goes over to (14) only when the imaginary part of k lies between $\pm 1/2a$. Above this region $S(k)\rightarrow\infty$ and below this region $S(k)\rightarrow 0$.

This is not the case, however, with the derivative of S with respect to $|k|$ at a point where (29) is satisfied. At such a point

$$\frac{dS}{d|k|}=-\exp(-2ikR)\frac{\dfrac{d\rho}{d|k|}\dfrac{d}{d\rho}\{J_{-i\rho}(\alpha)J_{i\rho+1}[\alpha\exp(-R/2a)]+J_{i\rho}(\alpha)J_{-i\rho-1}[\alpha\exp(-R/2a)]\}}{J_{-i\rho}(\alpha)J_{i\rho-1}[\alpha\exp(-R/2a)]+J_{i\rho}(\alpha)J_{-i\rho+1}[\alpha\exp(-R/2a)]}.$$

But for large values R

$$\frac{d}{d\rho}\{J_{-i\rho}(\alpha)J_{i\rho+1}[\alpha\exp(-R/2a)]\}\sim 0,$$

$$\frac{d}{d\rho}\{J_{i\rho}(\alpha)J_{-i\rho-1}[\alpha\exp(-R/2a)]\}\sim\frac{dJ_{i\rho}(\alpha)}{d\rho}J_{-i\rho-1}[\alpha\exp(-R/2a)],$$

$$J_{-i\rho}(\alpha)J_{i\rho-1}[\alpha\exp(-R/2a)]+J_{i\rho}(\alpha)J_{-i\rho+1}[\alpha\exp(-R/2a)]\sim J_{-i\rho}(\alpha)J_{i\rho-1}[\alpha\exp(-R/2a)],$$

so that

$$\frac{dS}{d|k|}\sim-\exp(-2ikR)\frac{dJ_{i\rho}(\alpha)}{d|k|}\frac{J_{-i\rho-1}[\alpha\exp(-R/2a)]}{J_{-i\rho}(\alpha)J_{i\rho-1}[\alpha\exp(-R/2a)]}\rightarrow-\left(\frac{\alpha}{2}\right)^{-2i\rho}\frac{\Gamma(i\rho)}{\Gamma(-i\rho)}\frac{dJ_{i\rho}(\alpha)}{d|k|}\Big/J_{-i\rho}(\alpha),$$

which is just the derivative of Eq. (14) with respect to $|k|$, whether the imaginary part of k is smaller or larger than $-1/2a$. From Eq. (9) we see that the expression $c_n\exp(-|k_n|r)$ represents the correct asymptotic behavior of the wave function for all the discrete states as $R\rightarrow\infty$. Now we have seen above that Eq. (28) tends to Eq. (14) as $R\rightarrow\infty$ for real values of k corresponding to positive energy states. It follows therefore that the S matrix for the cut-off exponential potential gives the correct asymptotic expression of the wave function for all the s states in the limit $R\rightarrow\infty$.

It is of interest to observe that for large values of R Eq. (28) differs very little from the expression

$$S(k)=-\exp(-2ikR)\times\frac{J_{i\rho}(\alpha)J_{-i\rho-1}[\alpha\exp(-R/2a)]}{J_{-i\rho}(\alpha)J_{i\rho-1}[\alpha\exp(-R/2a)]},\qquad(30)$$

when k is real; but the behavior of Eq. (30) is quite different from that of Eq. (28) when k is complex. This example shows that the analytic continuation in the eigenvalue problem has to be carried out with great caution.

A somewhat different situation occurs in the case of the Coulomb potential cut off at a large distance R. As shown by Møller, we have for the s states

$$S(k)=(2kR)^{-2i/ka}\frac{\Gamma(1+i/ak)}{\Gamma(1-i/ak)},\qquad(31)$$

where a is a negative constant for an attractive field. The eigenvalues are determined by the poles where

$$\Gamma(1+i/ak)=\infty,$$

from which we have

$$i/ak=-n\quad(n=1,2,3\cdots).$$

In the vicinity of the point $k=1/ian$,

$$S(k)\sim(-1)^{n+1}(2kR)^{2n}[\Gamma(n+1)]^{-2}k/(k-1/ani).$$

Hence by Eq. (7)

$$|c_n|^2=2\pi|k_n|(2R|k_n|)^{2n}[\Gamma(n+1)]^{-2}. \quad (32)$$

As $R\rightarrow\infty$, $S(k)$ tends to ∞ or 0 according as k is above or below the real axis, and $|c_n|\rightarrow\infty$. The expression

$$|c_n|\exp(-|k_n|R)=(2\pi|k_n|)^{\frac{1}{2}}(2R|k_n|)^n \times\Gamma(n+1)^{-1}\exp(-|k_n|R), \quad (33)$$

however, gives just the asymptotic value of $u_n(r)$ at $r=R$, as can be seen from the well-known expression for the radial wave function of the s states

$$u_n(r)=N_n r\exp(-|k_n|r)L_n{}^1(2|k_n|r),$$

where

$$N_n=[(2|k_n|)^3(n-1)!/2n(n!)^3]^{\frac{1}{2}}$$

and $L_n{}^1$ is an associated Laguerre polynomial.*

I wish to express my sincere gratitude to Professor Pauli for his advice on this work.

* *Note added in proof.*

The eigenvalues given by Eq. (18) are redundant because they are not given by the current scheme of quantum theory. They appear only when we determine the eigenvalues from the expression of $S(k)$ given by Eq. (14) without considering the behavior of the wave function in Eq. (12). Dr. D. ter Haar has recently informed me that according to a recent investigation of R. Jost, it is not sufficient to discard the redundant zeros in all cases on the basis of the inequality (21). It should be noted that the conclusion of the present paper, namely that Heisenberg's general condition given by Eq. (6) is not satisfied by the expression of $S(k)$ given by Eq. (14), is independent of the sign of inequality (21), and therefore holds even when the sign of (21) is changed.

PHYSICAL REVIEW VOLUME 71, NUMBER 3 FEBRUARY 1, 1947

The Invariant Form of Quantum Equations and the Schroedinger-Heisenberg Parallelism

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(Received October 30, 1946)

Some years have passed since the appearance of Dirac's striking interpretation of the Heisenberg-Schroedinger parallelism in the equations of motion, and yet it appears that there still remain obscure points which have led to misunderstanding. Although the Schroedinger method suffices to deal with many practical problems, the flexibility of the Dirac-Jordan representation theory, aside from its intrinsic unity and beauty, recommends it to general theoretical investigation. The present paper considers the invariant form of the equations of motion in relation to the Schroedinger-Heisenberg pictures of quantum mechanics insofar as the latter refer to the "pictured" intrinsic motion of states (vectors) and observables (Hermitian operators). The discussion is divided roughly into 5-sections: Operator and Vector Transforms, Contact Transformations, Heisenberg-Schroedinger Operators, Equations of Motion and Invariant Properties, and the Density Operator and Operator Spur. Where possible, quasi-geometrical diagrams are given to illustrate the relation and transition between the several "pictures of the motion."

Notation:†

$\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\mathbf{q}$, etc. (boldface type) = operators.

$|\rangle$ = state or coordinate vector in Hilbert space.

$\langle| = |\rangle^*$ = adjoint vector.

$|\rangle_\tau$ = transformed vector.

$\langle|\boldsymbol{\alpha}|\rangle=\langle|\cdot\boldsymbol{\alpha}\cdot|\rangle$ = general matrix element.

$|\alpha'\rangle$, α' = prototype eigenvector and eigenvalue belonging to operator $\boldsymbol{\alpha}$.

A. OPERATOR AND VECTOR TRANSFORMS

WHEN two dynamical variables $\boldsymbol{\alpha}_\tau$ and $\boldsymbol{\alpha}$ are related by an equation of the form

$$\boldsymbol{\alpha}_\tau=\mathbf{U}\boldsymbol{\alpha}\mathbf{U}^{-1}, \quad (1)$$

then we say that $\boldsymbol{\alpha}_\tau$ is the transform of $\boldsymbol{\alpha}$ under the similarity or collineatory transformation

† The notation here is that used in the author's forthcoming book on *Perturbation Calculus and Representation Theory*.