

## Simple Theorem on Hermitian Matrices and an Application to the Polarization of Vector Particles

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It is proven that a necessary and sufficient condition for an  $n$ -dimensional Hermitian matrix  $\rho$  to be positive definite is that it be expressible in the form  $\rho = OEO^\dagger$ , where  $O$  is a complex orthogonal matrix and  $E$  is a diagonal matrix with positive elements. This accomplishes a parametrization since  $O$  has  $n^2 - n$  real parameters and  $E$  has  $n$  of them. The proof is constructive, giving  $O$  and  $E$ . It is further shown that the limit forms of this expression yield all the non-negative definite matrices. The parametrization for the polarization matrix of a spin-one particle is given explicitly.

### I. INTRODUCTION

A PROBLEM of general interest and of immediate practical importance in the case of a density matrix is to be able to parametrize a Hermitian matrix in such a way that it is non-negative definite. Apparently it has been solved only for two-dimensional matrices.<sup>1</sup> In Sec. II, we present a theorem which accomplishes the parametrization of any  $n$ -dimensional Hermitian positive definite matrix. We then show in Sec. III that the limit values of the set of positive definite matrices include all the non-negative definite matrices and only these. In Sec. IV, as an application, the polarization matrix of a spin-one particle is expressed in terms of convenient parameters. This is necessary for an efficient study of the decay of vector particles.<sup>2</sup> In an Appendix an alternative parametrization of the positive definite matrices is given.

### II. STATEMENT AND PROOF OF THE THEOREM

A Hermitian matrix  $\rho$  is called positive definite if and only if<sup>3</sup>  $V^\dagger \rho V = \text{real} > 0$  for any vector  $V \neq 0$ . Let  $\rho$ ,  $O$ , and  $E$  be  $n$ -dimensional square matrices, such that  $\rho$  is Hermitian,<sup>4</sup>  $O$  is a proper complex orthogonal matrix,  $O^T = O^{-1}$ ,  $|O| = 1$ , and  $E$  is a diagonal matrix, whose diagonal elements  $E_i$  are real and positive. We shall prove the *Theorem*: A necessary and sufficient condition for  $\rho$  be positive definite is that

$$\rho = OEO^\dagger. \tag{1}$$

This is more restrictive than the usual diagonalization by means of a unitary matrix, since a unitary matrix has  $n^2$  independent real parameters, whereas an orthogonal matrix has  $n^2 - n$ . These, together with the  $n$  diagonal elements of  $E$ , provide the required parametrization.

<sup>1</sup> A special case of spin 1 (3 dimensions) has been treated by W. Larkin, Phys. Rev. **98**, 139 (1955). The result is displayed graphically by J. Raynal, Centre d'Etudes Nucléaires de Saclay, Report CEA No. 2287 (unpublished).

<sup>2</sup> M. Jacob and A. Morel, Phys. Letters **7**, 350 (1963).

<sup>3</sup> We use the notations  $(A^\dagger)_{ij} = (A^*)_{ji}$  and  $(A^T)_{ij} = A_{ji}$ , where  $A$  is any matrix and asterisk means complex conjugate.

<sup>4</sup> It is not actually necessary to assume the  $\rho$  is Hermitian, since a necessary and sufficient condition for the Hermiticity of any matrix  $\rho$  is that  $V^\dagger \rho V = \text{real}$  for any vector  $V$ .

To prove the sufficiency we note that Eq. (1) defines a non-negative form, so the eigenvalues  $\lambda_i$  of  $\rho$ , that is, the roots of  $|\rho - \lambda I| = 0$ , are non-negative,  $\lambda_i \geq 0$ . Furthermore,

$$\prod_{i=1}^n \lambda_i = |\rho| = |OEO^\dagger| = |E| = \prod_{i=1}^n E_i > 0,$$

so  $\lambda_i > 0$  for all  $i$ .

Let us now prove the necessity. We begin by re-writing Eq. (1) in terms of its matrix elements,

$$\rho_{ik}^* = OE, \quad \sum_j \rho_{ij} O_{jk}^* = O_{ik} E_k.$$

For each value of  $k$ , we thus have the equation

$$\sum_j \rho_{ij} V_j^* = V_i E. \tag{2}$$

We will establish necessity by showing the existence of  $n$  positive numbers  $E$  and corresponding vectors  $V$  satisfying Eq. (2), whose array forms an orthogonal matrix. For convenience in the following, we will call vectors  $V$  and numbers  $E$  satisfying Eq. (2) ortho-vectors and ortho-values of the Hermitian matrix  $\rho$ .

Let  $\rho = S + iA$  and  $V = R + iI$ , where  $S$  and  $A$  are, respectively, symmetric and antisymmetric real matrices and  $R$  and  $I$  are real vectors. Then we have

$$(S + iA)(R - iI) = (R + iI)E. \tag{3a}$$

If  $E$  were real, we would have

$$SR + AI = RE, \quad AR - SI = IE,$$

or

$$\begin{pmatrix} S & +A \\ A & -S \end{pmatrix} \begin{pmatrix} R \\ I \end{pmatrix} = \begin{pmatrix} S & -A \\ A & S \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} R \\ I \end{pmatrix} = E \begin{pmatrix} R \\ I \end{pmatrix}, \tag{3b}$$

in an obvious matrix notation.

The problem has been reduced to finding eigenvalues and eigenvectors in the usual sense, for the symmetric matrix  $\begin{pmatrix} S & -A \\ A & S \end{pmatrix}$ , with the indefinite metric  $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ . Every solution of Eq. (3b) is a solution of Eq. (3a), although the converse is not true if  $R$ ,  $I$ , and  $E$  are not real. We define the ortho-values  $E$  of the Hermitian

matrix  $\rho$  to be the solutions of

$$\begin{vmatrix} S-E & A \\ A & -S-E \end{vmatrix} = (-1)^n |S-E| \times |S+E| - |A|^2 = 0. \quad (4)$$

This equation is of order  $2n$  in  $E$ , but only even powers of  $E$  appear in Eq. (4), so that if  $E$  is a root, so is  $-E$ . This occurs because if  $V$  and  $E$  are solutions of Eq. (2), so are  $iV$  and  $-E$ .

Let us show that no null values of  $E$  are possible. For assume  $E=0$  were a solution of Eq. (4). Then Eq. (3b) yields real vectors,  $R$  and  $I$ , so that we would have, for  $V=R+iI$ ,

$$V \cdot \rho \cdot V^* = 0,$$

which violates the positivity hypothesis. (Here and in the following we use the dot symbol to indicate summation over like indices.) Similarly no complex roots of  $E$  are possible. For assume there is a complex root  $E$ , with corresponding (complex) solution  $R$  and  $I$  of Eq. (3b). Then so is  $E^*$ , corresponding to  $R^*$  and  $I^*$ , since  $S$  and  $A$  are real. They satisfy

$$\rho \cdot (R - iI) = E(R + iI), \quad (5)$$

$$\rho \cdot (R^* - iI^*) = E^*(R^* + iI^*). \quad (6)$$

The Hermitian conjugate of the last equation reads

$$(R + iI) \cdot \rho = E(R - iI). \quad (7)$$

We now multiply Eq. (5) by  $(R - iI)^*$  on the left and obtain

$$E(R^* + iI^*) \cdot (R + iI) = \text{real} > 0.$$

We likewise multiply Eq. (7) on the right by  $(R + iI)^*$ , and obtain

$$E(R - iI) \cdot (R^* - iI^*) = \text{real} > 0.$$

Adding the last two inequalities we find

$$2E(R^* \cdot R - I^* \cdot I) = \text{real} > 0,$$

which states that  $E$  is a real number, contrary to the assumption that it is complex.

Consequently, the roots of Eq. (4) are all nonzero and real;  $n$  positive numbers, and their negatives. We consequently obtain  $n$  solutions  $V$  of Eq. (2), corresponding to  $n$  positive ortho-values  $E$ .

Suppose two ortho-vectors  $V_1$  and  $V_2$  correspond to distinct values,  $E_1$  and  $E_2$ ,  $E_1 \neq E_2$ . They satisfy

$$\rho \cdot V_1^* = E_1 V_1, \quad (8)$$

$$\rho \cdot V_2^* = E_2 V_2. \quad (9)$$

We contract Eq. (9) on the left with  $V_1$ , and contract the Hermitian conjugate of Eq. (8) on the right with  $V_2^*$  and subtract, thereby obtaining

$$E_2 V_2 \cdot V_1 - E_1 V_2^* \cdot V_1^* = 0. \quad (10)$$

We now rewrite this last equation, making the substitution  $1 \leftrightarrow 2$  everywhere:

$$E_1 V_2 \cdot V_1 - E_2 V_2^* \cdot V_1^* = 0. \quad (11)$$

We multiply Eq. (10) by  $E_2$  and Eq. (11) by  $E_1$  and subtract, thereby finding

$$(E_2^2 - E_1^2) V_2 \cdot V_1 = 0.$$

So for  $E_1 \neq E_2$ ,

$$V_2 \cdot V_1 = 0, \quad (12)$$

that is, ortho-vectors corresponding to different ortho-values are orthogonal, as expected.

Let us now consider the set of ortho-vectors belonging to the same ortho-value. By inspection of Eq. (2) it is clear that they form a linear vector space over the reals. So there is no phase arbitrariness in the ortho-vectors, which is the principle distinction between them and eigenvectors. From

$$V \cdot \rho \cdot V^* = EV^2, \quad (13)$$

we see that lengths of ortho-vectors are positive numbers. If  $V_1$  and  $V_2$  belong to the same ortho-value  $E$  then

$$V_1 \cdot \rho \cdot V_2^* + V_2 \cdot \rho \cdot V_1^* = 2E(V_1 \cdot V_2), \quad (14)$$

and we see that dot products of ortho-vectors belonging to the same ortho-value are real. Consequently, we may orthogonalize linearly independent ortho-vectors corresponding to the same ortho-value:  $V_2' = V_2 - V_1^{-2} V_1 \cdot V_2 V_1$  is orthogonal to  $V_1$ , and is also an ortho-vector. We may normalize the vectors to unit length using real normalization constants.

The ortho-vectors  $V_i$  thereby obtained now form an orthonormal set; with at least one vector corresponding to each discrete ortho-value. However, in the case of an  $r$ -fold root of Eq. (4), the system of equations (3b) does not by itself guarantee the existence of more than one linearly independent ortho-vector belonging to it, in which case, the orthonormal set may span a linear vector space of dimension  $p \leq n$ . Let us suppose  $p < n$ . We arbitrarily choose a set of  $q$  orthonormal vectors  $V_i$  which complete the orthonormal set,  $p + q = n$ . We now form the orthogonal matrix  $O_1$ , which is the columnar array of column vectors  $O_1 = (V_i U_i)$ . Then  $\rho' = O_1^T \rho O_1^*$  is also a positive definite Hermitian matrix of the form

$$\begin{bmatrix} E_1 & & & 0 \\ & \cdot & & \\ & & E_p & \\ 0 & & & \rho_1 \end{bmatrix}.$$

The  $q$ -dimensional matrix  $\rho_1$  is positive definite, and we may apply our reasoning to it and obtain at least one new ortho-vector  $W$  and corresponding ortho-value  $E$ , of  $\rho'$ ,  $\rho' W^* = EW$ . But since  $\rho' = O_1^T \rho O_1^*$ , we have

$$O_1^T \rho O_1^* W^* = EW$$

or

$$\rho(O_1 W)^* = E(O_1 W),$$

and  $O_1 W$  is an additional ortho-vector of  $\rho$  contrary

to the assumption. Consequently the columnar array of ortho-vectors  $V$  forms an orthonormal matrix  $O$ , satisfying

$$\rho O^* = OE$$

or

$$\rho = OEO^\dagger.$$

By interchanging two of the columns, if necessary, we have  $|O| = 1$ . This completes the proof of the theorem.

### III. REPRESENTATION OF THE SEMIDEFINITE MATRICES

The theorem of the preceding section makes available for the parametrization of positive definite matrices, the several known methods of parametrization of proper orthogonal matrices. Two useful forms are

$$O = \exp A$$

and

$$O = (1 - A)/(1 + A),$$

where  $A$  is an arbitrary antisymmetric matrix. Also, since the  $n$ -dimensional proper orthogonal matrices form a Lie group, one may parametrize them in terms of the generators  $G_i$  of the infinitesimal Lie group:

$$O = \prod_i \exp(\theta_i G_i).$$

We may also uniquely factor  $O$  into an orthogonal real matrix  $O_r$  and a positive definite Hermitian orthogonal matrix  $O_h$ ,

$$O = O_r O_h, \tag{15}$$

where

$$O_h = [O^\dagger O]^{1/2}. \tag{16}$$

Equation (1) as it stands has the disadvantage for parametrization that the elements  $O_{ij}$  of  $O$  are unbounded for fixed values of  $\text{tr} \rho$ , whereas, as we shall see, the elements of  $\rho$  are in fact bounded by  $\text{tr} \rho$ . A slight modification of the formula is convenient. In terms of components, Eq. (1) reads

$$\rho_{ij} = \sum_k E_k O_{ik} O_{jk}^*. \tag{17}$$

We have

$$\text{tr} \rho = \sum_k E_k \sum_i O_{ik} O_{ik}^* = \sum_k E_k (O^\dagger O)_{kk}.$$

This suggests introducing the quantities

$$a_k \equiv (O^\dagger O)_{kk} \tag{18}$$

and

$$\mu_k = E_k a_k. \tag{19}$$

We note that when  $O$  has been factored according to Eq. (15),  $O = O_r O_h$ , then

$$a_k = (O^\dagger O)_{kk} = (O_h^2)_{kk}. \tag{20}$$

We have

$$a_k = \sum_i O_{ik}^* O_{ik} \geq \text{Re} \sum_i O_{ik}^2 = 1$$

or

$$a_k = \text{real} \geq 1, \tag{21}$$

so

$$\mu_k = \text{real} > 0, \tag{22}$$

and

$$\text{tr} \rho = \sum_k \mu_k. \tag{23}$$

The  $\mu_k$  will prove to be more convenient as parameters than the  $E_k$ . Let us also define the positive semidefinite Hermitian matrices  $\rho_k$ ,

$$(\rho_k)_{ij} \equiv a_k^{-1} O_{ik} O_{jk}^*, \tag{24}$$

so that we have

$$\rho = \sum_k \mu_k \rho_k. \tag{25}$$

The significance of this last equation is that each  $\rho_k$  is a projection operator onto a one-dimensional subspace, as we shall now verify. For we have

$$\begin{aligned} (\rho_k^2)_{im} &= a_k^{-2} \sum_j O_{ik} O_{jk}^* O_{jm} O_{mk}^* = a_k^{-1} O_{ik} O_{mk}^* \\ &= (\rho_k)_{im}, \end{aligned} \tag{26}$$

which shows that  $\rho_k$  is a projection operator, and

$$\text{tr} \rho_k = \sum_i a_k^{-1} O_{ik} O_{ik}^* = 1, \tag{27}$$

which shows that it projects onto a one-dimensional subspace. However, it is *not* true in general that  $\rho_k \rho_l = 0$  for  $k \neq l$ .

The  $\mu_k$  are bounded by Eqs. (22) and (23). The  $\rho_k$  satisfy

$$|(\rho_k)_{ij}| \leq \frac{1}{2}(1 + \delta_{ij}), \tag{28}$$

because, on the one hand,  $\text{tr} \rho_k = 1$  and  $(\rho_k)_{ii} = \text{real} \geq 0$ , and, on the other hand, because

$$\begin{aligned} |(\rho_k)_{ij}| &= |O_{ik}| |O_{jk}| \\ &\times [ |O_{ik}|^2 + |O_{jk}|^2 + \sum_{l \neq ij} |O_{lk}|^2 ]^{-1/2} \leq \frac{1}{2}. \quad (i \neq j) \end{aligned}$$

These bounds correspond to the bound on  $\rho_{ij}$  of

$$|\rho_{ij}| \leq \sum_k \mu_k |(\rho_k)_{ij}| = \frac{1}{2} \sum_k \mu_k (1 + \delta_{ij})$$

or

$$|\rho_{ij}| \leq \frac{1}{2}(1 + \delta_{ij}) \text{tr} \rho. \tag{29}$$

A density matrix may be either a positive definite, or a positive semidefinite Hermitian matrix. So far we have obtained only the positive definite matrices. However, it is a simple matter to show that the limit values of the set of positive definite matrices include all the positive semidefinite matrices and only these. For any given positive semidefinite matrices  $\rho_s$  may be obtained as the limit of a sequence of positive definite matrices. This may be achieved for example by writing it in terms of its eigenvalues,  $\lambda_i = \text{real} \geq 0$ , in the form

$\rho_s = U\lambda U^\dagger$ , where  $U$  is unitary and  $\lambda_{ij} = \lambda_i \delta_{ij}$ . The required sequence is obtained by taking a sequence of positive  $\lambda_i$  which converges to the required non-negative values. Conversely, consider any sequence  $\rho_n$  of positive definite matrices and let  $V$  be any nonvanishing vector. We have  $V^\dagger \rho_n V = \text{real} > 0$ . Let the matrix  $\rho$  be a limit of the sequence  $\rho_n$ . Then for any  $V$ , we have  $V^\dagger \rho V = \text{real} \geq 0$ , which is characteristic of the positive semidefinite matrices. The assertion is thereby proven.

Consequently, whenever the variables that parameterize the positive definite matrices range over open intervals, we may close the intervals and thereby parameterize positive semidefinite matrices, provided that the matrices  $\rho$  converge to unique values as the variables approach their end points. This will be useful in the next section.

#### IV. POLARIZATION MATRICES FOR VECTOR PARTICLES

Let us now consider the density matrix in the spin space of a particle, or as it is often called, the polarization matrix, and take the case of spin-one. The density matrix  $\rho$ , and the orthogonal matrix  $O$  are then 3-dimensional. The irreducible 3-dimensional representations of the homogeneous Lorentz group are constituted by the 3-dimensional complex orthogonal matrices, so in this case, the orthogonal matrix  $O$  may be interpreted as a Lorentz transformation and the orthovalues are Lorentz invariants. (We intend to return shortly, in another publication, to the spinorial, or covariant, representations of polarization matrices.)

Let us set  $O = O_r O_h$ , according to Eq. (15). We may then write the most general 3-dimensional orthogonal matrix in the form,

$$O_r = \exp(\epsilon_{ijl} \hat{\theta}_l \theta) = \delta_{ij} + \epsilon_{ijl} \hat{\theta}_l \sin \theta + (\hat{\theta}_i \hat{\theta}_j - \delta_{ij})(1 - \cos \theta), \quad (30)$$

$$O_h = \exp(i \epsilon_{ijl} \hat{v}_l \psi) = \delta_{ij} + i \epsilon_{ijl} \hat{v}_l \sinh \psi + (\hat{v}_i \hat{v}_j - \delta_{ij})(1 - \cosh \psi), \quad (31)$$

where  $\hat{\theta}$  and  $\hat{v}$  are unit vectors,  $0 \leq \theta \leq \pi$ ,  $\tanh \psi = v$  and  $0 \leq v < 1$ . The density matrix is given by Eqs. (24) and (25), with  $a_k$  given by Eq. (20),

$$a_k = (O_h^2)_{kk} = 1 + (\hat{v}_k^2 - 1)(1 - \cosh 2\psi), \quad (32)$$

and  $\mu_k \geq 0$ ,  $\sum \mu_k = 1$ . By an appropriate choice of the coordinate system, we may set  $O_r = 1$ .

Let us introduce the new variables  $p_i = v_i(1 - v^2)^{-1/2}$ , so parameter space is all of  $p$  space. Then

$$(O_h)_{ik} = \delta_{ik} + i \epsilon_{ikl} p_l + (\delta_{ik} p^2 - p_i p_k)(p_0 + 1)^{-1} \quad (33)$$

and

$$a_k = 1 + 2(p^2 - p_k^2), \quad (34)$$

where  $p^2 \equiv p_1^2 + p_2^2 + p_3^2$  and  $p_0 \equiv (1 + p^2)^{1/2}$ . When these

expressions are substituted into Eq. (24), one obtains

$$(\rho_k)_{ij} = \frac{1}{3} \delta_{ij} + i \sum_n \epsilon_{ijn} \left\{ \frac{p_n}{2(p_0 + 1)} \left( 1 - \frac{1}{a_k} \right) + \frac{p_n}{a_k} (1 - \delta_{nk}) \right\} + \left\{ \frac{\delta_{ik} \delta_{jk}}{a_k} + \delta_{ij} \left( \frac{1}{6} - \frac{1}{2a_k} \right) - \frac{p_i p_j}{2(p_0 + 1)^2} \left( 1 - \frac{1}{a_k} \right) - \frac{p_i p_j}{p_0 + 1} \left[ (1 - \delta_{ik}) + (1 - \delta_{jk}) \right] \frac{1}{a_k} \right\}, \quad (35)$$

in which there is no summation over repeated indices, except where indicated. The first term is scalar and represents the normalization, the second is antisymmetric and represents the linear polarization, whereas the last term is traceless and symmetric and represents the tensor or quadrupole polarization. We may write Eq. (35) more explicitly in the form

$$\rho_{ij} = \sum_k \mu_k \left\{ \frac{1}{3} \delta_{ij} + i \sum_n \epsilon_{ijn} \left[ \frac{p_n}{2(p_0 + 1)} \left( 1 - \frac{1}{a_k} \right) + (p_n - \delta_{nk} p_k) \frac{1}{a_k} \right] + \left[ \frac{1}{\delta_{ij}} + \delta_{ij} \left( \frac{1}{6} - \frac{1}{2a_k} \right) - \frac{p_i p_j}{2(p_0 + 1)^2} \left( 1 - \frac{1}{a_k} \right) + \frac{p_i p_j}{(p_0 + 1)} \left( \frac{1}{a_i} + \frac{1}{a_j} - \frac{2}{a_k} \right) \right] \right\}. \quad (36)$$

Suppose now that the spin-one particle is produced in a parity conserving two-body reaction, in which the incident particles are unpolarized. Let the  $z$  axis be perpendicular to the production plane and let the  $x-y$  axes lie in it, so that  $\rho_{xz} = \rho_{yz} = 0$ . Then  $\rho$  may be obtained from its diagonal form by a complex rotation about the  $z$  axis. The real part of the rotation may be eliminated by a suitable choice of the  $x$  axis. The imaginary rotation is given by

$$O_h = \begin{pmatrix} \cosh \psi & i \sinh \psi & 0 \\ -i \sinh \psi & \cosh \psi & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} (1 - v^2)^{-1/2} & i v (1 - v^2)^{-1/2} & 0 \\ -i v (1 - v^2)^{-1/2} & (1 - v^2)^{-1/2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (37)$$

where  $-1 < v < 1$ , and

$$a_k = (O_h^2)_{kk} = (\cosh 2\psi, \cosh 2\psi, 1) = \left( \frac{1 + v^2}{1 - v^2}, \frac{1 + v^2}{1 - v^2}, 1 \right).$$

Then from Eqs. (24) and (25) we find

$$\rho = \begin{pmatrix} (\mu_1 + \mu_2 v^2)(1 + v^2)^{-1} & i(\mu_1 + \mu_2)v(1 + v^2)^{-1} & 0 \\ -i(\mu_1 + \mu_2)v(1 + v^2)^{-1} & (\mu_1 v^2 + \mu_2)(1 + v^2)^{-1} & 0 \\ 0 & 0 & \mu_3 \end{pmatrix}. \quad (38)$$

The range of the parameters is  $\mu_i \geq 0$ , with  $\sum \mu_i = 1$ , and  $-1 \leq v \leq 1$ .

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#### APPENDIX

An alternative parametrization of a positive definite Hermitian matrix  $\rho$  is

$$\rho = \exp H, \quad (17)$$

where  $H$  is any Hermitian matrix. For let  $H$  be diagonalized by a unitary transformation, so that its diagonal

elements  $h_i$  are real numbers. Then  $\rho$ , as defined by Eq. (17) will also be diagonal, with diagonal elements  $\lambda_i = \exp(h_i)$  which are real positive numbers. Conversely, let  $\rho$  be a positive definite Hermitian matrix, diagonalized by the unitary matrix  $U$ , and with real positive eigenvalues  $\lambda_i$ . Let  $H_d$  be a diagonal matrix, with diagonal elements  $h_i = \ln \lambda_i$ , which are real numbers. Then  $H \equiv UH_dU^\dagger$  is Hermitian and  $\rho$  is given by Eq. (17). We observe that there is one and only one logarithm of a positive definite Hermitian matrix, which is Hermitian. This parametrization is perhaps less convenient than the one discussed in the text. In fact any mapping  $f$  of the whole real line allows the parametrization  $\rho = f(H)$ .

## Scattering Resonances and Metastable States in Wave Equations

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In the neighborhood of scattering resonances, the plane-wave solutions are strongly altered and low-order perturbation theory breaks down. Instead of calculating and using the exact scattering solutions there are many advantages to introducing the quasistationary concept of metastable localized eigenfunctions, by means of which the nonperturbative behavior near resonances can be described, whereas nonlocalized features are given by plane-wave functions. It is shown how metastable eigenfunctions can be defined in a natural way without arbitrariness. It is found that a number of general relations have to be satisfied by the metastable functions, which helps to approximate them in the case of a special problem.

### I. INTRODUCTION

IN an unrestricted and uniform, but not necessarily isotropic, space or lattice, all wave equations (classical, quantum-mechanical, continuous, or discrete) have plane-wave eigensolutions. They are basic functions of irreducible representations to the respective space group and can only be normalized to the  $\delta$  function.

If there is a localized region of disturbance, there is always some difficulty in handling both localized and nonlocalized features simultaneously. The wave functions for discrete energy levels are necessarily localized. For continuous (or quasicontinuous) energy sequences, on the other hand, the plane-wave solutions may be used for a low-order perturbation theory. Such a procedure breaks down, however, if there are scattering resonances, i.e., if the wave amplitude in the disturbed region exceeds strongly the amplitude outside. One has the phenomenon of a "quasilocalized" state. Yet, belonging to a continuous set of eigenvalues, it is impossible to normalize an exact eigenfunction to a finite value.

It is therefore advisable to abandon the rigid concept of stationary solutions in favor of a metastable solution

which can be normalized and has, because of its slow decay, almost the features of a stationary state. Provided that it is possible to define (i.e., to localize) in a natural way the metastable function  $\phi(0)$  belonging to some given scattering resonance, and also that we know the dissipation  $\phi(t)$  of this localized state in time, such a concept has two essential advantages:

(a) Let  $\psi(0)$  be an arbitrary wave packet at  $t=0$ ,  $\langle \psi(0) | \phi(0) \rangle$  its projection onto the normalized metastable state. Then one can show that the difference  $\Delta\psi(0) = \psi(0) - \langle \psi(0) | \phi(0) \rangle \phi(0)$  proceeds in time very nearly as if there were no scattering at all,

$$\Delta\psi(t) = \int a(\mathbf{k}) \phi_{\mathbf{k}}^{(0)} e^{-i\omega(\mathbf{k})t} d^3k, \quad (1)$$

$$a(\mathbf{k}) = \langle \Delta\psi(0) | \phi_{\mathbf{k}}^{(0)} \rangle, \quad (1a)$$

where  $\phi_{\mathbf{k}}^{(0)}(\mathbf{r})$  are the eigensolutions of the uniform space. We may, therefore, write the time behavior of the whole packet  $\psi(0)$  as

$$\psi(t) = \langle \psi(0) | \phi(0) \rangle \phi(t) + \int a(\mathbf{k}) \phi_{\mathbf{k}}^{(0)} e^{-i\omega(\mathbf{k})t} d^3k. \quad (2)$$

If there is more than one resonance, we have naturally to consider the projections to the other metastable

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