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CONDITIONS ON DENSITY MATRIX ELEMENTS AND THEIR APPLICATION IN RESONANCE PRODUCTION

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Abstract

We obtain model-independent upper bounds on the off-diagonal elements of the density matrices. They follow simply from a geometrical interpretation of these quantities.

The spin-density matrix of a resonance is determined by measuring the angular distribution of its decay products, but very often not all the matrix elements can be found in this way. For example, the Im ρ_{10} of the vector mesons cannot be measured. It is therefore not possible to bring such a matrix into a diagonal form and check whether it actually has no negative eigenvalues. There are other conditions for a density matrix to be positive semi-definite; for example, in a multipole expansion the multipole parameters have to satisfy certain inequalities[(1)].

Here, we point out some very simple conditions for the density matrix elements (see (7)), which seem to be not well-known. They should be useful to check whether the background is correctly considered. They can also be used as subsidiary conditions to insure that the measured spin-density matrix is positive semi-definite. For the vector mesons we give a simple parametrization of the measurable matrix elements, which incorporates these conditions.

The elements of any n x n density matrix ρ can always be written as scalar products of n (complex) vectors $v_1 , \ldots , v_n$ [(*)]

$$\rho_{ij} = (v_i , v_j) = (v_j , v_i)^* = \rho^*_{ji} \tag{1}$$

(*) The inverse statement is also true. If the elements of a matrix ρ can be written in the form (1), then ρ is positive semi-definite. This is proved by showing that $X^+ \rho X$ = real $\geq$ o for any vector X:

$$X^+\rho X = \sum_{ij} x_i^* \rho_{ij} x_j = \sum_{ij} x_i^* (v_i, v_j)x_j = (\sum_i x_i v_i, \sum_j x_j v_j) = (\omega,\omega) \geq o.$$

This can be seen easily as follows: Consider an ensemble (incoherent mixture) of N normalized pure states $|\psi_s\rangle$ (s = 1, ..., N), each occurring with a statistical weight (probability) $p_s \geqslant 0$. The states need not be orthogonal. The density matrix describing this ensemble[2] is a weighted sum over projection operators onto the different states

$$\rho = \sum_{s=1}^{N} p_s \, |\psi_s\rangle\langle\psi_s|$$

The spectral representation of the Hermitian ρ is a special case of this equation. If we choose n-dimensional orthonormal basis states $|m\rangle$, then the matrix elements of ρ are

$$\rho_{m\,m'} \equiv \langle m|\rho|m'\rangle = \sum_{s=1}^{N} p_s \, \langle m|\psi_s\rangle\langle\psi_s|m\rangle$$

We may then choose our vectors v_m to be

$$v_m = (\sqrt{p_1}\,\langle\psi_1|m\rangle,\ \sqrt{p_2}\,\langle\psi_2|m\rangle,\ \ldots\ldots,\ \sqrt{p_N}\,\langle\psi_N|m\rangle)$$

From the definition (1) we obtain immediately two conditions by using the Schwarz inequality

$$|\rho_{ij}| = |(v_i, v_j)| \leq |v_i|\,|v_j| = (\rho_{ii}\,\rho_{jj})^{1/2} \tag{2}$$

and

$$\begin{aligned} |\rho_{mj} \pm \rho_{nj}| &= |(v_m \pm v_n, v_j)| \leq |v_m \pm v_n|\,|v_j| \\ &= (|v_m|^2 + |v_n|^2 \pm 2\,\mathrm{Re}(v_m, v_n))^{1/2}\,|v_j| \\ &= [(\rho_{mm} + \rho_{nn} \pm 2\,\mathrm{Re}\,\rho_{mn})\,\rho_{jj}]^{1/2} \end{aligned} \tag{3}$$

where $|v_i| = (v_i, v_i)^{1/2}$ denotes the length of the vector v_i.

We now consider spin density matrices of particles produced in a two-body reaction. Parity-invariance for the production mechanism gives the symmetry relations [3,4]

$$\rho_{mm'} = (-1)^{m-m'} \rho_{-m,-m'} \qquad (4)$$

where m and m' are the projection of the spin of the particle onto a certain direction. Since ρ is Hermitian, it follows from (4) that $\rho_{m,-m}$ is real (pure imaginary) for integer (half-integer) spin. If parity is conserved, condition (3) will then read

$$|\rho_{mj} \pm \rho_{-mj}| \leq \begin{cases} [2(\rho_{mm} \pm \rho_{m,-m})\rho_{jj}]^{1/2} & \text{for m integer} \\ [2\rho_{mm}\rho_{jj}]^{1/2} & \text{for m half-integer} \end{cases} \qquad (5)$$

so that an <u>actual</u> violation of (6) will mean parity violation. For j = 0 eq. (4) yields $2\rho_{mo} = \rho_{mo} + (-1)^m \rho_{-mo}$, and we get the following interesting condition

$$\rho_{mo} \leq [1/2(\rho_{mm} + (-1)^m \rho_{m,-m})\rho_{oo}]^{1/2} \qquad (6)$$

which is much stronger than (2). It reduces to (2) only when $\rho_{mm} = (-1)^m \rho_{m,-m}$.

From a number of current experiments in high energy physics we quote in Table 1 some data on spin-density matrix elements to illustrate the practical importance of the above conditions. We shall consider vector mesons and $N^*_{3/2}$-resonances, for which we give the upper bounds explicitely:

<u>Vector Mesons</u>

$$|\rho_{1,-1}| \leq \rho_{11} = (1 - \rho_{oo})/2 \leq 0.5 \qquad (7.1)$$

$$|\rho_{10}| \leq [1/2(\rho_{11} - \rho_{1,-1})\rho_{oo}]^{1/2} \leq 1/\sqrt{8} \simeq 0.353 \qquad (7.2)$$

<u>N*3/2 Resonances</u>

$$|\rho_{\frac{3}{2}\frac{1}{2}}| \text{ or } |\rho_{\frac{3}{2},-\frac{1}{2}}| \leq (\rho_{\frac{3}{2}\frac{3}{2}}\rho_{\frac{1}{2}\frac{1}{2}})^{1/2} = [\rho_{\frac{3}{2}\frac{3}{2}}(0.5-\rho_{3/2\,3/2})]^{1/2} \leq 0.25 \qquad (7.3)$$

$$|\rho_{\frac{3}{2}\frac{1}{2}} - \rho_{\frac{3}{2},-\frac{1}{2}}| \leq (2\,\rho_{\frac{3}{2}\frac{3}{2}}\;\rho_{\frac{1}{2}\frac{1}{2}})^{1/2} \leq 1/\sqrt{8} \simeq 0.353 \qquad (7.4)$$

$$|Re\;\rho_{\frac{3}{2}\frac{1}{2}}| \leq [(0.5 - 2\,|Re\;\rho_{\frac{3}{2},-\frac{1}{2}}|\,\rho_M]^{1/2}, \qquad \rho_M \equiv Min(\rho_{\frac{1}{2}\frac{1}{2}},\rho_{\frac{3}{2}\frac{3}{2}}) \qquad (7.5)$$

$$|Re\;\rho_{\frac{3}{2},-\frac{1}{2}}| \leq [(0.5 - 2\,|Re\;\rho_{\frac{3}{2}\frac{1}{2}}|\,\rho_M]^{1/2} \qquad (7.6)$$

The inequalities (7.5)and (7.6)follows from (3) by noting that $\rho_{-\frac{1}{2}\frac{1}{2}}$ and $\rho_{-\frac{3}{2}\frac{3}{2}}$ are pure imaginary, so that $|Re\;\rho_{\frac{3}{2}\frac{1}{2}}| \leq |\rho_{\frac{3}{2}\frac{1}{2}} \pm \rho_{-\frac{1}{2}\frac{1}{2}}|$ etc.

Data set No.	Reaction	Incident Momentum GeV/c	Scattering angle or momentum transfer	Spin-density matrix	Ref.
1	$\gamma P \to \rho^0 P$	$1.8 < E_\gamma < 2.5$	$0.7 < \cos\theta < 0.9$	$\rho_{00} = 0.41 \pm 0.07$ $\rho_{1,-1} = 0.35 \pm 0.05$ (') Re $\rho_{10} = -0.12 \pm 0.03$	(5)
2	$\gamma P \to \rho^0 P$	$1.8 < E_\gamma < 2.5$	$0.8 < \cos\theta < 0.96$	$\rho_{00} = 0.56 \pm 0.14$ $\rho_{1,-1} = 0.26 \pm 0.06$ (')	(6)
3	$\pi^+ P \to \rho^+ P$	4	$\Delta^2 < 0.3$ GeV^2	$\rho_{00} = 0.70 \pm 0.08$ $\rho_{1,-1} = 0.17 \pm 0.08$(') Re $\rho_{10} = 0.07 \pm 0.07$	(7)
4	$K^- P \to K^{*-} P$	5	$0.9 < \cos\theta < 1$	$\rho_{00} = 0.34 \pm 0.08$ $\rho_{1,-1} = 0.35 \pm 0.06$(') Re $\rho_{10} = 0.01 \pm 0.04$	(8)
5	$K^+ P \to K^0 N^{*++}$	3	$0.02 < \Delta^2 < 0.16$ GeV^2	$\rho_{\frac{3}{2}\frac{3}{2}} = 0.20 \pm 0.08$ ('') Re $\rho_{\frac{3}{2},-\frac{1}{2}} = 0.25 \pm 0.08$ (''') Re $\rho_{\frac{3}{2}\frac{1}{2}} = 0.12 \pm 0.08$	(9)
6	$\pi^+ P \to \pi^0 N^{*++}$	4	$\Delta^2 < 0.3$ GeV^2	$\rho_{\frac{3}{2}\frac{3}{2}} = 0.40 \pm 0.06$ ('') Re $\rho_{\frac{3}{2},-\frac{1}{2}} = 0.21 \pm 0.08$	(7)

Table 1: Some spin-density matrix elements given in the Gottfried-Jackson frame

(') This violates condition (7.1) and hence we cannot calculate the upper bound of ρ_{10} according to (7.2) because the argument of the square root becomes negative.

('') This violates condition (7.3). Note that if Re$\rho_{3/2,-1/2} = 0$, then $|\rho_{3/2\ 3/2}| = |\rho_{1/2\ 1/2}| = 0.25$ and $|\rho_{3/2\ 1/2}| = 0$.

(''') This violates condition (7.5).

We conclude from these data that:

a) In many experiments the off-diagonal elements actually reach their upper bounds given in (7).

b) In the quoted results the nondiagonal elements exceed their upper bounds, although the deviations are generally small compared to the experimental errors. Sometimes these conditions will still be violated by a small amount even if we choose the most favourable values within the experimental errors. For example, consider the data set No. 1. We choose for ρ_{00} and $\rho_{1,-1}$ their smallest possible values in order to make $\rho_{11} - \rho_{1,-1}$ as large as possible. This gives, according to (7.2)

$$|\rho_{10}| \leq \left(1/2 \, (0.33 - 0.30) \, 0.34 \right)^{1/2} \simeq 0.07.$$

The experimental value is Re $\rho_{10} = -\,0.12 \pm 0.03$.

These small deviations are probably due to background. Since the background effects are very difficult to estimate, our conditions should be useful as a check for such estimates. If the measured value of some density-matrix element lies near it upper bound, our conditions should be imposed as subsidiary conditions to insure that the measured spin density-matrix is positive semi-definite.

c) From the angular distribution of the decay products of vector mesons V and $N^*_{3/2}$-resonances one can determine the real parts of ρ_{10}, $\rho_{3/2\;1/2}$ and $\rho_{3/2,-1/2}$ but not their imaginary parts. The data in Table 1 on the vector mesons indicate that $\rho_{1,-1} = \rho_{11} - \Delta_{11}$, where Δ_{11} should be smaller or equal to the experimental errors. Therefore, in such cases

$$|\rho_{10}| \leq \left(1/2 \;\; \Delta_{11} \; \rho_{00}\right)^{1/2} \leq \left(\Delta_{11}/2 \right)^{1/2}$$

For example, if $\rho_{00} \simeq 0.4$ and the experimental errors $\simeq 0.05$, we can predict that $|\mathrm{Im}\; \rho_{10}| \leq |\rho_{10}| \leq 0.1$. Naturally, if ρ_{00} or the experimental errors were smaller, we would get a smaller upper bound on Im ρ_{10}. Similar considerations can be applied for the unmeasurable spin density-matrix elements of $N^*_{3/2}$.

It is easier to impose subsidiary conditions if a suitable parameterization of the relevant quantities can be found, which insures that the conditions are satisfied. For the vector mesons there are three measurable quantities $\rho_{oo}, \rho_{1,-1}$ and Re ρ_{10}, and we parametrize them in terms of three angles α, β and γ.

$$\rho_{oo} = \sin^2 \alpha$$

$$\rho_{1,-1} = \rho_{11} \cos 2\beta \qquad (0 \leq \beta \leq \tfrac{\pi}{2}) \qquad (8)$$

$$\mathrm{Re}\; \rho_{10} = (\rho_{11}\, \rho_{oo})^{1/2} \sin\beta \cos\gamma \qquad (0 \leq \gamma \leq \pi)$$

This parameterization holds when parity is conserved in the production process and hence it satisfies conditions (7.1) and (7.2). For the $N^*_{3/2}$ we were unable to find a similar parameterization for the $\rho_{3/2,3/2}$, Re $\rho_{3/2,-1/2}$ and Re $\rho_{3/2,1/2}$ in terms of three variables only.

We finally remark that the above conditions should also be useful for the theoretician, who wants to describe a measured spin density-matrix. For example , if the data show that $\rho_{1,-1} \simeq \rho_{11}$ holds for a certain s and t, then he knows that the vectors v_1 and v_{-1} have to be parallel at this point. This will give him useful conditions on the scattering amplitudes, since the components of v_m are usually related directly to these scattering amplitudes. For example, if the above relation holds in the Gottfried-Jackson system(4), then the components of v_m can be chosen equal to the helicity amplitudes in the t-channel (except for a normalization factor), so that $\rho_{1,-1} \simeq \rho_{11}$ would imply(*) $\langle 1\, \lambda_{\bar{c}} | F^t | \lambda_{\bar{b}}\, \lambda_a \rangle \simeq \langle -1\, \lambda_{\bar{c}} | F^t | \lambda_{\bar{b}}\, \lambda_a \rangle$ for all helicities λ_i's . If for a certain set of λ_i's this condition cannot be satisfied, then the amplitudes on both sides have to be very small.

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(*) see eq.(10) of Ref. (4)

Appendix A

An n-dimensional positive semi-definite hermitian matrix ρ, depends, in general, on n^2 real variables. However, these variables are not completely free, since they have to satisfy certain conditions to insure that ρ has no negative eigenvalues. It is therefore useful to parametrize them in terms of n^2 parameters so that these conditions are automatically satisfied.

Such a parametrization was given recently by Zwanziger[10]. He proved that a Hermitian matrix ρ is then and only then positive semi-definite if it has the following representation

$$\rho_{nm} = \sum_i O_{ni} E_i O^{\dagger}_{im} \qquad \text{(A.1)}$$

where $E_i \geq o$ ($i=1,\ldots,n$) and O is an orthogonal (complex) matrix (i.e. $O^T = O^{-1}$). Since O can be parametrized in terms of n^2-n variables, the right-hand side of (A.1) provides a possible parametrization of ρ.

Another parametrization follows from expressing the vectors v_i of (1) in terms of complex hyperspherical coordinates(*) with the polar axes e_k ($k=1,\ldots,n$) chosen such that v_i is a linear combination of $e_1,\ldots e_i$ only.

$$v_1 = |v_1| \; e_1 \qquad\qquad 0 \leq \theta_{ij} \leq \pi$$

$$v_2 = |v_2| \; (e_1 \cos\theta_{12} e^{i\phi_{12}} + e_2 \sin\theta_{12}) \qquad 0 \leq \phi_{ij} \leq \pi$$

$$\cdots\cdots \qquad\qquad \cdots\cdots$$

$$\begin{aligned} v_i = |v_i| \; (&e_1 \cos\theta_{1i} e^{i\phi_{1i}} + e_2 \sin\theta_{1i} \cos\theta_{2i} e^{i\phi_{2i}} + \ldots \\ &+ e_{i-1} \sin\theta_{1i} \sin\theta_{21} \ldots \sin\theta_{i-2,i} \cos\theta_{i-1,i} e^{i\phi_{i-1,i}} \\ &+ e_i \sin\theta_{1i} \sin\theta_{2i} \ldots \sin\theta_{i-2,i} \sin\theta_{i-1,i}). \end{aligned} \qquad \text{(A.2)}$$

(*) For real hyperspherical coordinates, see for example Erdélyi[11]

This leads to the "Cholesky decomposition"[(12)] of ρ in terms of a triangular matrix V

$$\rho = V^{\dagger}V \qquad \text{(A.3)}$$

and gives at the same time a parametrization of the matrix elements

$$V_{ij} = (e_i, v_j)$$

in terms of n^2-n angles and n diagonal elements $\rho_{ii} = |v_i|^2$.

A third parametrization may be obtained from the spectral representation

$$\rho_{nm} = \sum_i U_{ni}\ \lambda_i\ U^{\dagger}_{im}, \qquad UU^{\dagger} = 1 \qquad \text{(A.4)}$$

where the $\lambda_i \geq 0$ are the eigenvalues of ρ. The eigenvectors of ρ are determined only up to phase factors $e^{i\phi_i}$, i.e. we obtain the same matrix ρ by using the unitary matrix $U'_{ni} = U_{ni}e^{i\phi_i}$ with ϕ_i arbitrary. Therefore, we can impose n conditions to fix these phases in a certain way, for example by demanding that the diagonal elements U_{ii} be real and non-negative. These additional conditions on U will make it depend on n^2-n variables only instead of n^2. Thus (A.4) will provide a third parametrization of ρ, if we can express U explicitly in terms of n^2-n variables.

We illustrate the above three representations for the simple case of 2 x 2 matrices.

Let

$$\rho = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \qquad \begin{matrix} a,b \text{ real} \geq o \\ |c|^2 \leq ab \end{matrix}$$

Then we have:

I. The spectral representation

$$\rho = U\Lambda U^{\dagger}$$

with

$$\Lambda = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \qquad U = \begin{pmatrix} \cos\alpha & -\sin\alpha e^{i\beta} \\ \sin\alpha e^{-i\beta} & \cos\alpha \end{pmatrix}$$

$$\lambda_{\pm} = \frac{a+b}{2} \pm \sqrt{\left(\frac{a-b}{2}\right)^2 + |c|^2} \geq 0, \qquad \lambda_+\lambda_- = \det\rho$$

$$\cos\alpha = \sqrt{\frac{\lambda_+ - b}{\lambda_+ - \lambda_-}}, \qquad \sin\alpha = \sqrt{\frac{\lambda_+ - a}{\lambda_+ - \lambda_-}}$$

$$e^{i\beta} = c/|c|$$

II. The Zwanziger representation

$$\rho = OEO^{\dagger}$$

with

$$E = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}, \qquad O = O_r O_h \text{ and } O_h^{\dagger} = O_h$$

$$O_r = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}, \qquad O_h = \begin{pmatrix} \cosh\chi & i\sinh\chi \\ -i\sinh\chi & \cosh\chi \end{pmatrix}$$

$$E_{\pm} = \sqrt{\left(\frac{a+b}{2}\right)^2 - (\mathrm{Im}c)^2} \pm \sqrt{\left(\frac{a-b}{2}\right)^2 + (\mathrm{Re}c)^2} \geq 0$$

$$E_+E_- = \det\rho$$

$$\cos 2\phi = \frac{a-b}{E_+ - E_-}, \qquad \cosh 2\chi = \frac{a+b}{E_+ + E_-}$$

$$\mathrm{sign}(\cos\phi) = \mathrm{sign}(\cosh\chi) = +1$$

$$\mathrm{sign}(\sin\phi) = \mathrm{sign}(\mathrm{Re}\, c)$$

$$\mathrm{sign}(\sinh\chi) = \mathrm{sign}\,(\mathrm{Im}\, c)$$

The matrices O_r or O_h will be equal to unity, if Re c or Im c vanish so that the unitary and the orthogonal representations coincide for real ρ.

3. The triangular representation

$$\rho = V^{\dagger}V$$

with

$$V = \begin{pmatrix} \sqrt{a} & \sqrt{b}\,\cos\theta_{12}e^{i\phi_{12}} \\ 0 & \sqrt{b}\,\sin\theta_{12} \end{pmatrix}$$

$$\cos\theta_{12} = |c|/\sqrt{ab}, \qquad e^{i\phi_{12}} = c/|c|.$$

Appendix B

In Appendix A we gave the parametrization of the <u>general</u> n-dimensional density matrix ρ in terms of n^2 variables. But very often there are some symmetry conditions on the elements of ρ, which reduce the number of independent variables. These conditions will generally lead to rather complicated relations between the different angles and it will be difficult to eliminate the unnecessary variables.

An even more difficult problem arises in physical applications, when some of the matrix elements cannot be measured. In such cases it is desirable to express N ($N < n^2$) measurable quantities in terms of only N variables. We have solved this problem for the spin-density matrix of vector mesons, but we did not succeed in finding similar solutions for the more general cases.

From (A.2) and (A.3) we obtain

$$\rho_v^* = \left(\begin{array}{c|c|l} \rho_{11} & \sqrt{\rho_{11}\rho_{00}}\cos\theta_{10} e^{i\phi_{10}} & \sqrt{\rho_{11}\rho_{-1-1}}\cos\theta_{1-1} e^{i\phi_{1-1}} \\ \hline \rho^*_{10} & \rho_{00} & \sqrt{\rho_{00}\rho_{-1-1}}\left(\cos\theta_{10}\cos\theta_{1-1} e^{i(\phi_{1-1}-\phi_{10})} \right. \\ & & \left. + \sin\theta_{10}\sin\theta_{1-1}\cos\theta_{0-1} e^{i\phi_{0-1}}\right) \\ \hline \rho^*_{1-1} & \rho^*_{0-1} & \rho_{-1-1} \end{array}\right)$$

where we have used the notation v_0 and v_{-1} instead of v_2 and v_3. The symmetry relations(4) will lead to

$$\phi_{1,-1} = 0$$

$$\cos\theta_{10}(1 + \cos\theta_{1-1}) = - \sin\theta_{10} \sin\theta_{1-1} \cos\theta_{0-1} e^{-i(\phi_{10} + \phi_{0-1})}$$

so that, unless $\sin\theta_{10}\ \sin\theta_{1-1}\ \cos\theta_{0-1}$ vanishes, we must have $\sin(\phi_{10} + \phi_{0-1}) = 0$, and we may choose $\phi_{10} = \pi - \phi_{o-1}$ to get

$$\mathrm{ctg}\theta_{10}\ \mathrm{ctg}(\theta_{1-1}/2) = +\cos\theta_{0-1}$$

Hence

$$\cos\theta_{10} = \sin(\theta_{1-1}/2)\cos a$$

with

$$\cos^2 a = (1 + \cos^2(\theta_{1-1}/2)\ \mathrm{tg}^2\ \theta_{o-1})^{-1}$$

The angle a can assume all values between o and π for any given $\theta_{1-1} \neq \pi$, if we choose θ_{0-1} appropriately. Therefore, we can introduce a new parameter γ such that $\cos\gamma = \cos a\ \cos\phi_{10}$. This gives the desired parametrization of the measurable matrix elements ρ_{00}, $\mathrm{Re}\rho_{10}$ and ρ_{1-1} in terms of the three parameters ρ_{00}, θ_{1-1} and γ.

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