Congruences and Canonical Forms for a Positive Matrix: Application to the Schweinler-Wigner Extremum Principle

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It is shown that a $N \times N$ real symmetric [complex hermitian] positive definite matrix V is congruent to a diagonal matrix modulo a pseudo-orthogonal [pseudo-unitary] matrix in $SO(m,n)$ [$SU(m,n)$], for any choice of partition $N = m + n$. It is further shown that the method of proof in this context can easily be adapted to obtain a rather simple proof of Williamson's theorem which states that if N is even then V is congruent also to a diagonal matrix modulo a symplectic matrix in $Sp(N, \mathcal{R})$ [$Sp(N, \mathcal{C})$]. Applications of these results considered include a generalization of the Schweinler-Wigner method of 'orthogonalization based on an extremum principle' to construct pseudo-orthogonal and symplectic bases from a given set of linearly independent vectors.

I. INTRODUCTION

It is well known that a N-dimensional real symmetric [complex hermitian] matrix V is congruent to a diagonal matrix modulo an orthogonal [unitary] matrix [1]. That is, $V = S^{\dagger}DS$ where D is diagonal and $S \in SO(N)$ [$S \in SU(N)$]. If, in addition, V is also positive definite, new possibilities arise for establishing its congruence to a diagonal matrix. For N even, it was shown by Williamson [2] some sixty years ago, and subsequently by several authors [3,4], that such a V is also congruent to a diagonal matrix modulo a symplectic matrix in $Sp(N, \mathcal{R})$ [$Sp(N, \mathcal{C})$]. That is, $V > 0$ implies $V = S^{\dagger}D'S$ where D' is diagonal and $S \in Sp(N, \mathcal{R})$ [$S \in Sp(N, \mathcal{C})$]. Williamson's theorem has recently been exploited in defining quadrature squeezing and symplectically covariant formulation of the uncertainty principle for multimode states [5]. In this work we establish yet another kind of congruence of a real symmetric [complex hermitian] positive definite matrix to a diagonal matrix valid, for both odd and even dimensions. We show

that an N-dimensional real symmetric [complex hermitian] positive definite matrix V is congruent to a diagonal matrix modulo a pseudo-orthogonal [pseudo-unitary] matrix. That is, $V > 0$ implies $V = S^{\dagger}D''S$ where D'' is diagonal and $S \in SO(m,n)$ [$S \in SU(m,n)$], for any choice of partition $N = m + n$. A simple proof of this result is given. The strategy adopted in proving this result, with appropriate modification, works for the Williamson case as well, and affords a particularly simple proof of Williamson's theorem. Needless to add that the diagonal entries of neither D' nor D'' correspond to the eigenvalues of V.

The theorems established here play a crucial role in enabling one to construct pseudo-orthogonal and symplectic bases from a given set of linearly independent vectors via an extremum principle in the spirit of the work of Schweinler and Wigner [6]. In an important contribution to the age old "orthogonalization problem" – the problem of constructing an orthonormal set of vectors from a given set of linearly independent vectors – Schweinler and Wigner proposed an orthonormal basis which, unlike the familiar Gram-Schmidt basis (which depends on the particular initial order in which the given linearly independent vectors are listed), treats all the linearly independent vectors on an equal footing and has since found important application in wavelet analysis [7]. More significantly, they showed that this special basis follows from *an extremum principle*. In this work, we exploit our results on congruence to obtain generalizations of the Schweinler-Wigner exremum principle leading to pseudo-orthogonal and symplectic bases from a given set of linearly independent vectors. Conversely, the extremum principle, once formulated, can be interpreted as a procedure for finding the appropriate congruence transformation to effect the desired diagonalization.

II. CONGRUENCE OF A POSITIVE MATRIX UNDER PSEUDO-ORTHOGONAL [PSEUDO-UNITARY] TRANSFORMATIONS

The fact that a real symmetric [complex hermitian] matrix is congruent to a diagonal matrix modulo an orthogonal [unitary] matrix is well known. While congruence coincides with conjugation in the real orthogonal and complex unitary cases, they become distinct when more general sets of transformations are involved. A question which naturally arises is whether congruence to

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a diagonal form can also be achieved through a pseudo orthogonal [pseudo-unitary] transformation. The answer to this question turns out to be in the affirmative with the caveat that the matrix in question be positive definite, and can be formulated as the following theorem:

Theorem 1: Let V be a real symmetric positive definite matrix of dimension N. Then, for any choice of partition $N = m + n$, there exists an $S \in SO(m,n)$ such that

$$S^T V S = D^2 = \text{diagonal (and } > 0). \qquad (1)$$

Proof: We begin by recalling that the group $SO(m,n)$ consists of all real matrices which satisfy $S^T g S = g$, $\det S = 1$, where $g = \text{diag}(\underbrace{1, 1, \cdots, 1}_{m}, \underbrace{-1, \cdots, -1}_{n})$.
Consider the matrix $V^{-1/2} g V^{-1/2}$ constructed from the given matrix V. Since $V^{-1/2} g V^{-1/2}$ is real symmetric, there exists a rotation matrix $R \in SO(N)$ which diagonalizes $V^{-1/2} g V^{-1/2}$:

$$R^T V^{-1/2} g V^{-1/2} R = \text{diagonal} \equiv \Lambda. \qquad (2)$$

This may be viewed also as a congruence of g using $V^{-1/2} R$, and signatures are preserved under congruence. (Indeed, signatures are the only invariants if we allow congruence over the full linear group $GL(N,\mathcal{R})$). As a consequence, the diagonal matrix Λ can be expressed as the product of a positive diagonal matrix and g:

$$R^T V^{-1/2} g V^{-1/2} R = D^{-2} g = D^{-1} g D^{-1}. \qquad (3)$$

Here D is diagonal and positive definite.

Taking the inverse of the matrices on both sides of (3) we find that the diagonal entries of $g D^2 = D^2 g$ are the eigenvalues of $V^{1/2} g V^{1/2}$ and that the columns of R are the eigenvectors of $V^{1/2} g V^{1/2}$. Since $V^{1/2} g V^{1/2}$, gV, and Vg are conjugate to one another, we conclude that D^2 is determined by the eigenvalues of $gV \sim Vg$.

Define $S = V^{-1/2} RD$. It may be verified that S satisfies the following two equations:

$$\begin{aligned} S^T g S &= g, \\ S^T V S &= D^2 = \text{diagonal}. \end{aligned} \qquad (4)$$

The first equation says that $S \in SO(m,n)$ and the second says that V is diagonalized through congruence by S. Hence the proof.

group $SO(m,n)$ by $SU(m,n)$, and $R \in SO(N)$ by $U \in SU(N)$ in the statement and proof of the above theorem, we have the following theorem which applies to the complex case.

Theorem 2: Let V be a hermitian positive definite matrix of dimension N. Then, for any partition $N = m+n$, there exists an $S \in SU(m,n)$ such that

$$S^\dagger V S = D^2 = \text{ diagonal (and } > 0). \qquad (5)$$

III. A SIMPLE PROOF OF WILLIAMSON'S THEOREM

It turns out that the above procedure when applied to the real symplectic group of linear canonical transformations leads a particularly simple proof of Williamsons's theorem.

Theorem 3: Let V be a $2n$-dimensional real symmetric positive definite matrix. Then there exists an $S \in Sp(2n, \mathcal{R})$ such that

$$\begin{aligned} S^T V S &= D^2 > 0, \\ D^2 &= \text{diag}(\kappa_1, \kappa_2, \cdots, \kappa_n, \kappa_1, \kappa_2, \cdots, \kappa_n). \end{aligned} \qquad (6)$$

Proof: Note that the $2n$-dimensional diagonal matrix D has only n independent entries. The group $Sp(2n, \mathcal{R})$ consits of all real matrices S which obey the condition

$$S^T \beta S = \beta, \quad \beta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad (7)$$

with 1 and 0 denoting the $n \times n$ unit and zero matrices respectively. Even though $S^T \beta S = \beta$ may appear to suggest that $\det S = \pm 1$, it turns out that $\det S = 1$. In other words, $Sp(2n, \mathcal{R})$ consists of just one connected (though not simply connected) piece. Indeed, for every $n \geq 1$ the connectivity property of $Sp(2n, \mathcal{R})$ is the same as that of the circle.

The most general $S \in GL(2n, \mathcal{R})$ which solves $S^T V S = D^2$ is $S = V^{-1/2} RD$, where $R \in O(2n)$. Note that none of the factors D, R or $V^{-1/2}$ is an element of $Sp(2n, \mathcal{R})$. However, a V-dependent choice of D, R can be so made that the product $V^{-1/2} RD$ is an element of $Sp(2n, \mathcal{R})$ as we shall now show.

Since $\beta^T = -\beta$, it follows that $\mathcal{M} = V^{-1/2} \beta V^{-1/2}$ is antisymmetric. Hence there exists an $R \in SO(2n)$ such that [8]

$$R^T V^{-1/2} \beta V^{-1/2} R = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}, \quad \Omega = \text{diagonal} > 0. \qquad (8)$$

Define a diagonal positive definite matrix

$$D = \begin{pmatrix} \Omega^{-1/2} & 0 \\ 0 & \Omega^{-1/2} \end{pmatrix}. \qquad (9)$$

Then we have

$$D R^T V^{-1/2} \beta V^{-1/2} RD = \beta. \qquad (10)$$

Now define $S = V^{-1/2} RD$. It may be verified that S enjoys the following properties:

$$\begin{aligned} S^T \beta S &= \beta, \\ S^T V S &= D^2 = \text{diagonal}. \end{aligned} \qquad (11)$$

The first equation says that $S \in Sp(2n, , \mathcal{R})$ and the second one says that V is diagonalized by congruence

through S. This completes the proof of the Williamson theorem. To appreciate the simplicity of the present the reader may like to compare it with two recently published proofs of the Williamson theorem [4].

We wish to explore the structure underlying the above proof a little further so that the relationship between D and S in (11) on the one hand and the eigenvalues and eigenvectors of βV^{-1} (or $V^{-1/2}\beta V^{-1/2}$) on the other becomes transparent. Again consider the matrix $\mathcal{M} = V^{-1/2}\beta V^{-1/2}$. It is a real, non-singular, anti-symmetric matrix and hence its eigenvalues $i\omega_\alpha$ and eigenvectors η_α have the following properties:

$$\begin{aligned} \mathcal{M}\eta_\alpha &= i\,\omega_\alpha\eta_\alpha\,, \quad \alpha = 1,\cdots,2n; \\ \omega_k &> 0\,, \quad k = 1,\cdots,n\,; \quad \omega_{n+k} = -\omega_k\,; \\ \eta_{n+k} &= \eta_k^*\,; \quad k = 1,\cdots,n\,. \end{aligned} \quad (12)$$

The eigenvectors η_α can be chosen to be orthonormal even when the eigenvalues $i\omega_\alpha$ are degenerate. Arrange the eigenvectors η_α as columns of a matrix U. The matrix U thus obtained clearly belongs to the unitary group $U(2n)$, and satisfies

$$U^\dagger \mathcal{M} U = \Lambda, \quad \Lambda = \begin{pmatrix} i\Omega & 0 \\ 0 & -i\Omega \end{pmatrix}, \quad (13)$$

where $\Omega = \mathrm{diag}(\omega_1,\cdots,\omega_n) > 0$. Now define the following $2n \times 2n$ unitary matrices

$$\Sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \Delta = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}. \quad (14)$$

These two matrices have the properties $\Sigma^2 = 1$, $U\Sigma = U^*$, and $\Sigma\Delta = \Delta^*$ (* denotes complex cojugate of a matrix). As a useful consequence of these properties we have

$$U^*\Delta^* = U^*\Sigma\Sigma\Delta^* = U\Delta. \quad (15)$$

We find that the unitary matrix $U\Delta$ is real: $U\Delta \in O(2n)$.

Now consider $S = V^{-1/2}U\Delta D$, where D is a diagonal matrix to be determined. It follows from the definition of S and the reality of $U\Delta \in O(2n)$ that

$$S^T V S = S^\dagger V S = D^2\,. \quad (16)$$

Further, recalling that $U^\dagger \mathcal{M} U = \Lambda$ we obtain

$$\begin{aligned} S^T \beta S = S^\dagger \beta S &= D\Delta^\dagger U^\dagger \mathcal{M} U\Delta D \\ &= D\Delta^\dagger \Lambda\Delta D = D\begin{pmatrix} O & \Omega \\ -\Omega & O \end{pmatrix}D\,. \quad (17) \end{aligned}$$

It is now evident that the following choice for D ensures that S is an element of $S \in Sp(2n,\mathcal{R})$:

$$D = \begin{pmatrix} \Omega^{-1/2} & O \\ O & \Omega^{-1/2} \end{pmatrix}. \quad (18)$$

This completes our analysis of the manner in which S and D are related to the eigenvalues and eigenvectors of the matrix βV^{-1}.

As in the pseudo-orthogonal case, by replacing the superscript ^{T} by † in the statement and proof of Theorem 3, one obtains the following result.

Theorem 4: Let V be a $2n$-dimensional hermitian positive definite matrix. Then there exists an $S \in Sp(2n,\mathcal{C})$ such that

$$\begin{aligned} S^\dagger V S &= D^2 > 0\,, \\ D^2 &= \mathrm{diag}(\kappa_1,\kappa_2,\cdots,\kappa_n,\kappa_1,\kappa_2,\cdots,\kappa_n). \quad (19) \end{aligned}$$

An immediate consequence of the theorems stated above is that for a real symmetric [complex hermitian] positive definite matrix we can not talk about *the* canonical form under congruence, for there are $m + n$ possible choices of $SO(m,n)$ $[SU(m,n)]$, and in the case of even dimension one more choice coming from Williamson's theorem. Needless to add that for the same matrix V, the diagonal matrix D will be different for different choices.

IV. ORTHOGONALZATION PROCEDURES

Assume that we are given a set of linearly independent N-dimensional vectors $v_1,\cdots,v_N$. Let G denote the associated Gram matrix of pairwise inner products: $G_{ij} = (v_i, v_j)$. The Gram matrix is hermitian by construction, and positive definite by virtue of the linear independence of the given vectors. The orthogonalization problem, i.e., constructing a set of orthonormal vectors out of the given set of linearly independent vectors, amounts to finding a matrix S that solves

$$S^\dagger G S = 1, \quad \textbf{\textit{i.e.}}, \quad G^{-1} = SS^\dagger. \quad (20)$$

Each such S defines an orthogonalization procedure.

Let us arrange the set of N vectors as the entries of a row $\mathbf{v} = (v_1, v_2, \cdots, v_N)$, and let $\mathbf{z} = (z_1, z_2, \cdots, z_N)$ represent a generic orthonormal basis. The orthonormal set of vectors $\mathbf{z}$ corresponding to a chosen S are related to the given set of linearly independent vectors through $\mathbf{z} = \mathbf{v}S$. Clearly, there are infinitely many choices for S satisfying (20): given an S satisfying (20), any $S' = SU$ where U is an arbitrary unitary matrix also satifies (20). Thus the freedom available for the solution of the orthonormalization problem is exactly as large as the unitary group $U(N)$, and this was to be expected.

Schweinler and Wigner [6] posed and answered the following question: is there a way of descriminating between various choices of S that solves (20) and hence between various orthogonalization procedures? They argued that a particular choice of orthogonalization procedure should correspond ultimately to the extremization of a suitable scalar function over the manifold of all orthonormal bases, with the given linearly independent vectors appearing as parameters in the function. Different choices of onthonormal bases will then correspond to different functions to be extremized. They preferred the function to be symmetric under permutation of the

given vectors. As an example they considered the following function which is quartic in the given vectors:

$$gm(\mathbf{z}) = \sum_k \left(\sum_l |(z_k, v_l)|^2 \right)^2 . \qquad (21)$$

They showed that the extremum (maximum in this case) value of $m(\mathbf{z})$ is given by $\mathrm{tr}(G^2)$, and this value corresponds to the orthonormal basis $\mathbf{z} = \mathbf{v} U_0 P^{-1/2}$, where U_0 is the unitary matrix which diagonalizes G: $U_0^\dagger G U_0 = P$. We may refer to this as the Schweinler-Wigner basis, and the function $m(\mathbf{z})$ as the Schweinler-Wigner quartic form. It is clear that U_0 and hence the Schweinler-Wigner basis is essentially unique if the eigenvalues of the Gram matrix G are all distinct. We may note in passing that, unlike the Gram-Schmidt orthogonalization procedure, the Schweinler-Wigner procedure is democratic in that it treats all the linearly independent vectors $\mathbf{v}$ on an equal footing.

The content of the work of Schweinler and Wigner has recently been reformulated [9] in a manner that offers a clearer and more general picture of the Schweinler-Wigner quartic form $m(\mathbf{z})$ and of the orthonormal basis which maximizes it. This perspective on the orthogonalization problem plays an important role in our generalizations of the Schweinler-Wigner extremum principle, and hence we summarise it briefly.

Since every orthonormal basis is the eigenbasis of a suitable hermitian operator, it is of interest to characterize the Schweinler-Wigner basis in terms of such an operator. Given linearly independent N-dimensional vectors $\mathbf{v} = (v_1, v_2, \cdots, v_N)$, the operator $\hat{M} = \sum_j v_j v_j^\dagger$ is hermitian positive definite. In a *generic orthonormal* basis $\mathbf{z}$, it is represented by a hermitian positive definite matrix $M(\mathbf{z})$: $M(\mathbf{z})_{ij} = (z_i, \hat{M} z_j)$. Under a change of orthonarmal basis $\mathbf{z} \to \mathbf{z}' = \mathbf{z}S$, $M(\mathbf{z})$ transforms as follows

$$M(\mathbf{z}) \to M(\mathbf{z}') = S^\dagger M(\mathbf{z})S , \quad S \in U(N) . \qquad (22)$$

Recall that $U(N)$ acts transitively on the set of all orthonormal bases and that $\mathrm{tr}(M(\mathbf{z})^2) = \sum_{j,k} |M(\mathbf{z})_{jk}|^2$ is invariant under such a change of basis, and hence is en-dependent of $\mathbf{z}$. The Schweinler-Wigner quartic form $m(\mathbf{z})$ can easily be identified as $\sum_k (M(\mathbf{z})_{kk})^2$. In view of the above invariance, maximization of $\sum_k (M(\mathbf{z})_{kk})^2$ is the same as minimization of $\sum_{j \neq k} |M(\mathbf{z})_{jk}|^2$. The absolute minimum of $\sum_{j \neq k} |M(\mathbf{z})_{jk}|^2$ equals zero, and obtains when $M(\mathbf{z})$ is diagonal. Thus, the orthonormal basis which maximizes $\sum_k (M(\mathbf{z})_{kk})^2$ is the same as the one in which

$\hat{M}$ is diagonal, and we arrive at the following important conclusion of Ref.[9]:

Theorem 5: The distinquished orthonormal basis which extremizes the Schweinler-Wigner quartic form $m(\mathbf{z})$ over the manifold of all orthonormal bases is the same as the orthonormal basis in which the positive definite matrix $M(\mathbf{z})$ becomes diagonal.

Important for the above structure is the fact that the invariant $\mathrm{tr}(M(\mathbf{z})^2)$ is the sum of non-negative quantities, and therefore a part of it is necessarily bounded. It is precisely this property, which can be traced to the underlying unitary symmetry, that is not available when we try to generalize the Schweinler-Wigner procedure to construct pseudo-orthonormal and symplectic bases wherein the underlying symmetries are the noncompact groups $SO(m,n)$ and $Sp(2n, \mathcal{R})$ respectively..

V. LORENTZ BASIS WITH AN EXTREMUM PROPERTY

In this Section we show how the Schweinler-Wigner procedure can be generalized to construct pseudo-orthonormal basis based on an extremum principle. We begin with the case of real vectors.

We are given a set of linearly independent real N-dimensional vectors $\mathbf{v} = (v_1, \cdots, v_N)$ and we want to construct out of it a pseudo-orthonormal basis $[SO(m,n)$ Lorentz basis with $N = m + n]$, i.e., a set of vectors $\mathbf{z} = (z_1, \cdots, z_N)$ satisfying

$$(z_k, g z_l) = g_{kl} , \quad g = \mathrm{diag}(\underbrace{1, 1, \cdots, 1}_{m}, \underbrace{-1, \cdots, -1}_{n}). \qquad (23)$$

Let $\hat{M} = \sum_j v_j v_j^T$ as before, and let the symmetric positive definite matrix $M(\mathbf{z})$: $M(\mathbf{z})_{ij} = (z_i, \hat{M} z_j)$ represent $\hat{M}$ in a *generic pseudo-orthonormal* basis $\mathbf{z}$. Under a pseudo-orthogonal change of basis $\mathbf{z} \to \mathbf{z}' = \mathbf{z}S$, the matrix $M(\mathbf{z})$ transforms as follows:

$$M(\mathbf{z}) \to M(\mathbf{z}') = S^T M(\mathbf{z})S , \quad S \in SO(m,n) . \qquad (24)$$

Since $S^T g S = g$ (or $g S^T = S^{-1} g$) by definition, we have

$$S : \quad g M(\mathbf{z}) \to g M(\mathbf{z}') = S^{-1} g M(\mathbf{z})S . \qquad (25)$$

That is, as $M(\mathbf{z})$ undergoes congruence, $g M(\mathbf{z})$ undergoes conjugation. Thus, $\mathrm{tr}(g M(\mathbf{z}))^l$, $l = 1, 2, \cdots$, are invariant. In what follows we shall often leave implicit the dependence of M on the generic pseudo-orthonormal basis $\mathbf{z}$.

Consider the invariant $\mathrm{tr}(g M(\mathbf{z}) g M(\mathbf{z}))$ corresponding to $l = 2$. Write $M = M^{\mathrm{even}} + M^{\mathrm{odd}}$ where

$$M^{\mathrm{even}} = \frac{1}{2}(M + g M g) , \quad M^{\mathrm{odd}} = \frac{1}{2}(M - g M g) . \qquad (26)$$

In the above decomposition we have exploited the fact that g is, like parity, an *involution*.

With M expressed in the (m, n) block form

$$M = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}, \ A^T = A, \ B^T = B, \qquad (27)$$

we have

$$M^{\text{even}} = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}, \ M^{\text{odd}} = \begin{pmatrix} 0 & C \\ C^T & 0 \end{pmatrix}. \qquad (28)$$

Symmetry of M implies that M^{odd} and M^{even} are symmetric. Further, M^{odd} and M^{even} are trace orthogonal: $\text{tr}(M^{\text{odd}} M^{\text{even}}) = 0$. Thus,

$$\text{tr}(gMgM) = \text{tr}(M^{\text{even}})^2 - \text{tr}(M^{\text{odd}})^2, \qquad (29)$$

which can also be written as

$$\text{tr}(MgMg) = \text{tr}(M^2) - 2\text{tr}(M^{\text{odd}})^2. \qquad (30)$$

A few observations are in order:

- In contradistinction to the original unitary case, the invariant in the present case is no more a sum of squares. This can be traced to the non-compactness of the underlying $SO(m, n)$ symmetry. As one consequence, $\sum_k (M_{kk})^2$ is not bounded. As an example, consider the simplest case $m = 1, \ n = 1$ and let

$$M = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \ a, b > 0. \qquad (31)$$

Under congruence by the $SO(1, 1)$ element

$$S = \begin{pmatrix} \cosh \mu & \sinh \mu \\ \sinh \mu & \cosh \mu \end{pmatrix}, \qquad (32)$$

the value of $\sum_k (M_{kk})^2$ changes from $a^2 + b^2$ to $a^2 + b^2 + 2ab \sinh^2 \mu \cosh^2 \mu$, which grows with μ without bounds, showing that $\sum_k (M_{kk})^2$ and hence $\text{tr}(M^2)$ is not bounded. Thus, in contrast to the unitary case, extremization of the Schweinler-Wigner quartic form $\sum_k (M_{kk})^2$ will make no sense in the absence of further restrictions.

- The structure of the invariant $\text{tr}(gMgM)$ in (30) suggests the further restriction needed to be imposed: within the submanifold of pseudo-orthogonal bases $\mathbf{z}$ which keep $\text{tr}(M(\mathbf{z})^{\text{odd}})^2$ (and hence $\text{tr}(M(\mathbf{z})^2)$) at a fixed value we can maximize $\sum_k M(\mathbf{z})_{kk}^2$. In particular we can do this within the submanifold which minimizes $\text{tr}(M(\mathbf{z})^{\text{odd}})^2$, and hence $\text{tr}(M(\mathbf{z})^2)$. Clearly, zero is the absolute minimum of the nonnegative object $\text{tr}(M(\mathbf{z})^{\text{odd}})^2$. But

by theorem 1 there exists a Lorentz basis $\mathbf{z}$ in which $M(\mathbf{z})$ is diagonal and hence $M(\mathbf{z})^{\text{odd}} = 0$. Thus the minimum $\text{tr}(M(\mathbf{z})^{\text{odd}})^2 = 0$, and hence the minimum of $\text{tr}(M(\mathbf{z})^2)$, namely $\text{tr}(gM(\mathbf{z})gM(\mathbf{z}))$, is attainable.

The above observations suggest the following *two step analogue of the Schweinler-Wigner extremum principle for Lorentz bases*. Choose the submanifold of Lorentz bases which minimize the quartic form $\text{tr}(M(\mathbf{z})^{\text{odd}})^2$, and maximize the Schweinler-Wigner quartic form $m(\mathbf{z}) = \sum_k (M(\mathbf{z})_{kk})^2$ within this submanifold. Clearly, the first step takes M to a block-diagonal form, and the second one diagonalizes it. Thus we have established the following generalization of Theorem 5 to the pseudo-orthonormal case:

Theorem 6: The distinguished pseudo-orthonormal basis which extremizes the "Schweinler-Wigner" quartic form $m(\mathbf{z})$ over the submanifold of pseudo-orthonormal bases which minimize the quartic form $\text{tr}(M(\mathbf{z})^2)$ is the same as the pseudo-orthonormal basis in which the positive definite matrix $M(\mathbf{z})$ becomes diagonal.

The submanifold under reference consists of Lorentz bases which are related to one another through the maximal compact (connected) subgroup of $SO(m, n)$, namely $SO(m) \times SO(n)$. This subgroup consists of matrices of the block-diagonal form

$$\begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix}, \quad R_1 \in SO(m), \ R_2 \in SO(n), \qquad (33)$$

and this is precisely the subgroup of $SO(m, n)$ transformations that do not mix the even and odd parts of $M(\mathbf{z})$.

To conclude this Section we may note that the above construction carries over to the complex case, with obvious changes like replacing ^{T} by † and $SO(m, n)$ by $SU(m, n)$.

VI. SYMPLETIC BASIS WITH AN EXTREMUM PROPERTY

Our construction in the pseudo-orthogonal case suggests a scheme by which the Schweinler-Wigner extremum principle principle can be generalized to construct a symplectic basis. Suppose that we are given a set of linearly independent vectors $\mathbf{v} = (v_1, v_2, \cdots, v_{2n})$ in $\mathcal{R}^{2n}$. The natural symplectic structure in R^{2n} is specified by the standard symplectic "metric" β defined in (7). Let $\mathbf{z} = (z_1, z_2, \cdots, z_{2n})$ denote a generic symplectic basis. That is, $(z_j, \beta z_k) = \beta_{jk}, \ j, k = 1, 2, \cdots, 2n$. The real symlectic group $Sp(2n, R)$ acts transitively on the set of all symplectic bases.

To generalize the Schweinler-Wigner principle to the symplectic case, we begin be defining $\hat{M} = \sum_{j=1}^{2n} v_j v_j^T$. Let

$M(\mathbf{z})$: $M(\mathbf{z})_{ij} = (z_i, \hat{M}z_j)$ be the symmetric positive definite matrix representing the operator $\hat{M}$ in a *generic symplectic* basis $\mathbf{z}$. Under a symplectic change of basis $\mathbf{z} \to \mathbf{z}' = \mathbf{z}S$, $S \in Sp(2n, \mathcal{R})$, the matrix $M(\mathbf{z})$ undergoes the following transformation:

$$M(\mathbf{z}) \to M(\mathbf{z}') = S^T M(\mathbf{z}) S, \quad S \in Sp(2n, R). \quad (34)$$

Since $S^T \beta S = \beta$ implies $\beta S^T = S^{-1}\beta$, we have

$$S : \quad \beta M(\mathbf{z}) \to \beta M(\mathbf{z}') = S^{-1}\beta M(\mathbf{z}) S. \quad (35)$$

That is, under a symplectic change of basis $M(\mathbf{z})$ undergoes congruence, but $\beta M(\mathbf{z})$ undergoes conjugation. Hence $\mathrm{tr}(\beta M(\mathbf{z}))^{2l}$, $l = 1, 2, \cdots, n$ are invariant (Note that $\mathrm{tr}(\beta M(\mathbf{z}))^{2l+1} = 0$ in view of $\beta^T = -\beta$, $M(\mathbf{z})^T = M(\mathbf{z})$).

Since $i\beta$ is an *involution* we can use it to separate $M(\mathbf{z})$ into even and odd parts :

$$M(\mathbf{z}) = M(\mathbf{z})^{\mathrm{even}} + M(\mathbf{z})^{\mathrm{odd}},$$
$$M(\mathbf{z})^{\mathrm{even}} = \frac{1}{2}(M(\mathbf{z}) + \beta M(\mathbf{z})\beta^T),$$
$$M(\mathbf{z})^{\mathrm{odd}} = \frac{1}{2}(M(\mathbf{z}) - \beta M(\mathbf{z})\beta^T). \quad (36)$$

The even and odd parts of $M(\mathbf{z})$ satisfy the symmetry properties

$$\beta M(\mathbf{z})^{\mathrm{even}}\beta^T = M(\mathbf{z})^{\mathrm{even}}, \quad \beta M(\mathbf{z})^{\mathrm{odd}}\beta^T = -M(\mathbf{z})^{\mathrm{odd}}. \quad (37)$$

Further, $M(\mathbf{z})^{\mathrm{odd}}$ and $M(\mathbf{z})^{\mathrm{even}}$ are trace orthogonal: $\mathrm{tr}\left(M(\mathbf{z})^{\mathrm{odd}} M(\mathbf{z})^{\mathrm{even}}\right) = 0$.

The structure of the even and odd parts of $M(\mathbf{z})$ may be appreciated by writing $M(\mathbf{z})$ in the block form

$$M(\mathbf{z}) = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}, \ A^T = A, \ B^T = B. \quad (38)$$

We have

$$M(\mathbf{z})^{\mathrm{even}} = \begin{pmatrix} \frac{1}{2}(A+B) & \frac{1}{2}(C - C^T) \\ -\frac{1}{2}(C - C^T) & \frac{1}{2}(A+B) \end{pmatrix},$$
$$M(\mathbf{z})^{\mathrm{odd}} = \begin{pmatrix} \frac{1}{2}(A-B) & \frac{1}{2}(C + C^T) \\ \frac{1}{2}(C + C^T) & \frac{1}{2}(B-A) \end{pmatrix}. \quad (39)$$

Now consider the invariant $-\mathrm{tr}(\beta M(\mathbf{z})\beta M(\mathbf{z})) = \mathrm{tr}(\beta^T M(\mathbf{z})\beta M(\mathbf{z}))$. We have

$$\mathrm{tr}(\beta^T M(\mathbf{z})\beta M(\mathbf{z})) = \mathrm{tr}(M(\mathbf{z})^{\mathrm{even}})^2 - \mathrm{tr}(M(\mathbf{z})^{\mathrm{odd}})^2, \quad (40)$$

which can also be written as

$$\mathrm{tr}(\beta^T M(\mathbf{z})\beta M(\mathbf{z})) = \mathrm{tr}(M(\mathbf{z})^2) - 2\mathrm{tr}(M(\mathbf{z})^{odd})^2. \quad (41)$$

The structural similarity of this invariant to that in the pseudo-orthogonal case should be appreciated.

Now, by an argument similar to the pseudo-orthogonal case one finds that, owing to the noncompactness of $Sp(2n, \mathcal{R})$, the function $\mathrm{tr}(M(\mathbf{z})^2)$ and hence the Schweinler-Wigner quartic form $\sum_{k=1}^{2n}(M(\mathbf{z})_{kk})^2$ is unbounded if $\mathbf{z}$ is allowed to run over the entire manifold of all symplectic bases. For instance, in the lowest dimensional case $n = 1$ with M chosen to be

$$M = \begin{pmatrix} a & u \\ d & b \end{pmatrix}, \ a, b > 0, \ ab - ud > 0, \quad (42)$$

under congruence by the $Sp(2,,\mathcal{R})$ matrix

$$S = \begin{pmatrix} \mu & 0 \\ 0 & 1/\mu \end{pmatrix}, \quad (43)$$

the value of $\sum_k (M_{kk})^2$ changes from $a^2 + b^2$ to $\mu^2 a^2 + (1/\mu^2)b^2$ which, by an appropriate choice of μ, can be made as large as one wishes.

However, it follows from (41) that over the submanifold of symplectic bases which leave $\mathrm{tr}(M(\mathbf{z})^{\mathrm{odd}})^2$ fixed, the function $\mathrm{tr}(M(\mathbf{z})^2)$ remains invariant and so the quartic form $\sum (M(\mathbf{z})_{kk})^2$ is bounded within this restricted class of symplectic bases and hence can be maximised. In particular the nonnegative $\mathrm{tr}(M(\mathbf{z})^{\mathrm{odd}})^2$ can be chosen to take its minimum value. Williamson theorem implies that there are symplectic bases which realize the absolute mimumum $\mathrm{tr}(M(\mathbf{z})^{\mathrm{odd}})^2 = 0$.

We can now formulate the *analogue of the Scweinler-Wigner extremum principle for symplectic bases* in the following way: Take the subfamily of symplectic bases in which $\mathrm{tr}(M(\mathbf{z})^{\mathrm{odd}})^2$ and hence $\mathrm{tr}(M(\mathbf{z})^2)$is minimum. [This minimum of $\mathrm{tr}(M(\mathbf{z})^2)$ equals the invariant $\mathrm{tr}(\beta^T M(\mathbf{z})\beta M(\mathbf{z}))$]. Then maximise the Schweinler-Wigner quartic form $m(\mathbf{z}) = \sum_k (M(\mathbf{z})_{kk})^2$ within this submanifold of symplectic bases. This will lead, not just to a basis in which $M(\mathbf{z})$ is diagonal, but to one where $M(\mathbf{z})$ has the Williamson canonical form $M(\mathbf{z}) = \mathrm{diag}(\kappa_1, \cdots, \kappa_n; \kappa_1, \cdots, \kappa_n)$. We have thus established the following generalization of the Schweinler-Wigner extremum principle to the symplectic case.

Theorem 7: The distinquished symplectic basis which extremizes the "Schweinler-Wigner" quartic form $m(\mathbf{z})$ over the submanifold of symplectic bases which minimize the quartic form $\mathrm{tr}(M(\mathbf{z})^2)$ is the same as the symplectic basis in which the positive definite matrix $M(\mathbf{z})$ assumes the Williamson canonical diagonal.

Note that once $M(\mathbf{z})^{\mathrm{odd}} = 0$ is reached, as implied by $\mathrm{tr}(M(\mathbf{z})^{\mathrm{odd}})^2 = 0$, $M(\mathbf{z})$ has the special even form

$$\begin{pmatrix} A & C \\ -C & A \end{pmatrix}, \ A^T = A, \ C^T = -C, \quad (44)$$

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so that $A + iC$ is hermitian. The subgroup of symplectic transformations which do not mix $M(\mathbf{z})^{\text{even}}$ with $M(\mathbf{z})^{\text{odd}}$, and hence maintain the property $M(\mathbf{z})^{\text{odd}} = 0$ have the special form

$$S = \begin{pmatrix} X & Y \\ -Y & X \end{pmatrix}, \quad X + iY \in U(n). \qquad (45)$$

This subgroup, isomorphic to the unitary group $U(n)$, is the maximal compact subgroup [10] of $Sp(2n, \mathcal{R})$. Thus, diagonalizing $M(\mathbf{z})$ using symplectic change of basis, after it has reached the even form, is the same as diagonalizing an n-dimensional hermitian matrix using unitary transformations.

VII. CONCLUDING REMARKS

To conclude, we have shown that an $N \times N$ real symmetric [complex hermitian] positive definite matrix is congruent to a diagonal form modulo a pseudo-orthogonal [pseudo-unitary] matrix belonging to $SO(m, n)$ $[SU(m, n)]$, for any choice of partition $N = m + n$. The method of proof of this result is adapted to provide a simple proof of Williamson's theorem. An important consequence of these theorems is that while a real-symmetric [complex-hermitian] positive definite matrix has a unique diagnal form under conjugation, it has several different canonical diagnal forms under congruence. The theorems developed here are used to formulate an extremum principle a lá Schweinler and Wigner for constructing pseudo-orthonormal[pseudo-unitary] and symplectic bases from a given set of linearly independent vectors. Conversely, the extremum principle thus formulated can be used for finding the congruence transformation which brings about the desired diagonalization.

It is interesting that pseudo-orthonormal basis and symplectic basis could be constructed by extremizing *precisely the same Schweinler-Wigner quartic form* $m(\mathbf{z}) = \sum_k (M(\mathbf{z})_{kk})^2$ that was originally used to construct orthonormal basis in the unitary case. However, it must be borne in mind that the similarity in the structure of the quartic form to be extremized in the three cases considered is only at a formal level. In reality, the three quartic forms are very different objects, for they are functions over topologically very different manifolds: $\mathbf{z}$ runs over the group manifold $U(N)$ of orthogonal frames in the original Schweinler-Wigner case, the group manifold $SO(m, n)$ of pseudo-orthogonal frames in the Lorentz case, and over the group manifold $Sp(2n, \mathcal{R})$ in the symplectic case. This has the consequence that, unlike the orthogonal case, this quartic form is unbounded in the noncompact $SO(m, n)[SU(m, n)]$ and $Sp(2n, \mathcal{R})[Sp(2n, \mathcal{C})]$ cases. Insight into the structure of these groups was used to achieve constrained extremization within a natural maximal compact submanifold.

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[8] Just as diagonal form is the canonical form for real symmetric matrices uner rotation, $i\sigma_2 \bigotimes K$, with K diagonal, is the canonical form for a real antisymmetric matrix under rotation. Further K can be chosen to be nonnegative, in general, and positive definite when the antisymmetric matrix is nonsingular.

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