ON SPECTRAL CONDITION OF J-HERMITIAN OPERATORS

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Abstract

The spectral condition of a matrix H is the infimum of the condition numbers $\kappa(Z) = \|Z\|\|Z^{-1}\|$, taken over all Z such that $Z^{-1}HZ$ is diagonal. This number controls the sensitivity of the spectrum of H under perturbations. A matrix is called J-Hermitian if $H^* = JHJ$ for some $J = J^* = J^{-1}$. When diagonalizing J-Hermitian matrices it is natural to look at J-unitary Z, that is, those that satisfy $Z^*JZ = J$. Our first result is: if there is such J-unitary Z, then the infimum above is taken on J-unitary Z, that is, the J unitary diagonalization is the most stable of all. For the special case when J-Hermitian matrix has definite spectrum, we give various upper bounds for the spectral condition, and show that all J-unitaries Z which diagonalize such a matrix have the same condition number. Our estimates are given in the spectral norm and the Hilbert–Schmidt norm. Our results are, in fact, formulated and proved in a general Hilbert space (under an appropriate generalization of the notion of 'diagonalising') and they are applicable even to unbounded operators. We apply our theory to the Klein–Gordon operator thus improving a previously known bound.

1 Introduction and preliminaries

Let X be a Hilbert space over the real or complex field Φ with the scalar product (x, y) linear in the second variable.[1] All operators in X will be linear, everywhere defined and bounded, if not specified otherwise. An operator in X is called non-singular, if it has an everywhere defined and bounded inverse. If X has a finite dimension n then X will be automatically identified with the standard Φ^n with $(x, y) = x^*y$ and linear operators in X will be identified with matrices of order n. An operator J in X is called *fundamental symmetry* if

$$J = J^* = J^{-1}$$

holds. The operators

$$P_+ = (I + J)/2 \ , \ P_- = (I - J)/2$$

are the corresponding *fundamental projections.* A principal subject of our considerations will be the so-called *J-Hermitian* operators, characterized by the relation

$$H^* = JHJ.$$

This just means that the operator

$$G = JH \tag{1.1}$$

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[1]This, together with other notational conventions and terminology are taken from [7].

is Hermitian. Another important class of operators closely related to the J-Hermitians are the J-*unitary* operators[2], defined by

$$U^*JU = J \quad \text{and} \quad UJU^* = J.$$

Obviously all J-unitaries form a multiplicative group, which is non-bounded for J indefinite. With H J-Hermitian and U J-unitary the similarity

$$H^{'} = U^{-1}HU$$

preserves the J-hermiticity and this is the basis of the use of the J-unitarity in the spectral theory of J-Hermitian operators ([12, 6]) as well in numerical algorithms with such matrices ([18, 19, 20, 13]).

Let $\kappa(H) = \|H\|\,\|H^{-1}\|$ denote the condition number of a non-singular operator H. If J is indefinite then the condition number of a J-unitary U, $\kappa(U) = \|U\|\,\|U^{-1}\|$ can be arbitrarily high, in fact, we have

$$\kappa(U) = \|U\|\,\|JU^*J\| = \|U\|^2.$$

Note that for a J-unitary U the value $\kappa(U)$ equals 1 if and only if $UJ = JU$ or, equivalently, U is both unitary and J-unitary. In want of a better term we shall call such matrices and operators *jointly unitary*. Similarly, we call a J-Hermitian commuting with J *jointly Hermitian*. Such operator is Hermitian in the ordinary sense.

Suppose now that a matrix Z diagonalizes a J-Hermitian H, that is, $H^{'} = Z^{-1}HZ$ is diagonal. In Numerical Linear Algebra this matrix is commonly called 'the matrix of eigenvectors' for H. The notion of 'diagonalization' can be given a natural meaning in an arbitrary, even infinite dimensional Hilbert space: we just ask that $Z^{-1}HZ$ is Hermitian, and this is the way we state and prove our theorems below. Indeed, once we have obtained a Hermitian matrix $Z^{-1}HZ$, it can further be diagonalized by a unitary similarity which does not change the condition number. From the numerical point of view we are interested in the *spectral condition* of a J-Hermitian H, defined by

$$\inf \kappa(Z), \tag{1.2}$$

where the infimum is taken over all non-singular matrices diagonalizing H. This number is known to control the sensitivity of the spectrum of H under perturbations. Our article gives information on this quantity. Our results, as well as the organization of the paper, can be summarized as follows:

- In Section 2 we first consider an important class of J-Hermitian operators H, namely those with "definite spectrum". Such operators are called strongly stable by Krein ([8]). We show that all J-unitary U diagonalizing such an H *have the same condition.*

- In Section 3 we compare J-unitaries which diagonalize a J-Hermitian H with other non-singulars that do the same. The answer is: J-unitaries are always the best. This remains so even if we drop the condition of definite spectrum and consider all similarities reducing H to a given block-diagonal form. Thus, in addition to preserving J-hermiticity, the J-unitary similarity is also the most stable one.

- In Section 4 we give a bound for $\kappa(U)$ in the important special case where $G = JH$ is itself positive definite. The bound reads

$$\kappa(U) \leq \min \sqrt{\kappa(D^*GD)},$$

where the minimum is taken over all non-singular D which commute with J. This result has applications in the perturbation and error analysis in the standard Hermitian eigenvalue problem ([2, 18, 22, 13]) and it confirms a conjecture, obtained by numerical evidence, acquired in [13]. This bound is attainable.

[2]For $\Phi = \mathbf{R}$ the terms *J-symmetric, J-orthogonal*, respectively, are more common.

- In Section 5 we consider another, somewhat larger subclass with definite spectrum, characterized by
$$\inf_{\|x\|=1}(|(x,Gx)|+|(x,Jx)|)>0,$$
(G from (1.1)) which is well-known to be equivalent to the existence of a real μ such that $J(H-\mu I)$ is positive definite. Such operators will be called *J-definite.* In addition, H, or at least some part of it, is supposed to be of trace class. We obtain an estimate for the Hilbert-Schmidt distance of a diagonalizing U from a point from the (standard) unit sphere.

- In Section 6 we apply our theory to the operators of the Klein-Gordon type studied in [15], [16], [17] and improve a bound, obtained in [16]. The unboundedness of the operator involved is conveniently overcome by a simple cut-off argument.

A standard representation of the fundamental symmetry is given by
$$J=\begin{pmatrix} I & 0\\ 0 & -I\end{pmatrix}. \tag{1.3}$$
Here the diagonal blocks need not have the same dimension and one of them may be void. Other common forms of J are
$$\begin{pmatrix} 0 & I\\ I & 0\end{pmatrix} \text{ or } \begin{pmatrix} 0 & iI\\ -iI & 0\end{pmatrix},$$
where the respective identities have necessarily the same size. For the block form (1.3) a jointly unitary looks like
$$\begin{pmatrix} U_1 & 0\\ 0 & U_2\end{pmatrix},$$
where U_1 and U_2 are unitary. Similarly, a jointly Hermitian looks like
$$\begin{pmatrix} H_1 & 0\\ 0 & H_2\end{pmatrix},$$
where H_1 and H_2 are Hermitian. Of course, a jointly Hermitian H can be diagonalized by a jointly unitary U. There is no loss of generality in representing a general J in the form (1.3) and we will often use it in our proofs. On the other hand, in applications - be it for finite matrices or differential operators - other forms of J may be more convenient.

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2 Operators with definite spectrum

A J-Hermitian operator H is said to have a *definite spectrum* if its spectrum $\sigma(H)$ can be divided into two disjoint parts σ_+ and σ_- with finite distance such that the corresponding Dunford spectral projections Q_+ and Q_- satisfy $\pm(x,JQ_\pm x)\geq 0$. Krein ([8]) calls such operators strongly stable because the reality of their spectrum and their diagonalizability survive small J-Hermitian perturbations. Another characterization of these operators is the existence of a real polynomial p such that $Jp(H)$ is positive definite ([9], [10], [11]). Obviously, J-definite operators have definite spectrum and in this case we have
$$\sigma_- < \sigma_+.$$

Let H have definite spectrum and set
$$K=Q_+-Q_-. \tag{2.1}$$
Then $K=f(H)$ where
$$f(\lambda)=\begin{cases} +1, & \text{around } \sigma_+\\ -1, & \text{around } \sigma_-\end{cases} \tag{2.2}$$
We will call f *the natural sign function* of H. It is immediately seen that K is J-Hermitian and that JK is positive definite.

Theorem 2.1 *Let H be J-Hermitian with definite spectrum. Then there exists a unique U which is simultaneously J-unitary and Hermitian positive definite and such that*

$$H_0 = U^{-1} H U \tag{2.3}$$

is jointly Hermitian. Further, any J-unitary V for which $H_1 = V^{-1}\ HV$ is jointly Hermitian has the form

$$V = UV_0$$

where V_0 is jointly unitary. Also,

$$\kappa(V) = \kappa(U) = \|K\|,$$

where K is given by (2.1).

Proof. Set

$$U = (JK)^{-1/2}.$$

Then it immediately follows

$$U^* JU = UJU = (JK)^{-1/2} J (JK)^{-1/2} = (JK)^{-1/2} J (KJ)^{1/2} = (JK)^{-1/2} (JK)^{1/2} J = J,$$

that is, U is J-unitary. Thus, H_0 is J-Hermitian, which means that

$$JKH = H^* JK,$$

(note that H and K commute) or, equivalently

$$H_0 = (JK)^{1/2} H (JK)^{-1/2} = (JK)^{-1/2} H^* (KJ)^{1/2} = H_0^*.$$

Therefore, H_0 is jointly Hermitian.

Let now V be any J-unitary such that

$$H_1 = V^{-1} HV,$$

is jointly Hermitian. Then $K_1 = V^{-1} KV$ is jointly Hermitian (note that $K_1 = f(H_1)$). Also,

$$JK_1 = JV^{-1} KV = V^* V^{-*} JV^{-1} KV = V^* JKV$$

is positive definite. This, together with

$$(JK_1)^{-1} = K_1 J = JK_1$$

implies $K_1 = J$. Thus, $V^{-1} KV = J$ and

$$U^{-1} VJ = U^{-1} KV = U^{-1} KUU^{-1} V = JU^{-1} V,$$

hence $V_0 = U^{-1} V$ is jointly unitary. The equalities

$$\|V\| = \|U\| = \|K\|^{1/2}$$

are then immediate.

It remains to prove the uniqueness of U. This follows from a simple decomposition formula: any J-unitary U in the representation (1.3) can be decomposed as

$$U = U_0 Y(W) = Y(W') U_0, \tag{2.4}$$

where

$$U_0 = \begin{pmatrix} U_+ & 0 \\ 0 & U_- \end{pmatrix}$$

with U_+ and U_- unitary,

$$Y(W) = \begin{pmatrix} \sqrt{I + WW^*} & W \\ W^* & \sqrt{I + W^*W} \end{pmatrix}.$$

and

$$W' = U_+ W U_-^*,$$

in particular, $Y(W)^{-1} = Y(-W)$). The proof is straightforward and uses just the block-wise written J-unitarity property (1.3) and the polar decomposition of U. **Q.E.D.**

Remark 2.2 The theorem above remains valid, if H is merely J-Hermitian with an "abstract sign" operator K with the properties

(i) JK is Hermitian and positive.

(ii) $K^2 = I$.

(iii) K bicommutes with H.

3 J-unitaries are the best

Now we would like to compare the conditions of all non-singular matrices Z that diagonalize or block diagonalize a given J-Hermitian matrix H. Here, too, definite spectrum will be particularly simple to handle. But even in the general case we show that as far as the condition is concerned, the J-unitaries are the best choice.

Theorem 3.1 *Let H be J-Hermitian with definite spectrum. Let Z be non-singular such that $H_1 = Z^{-1}HZ$ is Hermitian. Then $\kappa(Z) \geq \kappa(U)$, where U is the J-unitary from (2.3).*

Proof. The operators H_0 and H_1 are selfadjoint and similar. Then, as it is well known, they are unitarily similar, that is,

$$H_1 = U_0^{-1} H_0 U_0,$$

where H_0 is from (2.3) and U_0 is unitary. Now

$$H_1 = U_0^{-1} H_0 U_0 = Z^{-1} U H_0 U^{-1} Z.$$

By setting $T = U^{-1} Z U_0^{-1}$ we see that T (and also T^*) commutes with H_0 and also with $J = f(H_0)$, f from (2.2)[3]. Using this, the unitarity of U_0 and the J-unitarity of U we obtain

$$\kappa(Z)^2 = \kappa(UT)^2 = \|T^* U^* U T\| \, \|T^{-1} U^{-1} U^{-*} T^{-*}\| =$$

$$\begin{aligned} \|(TT^*)^{1/2} U^*\|^2 \|T^{-1} J U^* J J U J T^{-*}\| &= \|U (TT^*)^{1/2}\|^2 \|(TT^*)^{-1/2} U^*\|^2 \\ &\geq \|U (TT^*)^{1/2} (TT^*)^{-1/2} U^*\|^2 = \|UU^*\|^2 \\ &= \kappa(U)^2. \end{aligned}$$

Q.E.D.

We could pose the uniqueness question: if $\kappa(Z) = \kappa(U)$ for some Z with $Z^{-1}HZ$ Hermitian and U from (2.3), what can be said about Z? This does not seem to have a simple answer. Anyhow, such Z need not be J-unitary as is shown by the following example. Set

$$H = \begin{pmatrix} \cosh 2x & -\sinh 2x & 0 \\ \sinh 2x & -\cosh 2x & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$J = \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix}.$$

[3] This follows from the fact that H_0 is jointly Hermitian with definite spectrum.

By $H^2 = I$ it follows that $K = H$ and JH is positive definite. Set

$$Z = \begin{pmatrix} 2\cosh x & 2\sinh x & 0 \\ 2\sinh x & 2\cosh x & 0 \\ 0 & 0 & 3 \end{pmatrix},$$

$$U = \begin{pmatrix} \cosh x & \sinh x & 0 \\ \sinh x & \cosh x & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then

$$Z^{-1}HZ = U^{-1}HU = J,$$

U is J-unitary, and

$$\|Z\| = \max(3, 2e^{|x|}), \quad \|Z^{-1}\| = \max(1/3, e^{|x|}/2), \quad \kappa(U) = \|U\|^2 = e^{2|x|}.$$

Now, for $2e^{2|x|} > 3$ we have

$$\kappa(Z) = 2e^{|x|}\frac{1}{2}e^{|x|} = \kappa(U)$$

and Z is not J-unitary.

The situation is better if we take the Hilbert-Schmidt norm

$$\|Z\|_{HS} = \mathrm{Tr}(Z^*Z)^{1/2}.$$

In this case, of course the dimension n of the space X has to be finite. The corresponding condition $\kappa_{HS}(Z) = \|Z\|_{HS}\|Z^{-1}\|_{HS}$ satisfies the inequality

$$\kappa_{HS}(Z) \geq n,$$

where the equality holds if and only if Z is proportional to a unitary.

Theorem 3.2 *Let H be J-Hermitian with definite spectrum. Let Z be non-singular such that $H_1 = Z^{-1}HZ$ is Hermitian. Then $\kappa_{HS}(Z) \geq \kappa_{HS}(U)$, where U is the J-unitary from (2.3). Further, if the equality sign is attained, then Z is proportional to UV_0, where U is from (2.3) and V_0 is unitary.*

Proof. Taking Z, T and U as in the proof of Theorem 3.1 we obtain[4]

$$\kappa_{HS}(Z)^2 = \|U(TT^*)^{1/2}\|_{HS}^2\|(TT^*)^{-1/2}U^*\|_{HS}^2.$$

Let now V be a unitary matrix diagonalizing $(TT^*)^{1/2}$,

$$V^{-1}(TT^*)^{1/2}V = \mathrm{diag}(\xi_1, \ldots, \xi_n). \tag{3.1}$$

Setting $p_i = [V^{-1}U^*UV]_{ii}$ and using the Cauchy-Schwartz inequality we obtain

$$\begin{aligned} \kappa_{HS}(Z)^2 &= \left(\sum_i p_i\xi_i^2\right)\left(\sum_i p_i/\xi_i^2\right) \geq \left(\sum_i \sqrt{p_i\xi_i^2}\sqrt{p_i/\xi_i^2}\right)^2 = (\sum_i p_i)^2 \\ &= \left[\mathrm{Tr}(V^{-1}U^*UV)\right]^2 = [\mathrm{Tr}(U^*U)]^2 = \|U\|_{HS}^4 = \kappa_{HS}(U)^2. \end{aligned}$$

Conversely, $\kappa_{HS}(Z) = \kappa_{HS}(U)$ turns the inequality above into an equality. This means that the vectors

$$[\sqrt{p_i\xi_i^2}] \quad \text{and} \quad [\sqrt{p_i/\xi_i^2}]$$

[4]Here, too, we could continue by $\geq \|UU^*\|_{HS}^2$ but this expression can be less than $\|U\|^4$.

are proportional, that is, $\xi_i = \alpha$ for all i. Then (3.1) gives

$$TT^* = \alpha^2 I,$$

and

$$Z = UTU_0 = \alpha U \frac{T}{\alpha} U_0,$$

where $V_0 = \frac{T}{\alpha} U_0$ is unitary. **Q.E.D.**

If we drop the condition of definite spectrum then a J-Hermitian need not be J-unitarily diagonalizable or even reducible even in the finite dimensional space. This is shown by the trivial example

$$H = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \qquad J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

However, if a J-Hermitian H is reducible, that is, if $Z^{-1}HZ$ is, say, block-diagonal, then we can consider all non-singular Z which do the same reduction and ask for their conditions. We give now a precise definition of the reducibility which will be basic for our main theorem. We say that a J-Hermitian H is reducible, if there exists a J-Hermitian decomposition of the identity

$$Q_1, \ldots, Q_p$$

such that all Q_i commute with H. Note that Q_i may or may not be Dunford spectral projections. In this case there exists a J-unitary U such that

$$P_i = U^{-1} Q_i U, \qquad i = 1, \ldots, p \tag{3.2}$$

commute with J (and are therefore jointly Hermitian)[5]. Obviously, if H is a finite matrix, then the way from $U^{-1}HU$ to a really block diagonal matrix goes via another unitary similarity which does not change the condition. This definition of the reducibility is obviously the most general while still admitting J-unitary similarities. In the case

$$H = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

there is no J-unitary reducibility, that is, H is not reducible according to our definition above although H is normal and therefore unitarily diagonalizable. Our theory gives, of course, no results on such cases.

Theorem 3.3 *Let $Q_1, \ldots, Q_p$ be a J-Hermitian decomposition of the identity and let $Z^{-1}Q_iZ$ be Hermitian for all i. Then there exists a J-unitary V such that $V^{-1}Q_iV$ is Hermitian for all i and*

$$\kappa(V) \le \kappa(Z).$$

Proof. Take U and P_i from (3.2). Then there is a unitary U_0 such that $U_0^{-1}Z^{-1}Q_iZU_0 = P_i$ for all i. Setting $Z_1 = ZU_0$ we have

$$Z_1 P_i Z_1^{-1} = U P_i U^{-1}, \qquad i = 1, \ldots, p,$$

which means that $T = U^{-1}Z_1$ commutes with all P_i. We have

$$\kappa(Z)^2 = \kappa(Z_1)^2 = \operatorname{spr}(U^*UTT^*) \operatorname{spr}(J(TT^*)^{-1}JU^*U),$$

Until now the proof is quite similar to that of Theorem 3.1; the main difference is that here T need not commute with J.

[5]The proof of this fact for finite matrices is straightforward, a proof in a general Hilbert space was provided by P. Jonas, Berlin (private communication).

Since $JJTT^* = TT^*$ is positive definite the operator JTT^* has definite spectrum. By Theorem 2.1 there is a J-unitary V_0 such that

$$G_0 = V_0^{-1} JTT^* V_0$$

is jointly Hermitian and that V_0 commutes with all P_i. The latter follows from the fact that JTT^* commutes with all P_i. Then

$$G = G_0 J = JG_0 = V_0^* TT^* V_0$$

is jointly Hermitian and positive definite. Moreover,

$$J(TT^*)^{-1}J = J(V_0^{-*} G V_0^{-1})^{-1} J = JV_0 G^{-1} V_0^* J = V_0^{-*} G^{-1} V_0^{-1}.$$

Now

$$\begin{aligned}
\kappa(Z)^2 &= \operatorname{spr}(U^* U V_0^{-*} G V_0^{-1}) \operatorname{spr}(V_0^{-*} G^{-1} V_0^{-1} U^* U) \\
&= \|UV_0^{-*} G^{1/2}\|^2 \|G^{-1/2} V_0^{-1} U^*\|^2 \\
&\geq \|UV_0^{-*} V_0^{-1} U^*\|^2 = \|V\|^4 = \kappa(V)^2,
\end{aligned}$$

where $V = UV_0^{-*}$ is J-unitary and

$$V^{-1} Q_i V = V_0^* P_i V_0^{-*}, \qquad i = 1, \ldots, p,$$

since, as we know, V_0 commutes with all P_i. **Q.E.D.**

Theorem 3.4 *Theorem 3.1 above remains true, if κ is substituted by κ_{HS} ($\dim X = n < \infty$).*

The proof just combines the ideas of the proofs of Theorems 3.1 and 3.3 and is omitted.

4 J-positive case

In this section we consider a very special case of definite spectrum namely that of

$$H = JG$$

with G positive definite. The eigenvalue problem for H is obviously equivalent to the one of the Hermitian matrix $S = G^{1/2} J G^{1/2}$. It is an amazing and non-trivial fact that the eigenvalue problem for a given Hermitian matrix S has, in a sense, a more convenient perturbation and error analysis, if handled through H above with J from (1.3) (see [22, 13]).

Theorem 4.1 *Let H be such that $G = JH$ is Hermitian and positive definite. Then any J-unitary U with $U^{-1}HU$ jointly Hermitian satisfies*

$$\kappa(U) \leq \min \sqrt{\kappa(D^* G D)}, \tag{4.1}$$

where the minimum is taken over all non-singular D which commute with J.

Proof. We shall prove the bound (4.1) for $\kappa(U)$ in two stages: we shall first analyze the case when the bound is an equality, and then prove the bound itself. Our proof is modeled after the one for finite matrices, given in [14]. The only difference is with two steps, which are more technical in an infinite dimensional space. Represent J by (1.3); then any operator commuting with J is just block diagonal.

To prove our results we need the following lemma.

Lemma 4.2 *Let*

$$G = \begin{pmatrix} I & \Psi \\ \Psi^* & I \end{pmatrix} \tag{4.2}$$

be positive definite, that is, $\|\Psi\| < 1$. *Then*

$$\kappa(G) = \min \kappa(D^* G D),$$

where the minimum is taken over all non-singular D *which commute with* J.

This lemma was proved in [4] (see also [3]) for finite matrices. Our proof is modified to accommodate infinite dimensionality.

Proof of Lemma 4.2. We first prove the identity

$$\kappa(G) = \frac{1 + \|\Psi\|}{1 - \|\Psi\|} = \mathrm{spr}(JG^{-1}JG) = \|JG^{-1}JG\| \tag{4.3}$$

Indeed, writing $G = I + G_0$ we obviously have

$$JG_0J = -G_0 \quad , \quad JGJ = I - G_0,$$

so $\sigma(G)$ lies symmetrically with respect to 1 with

$$0 < \min \sigma(G) = 1 - \|\Psi\| < \max \sigma(G) = 1 + \|\Psi\| < 2.$$

Thus,

$$\kappa(G) = \frac{1 + \|\Psi\|}{1 - \|\Psi\|}.$$

Set

$$\Delta = \Delta(\Psi) = \begin{pmatrix} I - \Psi\Psi^* & 0 \\ 0 & I - \Psi^*\Psi \end{pmatrix}.$$

The following properties are immediately seen

- Δ is Hermitian and non-singular;
- Δ commutes with G and J;
- G^{-1} is given by
$$G^{-1} = \Delta^{-1}JGJ = JGJ\Delta^{-1}.$$

Thus,

$$JG^{-1}JG = J\Delta^{-1}JGJ^2G = G\Delta^{-1}G$$

hence $JG^{-1}JG$ is Hermitian and positive definite.

As it is known (see e.g. [23]) a point λ belongs to the spectrum of a Hermitian operator A, if and only if there is a sequence of vectors z_k not converging to zero, such that

$$Az_k - \lambda z_k \to 0.$$

Such z_k is called a singular sequence. So take any singular sequence z_k with

$$Gz_k - \lambda z_k \to 0. \tag{4.4}$$

This is equivalent to

$$JGJJz_k - \lambda J z_k \to 0.$$

or, by $JGJ = I - G_0 = 2I - G$, to

$$G^{-1}Jz_k - \frac{Jz_k}{2 - \lambda} \to 0. \tag{4.5}$$

Using (4.4) and (4.5) for $\lambda = 1 + \|\Psi\|$ we obtain

$$JG^{-1}JGz_k - \frac{1+\|\Psi\|}{1-\|\Psi\|}z_k \to 0,$$

that is, $\kappa(G)$ belongs to the spectrum of $JG^{-1}JG$. Hence

$$\|JG^{-1}JG\| = \mathrm{spr}(JG^{-1}JG) \geq \kappa(G).$$

Conversely, since J is unitary we have

$$\|JG^{-1}JG\| \leq \kappa(G)$$

and (4.3) follows. Now, as in [4], for any non-singular D which commutes with J we have

$$\begin{aligned}
\kappa(G) &= \mathrm{spr}(JG^{-1}JG) = \mathrm{spr}(D^{-1}JG^{-1}JGD) \leq \|D^{-1}JG^{-1}JGD\| \\
&= \|JD^{-1}JG^{-1}D^{-*}JD^*GD\| \leq \|(D^*GD)^{-1}\|\,\|D^*GD\| \\
&= \kappa(D^*GD).
\end{aligned}$$

Q.E.D.

The following lemma shows that the bound (4.1) becomes an equality for matrices of the form (4.2).

Lemma 4.3 *Let J and G be given by (1.3) and (4.2), respectively. Let U be J-unitary such that U^*GU is jointly Hermitian. Then*

$$\kappa(U) = \sqrt{\kappa(G)} = \sqrt{\min \kappa(D^*GD)}, \tag{4.6}$$

where the minimum is taken over all non-singular D which commute with J.

Proof of Lemma 4.3. The second equality in (4.6) follows from Lemma 4.2. We take V in the form

$$V = V(T) = MW = WM, \tag{4.7}$$

with

$$M = \begin{pmatrix} (I-TT^*)^{-1/2} & 0 \\ 0 & (I-T^*T)^{-1/2} \end{pmatrix} \quad \text{and} \quad W = \begin{pmatrix} I & T \\ T^* & I \end{pmatrix},$$

where $\|T\| < 1$.[6] The commutativity of the product in (4.7) follows from the identity

$$T(I-T^*T)^{-1/2} = (I-TT^*)^{-1/2}T,$$

which, in turn, follows from a more general identity

$$Af(BA) = f(AB)A$$

for any operator function f. This identity is often used in our proofs. The operator V is obviously J-unitary, Hermitian and positive definite. The same is obviously the case for $V^{1/2}$, its positive definite square root. Also obvious is the relation

$$V(T)^{-1} = V(-T) = JV(T)J.$$

Now take

$$U = \sqrt{V(-\Psi)}$$

with Ψ as in Lemma 4.2. Then U obviously commutes with G and

$$S = U^*GU = UGU = VG = \begin{pmatrix} \sqrt{I-\Psi\Psi^*} & 0 \\ 0 & \sqrt{I-\Psi^*\Psi} \end{pmatrix}. \tag{4.8}$$

[6]Obviously, $Y(W)$ may be identified with $V(T)$ from (2.4) with $W = T(I+T^*T)^{-1/2}$.

We have to determine the norm of U or, equivalently, that of V. First,

$$\|V\| \leq \|M\|\|W\| = (1 + \|T\|) \cdot \frac{1}{\sqrt{1 - \|T\|^2}} = \sqrt{\frac{1 + \|T\|}{1 - \|T\|}}.$$

Further, $V^{-1}M = W^{-1}$ so

$$\frac{1}{1 - \|T\|} = \|W^{-1}\| \leq \|V^{-1}\|\|M\| = \|V\|\|M\| \leq \|V\| \frac{1}{\sqrt{1 - \|T\|^2}}.$$

Thus,

$$\|V\| = \sqrt{\frac{1 + \|T\|}{1 - \|T\|}},$$

and the statement follows from (4.3). **Q.E.D.**

We now turn back to the proof of Theorem 4.1. For G positive definite and J as in (1.3) we may write

$$G = \begin{pmatrix} G_{11} & G_{12} \\ G_{12}^* & G_{22} \end{pmatrix}.$$

By taking

$$D_0 = \begin{pmatrix} G_{11}^{-1/2} & 0 \\ 0 & G_{22}^{-1/2} \end{pmatrix}.$$

we have $JD_0 = D_0 J$ and

$$\hat{G} = D_0 G D_0$$

is of the form (4.2). Let $\hat{U}$ be the J-unitary from Lemma 4.3, that is, $\hat{U}$ is also Hermitian and positive definite and

$$\hat{S} = \hat{U}\hat{G}\hat{U} = \hat{G}\hat{U}^2$$

is as in (4.8). Now, according to Theorem 2.1 there is a J-unitary U such that

$$U^* G U = \Delta$$

is jointly Hermitian, that is, block-diagonal. Set

$$Z = D_0^{-1}\hat{U}\hat{S}^{-1/2}.$$

Obviously, $Z^* G Z = I$ and, thus,

$$Z = U\Delta^{-1/2}Q^*,$$

with Q unitary and

$$Z^* J Z = QJ\Delta^{-1}Q^*. \tag{4.9}$$

By $\kappa(U) = \|UU^*\|$ we have

$$\kappa(U) = \operatorname{spr}(ZQ\Delta Q^* Z^*). \tag{4.10}$$

Inverting (4.9) gives

$$Z^{-1}JZ^{-*} = Q\Delta J Q^* = Q\Delta Q^* QJQ^*,$$

which, inserted in (4.10), gives

$$\kappa(U) = \operatorname{spr}(ZZ^{-1}JZ^{-*}QJQ^*Z^*) = \operatorname{spr}(QJQ^*Z^*JZ^{-*}).$$

Furthermore,

$$Z^* J Z^{-*} = \hat{S}^{-1/2}\hat{U}D_0^{-1}JD_0\hat{U}^{-1}\hat{S}^{1/2} = \hat{U}^2 J.$$

Here we have used the following facts:

- $\hat{U}$ is J-unitary and Hermitian;
- D_0 and $\hat{S}$ commute with J;
- $\hat{S}$ and $\hat{U}$ commute.

The last fact is an immediate consequence of the construction of $\hat{S}$ and $\hat{U}$ in Lemma 4.3. Altogether we have

$$\kappa(U) = \operatorname{spr}(QJQ^*\hat{U}^2J) \leq \|QJQ^*\hat{U}^2J\| \leq \|\hat{U}^2\| = \|\hat{U}\|^2 = \kappa(\hat{U}) = \sqrt{\kappa(\hat{G})},$$

where we have used Lemma 4.3 as well as the fact that both QJQ^* and J are unitary. **Q.E.D.**

5 Trace estimates

In the finite dimensional case it is known ([20]) that the transformation (2.3) is trace reducing in the sense that $\operatorname{Tr}(JH) - \operatorname{Tr}(JH_0) \geq 0$, the equality taking place, if and only if H itself is already Hermitian. Moreover, this trace difference controls the corresponding transformation U. We prove here a corresponding result under milder conditions on H, namely, that $H - H_0$ or, better still, only some parts of $JH - JH_0$, be of trace class.

Theorem 5.1 *Let H be J-definite, let U and H_0 be as in Theorem 2.1 and f be the natural sign function from (2.2). Then*

(i)

$$P_+(f(H) - J)P_+ \geq 0 \quad , \quad P_-(f(H) - J)P_- \leq 0,$$

and the following are equivalent

- *any of the inequalities above becomes an equality*
- *H is jointly Hermitian[7];*

(ii) furthermore, the properties

- *$U - I$ is Hilbert-Schmidt,*
- *any of the four operators $P_\pm(H - H_0)P_\pm$, $P_\pm(f(H) - J)P_\pm$ is of trace class*

are equivalent;

(iii) in the latter case we have

$$\|U - I\|_{HS}^2 \leq \frac{\operatorname{Tr} P_+(H - H_0)P_+ - \operatorname{Tr} P_-(H - H_0)P_-}{d}, \tag{5.1}$$

where d is the distance between σ_- and σ_+.

Before starting the proof we note that (5.1) simplifies, if $H - H_0$ is of trace class (this is always true for finite matrices); in this case we have

$$\|U - I\|_{HS}^2 \leq \frac{\operatorname{Tr}(JH - JH_0)}{d}, \tag{5.2}$$

Proof. We use again the representation (1.3) with

$$P_+ = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \qquad P_- = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}.$$

[7] Here and in the following "$\leq$" is the standard sesquilinear form ordering of Hermitian operators. Note that the involved operators are, in fact, jointly Hermitian).

Since U is Hermitian and positive definite, in its representation (2.4) we have $U_0 = I$ and

$$H = UH_0U^{-1} = Y(W)H_0Y(-W)$$

with

$$H_0 = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix},$$

where $\Lambda_\pm$ is Hermitian with the spectrum $\sigma_\pm$. Now,

$$\begin{aligned} H &= Y(W)\begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix}Y(-W) \qquad (5.3)\\ &= \begin{pmatrix} \sqrt{I+WW^*}\Lambda_+\sqrt{I+WW^*} - W\Lambda_-W^* & -\sqrt{I+WW^*}\Lambda_+W + W\Lambda_-\sqrt{I+W^*W} \\ W^*\Lambda_+\sqrt{I+WW^*} - \sqrt{I+W^*W}\Lambda_-W^* & \sqrt{I+W^*W}\Lambda_-\sqrt{I+W^*W} - W^*\Lambda_+W \end{pmatrix}. \end{aligned}$$

Also,

$$f(H_0) = U^{-1}f(H)U = J$$

and

$$f(H) = Y(W)JY(-W) = \begin{pmatrix} I+2WW^* & * \\ * & -I-2W^*W \end{pmatrix}.$$

Here the diagonal blocks of $f(H) - J$ are positive and negative, respectively, and they vanish, if and only if $W = 0$. This proves (i). Furthermore, these blocks are of trace class if and only if WW^* (and then also W^*W) is of trace class, that is, if W is a Hilbert-Schmidt operator. Moreover, this operator is positive and it vanishes if and only if H itself is jointly Hermitian. If W is Hilbert-Schmidt, by writing $\sqrt{1+a} = 1 + a(\sqrt{1+a}+1)^{-1}$ we have

$$\begin{aligned} \sqrt{I+WW^*}\Lambda_+\sqrt{I+WW^*} - \Lambda_+ &= WW^*(\sqrt{I+WW^*}+I)^{-1}\Lambda_+\sqrt{I+WW^*} + \\ &\quad + \Lambda_+WW^*(\sqrt{I+WW^*}+I)^{-1}, \end{aligned}$$

which is certainly of trace class, and its trace equals

$$\mathrm{Tr}(\Lambda_+WW^*(\sqrt{I+WW^*}+I)^{-1}(\sqrt{I+WW^*}+I)) = \mathrm{Tr}(W^*\Lambda_+W).$$

Altogether

$$\begin{gathered} \mathrm{Tr}\, P_+(H-H_0)P_+ = \mathrm{Tr}(W^*\Lambda_+W) - \mathrm{Tr}(W\Lambda_-W^*) \geq \\ \min\sigma_+\,\mathrm{Tr}(W^*W) - \max\sigma_-\,\mathrm{Tr}(WW^*) = d\|W\|_{HS}^2 \end{gathered}$$

(and similarly with P_-). The estimate (5.1) now follows from

$$\|Y(W) - I\|_{HS}^2 \leq 2\|W\|_{HS}^2,$$

which is directly verified. The only thing which remains to be proved is that the trace-class property of $P_\pm(H-H_0)P_\pm$ implies the same for WW^* (or W^*W). We have

$$P_+(H-H_0)P_+ = \begin{pmatrix} S & 0 \\ 0 & 0 \end{pmatrix},$$

$$S = \sqrt{I+WW^*}\Lambda_+\sqrt{I+WW^*} - W\Lambda_-W^* - \Lambda_+,$$

and thus the trace class property of $P_+(H-H_0)P_+$ is equivalent to the same for S. Without loss of generality we assume that $\pm\Lambda_\pm$ is positive definite. To get rid of matrix square roots we use a transformation introduced in [21]. We set

$$\nu = (I+\sqrt{I+WW^*})^{-1}W\,.$$

Then

$$\begin{gathered} W = 2(I-\nu\nu^*)^{-1}\nu, \qquad \|\nu\| < 1, \\ \sqrt{I+WW^*} = (I+\nu\nu^*)(I-\nu\nu^*)^{-1}, \end{gathered}$$

and hence

$$2\nu\nu^*\Lambda_+ + 2\Lambda_+\nu\nu^* - 4\nu\nu^*\Lambda_-\nu\nu^* = (I+\nu\nu^*)S(I+\nu\nu^*), \qquad (5.4)$$

where the right hand side is again of trace class. We need the following

Lemma 5.2 *Let*

$$Z = BA + AB + C$$

be of trace class, A,B,C Hermitian, A,C positive and B positive definite. Then A and C are of trace class also.

Proof. The equation

$$BA + AB = Z - C$$

with the unknown A has the unique solution

$$A = \int_0^\infty e^{-Bt}(Z - C)e^{-Bt}dt\,,$$

where the integral is absolutely convergent in the operator norm due to the positive definiteness of B. This may be written as

$$A + \int_0^\infty e^{-Bt}Ce^{-Bt}dt + \int_0^\infty e^{-Bt}Z_-e^{-Bt}dt = \int_0^\infty e^{-Bt}Z_+e^{-Bt}dt\,, \tag{5.5}$$

where $Z_\pm$ is the positive and negative part of Z, respectively. Both Z_+ and Z_- are again Hermitian, positive and of trace class. Here the right hand side is positive and of trace class since the function under the integral sign is obviously continuous and exponentially bounded in the trace norm. Since all terms on the left hand side of (5.5) are positive, we conclude that all of them and, in particular, A, must be of trace class. The same property for C is now obvious. **Q.E.D.**

We apply the above lemma to the formula (5.4) and obtain the trace class property of $\nu\nu^*$ or, equivalently, of WW^*. The case with P_- is analogous.

Q.E.D.

This result is applicable to operators with discrete spectrum. In this case $U^{-1}HU$ has an orthonormal eigenbasis e_k and $f_k = e_k + (U - I)e_k$ is an eigenbasis of H. Now, f_k is more than just Riesz basis, it is 'quadratically close to orthogonal' in the sense that $\sum_k \|f_k - e_k\|^2$ is finite and bounded by (5.1) (such bases are considered in [5], Ch. VI).

6 Klein-Gordon operators

A Klein-Gordon operator is given formally as

$$H = \begin{pmatrix} \epsilon^{1/2}V\epsilon^{-1/2} & \epsilon \\ \epsilon & \epsilon^{-1/2}V\epsilon^{1/2} \end{pmatrix},$$

where V is symmetric and ϵ is selfadjoint and positive definite (both V and ϵ may be unbounded). We assume that $\mathcal{D}(V) \supseteq \mathcal{D}(\epsilon)$ and

$$\|A\| < 1 \quad \text{for} \quad A = V\epsilon^{-1}. \tag{6.1}$$

Typically, the underlying space will be $L^2(R^n)^2$, ϵ^2 will be the selfadjoint realisation of $1 - \Delta$ and V will be a potential ([17]). The formal expression above is given a rigorous meaning as a product

$$H = \begin{pmatrix} \epsilon^{1/2} & 0 \\ 0 & \epsilon^{1/2} \end{pmatrix} \begin{pmatrix} A & I \\ I & A^* \end{pmatrix} \begin{pmatrix} \epsilon^{1/2} & 0 \\ 0 & \epsilon^{1/2} \end{pmatrix}$$

(this definition is equivalent with the pseudo-Friedrichs construction from [16]). Here every factor has a bounded inverse and thus

$$H^{-1} = \begin{pmatrix} \epsilon^{-1/2} & 0 \\ 0 & \epsilon^{-1/2} \end{pmatrix} \begin{pmatrix} -A^* & I \\ I & -A \end{pmatrix} \begin{pmatrix} (I - AA^*)^{-1} & 0 \\ 0 & (I - A^*A)^{-1} \end{pmatrix} \begin{pmatrix} \epsilon^{-1/2} & 0 \\ 0 & \epsilon^{-1/2} \end{pmatrix}.$$

Setting

$$J = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \qquad G = JH, \tag{6.2}$$

the operator G, given formally as

$$G = \begin{pmatrix} \epsilon & \epsilon^{-1/2} V \epsilon^{1/2} \\ \epsilon^{1/2} V \epsilon^{-1/2} & \epsilon \end{pmatrix},$$

is obviously selfadjoint and positive definite.[8] Ignoring the unboundedness of the operators involved, according to Theorem 4.1 we would take

$$D = \begin{pmatrix} \epsilon^{-1/2} & 0 \\ 0 & \epsilon^{-1/2} \end{pmatrix},$$

thus obtaining

$$\hat{G} = DGD = \begin{pmatrix} I & A^* \\ A & I \end{pmatrix}$$

with the condition number $\frac{1+\|A\|}{1-\|A\|}$. Thus, the condition number of a J-unitary U, with $U^{-1}HU$ jointly selfadjoint[9] would be bounded as

$$\kappa(U) \leq \sqrt{\frac{1+\|A\|}{1-\|A\|}} = \sqrt{\frac{1+\|V\epsilon^{-1}\|}{1-\|V\epsilon^{-1}\|}}, \tag{6.3}$$

thus improving the estimate

$$\kappa(U) \leq \frac{1}{1-\|V\epsilon^{-1}\|}$$

from [16]. The improvement is particularly strong when the denominators above approach zero.[10]

The plausibility of our argument comes from the fact that the key estimate (4.1) allows D's with arbitrary norms. This suggests a rigorous proof via a regularization step. For any $d > 0$ we approximate H by

$$H_d = \begin{pmatrix} \epsilon_d^{1/2} V_d \epsilon_d^{-1/2} & \epsilon_d \\ \epsilon_d & \epsilon_d^{-1/2} V_d^* \epsilon_d^{1/2} \end{pmatrix} = \begin{pmatrix} \epsilon_d^{1/2} & 0 \\ 0 & \epsilon_d^{1/2} \end{pmatrix} \begin{pmatrix} A & I \\ I & A^* \end{pmatrix} \begin{pmatrix} \epsilon_d^{1/2} & 0 \\ 0 & \epsilon_d^{1/2} \end{pmatrix},$$

$$\epsilon_d = f_d(\epsilon) \quad , \quad f_d(t) = \begin{cases} t, & t \leq d, \\ d, & t > d, \end{cases}$$

$$V_d = V\epsilon^{-1}\epsilon_d.$$

Now everything is bounded, our theory applies and the estimates above become rigorous (the fact that V_d is not symmetric makes no difficulty). The following facts are obvious

- H_d, H_d^{-1}, $G_d = JH_d$, G_d^{-1} are bounded and G_d is Hermitian and positive definite.
- $V_d\epsilon_d^{-1} = V\epsilon^{-1}$.
- $H_d^{-1} \to H^{-1} \quad , \quad d \to \infty$.

[8] A formulation of the Klein-Gordon operator using J of the form (1.3) leads to more complicated expressions ([15]). The underlying Hilbert space topology is not uniquely defined by the formal Klein-Gordon differential equation and this may lead to different predictions. Our present definition is based on the so-called *number norm*, which is natural for quantum mechanical interpretation ([17]).

[9] In accordance with our current terminology *jointly selfadjoint* means selfadjoint and commuting with J.

[10] The fact that the condition number may grow as the reciprocal of the square root of the distance to the 'non-definite' operators was observed in [20].

- The J-unitary U_d making H_d jointly Hermitian, is bounded as

$$\kappa(U_d) = \|\operatorname{sign} H_d\| \le \sqrt{\frac{1+\|A\|}{1-\|A\|}}\,.$$

Here the symbol $'\to'$ means the strong convergence of bounded operators. By the uniform bound above any spectral projection $E_d(\Delta)$ (Δ a Borel set) of H_d^{-1} is bounded as

$$\|E_d(\Delta)\| \le \sqrt{\frac{1+\|A\|}{1-\|A\|}}\,.$$

Now we are in a position to use classical result of Bade ([1], Th. 2.6), applied to H_d^{-1} (H_d^{-1} and H_d have the same spectral projections). Accordingly, H^{-1} (and therefore H) is scalar type operator and

$$\operatorname{sign} H_d \to \operatorname{sign} H^{-1} = \operatorname{sign} H\,,$$

due to the fact that zero is not an eigenvalue of H^{-1}. Furthermore, $J \operatorname{sign} H_d^{-1} = J \operatorname{sign} H_d$ is positive definite and this remains valid for the strong limit $J \operatorname{sign} H^{-1}$ (note that both J and $\operatorname{sign} H^{-1}$ are non-singular). So, according to Theorem 2.1 and Remark 2.2

$$U = (J \operatorname{sign} H^{-1})^{1/2}$$

is J-unitary and $U^{-1}H^{-1}U$ is jointly Hermitian, and therefore the inverse $U^{-1}HU$ is jointly selfadjoint. We summarize:

Theorem 6.1 *Let H be a Klein-Gordon operator satisfying (6.1). Then there exists a J-unitary U, satisfying (6.3) and such that $U^{-1}HU$ is jointly selfadjoint (J is defined by (6.2)).*

Note that the theorem above also gives the existence of U and the proof is independent of the one in [16].

Remark 6.2 The estimate (6.3) can be strengthened by replacing the expression $\|V\epsilon^{-1}\|$ by

$$\beta = \inf_{\alpha \text{ real}} \|(V-\alpha I)\epsilon^{-1}\|\,.$$

This is immediately seen from the formal expression

$$H = \alpha I + \begin{pmatrix} \epsilon^{1/2}(V-\alpha I)\epsilon^{-1/2} & \epsilon \\ \epsilon & \epsilon^{-1/2}(V-\alpha I)\epsilon^{1/2} \end{pmatrix}.$$

Thus, in our theorem above the condition in (6.1) can be replaced by the weaker one

$$\beta < 1\,.$$

The same approximation works with the trace results from Section 5 under the assumption that $\epsilon^{-1}V\epsilon^{-1}$ be of trace class. We omit the details.

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