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THE ROTATION OF EIGENVECTORS BY A PERTURBATION. III*

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Abstract. When a Hermitian linear operator is slightly perturbed, by how much can its invariant subspaces change? Given some approximations to a cluster of neighboring eigenvalues and to the corresponding eigenvectors of a real symmetric matrix, and given an estimate for the gap that separates the cluster from all other eigenvalues, how much can the subspace spanned by the eigenvectors differ from the subspace spanned by our approximations? These questions are closely related; both are investigated here. The difference between the two subspaces is characterized in terms of certain angles through which one subspace must be rotated in order most directly to reach the other. These angles unify the treatment of natural geometric, operator-theoretic and error-analytic questions concerning those subspaces. Sharp bounds upon trigonometric functions of these angles are obtained from the gap and from bounds upon either the perturbation (1st question) or a computable residual (2nd question). An example is included.

CONTENTS

Introduction. Given an invariant subspace of a Hermitian matrix and the corresponding invariant subspace of a perturbed matrix, the object is to bound the amount by which the two subspaces differ as a function of the magnitudes of the perturbation and of the gaps between appropriate parts of the spectra. This paper centers on four theorems of that sort. They will be referred to as the $\sin\theta$ theorem, the $\tan\theta$ theorem, the $\sin 2\theta$ theorem, and the $\tan 2\theta$ theorem. None of these theorems implies any of the others; each gives, under hypotheses of a particular form, the best possible bound on the angle between perturbed and unperturbed subspaces.

Theorems of the same sort were considered, along with other matters, in the earlier papers in this series (by Davis alone) [5], [6]. Our $\sin 2\theta$ and $\tan 2\theta$ theorems are extensions of Theorem 6.1 of [6]. The $\sin\theta$ and $\tan\theta$ theorems are of a new type. All four theorems are applicable for infinite- as well as finite-dimensional spaces.

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All four theorems assert bounds on trigonometric functions of the angle between two subspaces, expressed as norms of suitable operators. Whereas in the earlier papers such bounds could be asserted only upon these operators' bound norm, we are now able to do it for arbitrary unitary-invariant norms.

We have tried to give in § 1 and § 2 a statement of the problem which is more than just definitions and statement of results. Since the problem is of interest both for perturbation theory and for numerical analysis, we have tried to explain our formulations in terms natural to both motivations. We have also explained the significance of giving bounds for arbitrary unitary-invariant norms.

This discussion must be based on the geometry of a pair of subspaces. That topic has by now a considerable literature; nevertheless we give, in § 1 and § 3, a fairly self-contained exposition, with some new features. A major idea, both intuitively and computationally, is that of the "direct rotation" carrying one subspace to another. Section 4 treats extremal properties of this rotation; it includes the resolution of a problem left open in [3, Section 7]. Section 4 is not required for the rest of the paper.

The chief new idea in the proofs of the four main theorems is embodied in a simple inequality for binomials $AX - XB$. This is given separate treatment in § 5 because of its apparent independent interest.

The main theorems, stated in § 2, are proved in § 6–§ 7. This development is continued in § 8.

Most comparable eigenvector estimates in the literature (some significant papers are [16], [34], [10], [28]) differ from ours not only in notation but also in nature; they estimate only single eigenvectors, whereas we, like Swanson [30], estimate subspaces. We have tried to give, in § 9, a numerical example which will bring out the differences. The example is that used by Weinberger [34] to illustrate his eigenvector error bounds; our theorems also apply, in several different ways. This section can be read immediately after § 2.

Section 10 is devoted to open questions.

1. Introduction to the problem. Throughout the paper, $\mathscr{H}$ will denote a separable Hilbert space and its vectors will be denoted by x, y, etc.; the inner product of x with y, often written (x, y), will here be written y^*x. (On the other hand, $[x, y]$ will denote the linear subspace spanned by x and y.) It will usually not matter whether the space is real or complex, or whether its dimensionality is finite.

It also will usually not matter whether the reader chooses to regard the elements of $\mathscr{H}$ as column vectors. Furthermore, if he does, this does not oblige him to make any special choice of inner product. Thus $\mathscr{H}$ may have as elements complex n-component column vectors such as $x = (\xi_i)$ and $y = (\eta_i)$, with its inner product defined by the positive definite matrix (μ_{ij}): $y^*x = \sum_{i,j=1}^n \eta_i^* \mu_{ij} \xi_j$. One is still free to represent the linear functional y^* by a row vector in the usual way, although one must take for the jth component of y^*, not η_j^*, but $\sum_{i=1}^n \eta_i^* \mu_{ij}$. We shall sometimes insist that we are talking about matrices rather than operators, but we shall never insist that our operators are *not* matrices.

The subject throughout will be a bounded Hermitian operator A acting upon $\mathscr{H}$, together with a modified Hermitian operator $A + H$, where H will usually be thought of as small. The results and proofs also apply to unbounded self-adjoint A, provided the domain of H contains that of A. (Some of the results are vacuous when certain norms fail to exist, but we shall not need to make special mention of this.) We shall consider a subspace spanned by several eigenvectors of A. More generally, in the infinite-dimensional case where A need not have any eigenvectors but must have plenty of reducing subspaces, we shall be considering such a subspace. The customary way to specify such a subspace is by its projector; thus we write P for an operator such that $P^2 = P = P^*$ and $AP\mathscr{H} \subseteq P\mathscr{H}$. Extreme cases are the zero operator 0 and the identity operator 1, but these are not interesting. The projector complementary to a given P can be written $1 - P$ or $\tilde{P}$. Similar notations are used for projectors Q onto reducing subspaces of $A + H$.

Even the finite-dimensional reducing subspaces, which could be specified by lists of eigenvectors, may be more naturally specified by their projectors, if only to avoid the familiar predicament of not knowing which basis to use. When we do have an orthonormal basis $\{u_1, \cdots, u_m\}$ of a subspace, the projector P upon it may be written $P = \sum_1^m u_k u_k^*$ (whether or not the u_k are eigenvectors), and this extends to subspaces of countably infinite dimensionality.

Having fixed a reducing subspace $P\mathscr{H}$ of A, we shall study $A + H$ and other operators in terms of the orthogonal decomposition of $\mathscr{H}$ into $P\mathscr{H}$ and $\tilde{P}\mathscr{H}$. Let us explain the notation separately to the operator theorist and to the numerical analyst now, though we subsequently speak to both in the same terms.

First, viewing $\mathscr{H}$ as an arbitrary Hilbert space, we shall be systematically expressing every $x \in \mathscr{H}$ as $Px + \tilde{P}x$. However, we prefer to deal with pairs of vectors $\begin{pmatrix} x_0 \\ x_1 \end{pmatrix}$, not only so that familiar matrix ideas can be invoked, but also to avoid an inconvenient ambiguity: when we discuss (say) PAP, it seems to have all of $\tilde{P}\mathscr{H}$ as null vectors, but what really matters of its spectrum is the spectrum of its restriction to $P\mathscr{H}$. Consequently we define $E_0 : \mathscr{K}(E_0) \to \mathscr{H}$ and $E_1 : \mathscr{K}(E_1) \to \mathscr{H}$, isometric mappings of new Hilbert spaces into $\mathscr{H}$, having ranges $E_0\mathscr{K}(E_0) = P\mathscr{H}$ and $E_1\mathscr{K}(E_1) = \tilde{P}\mathscr{H}$. (Here we have introduced the notation $\mathscr{K}(\cdot)$ for the "source space" of an isometry. Later we shall also use the notations $\mathscr{N}(\cdot)$ for null space and $\mathscr{R}(\cdot)$ for range; $\mathscr{K}(E_j) = \mathscr{R}(E_j^*)$.) Now $E_0E_0^* = P$ and $E_1E_1^* = \tilde{P}$; on the other hand, $E_0^*E_0$ is the identity operator on $\mathscr{K}(E_0)$, $E_1^*E_0$ is the zero transformation on $\mathscr{K}(E_0)$ to $\mathscr{K}(E_1)$, and so on. Now we can write $x_0 = E_0^*x$, $x_1 = E_1^*x$ and

$$x = (E_0 \quad E_1)\begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = E_0x_0 + E_1x_1 \tag{1.1}$$

if we want to; or we can simply say x is represented by $\begin{pmatrix} x_0 \\ x_1 \end{pmatrix}$. Clearly $(E_0 \quad E_1)$ is an isometry onto $\mathscr{H}$, and $(E_0 \quad E_1)^{-1} = \begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix}$.

The corresponding notation for operators is

$$A = (E_0 \quad E_1)\begin{pmatrix} A_0 & 0 \\ 0 & A_1 \end{pmatrix}\begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix}, \qquad H = (E_0 \quad E_1)\begin{pmatrix} H_0 & B^* \\ B & H_1 \end{pmatrix}\begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix}. \tag{1.2}$$

These equations define the new operators appearing in them; for instance, $B = E_1^* H E_0$, an operator from $\mathscr{K}(E_0)$ to $\mathscr{K}(E_1)$.

The A_j and H_j are automatically Hermitian. Equations like (1.1) and (1.2) can be written more clearly if we agree that the sign $\simeq$ is to be read as "is represented by". Then we write

$$x \simeq \begin{pmatrix} x_0 \\ x_1 \end{pmatrix}, \quad A \simeq \begin{pmatrix} A_0 & 0 \\ 0 & A_1 \end{pmatrix}, \quad P \simeq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

and so on. The usual rules of matrix multiplication apply; for example,

$$PAP \simeq \begin{pmatrix} A_0 & 0 \\ 0 & 0 \end{pmatrix}$$

(and neither member here is the same as A_0).

When we decompose $\mathscr{H}$ according to a reducing subspace $Q\mathscr{H}$ of $A + H$ instead, then we shall want to define new isometries $F_0 : \mathscr{K}(F_0) \to \mathscr{H}$ and $F_1 : \mathscr{K}(F_1) \to \mathscr{H}$, with $F_0 F_0^* = Q$ and $F_1 F_1^* = \tilde{Q} = 1 - Q$. Now the notion of representing operators on $\mathscr{H}$ by 2×2 block matrices becomes treacherous, because there are more ways than one to represent them. The two ways of representing $A + H$ are

$$(1.3) \quad A + H = (E_0 \quad E_1) \begin{pmatrix} A_0 + H_0 & B^* \\ B & A_1 + H_1 \end{pmatrix} \begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix} = (F_0 \quad F_1) \begin{pmatrix} \Lambda_0 & 0 \\ 0 & \Lambda_1 \end{pmatrix} \begin{pmatrix} F_0^* \\ F_1^* \end{pmatrix}.$$

Nothing has been said about diagonalizing A_0 or Λ_0; choice of coordinate system in their respective spaces has not come up. No demand has been made that the reducing projectors P and Q be spectral projectors either; that is, so far A_0 may have spectrum in common with A_1, or Λ_0 with Λ_1.

In a limited sense, though, (1.3) expresses that $A + H$ has been diagonalized: P, or $(E_0 \quad E_1)$, afforded a representation of A as a diagonal 2×2 block matrix (1.2), and passing to Q, or $(F_0 \quad F_1)$, affords a representation of $A + H$ as a diagonal 2×2 matrix. See Fig. 1.

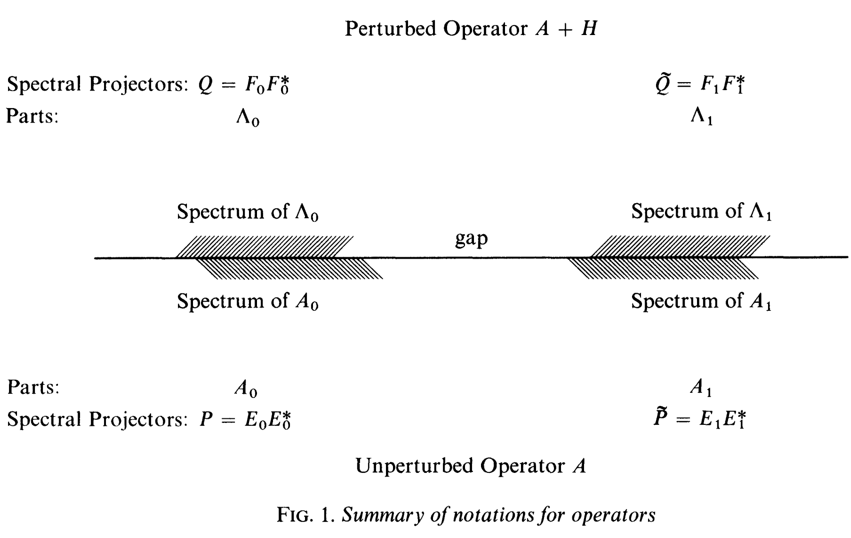

FIG. 1. *Summary of notations for operators*

To formulate the desired conclusion, that the subspaces $P\mathscr{H}$ and $Q\mathscr{H}$ are close, we must see how one can be changed to the other by a unitary transformation. The unitaries V in question, then, will be those such that

$$VP = QV, \qquad V\tilde{P} = \tilde{Q}V \tag{1.4}$$

(the second equality is a consequence of the first). This means first of all that the dimensions must agree:

$$\dim P\mathscr{H} = \dim Q\mathscr{H}, \qquad \dim \tilde{P}\mathscr{H} = \dim \tilde{Q}\mathscr{H} \tag{1.5}$$

(the second equality is a consequence of the first if $\dim P\mathscr{H}$ is finite). Given (1.5), there surely exist solutions of (1.4).

Now (1.4) is equivalent to $VE_jE_j^* = F_jF_j^*V$. Define $W_j : \mathscr{H}(E_j) \to \mathscr{H}(F_j)$ by $W_j = F_j^*VE_j$. It is an isometry onto, because

$$W_j^*W_j = E_j^*V^*F_jF_j^*VE_j = E_j^*V^*VE_jE_j^*E_j = (E_j^*E_j)^2 = 1,$$

and similarly $W_jW_j^* = 1$. Conversely, if the W_j are any two such isometries onto then $V = F_0W_0E_0^* + F_1W_1E_1^*$ satisfies (1.4) and is related to the W_j in the same way. In words, any two unitary operators on $\mathscr{H}$ which take $P\mathscr{H}$ onto $Q\mathscr{H}$ differ only by unitary transformation within the coordinate subspaces.

We shall want names for the entries in the block matrix representation of V:

$$V \simeq \begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix}. \tag{1.6}$$

One computes

$$\begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix} = \begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix} V(E_0 \quad E_1) = \begin{pmatrix} E_0^*F_0 & E_0^*F_1 \\ E_1^*F_0 & E_1^*F_1 \end{pmatrix}\begin{pmatrix} W_0 & 0 \\ 0 & W_1 \end{pmatrix}. \tag{1.7}$$

Now a measure of how much $P\mathscr{H}$ differs from $Q\mathscr{H}$ should be a measure of how much this V must differ from the identity. But before pursuing this, we want to recapitulate our notation with interpretations suited to numerical analysis.

A numerical analyst, charged with the computation of (some) eigenvalues and eigenvectors of a Hermitian operator, frequently proceeds via a sequence of successively more refined approximations. At a typical stage in such a process, the following information will be before him. First, the operator itself. This is $A + H$ in our notation, and we do not care whether it is given as a matrix (in which case elements of $\mathscr{H}$ are column vectors), as an integral operator (in which case elements of $\mathscr{H}$ are functions), or whatever. The terms A and H will be separated from $A + H$ later. Second, the analyst has some putative eigenvectors $e_1, e_2, \cdots, e_m$. (We shall usually assume that these are exactly orthonormal.) They may not be *all* the putative eigenvectors he has computed at that step; they may just be a subset associated with closely bunched eigenvalues. In particular, m may be 1. Third, the analyst may compute the vectors $(A + H)e_j$ and their components $e_i^*(A + H)e_j$, should he need them.

Here is how we subsume this in our formulation. Let E_0 above be the row $(e_1 e_2 \cdots e_m)$, and let E_0^* be the column

$$\begin{pmatrix} e_1^* \\ e_2^* \\ \cdot \\ \cdot \\ e_m^* \end{pmatrix}.$$

This means a special choice of the space $\mathscr{K}(E_0)$; namely, it must be the m-space of m-component column vectors with the usual inner product. Our notation for this space will be $\mathbf{R}^m$. (If the given operator $A + H$ is an $n \times n$ matrix, so that $\mathscr{H}$ is $\mathbf{R}^n$, then each e_j is an n-component column vector, so E_0 is an $n \times m$ matrix.) The matrix of the $e_i^*(A + H)e_j$ is accordingly $E_0^*(A + H)E_0$, which is what we called $A_0 + H_0$ above.

What the numerical analyst has in mind, but has not computed yet, are of course m exact eigenvectors $f_1, \cdots, f_m$, again orthonormal, and their corresponding eigenvalues $\lambda_1, \cdots, \lambda_m$. This will be represented by $(A + H)F_0 = F_0\Lambda_0$ if we use the same treatment as for the e_j; let $\mathscr{K}(F_0)$ also be $\mathbf{R}^m$, so that F_0 is the row $(f_1 \cdots f_m)$, and let $\Lambda_0 = \operatorname{diag}(\lambda_1, \cdots, \lambda_m)$.

Now $P = E_0E_0^* = \sum_1^m e_je_j^*$ and $Q = F_0F_0^* = \sum_1^m f_jf_j^*$. The problem of error bounds for the eigenspace is just this: how far is $P\mathscr{H}$ from $Q\mathscr{H}$?

It may seem that one should ask, how far is e_j from $f_j, j = 1, \cdots, m$? This apparently natural alternative is not a well-defined question if all the λ_j are equal; and if they are very closely bunched, that question becomes unstable because of the sensitivity of the f_j to small perturbations in the given operator, whereas our problem still makes sense.

The numerical analyst also chooses, at each step, an $m \times m$ matrix intended to have eigenvalues approximating $\lambda_1, \cdots, \lambda_m$; this we call A_0. From this is computed the residual

$$R = (A + H)E_0 - E_0A_0 \tag{1.8}$$

(if $E_0 = F_0$ and $A_0 = \Lambda_0$ then $R = 0$).

Any choice of A_0 which makes R small will give good approximate eigenvalues. More explicitly, let the eigenvalues of A_0 in some order be $\alpha_1, \cdots, \alpha_m$ (since m is relatively small, think of these also as easily computable). Kahan has shown [15] that then there exists an ordered m-tuple $(\lambda_1, \cdots, \lambda_m)$ of eigenvalues of $A + H$ such that $\sum_1^m (\alpha_j - \lambda_j)^2 \leqq \|R\|_{\text{sq}}^2 \equiv \operatorname{tr} R^*R$ and $|\alpha_j - \lambda_j| \leqq \|R\|_1$ (bound norm) for $j = 1, \cdots, m$.

Thus in the numerical-analytic interpretation of the problem of rotation of eigenspaces, though the same operator-theoretic notation can be followed, there is a slight difference which will bear on the statements of our theorems. Instead of comparing a given operator $A + H$ to a simpler operator A on the same space and saying that the difference H between the two is small, we compare the given operator to an operator A_0 on a space of lower dimension and say that the residual R is small. In our notation A_0 is isometric-equivalent to a part of A (see (1.2)), and the numerical analyst would rather talk about that part than about A_1, which he does not compute. Similarly, R is essentially that part of the perturbation H which he does compute. To see the point of the notation better, the reader may want to check formally from (1.3) and (1.8) that R, left-multiplied by the isometry $\begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix}$, gives the first column of $\begin{pmatrix} H_0 & B^* \\ B & H_1 \end{pmatrix}$, which represents H (see (1.2)); or that $R = HE_0$.

In two of our main theorems we shall make hypotheses that the perturbation is off-diagonal. In one theorem, this means the strong assertion that both the H_j are zero; but the numerical analyst might prefer that nothing be said about the southeast corners of our block matrices; accordingly, another theorem has as its hypothesis of off-diagonality only $H_0 = 0$. It is a natural hypothesis because it means that, from the given $A + H$ and the computed vectors E_0, he obtains his A_0 by the simple rule $A_0 = E_0^*(A + H)E_0$, which is the $m \times m$ generalization of what, for $m = 1$, is known as the Rayleigh quotient. This is often a good choice, particularly in view of the fact that $R^*R = H_0^2 + B^*B$, so that the size of R is minimized when H_0 is taken to be zero. In the operator-theoretic interpretation of the problem we are less likely to have the option of declaring an H_j to be zero.

The measures we have chosen to use for magnitudes of operators are arbitrary unitary-invariant norms. There are three good surveys [12, Chaps. II-III], [21], [25] of the theory of such norms. However, we think it will be convenient to collect here some of the leading points.

The symbol $\|\cdot\|$, applied to bounded operators K from one Hilbert space to the same or another Hilbert space, stands for a norm which, beside having the usual properties

$$\|K\| \geqq 0,$$
$$\|K\| = 0 \Leftrightarrow K = 0,$$
$$\|\lambda K\| = |\lambda|\|K\|,$$
$$\|K + L\| \leqq \|K\| + \|L\|,$$

is unitary-invariant in the sense that

$$\|VKW\| = \|K\| \tag{1.9}$$

whenever V and W are unitary operators (on the respective spaces).

Normalization. We assume that $\|uv^*\| = \|u\| \cdot \|v\|$ for the operator uv^* of rank 1. (If this holds for one choice of nonzero u and v, it holds for all.)

Compatibility. If W is a contraction ($\|Wx\| \leqq \|x\|$ for all x) and V is a contraction, then $\|VKW\| \leqq \|K\|$. This follows easily from (1.10) below.

We recall that, for compact K, the "singular values" $\kappa_1 \geqq \kappa_2 \geqq \cdots$ of K are the square roots of the eigenvalues of K^*K. These are the same as the eigenvalues of KK^*, except perhaps for striking out a certain number of zeros. Now it follows from (1.9) that for any unitary-invariant norm, the value of $\|K\|$ depends only on the nonzero singular values of K.

Minimax characterization of singular values.

$$\kappa_k = \inf_{\mathscr{X}} \sup_x \|Kx\|, \tag{1.10}$$

where the infimum is over $(k-1)$-dimensional subspaces $\mathscr{X}$ of the domain space, and the supremum is over unit vectors $x \perp \mathscr{X}$. In particular, κ_1 is equal to the bound norm of K, which we write $\|K\|_1$, and we could write instead of (1.10) that $\kappa_k = \inf \|K|_{\mathscr{X}^\perp}\|_1$. These formulations are applicable to general bounded operators, not only compact ones, but for noncompact operators it might be more appropriate to deal instead with the spectral multiplicity function [13] of K^*K. Although we shall not assume our operators compact in most of this paper, we believe the most important applications are to compact operators.

Every unitary-invariant norm is obtained as a "symmetric gauge function" of the singular values; the converse also holds. For the details, see the references cited.

One of the most tractable of these norms is the Hilbert-Schmidt norm or square norm $\|\cdot\|_{sq}$: $\|K\|_{sq}^2 = \sum_k \kappa_k^2 = \operatorname{tr} K^*K$.

Particular unitary-invariant norms are

$$\|K\|_\nu = \kappa_1 + \kappa_2 + \cdots + \kappa_\nu, \qquad \nu = 1, 2, \cdots, \tag{1.11}$$

the sums of the ν highest singular values (whether or not there are that many nonzero ones). These include the bound norm $\|\cdot\|_1$. The norms (1.11) play a distinguished role: K and L being two operators, the inequality $\|K\| \leqq \|L\|$ holds for arbitrary unitary-invariant norms if and only if it holds for all the norms $\|\cdot\|_\nu$ (theorem of Ky Fan [12, Chap. III, Section 3]).

The following analogue of the Rayleigh–Ritz principle therefore becomes interesting:

$$\|K\|_\nu = \sup_\Omega \|K\Omega\|_\nu, \tag{1.12}$$

the supremum being over all projectors Ω onto ν-dimensional subspaces. For $\nu = 1$ this is evident, but even for higher ν it is readily reduced to familiar statements. We shall also use the alternative form

$$\|K\|_\nu = \sup_{\Omega,\Upsilon} \|\Upsilon K \Omega\|_\nu = \sup \operatorname{Re} \sum_{k=1}^{\nu} y_k^* K x_k, \tag{1.13}$$

the first supremum being over pairs of ν-projectors Ω, Υ, and the second supremum being over all orthonormal ν-tuples $\{x_1, \cdots, x_\nu\}$ and all orthonormal ν-tuples $\{y_1, \cdots, y_\nu\}$.

Extending error bounds to norms other than the bound norm improves them significantly. Saying an operator is smaller than ε everywhere is good if you can do it, but it may be more important and/or more feasible to say that it is smaller than $\varepsilon/10$ except on a subspace of small dimensionality. This sort of assertion involves the other unitary-invariant norms. On the other hand, we have not attempted extension of our theorems to norms other than the unitary-invariant. They seemed less interesting to us because they are less natural geometrically, although admittedly some of them are very convenient to evaluate in an adapted coordinate system.

Our measures of the amount of difference between the two subspaces $P\mathscr{H}$ and $Q\mathscr{H}$ will be unitary-invariant norms of suitable trigonometric functions of the angle Θ between them. This angle Θ will be a Hermitian operator. If we bound just its bound norm, we express that $P\mathscr{H}$ cannot have any unit vector too far from $Q\mathscr{H}$. But one may want to know whether *several different* vectors of $P\mathscr{H}$ have far to go to $Q\mathscr{H}$. It is to deal with this that we apply arbitrary unitary-invariant norms and an operator angle.

First, for nonzero vectors x and y the natural definition of angle is just the number

$$\angle(x, y) = \arc\cos \frac{\operatorname{Re}(y^*x)}{\|x\| \, \|y\|}. \tag{1.14}$$

This agrees with elementary definitions (in particular, $\angle(x, -x) = \pi$), and it preserves the useful formula

$$\|x + y\|^2 = \|x\|^2 + \|y\|^2 + 2\|x\| \, \|y\| \cos \angle(x, y).$$

But if we speak of the angle between their subspaces $[x] = xx^*\mathscr{H}$ and $[y] = yy^*\mathscr{H}$, we should mean something depending only on the subspaces themselves, and we can use again a number: $\inf \angle(u, v)$ taken over nonzero $u \in [x]$ and $v \in [y]$, which is equal to

$$\arc\cos \frac{|y^*x|}{\|x\| \, \|y\|}. \tag{1.15}$$

(If $y = -x$, this comes out 0 instead of π.)

For our more general P and Q, we want again something not dependent on choice of vectors within the subspaces. The entries C_j and S_j appearing in (1.6) are not determined by P and Q (not even up to unitary equivalence). We required that V map $P\mathscr{H}$ isometrically onto $Q\mathscr{H}$, but we did not say by which isometry, and similarly for $\tilde{P}\mathscr{H}$. To remove the leeway remaining is to specify a unitary operating within each of the coordinate subspaces—in the notation (1.7), to fix W_0 and W_1. As the W_j vary, the singular values of the C_j and S_j do not, because the $C_j^*C_j$ and the $S_j^*S_j$ are transformed by unitaries. Better yet, the $C_jC_j^*$ and $S_jS_j^*$ do not change at all. (This asymmetry of behavior is an artifact of our notation (1.7).) How appealing, then, to define operators

$$\Theta_j \equiv \arc\cos (C_jC_j^*)^{1/2} \geqq 0, \qquad j = 0, 1, \tag{1.16}$$

in more or less immediate extension of (1.15); to define further an operator $\Theta \geqq 0$ upon $\mathscr{H}$ by

$$\Theta \simeq \begin{pmatrix} \Theta_0 & 0 \\ 0 & \Theta_1 \end{pmatrix}; \tag{1.17}$$

and to use norms of one or other of these operators as measures of the difference between the subspaces. This works, in fact, with the modification that we shall bound not Θ nor Θ_j, but trigonometric functions thereof.

One of these trigonometric functions is already before us; the sine. Our S_0 is not exactly $\sin \Theta_0$, because it maps into the wrong space, but it is $\sin \Theta_0$ followed by an isometry, so $\|S_0\| = \|\sin \Theta_0\|$ for every unitary-invariant norm, and they have the same singular values $\sin \theta_1 \geqq \sin \theta_2 \geqq \cdots$. Here $\theta_1 \geqq \theta_2 \geqq \cdots$ are the singular values of Θ_0. It will appear that the nonzero singular values of Θ are the same, but each occurs twice: $\theta_1, \theta_1, \theta_2, \theta_2, \cdots$.

We collect here for reference, without proofs, the expressions in terms of Θ of several natural measures of difference between the subspaces $P\mathscr{H} = \mathscr{R}(E_0)$ and

$Q\mathscr{H} = \mathscr{R}(F_0)$:

$$\sup\{\|Qp - p\| : \|p\| = 1, p = Pp\} = \|\sin\Theta\|_1,$$

$$\sup\{\inf\{\|q - p\| : \|q\| = 1, q = Qq\} : \|p\| = 1, p = Pp\}$$
$$= 2\|\sin\tfrac{1}{2}\Theta\|_1,$$

$$\|\tilde{Q}P\| = \|\tilde{Q}E_0\| = \|\sin\Theta_0\| \qquad \text{(all norms)},$$

$$\|P - Q\| = \|\sin\Theta\| \qquad \text{(all norms)}.$$

One can make (1.6) look even more like the familiar matrix $\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$ of a rotation through angle θ in $\mathbf{R}^2$. Indeed we shall show in § 3 how to choose a partial isometry $J \simeq \begin{pmatrix} 0 & -J_0^* \\ J_0 & 0 \end{pmatrix}$, which plays the role of $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ or of the imaginary unit, so that

$$U \equiv \exp(J\Theta) = \cos\Theta + J\sin\Theta \simeq \begin{pmatrix} \cos\Theta_0 & -J_0^*\sin\Theta_1 \\ J_0\sin\Theta_0 & \cos\Theta_1 \end{pmatrix} \tag{1.18}$$

will be one of the unitaries (1.6) taking $P\mathscr{H}$ to $Q\mathscr{H} = UP\mathscr{H}$. The virtue of this U, the "direct rotation" of $P\mathscr{H}$ to $Q\mathscr{H}$, is not merely to make S_0 appear explicitly as something resembling a sine; it has much richer geometric significance: of all unitary V taking $P\mathscr{H}$ to $Q\mathscr{H} = VP\mathscr{H}$, the choice $V = U$ turns out to differ least from the identity. (See Section 4.) But U is not mentioned in our main theorems, which all pertain only to the numbers $\theta_1, \theta_2, \cdots$ via the norms of trigonometric functions of Θ and Θ_0.

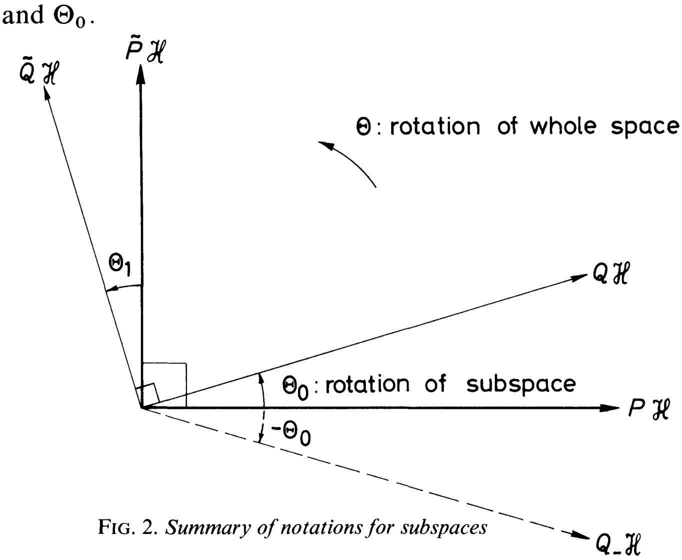

FIG. 2. *Summary of notations for subspaces*

2. Statement of the theorems.

THE SIN θ THEOREM. *Assume there is an interval $[\beta, \alpha]$ and a $\delta > 0$ such that the spectrum of A_0 lies entirely in $[\beta, \alpha]$ while that of Λ_1 lies entirely outside of $]\beta - \delta, \alpha + \delta[$ (or such that the spectrum of Λ_1 lies entirely in $[\beta, \alpha]$ while that of A_0 lies entirely outside of $]\beta - \delta, \alpha + \delta[$). Then for every unitary-invariant norm, $\delta\|\sin\Theta_0\| \leqq \|R\|$.*

(The hypotheses can be relaxed. In Theorem 6.1 below we give a more definitive formulation.)

We know that some kind of gap has to be hypothesized between spectra of parts of the operators in order for any closeness of eigenspaces to be concluded. In the past, it has been usual to require a gap between parts of a single operator, say between A_0 and A_1. (But see [5, Theorem 3.2] for an exception.) Here a part of A is separated from a part of $A + H$. Note also that the spectrum of Λ_1 is allowed to lie both above and below the spectrum of A_0.

This last advantage is lost in the following theorem, in which we make an off-diagonality hypothesis and gain a slight improvement in our bound. That is, the improvement is slight if all angles are small; in exceptional applications it might be important.

THE TAN θ THEOREM. *Assume there is an interval* $[\beta, \alpha]$ *and a* $\delta > 0$ *such that the spectrum of* A_0 *lies entirely in* $[\beta, \alpha]$ *while that of* Λ_1 *lies entirely in* $[\alpha + \delta, \infty[$. *Assume further that* $H_0 = 0$. *Then for every unitary-invariant norm,* $\delta\|\tan \Theta_0\| \leqq \|R\|$, $\delta\|\tan \Theta\| \leqq \|H\|$.

Now these two theorems answer most directly the numerical analyst's problem set forth in § 1; and the proofs below will make them seem like the central ones. Still, to the operator theorist it may look more natural to hypothesize as usual a gap in spectrum between A_0 and A_1, or between Λ_0 and Λ_1. We obtain close analogues of the first two theorems.

THE SIN 2θ THEOREM. *Assume there is an interval* $[\beta, \alpha]$ *and a* $\delta > 0$ *such that the spectrum of* Λ_0 *lies entirely in* $[\beta, \alpha]$ *while that of* Λ_1 *lies entirely outside of* $]\beta - \delta, \alpha + \delta[$. *Then for every unitary-invariant norm,* $\delta\|\sin 2\Theta_0\| \leqq 2\|R\|$, *and* $\delta\|\sin 2\Theta\| \leqq 2\|H\|$.

Just as before, a slight improvement in the bound results from an off-diagonality requirement, which now, however, must be imposed on $\tilde{P}\mathscr{H}$, not only on $P\mathscr{H}$.

THE TAN 2θ THEOREM. *Assume there is an interval* $[\beta, \alpha]$ *and a* $\delta > 0$ *such that the spectrum of* A_0 *lies entirely in* $[\beta, \alpha]$ *while that of* A_1 *lies entirely in* $[\alpha + \delta, \infty[$. *Assume further that* $H_0 = 0$, $H_1 = 0$. *Then for every unitary-invariant norm,* $\delta\|\tan 2\Theta_0\| \leqq 2\|R\|$, *and* $\delta\|\tan 2\Theta\| \leqq 2\|H\|$.

It was mentioned earlier that the constants in all four theorems are best possible; this is seen from the 2-dimensional case. Furthermore, one sees by taking a direct sum of 2-dimensional examples that, in any one of the theorems, equality in the conclusion can be attained simultaneously for all unitary-invariant norms.

One observes with no surprise that, if the perturbation H depends linearly upon a real parameter ε, then for $\varepsilon \to 0$ the conclusions of the four theorems are asymptotically the same.

Unbounded self-adjoint operators, important in several applications, are covered by our theorems or slight extensions thereof, although we must assume H or R bounded to draw useful inferences. The theorems above contain references to a finite interval $[\beta, \alpha]$; they remain valid after this interval is extended to $]-\infty, \alpha]$ and $]\beta - \delta, \alpha + \delta[$ to $]-\infty, \alpha + \delta[$. As long as the spectra of A_i and Λ_i satisfy their respective hypotheses concerning the gap δ, they may be otherwise unbounded without invalidating the theorems. However, to free our theorems from all inessential boundedness hypotheses, we have had to complicate the proofs substantially.

These complications have been confined to two passages—Theorem 5.2, and the Appendix to § 6—in order to avoid distracting those readers not concerned with the utmost generality.

3. Separation of two subspaces. In this section, A and $A + H$ are ignored. Attention is on the two projectors $P = E_0E_0^*$ and $Q = F_0F_0^*$. We shall construct an operator Θ embodying a complete set of unitary invariants for the pair P, Q, and an operator U giving a canonical choice of unitary mapping $P\mathscr{H}$ to $Q\mathscr{H}$. The two problems are closely related.

Notations and hypotheses of § 1 are conserved. Note that the symbol "$\simeq$" always means representation in terms of the decomposition by E_0 and E_1, never in terms of F_0 and F_1. Thus $P \simeq \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, whereas

$$Q = F_0F_0^* \simeq \begin{pmatrix} E_0^*F_0F_0^*E_0 & E_0^*F_0F_0^*E_1 \\ E_1^*F_0F_0^*E_0 & E_1^*F_0F_0^*E_1 \end{pmatrix}, \tag{3.1}$$

and similarly for $\tilde{Q} = F_1F_1^*$.

We have already remarked that the operator V of (1.4) and (1.6) is not determined uniquely; but we proved the relation (1.7) and noted as a consequence that the $C_jC_j^*$ and $S_jS_j^*$ *are* determined by P and Q. We defined $\theta_1, \theta_2, \cdots$ as the singular values, in descending order, of $\Theta_0 \equiv \arccos(C_0C_0^*)^{1/2}$; but we have not yet elucidated the way they appear in V. To do this, we write out the assumption that V is unitary:

$$V^*V \simeq \begin{pmatrix} C_0^*C_0 + S_0^*S_0 & -C_0^*S_1 + S_0^*C_1 \\ -S_1^*C_0 + C_1^*S_0 & S_1^*S_1 + C_1^*C_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.2}$$

$$VV^* \simeq \begin{pmatrix} C_0C_0^* + S_1S_1^* & C_0S_0^* - S_1C_1^* \\ S_0C_0^* - C_1S_1^* & S_0S_0^* + C_1C_1^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.3}$$

By a well-known general theorem (e.g., [12, Chap. I, Section 1.4] or [17, p. 334]), $C_0^*C_0$ and $C_0C_0^*$ become isometric-equivalent operators if restricted to the orthogonal complement of their null spaces. Now $\mathscr{N}(C_0^*C_0) = \mathscr{N}(C_0)$ is the eigenspace of $S_0^*S_0 = 1 - C_0^*C_0$ belonging to eigenvalue 1; similarly for $\mathscr{N}(C_0C_0^*)$ in relation to $S_1S_1^*$. The nonzero singular values of S_0, which are seen immediately from definitions to be equal to $\sin\theta_1, \sin\theta_2, \cdots$, will be the same as those of S_1^* (hence of S_1), unless $\dim \mathscr{N}(C_0) \neq \dim \mathscr{N}(C_0^*)$, in which case they will differ by beginning with strings of 1's of different lengths. This case will be excluded in most of the paper.

DEFINITION 3.1. A unitary solution $V \simeq \begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix}$ of $VP = QV$ will be called a *direct rotation* from $P\mathscr{H}$ to $Q\mathscr{H}$ if it satisfies the following additional conditions:

(i) $C_0 \geqq 0$, $C_1 \geqq 0$;
(ii) $S_1 = S_0^*$.

The symbol U will be reserved for direct rotations.

DEFINITION 3.2. Subspaces $P\mathscr{H}$ and $Q\mathscr{H}$ are said to be in *the acute case* if $P\mathscr{H} \cap \tilde{Q}\mathscr{H}$ and $\tilde{P}\mathscr{H} \cap Q\mathscr{H}$ are zero.

PROPOSITION 3.1. *In the acute case the direct rotation exists, is unique, and is characterized by property* (i) *alone.*

Proof. Under our hypothesis of equality of dimension (1.5), there surely exists some V with $VP = QV$. We write the polar resolution $C_0 = (C_0C_0^*)^{1/2}Z_0$, where Z_0 is a uniquely determined isometry from $\mathscr{R}(C_0^*)^-$ onto $\mathscr{R}(C_0)^-$. (The bar denotes closure.) To prove Z_0 is actually a unitary on $\mathscr{K}(E_0)$ we must show that C_0 and C_0^* have zero null space. Suppose $x_0 \in \mathscr{N}(C_0)$, and let $x \simeq \begin{pmatrix} x_0 \\ 0 \end{pmatrix}$. Then $x \in P\mathscr{H}$, which is taken to $Q\mathscr{H}$ by V, and on the other hand

$$Vx \simeq \begin{pmatrix} C_0x_0 \\ S_0x_0 \end{pmatrix} = \begin{pmatrix} 0 \\ S_0x_0 \end{pmatrix}.$$

Thus $Vx \in Q\mathscr{H} \cap \tilde{P}\mathscr{H}$, which is zero by hypothesis; hence $x = 0$. This proves $\mathscr{N}(C_0)$ is zero. If, on the other hand, $x_0 \in \mathscr{N}(C_0^*)$, then $V^*x \in \tilde{P}\mathscr{H}$ as before; since $\tilde{P}\mathscr{H}$ is taken to $\tilde{Q}\mathscr{H}$ by V, we have $x = VV^*x \in P\mathscr{H} \cap \tilde{Q}\mathscr{H}$. This proves $\mathscr{N}(C_0^*)$ is zero.

Now do the same for C_1, getting $C_1 = (C_1C_1^*)^{1/2}Z_1$.

Starting from our arbitrary solution V of (1.4) we can obtain a direct rotation U as $U = VZ^{-1}$, where $Z \simeq \begin{pmatrix} Z_0 & 0 \\ 0 & Z_1 \end{pmatrix}$. U is unitary because V and Z are; U satisfies (1.4) because V does and P reduces Z^{-1}. We have constructed U so as to satisfy (i). Uniqueness is also clear, because of the uniqueness of the polar resolutions of operators with zero null space.

It remains to prove (ii). In doing so, we may simplify the notation by starting with $V = U$, i.e., $C_j \geqq 0$, $Z_j = 1$ (for we have proved our U has the properties V had). From (3.2) and (3.3), we have

$$C_0S_1 = S_0^*C_1, \qquad C_0S_0^* = S_1C_1. \tag{3.4}$$

Eliminating S_0^* gives $C_0^2S_1 = S_1C_1^2$. From this we deduce that $f(C_0^2)S_1 = S_1f(C_1^2)$ for all polynomials f, hence also for f any continuous real function on $[0, 1]$. Choosing f to be the square root function, we deduce that $C_0S_1 = S_1C_1$. Comparing this with the first of equations (3.4) shows that S_1 and S_0^* must agree on the range of C_1. But we saw above that in the acute case $\mathscr{R}(C_1)$ is dense; hence $S_1 = S_0^*$, and the proof is complete.

PROPOSITION 3.2. *In the nonacute case, a direct rotation exists if and only if*

$$\dim P\mathscr{H} \cap \tilde{Q}\mathscr{H} = \dim \tilde{P}\mathscr{H} \cap Q\mathscr{H}. \tag{3.5}$$

It is not unique.

Remark. Since we are assuming (1.5), (3.5) will hold automatically if either $\dim P\mathscr{H}$ or $\dim \tilde{P}\mathscr{H}$ is finite. But suppose $\mathscr{H}$ is the space of square-summable sequences $(\cdots, a_{-1}, a_0, a_1, \cdots)$; $P\mathscr{H}$, the subspace of those with $a_n = 0$ for $n < 0$; and $Q\mathscr{H}$, the subspace of those with $a_n = 0$ for $n \leqq 0$. Then (1.5) holds, and an example of V satisfying (1.4) is the bilateral shift: $V(a_n) = (b_n)$ with $b_n = a_{n-1}$. But $P\tilde{Q}$ is the projector upon the subspace of sequences with $a_n = 0$ for $n \neq 0$, whereas $\tilde{P}Q = 0$; so (3.5) fails.

Proof. We pick up the proof from the acute case. There, starting from any V satisfying (1.4), we used the polar resolution of its entries C_0 and C_1. The polar resolution of C_0 (say) is determined except for $\mathcal{N}(C_0)$. We see that $\mathcal{N}(C_0)$ "represents" (in the sense of (1.1) and (1.2)) $V^{-1}(\tilde{P}\mathcal{H} \cap Q\mathcal{H})$, and similarly that $\mathcal{N}(C_0^*)$ represents $P\mathcal{H} \cap \tilde{Q}\mathcal{H}$, $\mathcal{N}(C_1)$ represents $V^{-1}(P\mathcal{H} \cap \tilde{Q}\mathcal{H})$, $\mathcal{N}(C_1^*)$ represents $\tilde{P}\mathcal{H} \cap Q\mathcal{H}$. These subspaces are no longer zero, but under the assumption (3.5) they have equal dimensionalities, so we can extend the isometry Z_0 to a unitary and it will take $\mathcal{N}(C_0)$ onto $\mathcal{N}(C_0^*)$. This extension is not unique (even if $\dim \mathcal{N}(C_0) = 1$), and the nonuniqueness will survive.

We do not extend Z_1 arbitrarily, lest we lose property (ii). Instead we observe that S_0 takes $\mathcal{N}(C_0)$ isometrically onto $\mathcal{N}(C_1^*)$ and S_1 takes $\mathcal{N}(C_1)$ isometrically onto $\mathcal{N}(C_0^*)$; accordingly we define Z_1 to be $S_0 Z_0^{-1} S_1$ on $\mathcal{N}(C_1)$, which is thereby mapped isometrically onto $\mathcal{N}(C_1^*)$, as required.

Now we define unitary $Z \simeq \begin{pmatrix} Z_0 & 0 \\ 0 & Z_1 \end{pmatrix}$ and $U = VZ^{-1}$ as before, and U will take $P\mathcal{H}$ to $Q\mathcal{H}$. The effect of the special choice of Z_1 is, as one readily computes, the following special property:

(iii) for $x \in P\mathcal{H} \cap \tilde{Q}\mathcal{H}$ or $x \in \tilde{P}\mathcal{H} \cap Q\mathcal{H}$ we have $U^2 x = -x$.

Contemplate Fig. 2, and imagine the angle between $P\mathcal{H}$ and $Q\mathcal{H}$ approaching $\pi/2$, and you will see why (iii) is a natural requirement.

We must still prove that our U satisfies (ii). A reformulation: we prove that if the V we started with satisfies (i) and (iii) then it satisfies (ii). As above, (3.4) shows that S_1 and S_0^* agree on the range of C_1. Let $x_1 \perp \mathcal{R}(C_1)$, $x \simeq \begin{pmatrix} 0 \\ x_1 \end{pmatrix}$. Then $x \in \tilde{P}\mathcal{H} \cap Q\mathcal{H}$, so by (iii), $Ux = -U^*x$. But $Ux \simeq \begin{pmatrix} -S_1 x_1 \\ 0 \end{pmatrix}$ and $U^*x \simeq \begin{pmatrix} S_0^* x_1 \\ 0 \end{pmatrix}$, so S_1 and S_0^* agree everywhere.

There remains the converse: If $U \simeq \begin{pmatrix} C_0 & -S_1 \\ S_0 & C_1 \end{pmatrix}$ is a direct rotation, (3.5) is to be proved. Let $x \in P\mathcal{H} \cap \tilde{Q}\mathcal{H}$; we shall prove $Ux \in \tilde{P}\mathcal{H} \cap Q\mathcal{H}$. In terms of the representations, this means $x \simeq \begin{pmatrix} x_0 \\ 0 \end{pmatrix}$ with $x_0 \in \mathcal{N}(C_0^*)$, but now by (i) this is $\mathcal{N}(C_0)$, so $x \in U^{-1}(\tilde{P}\mathcal{H} \cap Q\mathcal{H})$. This proves inequality one way in (3.5), and the argument the other way is the same.

We shall assume (3.5) as well as (1.5) except where stated otherwise. Consequently the direct rotation will always exist, and rather than the more general V of (1.6) we shall deal mostly with its direct special case

$$U \simeq \begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix}, \qquad C_j \geqq 0. \tag{3.6}$$

We can write as an alternative to (3.1)

$$Q = UPU^{-1} \simeq \begin{pmatrix} C_0 \\ S_0 \end{pmatrix} (C_0 \quad S_0^*) = \begin{pmatrix} C_0^2 & C_0 S_0^* \\ S_0 C_0 & S_0 S_0^* \end{pmatrix}. \tag{3.7}$$

Next, we relate the direct rotation to reflection in $P\mathscr{H}$, an idea which will be essential to § 7.

Define $X \equiv P - \tilde{P} \simeq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, the reflection in $P\mathscr{H}$; and

$$Q_- \equiv XQX \simeq \begin{pmatrix} C_0^2 & -C_0S_0^* \\ -S_0C_0 & S_0S_0^* \end{pmatrix},$$

the projector onto the mirror image of $Q\mathscr{H}$. We see at once that $U^{-1} = XUX$ and that this is the direct rotation of $P\mathscr{H}$ to $Q_-\mathscr{H}$.

The relation

$$U^2 = (Q - \tilde{Q})(P - \tilde{P}) \tag{3.8}$$

may be verified mechanically from (3.6) and (3.7), or else by $U^2X^{-1} = U^2X = U(UX) = U(XU^{-1}) = UPU^{-1} - U\tilde{P}U^{-1} = Q - \tilde{Q}$. We see from (3.8) that if P and Q are given, U^2 is very easy to compute. Consequently, the following proposition provides us with a welcome constructive definition of U.

PROPOSITION 3.3. *Any direct rotation of $P\mathscr{H}$ to $Q\mathscr{H}$ is a principal square root of $(Q - \tilde{Q})(P - \tilde{P})$, that is, a unitary square root with spectrum in the right half-plane. Any principal square root of $(Q - \tilde{Q})(P - \tilde{P})$ is a direct rotation of $P\mathscr{H}$ to $Q\mathscr{H}$ provided it takes $P\mathscr{H} \cap \tilde{Q}\mathscr{H}$ onto $\tilde{P}\mathscr{H} \cap Q\mathscr{H}$.*

The first assertion is clear, for a direct rotation (3.6) satisfies (3.8) and $U + U^* \simeq \begin{pmatrix} 2C_0 & 0 \\ 0 & 2C_1 \end{pmatrix} \geqq 0$. Conversely, consider V, a principal square root of U^2, with spectral resolution $V = \int_{-\pi/2}^{\pi/2} e^{i\lambda}\, d\Omega_\lambda$. It is well known (and obvious) that the family $\{\Omega_\lambda\}$ is determined uniquely by $U^2 = V^2 = \int_{-\pi}^{\pi} e^{i\mu}\, d\Omega_{\mu/2}$, except for ambiguity on that eigenspace of U^2 which belongs to eigenvalue -1. Now those x for which $(Q - \tilde{Q})(P - \tilde{P})x = -x$ are easily seen to be those for which $QPx = \tilde{Q}\tilde{P}x = 0$, namely, those in $(P\mathscr{H} \cap \tilde{Q}\mathscr{H}) + (\tilde{P}\mathscr{H} \cap Q\mathscr{H})$. On this subspace, we are making a special hypothesis ensuring $VP = QV$ and we just saw that $V^2 = -1$. But on the orthogonal complement of $(P\mathscr{H} \cap \tilde{Q}\mathscr{H}) + (\tilde{P}\mathscr{H} \cap Q\mathscr{H})$, we are in the acute case; the direct rotation exists and is a principal square root, so V must agree with it. From the fact that V is a direct rotation on each of two complementary reducing subspaces, it is easy to see it is direct on all $\mathscr{H}$.

PROPOSITION 3.4. *If $C_0^2 \geqq \frac{1}{2}$, then U^2 is the direct rotation of $Q_-\mathscr{H}$ to $Q\mathscr{H}$.*

First, $U^2Q_- = (Q - \tilde{Q})X^2QX = QX = QU^2$ by (3.8). We must still prove (i) and (ii), which for this case take the form $Q_-U^2Q_- \geqq 0$ and $(Q_-U^2\tilde{Q}_-)^* = -\tilde{Q}_-U^2Q_-$. In the matrix representation this is routine.

A glance at Fig. 2 will show why $C_0^2 \geqq \frac{1}{2}$ is essential.

Now we bring in the angle operators Θ_0, Θ_1, and $\Theta \simeq \begin{pmatrix} \Theta_0 & 0 \\ 0 & \Theta_1 \end{pmatrix}$. In terms of the direct rotation, (1.16) is simply $\Theta_j \equiv \arccos C_j$. Also, because (3.2) says that $S_0^*S_0 = 1 - C_0^2$ on $\mathscr{K}(E_0)$ while $S_0S_0^* = 1 - C_1^2$ on $\mathscr{K}(E_1)$, the two operators C_j^2 must be isometric-equivalent except for their eigenspaces belonging to eigenvalue 1; these may, and ordinarily will, have different dimensionality. In terms of the angles, $C_j = \cos \Theta_j$, and the two operators Θ_j must be isometric-equivalent except perhaps for different dimensionalities of their null spaces.

Now by the facts just proved, the polar resolution of S_0 is $S_0 = J_0(S_0^*S_0)^{1/2} = J_0 \sin \Theta_0$, where J_0 maps $\mathscr{R}(S_0^*)^- = \mathscr{R}(\Theta_0)^-$ isometrically onto $\mathscr{R}(S_0)^- = \mathscr{R}(\Theta_1)^-$. On $\mathscr{R}(\Theta_0)^-$, $S_0 = (S_0S_0^*)^{1/2}J_0$. We then set $J \simeq \begin{pmatrix} 0 & -J_0^* \\ J_0 & 0 \end{pmatrix}$, defining an operator J uniquely on $\mathscr{R}(\Theta)^-$. On that space it is unitary, indeed a square root of -1; its values elsewhere will not matter, so we arbitrarily set $J = 0$ on $\mathscr{N}(\Theta)$.

We are now able to write as in (1.18)

$$U = \cos \Theta + J \sin \Theta \simeq \begin{pmatrix} \cos \Theta_0 & -J_0^* \sin \Theta_1 \\ J_0 \sin \Theta_0 & \cos \Theta_1 \end{pmatrix};$$

and the left side can even be written $\exp J\Theta$, as one sees easily from the properties of J just established.

THEOREM 3.1. *For a pair of subspaces $P\mathscr{H}$, $Q\mathscr{H}$, subject to* $\dim P\mathscr{H} = \dim Q\mathscr{H}$, $\dim P\mathscr{H} \cap \tilde{Q}\mathscr{H} = \dim \tilde{P}\mathscr{H} \cap Q\mathscr{H}$, *a complete system of invariants under isometric equivalence is afforded by the spectral multiplicity functions of Θ_0, Θ_1. These are arbitrary Hermitian operators satisfying the following conditions: $0 \leqq \Theta_j \leqq \pi/2$; the dimensionalities of their domains sum to that of $\mathscr{H}$; and the spectral multiplicity functions of the Θ_j are the same except for a possible difference in the multiplicity of $\{0\}$.*

(For spectral multiplicity functions and equivalence of Hermitian operators, see [13]. In many cases it is just a matter of eigenvalues; see Corollary 3.1.)

We have shown how to construct the Θ_j from P and Q, and they satisfy the stated conditions. It remains to show how, given such Θ_j acting on spaces $\mathscr{K}_j$, the system consisting of space $\mathscr{H}$ and projectors P and Q may be recaptured in a way which is well-determined up to isometric equivalence.

By the identity of spectral multiplicity functions which we imposed, there exists some isometry J_0 of $\mathscr{R}(\Theta_0)^-$ onto $\mathscr{R}(\Theta_1)^-$ such that $J_0\Theta_0J_0^{-1}$ agrees on its domain with Θ_1. Choose any such. Take Hilbert space $\mathscr{H}$ of dimensionality $\dim \mathscr{K}_0 + \dim \mathscr{K}_1$ and choose any isometries $E_j: \mathscr{K}_j \to \mathscr{H}$ such that $\mathscr{R}(E_1)$ is the orthogonal complement of $\mathscr{R}(E_0)$. Define $P = E_0E_0^*$ and

$$Q = (E_0 \quad E_1)\begin{pmatrix} \cos^2 \Theta_0 & -J_0^* \sin \Theta_1 \cos \Theta_1 \\ J_0 \sin \Theta_0 \cos \Theta_0 & \sin^2 \Theta_1 \end{pmatrix}\begin{pmatrix} E_0^* \\ E_1^* \end{pmatrix}.$$

It is straightforward to verify that these P and Q do lead to the given Θ_j. This in turn gives the desired equivalence between two pairs of projectors associated with the same invariants. That is all there is to the proof.

COROLLARY 3.1. *For a pair of subspaces $P\mathscr{H}$, $Q\mathscr{H}$, subject to* $\dim P\mathscr{H} = \dim Q\mathscr{H}$, $\dim P\mathscr{H} \cap \tilde{Q}\mathscr{H} = \dim \tilde{P}\mathscr{H} \cap Q\mathscr{H}$ *and such that $P\tilde{Q}P$ is compact, a complete system of invariants under isometric equivalence is afforded by the eigenvalues (multiplicity counted) of Θ_0, Θ_1. The eigenvalues θ_i of Θ_0 are an arbitrary sequence satisfying $\pi/2 \geqq \theta_1 \geqq \theta_2 \geqq \cdots$ and approaching* 0, *together with a possible eigenvalue* 0. *The eigenvalues of Θ_1 must be the same except perhaps for the multiplicity of* 0.

There is no new idea here, and we leave to the reader the verification of this special case of the theorem. The hypothesis that $P\tilde{Q}P$ is compact is satisfied in particular when $\dim P\mathscr{H}$ is finite.

The picture one has in mind is that of the whole space decomposed into a direct sum of 2-dimensional subspaces, each of which has 1-dimensional intersections with both $P\mathscr{H}$ and $Q\mathscr{H}$. Then all the manipulation of projectors, etc., proceeds in each of these 2-subspaces separately from the others, because each is invariant under all the operators we introduce. This picture is hardly ever misleading, and Corollary 3.1 shows how generally it is exactly valid; but on the other hand Theorem 3.1 shows that it must be modified in the general case by the fact that Θ can have continuous spectrum. Let us collect a few more of the useful obvious properties of the picture. Notation: Let $\Omega(\cdot)$ denote the special resolution of Θ.

PROPOSITION 3.5. *Θ commutes with P, with Q, with J, and with U. For every eigenvalue θ, the eigenvectors x satisfy $\angle(x, Ux) = \theta$. In the acute case, for every eigenvalue θ, the eigenspace $\Omega(\{\theta\})$ is the unique maximal subspace with the properties* (a) *it reduces P and Q,* (b) *for every nonzero vector x of $P\mathscr{H}$ lying in it, $\angle(x, Qx) = \theta$,* and (c) *for every nonzero vector x of $\tilde{P}\mathscr{H}$ lying in it, $\angle(x, \tilde{Q}x) = \theta$.*

These are mostly routine verifications, given the definitions. To check that $U \leftrightarrow \Theta$, one may use the fact that $J \leftrightarrow \Theta$, which reduces to the fact that $J_0\Theta_0 = \Theta_1 J_0$. But by the construction of J, we have $J_0 \sin \Theta_0 = \sin \Theta_1 J_0$, and then we can take the arc sin on both sides by the same familiar argument applied at the end of the proof of Proposition 3.1.

We give one part of the proof in detail, because it involves some complications. Assume $\mathscr{X}$ is a subspace of $\mathscr{H}$ reducing P and Q, and $\mathscr{X} \nsubseteq \Omega(\{\theta\})\mathscr{H}$. We shall prove that $\mathscr{X}$ does not possess both properties (b) and (c).

Choose, as we may by assumption, $x \in \mathscr{X}$ having a nonzero component in $(\Omega(\{\theta\})\mathscr{H})^{\perp}$. We now compute

$$\cos^2 \Theta = PQP + \tilde{P}\tilde{Q}\tilde{P},$$

consequently $\mathscr{X}$ must reduce $\cos^2 \Theta$, and hence also every spectral projector of Θ. Therefore $0 \neq x - \Omega(\{\theta\})x \in \mathscr{X}$. There exist ϕ_1, ϕ_2, with either $\phi_1 \leqq \phi_2 < \theta$ or $\theta < \phi_1 \leqq \phi_2$, such that $0 \neq \Omega([\phi_1, \phi_2])x \equiv y \in \mathscr{X}$. Take $\phi_1 \leqq \phi_2 < \theta$, the other alternative goes the same. Not both Py and $\tilde{P}y$ are zero; both are in $\mathscr{X}$; and because $\Omega(\cdot) \leftrightarrow P$, both are in $\Omega([\phi_1, \phi_2])\mathscr{H}$; so say without loss of generality that there exists a unit vector $z = \Omega([\phi_1, \phi_2])z \in P\mathscr{H} \cap \mathscr{X}$. Set $z \simeq \begin{pmatrix} z_0 \\ 0 \end{pmatrix}$. Then $Qz \simeq \begin{pmatrix} C_0^2 z_0 \\ S_0 C_0 z_0 \end{pmatrix}$ and $Uz \simeq \begin{pmatrix} C_0 z_0 \\ S_0 z_0 \end{pmatrix}$, whence $Qz = (\cos \Theta)Uz$. Therefore

$$z^*Qz = z_0 C_0^2 z_0 \in [\cos^2 \phi_2, \cos^2 \phi_1],$$

$$\|Qz\|^2 = (Uz)^* \cos^2 \Theta Uz \in [\cos^2 \phi_2, \cos^2 \phi_1]$$

(the last relation uses the fact that Uz is still in $\Omega([\phi_1, \phi_2])\mathscr{H}$). Therefore $\cos \angle(z, Qz) \equiv \operatorname{Re} z^*Qz/\|Qz\| \geqq \cos^2 \phi_2/\cos \phi_1$. The whole argument so far is valid for any $\phi_1 \leqq \phi_2 < \theta$ such that $0 \neq \Omega([\phi_1, \phi_2])x$. But we can surely choose a fixed $\phi < \theta$ such that this will hold for $\phi_1 \leqq \phi \leqq \phi_2$ and arbitrarily small $\phi_2 - \phi_1$.

Taking this difference small enough will give $\cos^2 \phi_2/\cos \phi_1 > \cos \theta$, and property (b) fails, as asserted.

COROLLARY 3.2. *If the roles of P and Q are interchanged, Θ remains the same, while J is replaced by $-J$.*

Bibliographical note. It has been known for many years that two m-dimensional subspaces of real n-dimensional inner product space have m angles as a complete set of unitary invariants [14], [26]. A more modern treatment is in [11]. The extension to Hilbert space was given by Kreĭn, Krasnosel'skiĭ, and Mil'man [18, Section 3] and independently by Dixmier [7], [8]. A number of other independent developments of a rather similar theory followed [1], [2], [3], [17, Sections 1.4.6, 1.6.8], [29], [32], [35]. Most of these lacked references to earlier literature, and most of them did not include the infinite-dimensional case; most of them give, at least in the finite-dimensional case, some complete set of invariants for a pair of subspaces, and while they share an algebraic spirit there are many points of difference. Special mention must be made of Seidel's [27] careful geometric treatment of Euclidean and non-Euclidean theories together. The direct rotation was introduced by Davis [3] and Kato [17, Sections 1.4.6, 1.6.8], both motivated by perturbation theory and both influenced by Sz.-Nagy [23, Section 136]. Most of the novelty of the present treatment is in matters concerning the direct rotation.

4. Extremal properties of the direct rotation. The present section is not required for the rest of the paper.

We shall make the hypotheses of Theorem 3.1 and Corollary 3.1 (leaving to the reader the modifications entailed in the absence of compactness). The notation will be

$$U \simeq \begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix}, \quad V = UZ, \quad Z \simeq \begin{pmatrix} Z_0 & 0 \\ 0 & Z_1 \end{pmatrix}.$$

We have introduced the angles $\theta_1 \geqq \theta_2 \geqq \cdots$ associated with $P\mathscr{H}$ and $Q\mathscr{H}$. We showed how the sines of these angles can be recovered from any unitary taking $P\mathscr{H}$ to $Q\mathscr{H}$. Among these, the "direct rotation" U of Definition 3.1 was singled out in two respects: the simple canonical construction of it in terms of P and Q (see (3.8)) and the decomposition of the space by (1.18) and Theorem 3.1. But the motivation for the direct rotation was the notion of taking elements of $P\mathscr{H}$ to $Q\mathscr{H}$ by the most economical route. This notion cannot be taken naively, for if (say) $\theta_1 = \pi/4$, $\theta_2 = \pi/6$, then a unitary cannot take *every* unit vector in $P\mathscr{H}$ to the unit vector in $Q\mathscr{H}$ closest to it. It can almost do this, however, as we now show.

PROPOSITION 4.1. *Given any unitary V which maps $P\mathscr{H}$ onto $Q\mathscr{H}$, there exist orthonormal $v_1, v_2, \cdots \in P\mathscr{H}$ such that for all k, $\angle(v_k, Vv_k) \geqq \theta_k$. Equivalent statement: among all such V, the singular values $\lambda_1 \geqq \lambda_2 \geqq \cdots$ of $(1 - V)|_{P\mathscr{H}}$ are all minimized when $V = U$, and their values then are $\lambda_k = 2 \sin (\theta_k/2)$.*

COROLLARY 4.1. *For every unitary-invariant norm, $\|(1 - V)P\|$ is minimized when $V = U$.*

Before proving these statements, it is more pressing to explain their relationship. For any unit vector $x \in P\mathscr{H}$, say $x \simeq \begin{pmatrix} x_0 \\ 0 \end{pmatrix}$,

$$\begin{aligned} \cos \angle(x, Vx) &= \operatorname{Re} x^*Vx = x^*\tfrac{1}{2}P(V + V^*)Px \\ &= x_0^*\tfrac{1}{2}(C_0Z_0 + Z_0^*C_0)x_0. \end{aligned}$$

The main point is that we have a Hermitian operator, with a complete set of eigenvectors, on $P\mathscr{H}$, or on $\mathscr{K}(E_0)$, which represents it. For the $v_1, v_2, \cdots$ of Proposition 4.1, we will take $v_k \simeq \begin{pmatrix} v_{0k} \\ 0 \end{pmatrix}$, the v_{0k} being orthonormal eigenvectors belonging respectively to the eigenvalues $\cos\phi_1 \leqq \cos\phi_2 \leqq \cdots$ of $(C_0Z_0 + Z_0^*C_0)/2$. If in particular $V = U$, then $Z_0 = 1$, so $\phi_k = \theta_k$ and the v_{0k} can be the orthonormal eigenvectors u_{0k} of C_0. The task is to compare the general case with this case, proving $\phi_k \geqq \theta_k$.

The singular values λ_k of $(1 - V)|_{P\mathscr{H}}$ are the nonnegative square roots of the eigenvalues of this operator on $\mathscr{K}(E_0)$:

$$(1 - Z_0^*C_0 \quad - Z_0^*S_0^*)\begin{pmatrix} 1 - C_0Z_0 \\ -S_0Z_0 \end{pmatrix} = 2 - C_0Z_0 - Z_0^*C_0.$$

Hence in terms of the angles ϕ_k above, $\lambda_k^2 = 2 - 2\cos\phi_k$, or $\lambda_k = 2\sin(\phi_k/2)$. In terms of the relation between x and Vx, for $x \in P\mathscr{H}$, we may write

$$\lambda_k = \inf_{\mathscr{X}} \sup_{x} \|(1 - V)x\|, \tag{4.1}$$

where the infimum is over $(k-1)$-dimensional subspaces $\mathscr{X}$ of $P\mathscr{H}$, and the supremum is over unit vectors $x \in P\mathscr{H} \ominus \mathscr{X}$. The λ_k are minimax values of the distance a unit vector in $P\mathscr{H}$ is moved by V.

Since for every unitary-invariant norm $\|(1 - V)P\|$ is a monotone function of the (ordered) nonzero singular values of $(1 - V)P$, and these are just the nonzero λ_k, Corollary 4.1 follows from Proposition 4.1.

Proof of Proposition 4.1. In (4.1), fix $\mathscr{X}$ as that choice for which the minimum is attained (under our compactness hypothesis, this exists). Among the unit vectors $x \in P\mathscr{H} \ominus \mathscr{X}$ there is at least one which is a linear combination of the first k eigenvectors $u_1 \simeq \begin{pmatrix} u_{01} \\ 0 \end{pmatrix}, \cdots, u_k \simeq \begin{pmatrix} u_{0k} \\ 0 \end{pmatrix}$ of $PUP|_{P\mathscr{H}}$. To prove that $\lambda_k \geqq 2\sin(\theta_k/2)$, that is, that $\phi_k \geqq \theta_k$, it is enough to show that for this x,

$$\angle(x, Vx) \geqq \theta_k = \angle(u_k, Uu_k). \tag{4.2}$$

Now if $x \perp Q\mathscr{H}$, then in particular $x \perp Vx$, so $\angle(x, Vx) = \pi/2 \geqq \theta_k$. Otherwise, $Qx \neq 0$, and we use the familar fact that the unit vector y in $Q\mathscr{H}$ for which $\|x - y\|$ is minimized is $y = Qx/\|Qx\|$. In terms of angles, this says that $\angle(x, Vx) \geqq \angle(x, Qx)$. Refer to (3.7) for the relations $x^*Qx = x_0^*C_0^2x_0 = \|Qx\|^2$. Thus

$$\cos\angle(x, Qx) = (x_0^*C_0^2x_0)^{1/2} \leqq \cos\theta_k,$$

because $x_0 \in [u_{01}, \cdots, u_{0k}]$, and on that subspace $C_0^2 \leqq \cos^2\theta_k$. This establishes (4.2) for this x, completing the proof.

Here is an easy extremal property of U, differing from the one just proved in that the orthonormal set which is efficiently moved by U is freely chosen.

PROPOSITION 4.2. *Given any unitary V which maps $P\mathscr{H}$ onto $Q\mathscr{H}$, and given any orthonormal basis $\{v_1, v_2, \cdots\}$ of $P\mathscr{H}$, we have*

$$\sum_1^\infty \sin^2\angle(v_k, Vv_k) \geqq \sum_1^\infty \sin^2\theta_k.$$

Proof. Writing again $v_k \simeq \begin{pmatrix} v_{0k} \\ 0 \end{pmatrix}$, we have

$$\begin{aligned}\sum_k \sin^2 \angle(v_k, Vv_k) &= \sum_k (1 - \cos^2 \angle(v_k, Vv_k)) \\ &= \sum_k (1 - (\operatorname{Re} v_{0k}^* C_0 Z_0 v_{0k})^2) \\ &\geqq \sum_k (1 - |v_{0k}^* C_0 Z_0 v_{0k}|^2) \\ &\geqq \sum_k (1 - \sum_l |v_{0k}^* C_0 Z_0 v_{0l}|^2) \\ &= \sum_k (1 - v_{0k}^* C_0^2 v_{0k}) = \operatorname{tr} S_0^* S_0 \\ &= \sum \sin^2 \theta_k,\end{aligned}$$

even if the rightmost member is infinite. This completes the proof.

Again, we have equality for $V = U$, if the basis is well chosen.

Now one suspects on the basis of the 2-dimensional special case that the direct rotation may be more economical than other V in the way it moves *any* x, not just those x in $P\mathscr{H}$. The next two propositions are of this sort. They are a little messier than Proposition 4.1; also the results are weaker, and we will offer counterexamples showing why. Proposition 4.4 will concern extremal values of $\|1 - V\|$; Proposition 4.3, extremal values of $\|(1 - V^*)(1 - V)\|$. The two problems are of course closely related, though the conclusions differ; therefore, we discuss them together.

By the theorem of Ky Fan mentioned in § 1, we may prove the inequality $\|1 - V\| \geqq \|1 - U\|$ for all unitary-invariant norms by proving it for the particular norms (1.11), and the same for $\|(1 - V^*)(1 - V)\| \geqq \|(1 - U^*)(1 - U)\|$. Let $\lambda_1 \geqq \lambda_2 \geqq \cdots$ be the nonzero singular values of $1 - V$, then those of $(1 - V^*)(1 - V)$ are $\lambda_1^2 \geqq \lambda_2^2 \geqq \cdots$. We now set out to prove that $\lambda_1 + \cdots + \lambda_\nu$ or $\lambda_1^2 + \cdots + \lambda_\nu^2$ is minimized when $V = U$, for $\nu = 1, 2, \cdots$.

When $V = U$, the sequence of the λ_j will be $2 \sin(\theta_1/2), 2 \sin(\theta_1/2), 2 \sin(\theta_2/2)$, $2 \sin(\theta_2/2), \cdots$, a sequence which, if not finite, approaches zero. Corresponding orthonormal eigenvectors of $(1 - U^*)(1 - U)$ will be $u_1, Ju_1, u_2, Ju_2, \cdots$, where $u_k \simeq \begin{pmatrix} u_{0k} \\ 0 \end{pmatrix}$ and the u_{0k} are the orthonormal eigenvectors of Θ_0.

For the more general V, we will not know where the vectors v lie which give the largest values to $\|(1 - V)v\|$, they might lie neither in $P\mathscr{H}$ nor in $\tilde{P}\mathscr{H}$. Nevertheless we have an inequality in one direction, given by (1.12). In that inequality, we choose $\Omega\mathscr{H}$ as $[x_1, \cdots, x_\nu]$, where x_1 and x_2 are in $\Omega_1\mathscr{H}$, x_3 and x_4 are in $\Omega_2\mathscr{H}$, and so on; here $\Omega_k\mathscr{H}$ is $[u_k, Ju_k]$ (if Θ_0 has no degenerate eigenvalues then simply $\Omega_k = \Omega(\{\theta_k\})$). Then (1.12) says that

$$(4.3)\qquad \begin{aligned}\|K\|_\nu &\geqq \sum_{k=1}^{\nu/2} \|K\Omega_k\|_2, &\nu \text{ even},\\ \|K\|_\nu &\geqq \sum_{k=1}^{[\nu/2]} \|K\Omega_k\|_2 + \|K\Omega_{(\nu+1)/2}\|_1, &\nu \text{ odd}.\end{aligned}$$

Also, using a second set of comparison vectors specialized in exactly the same way as the x_k, we obtain from (1.13) that

$$\|K\|_\nu \geqq \sum_{k=1}^{\nu/2} \|\Omega_k K \Omega_k\|_2, \qquad \nu \text{ even},$$

(4.4)

$$\|K\|_\nu \geqq \sum_{k=1}^{[\nu/2]} \|\Omega_k K \Omega_k\|_2 + \|\Omega_{(\nu+1)/2} K \Omega_{(\nu+1)/2}\|_1, \qquad \nu \text{ odd}.$$

We shall apply (4.3) to $K = 1 - V$ and (4.4) to $K = (1 - V^*)(1 - V)$.

These drastic specializations are all right if we can prove the right-hand members are minimized by $V = U$; because then the known best orthonormal set satisfies the restriction, and the inequalities (4.3) and (4.4) become equalities.

For the same reason, the estimation of (4.3) or (4.4) may be done term by term: thus for (4.3), it suffices to show, if we can, that for each k, $\|K\Omega_k\|_2$ and $\|K\Omega_k\|_1$ are both minimized when $V = U$.

Let us simplify the notation, writing Ω for Ω_k, θ for θ_k, u for u_k. We know that $Uu = (\cos\theta)u + (\sin\theta)Ju$ and $UJu = (-\sin\theta)u + (\cos\theta)Ju$.

We are able to keep track of Vu and VJu to this limited extent: V may be written as U followed by a unitary taking $Q\mathscr{H}$ into $Q\mathscr{H}$ and $\tilde{Q}\mathscr{H}$ into $\tilde{Q}\mathscr{H}$ (in our previous notation, $V = (UZU^{-1})U$). Consequently we can write

$$Vu = a_0 Uu + b_0 w,$$

$$VJu = a_1 UJu + b_1 x,$$

($|a_j|^2 + |b_j|^2 = 1$) for unit vectors $w \in Q\mathscr{H} \ominus [Uu]$, $x \in \tilde{Q}\mathscr{H} \ominus [JUu]$. Because Ω commutes with Q, we even know that $\Omega w = \Omega x = 0$.

The rest of the proof mostly concerns operators reduced by the 2-subspace $\Omega\mathscr{H}$ and zero on its orthogonal complement. We simplify further by writing only the 2×2 matrix of such an operator's part in $\Omega\mathscr{H}$, referred to the basis $\{u, Ju\}$.

In particular,

$$\Omega V \Omega: \begin{pmatrix} a_0 \cos\theta & -a_1 \sin\theta \\ a_0 \sin\theta & a_1 \cos\theta \end{pmatrix}.$$

We have to consider not this, but the singular values $\mu_1 \geqq \mu_2$ of $(1 - V)\Omega$. Now μ_1^2, μ_2^2 are the eigenvalues of $\Omega(1 - V^*)(1 - V)\Omega = \Omega(2 - V^* - V)\Omega$. Hence $1 - \mu_1^2/2$, $1 - \mu_2^2/2$ are the eigenvalues of $\operatorname{Re}(\Omega V \Omega) = \Omega(V + V^*)\Omega/2$, which by the above may be written

$$\operatorname{Re}(\Omega V \Omega): \begin{pmatrix} (\operatorname{Re} a_0)\cos\theta & \frac{1}{2}(a_0^* - a_1)\sin\theta \\ \frac{1}{2}(a_0 - a_1^*)\sin\theta & (\operatorname{Re} a_1)\cos\theta \end{pmatrix}.$$

By a routine computation, the eigenvalues of this matrix are found to be

(4.5)

$$1 - \mu_1^2/2 = c\cos\theta - \sqrt{d^2 + e^2 \sin^2\theta},$$

$$1 - \mu_2^2/2 = c\cos\theta + \sqrt{d^2 + e^2 \sin^2\theta}.$$

These have been put in terms of real constants c, d, e, f defined by $a_0 + a_1 = 2c + i2e$, $a_0 - a_1 = 2d - i2f$. We know that $|a_j|^2 \leqq 1$; in terms of the new constants this becomes

$$(4.6)\qquad \begin{aligned}(c+d)^2+(e-f)^2 &\leqq 1,\\ (c-d)^2+(e+f)^2 &\leqq 1,\end{aligned}$$

so that $c^2+d^2+e^2+f^2 \leqq 1$ as well.

Now (4.5) already settles the questions as to the bound norm; for $\|(1-V)\Omega\|_1^2 = \mu_1^2 = \|\Omega(1-V^*)(1-V)\Omega\|_1$, and

$$\mu_1^2 \geqq 2-2c\cos\theta \geqq 2-2\cos\theta = \|(1-U)\Omega\|_1^2.$$

It remains to consider $\|(1-V)\Omega\|_2 = \mu_1+\mu_2$ and $\|\Omega(1-V^*)(1-V)\Omega\|_2 = \mu_1^2+\mu_2^2$.

The latter also comes directly from (4.5), by adding the two equations: $\mu_1^2+\mu_2^2 = 2(1-c\cos\theta)$, which is indeed minimized when $c=1$ (hence $d=e=f=0$, hence $V=U$). We have proved the following proposition.

PROPOSITION 4.3. *For every unitary-invariant norm,* $\|(1-V^*)(1-V)\|$ *is minimized when* $V=U$.

For many of these norms, $\|1-V\|$ can be expressed as $(\|(1-V^*)(1-V)\|')^{1/2}$ for different unitary-invariant $\|\cdot\|'$, hence will also be minimized when $V=U$. This applies in particular to the bound norm and the square norm. It does not apply to the sum of the singular values. For this norm and a host of others, the extremal property can fail for $\|1-V\|$. Here are two examples. Both are in 2-space, so $\Omega=1$, but we use the notations above.

Example 4.1. Take θ reasonably large, and take

$$V:\begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix},$$

the reflection exchanging $P\mathscr{H}$ with $Q\mathscr{H}$. Then $1-V$ has singular values $\mu_1=2$, $\mu_2=0$, while $1-U$ has of course the equal singular values $2\sin(\theta/2)$, $2\sin(\theta/2)$. But $\|1-V\|_2=2$ can be less than $\|1-U\|_2=4\sin(\theta/2)$; namely, this will happen if and only if $\theta>\pi/3$.

Example 4.2. Take any θ, and take $V=e^{i\delta}U$, $0\leqq\delta<\theta$. Curiously, the singular values of $1-V$ come out as $2\sin((\theta\pm\delta)/2)$, so that $\|1-V\|_2 = 4\sin(\theta/2)\cdot\cos(\delta/2)$, which is not minimized when $\delta=0$; quite the reverse.

Thus we see that in two respects the following result is best possible.

PROPOSITION 4.4. *Assume V a unitary taking $P\mathscr{H}$ onto $Q\mathscr{H}$ in a real space $\mathscr{H}$; assume also that $\Theta\leqq\pi/3$. Then $\|1-V\|$ is minimized, for every unitary-invariant norm, when $V=U$.*

Proof. Return now to the discussion around (4.5). We want to show $\mu_1+\mu_2$ is minimized when $V=U$. In (4.5) and (4.6) we must have $e=f=0$ because $\mathscr{H}$ is real. A bit of computation extracts from (4.5) the expression

$$(\mu_1+\mu_2)^2/4 = 1-c\cos\theta+\sqrt{(1-c\cos\theta)^2-d^2}.$$

For fixed θ and $|c|$, this will be minimized by taking $c\geqq 0$ and d^2 maximal. By (4.6), $|d|\leqq 1-c$. Thus we must show that

$$1-c\cos\theta+\sqrt{2c(1-\cos\theta)-c^2\sin^2\theta}\qquad (c\geqq 0)$$

is minimized when $c = 1$; that is, that it is $\geqq 2 - 2\cos\theta$. Unless $(2 - c)\cos\theta \leqq 1$, this is immediate, so make that supposition. We are to prove that

$$2c(1 - \cos\theta) - c^2 \sin^2\theta \geqq [1 - (2 - c)\cos\theta]^2,$$

which reduces to $c \geqq (2\cos\theta - 1)^2$ after $1 - c$ is divided out. By the supposition, $c \geqq 2 - \sec\theta$, so it is enough to prove $2 - \sec\theta \geqq (2\cos\theta - 1)^2$. The hypotheses provide that $\theta \leqq \pi/3$, and in that range the desired inequality does hold. Proposition 4.4 is proved.

If θ gets any larger, the conclusion fails because of Example 4.1; in complex space, it fails because of Example 4.2.

5. On the equation $AX - XB = C$. In this section only, we abandon the notations established in § 1, and we state our result in a more general setting.

THEOREM 5.1. *Let $\mathscr{X}$ and $\mathscr{Y}$ be Banach spaces; let operators A on $\mathscr{Y}$ and B on $\mathscr{X}$ satisfy $\|B\| \leqq \alpha$ and $\|A^{-1}\| \leqq (\alpha + \delta)^{-1}$ for some $\alpha \geqq 0$, $\delta > 0$, and for the bound norms on the respective spaces. For linear transformations from $\mathscr{X}$ to $\mathscr{Y}$, use any norm compatible with the bound norms. Assume $AX - XB = C$. Then $\|C\| \geqq \delta\|X\|$.*

Compatibility means the property that for every pair of contractions W on $\mathscr{X}$ and V on $\mathscr{Y}$, $\|VKW\| \leqq \|K\|$. In particular, the unitary-invariant norms for Hilbert spaces are compatible with the bound norm, as noted in § 1.

Proof. Compatibility implies that $\|XB\| \leqq \alpha\|X\|$ and $\|AX\| \geqq (\alpha + \delta)\|X\|$. The triangle inequality implies that $\|C\| \geqq \|AX\| - \|XB\|$. Combining these gives the result.

Note that the roles of A and B are symmetrical, so the hypotheses upon them may be interchanged.

There are much subtler results asserting that if A and B are unlike then C cannot be small [24], [20]. These grow out of the elementary observation that, for finite matrices, if A and B have disjoint spectra then C cannot be 0. But hypotheses concerning merely the separation of spectra cannot give conclusions as sharp as Theorem 5.1, even in relatively special circumstances.

Here is an adumbration of the difficulties. Suppose A and B are Hermitian matrices, possibly of different dimensions, and suppose $0 < \delta \leqq |\lambda - \mu|$ for every eigenvalue λ of A and μ of B. Let $C = AX - XB$. Then the inequality

$$\|C\|_{\mathrm{sq}} \geqq \delta\|X\|_{\mathrm{sq}} \quad (= \delta\sqrt{\operatorname{tr} X^*X}) \tag{5.1}$$

is easy to prove via the unitary diagonalization of A and B. However, sometimes $\|C\|_1 \ngeqq \delta\|X\|_1$. To be sure, we may infer from (5.1) that

$$\|C\|_1\sqrt{\operatorname{rank} C} \geqq \delta\|X\|_1; \tag{5.2}$$

and this inequality has been discovered independently and applied by G. W. Stewart III [28, Theorem 4.6] to obtain results similar to but slightly weaker than our sin θ Theorems 6.1 and 6.2. But inequality (5.2) does not promise much help for infinite-dimensional applications. Besides, (5.2) is not best possible unless rank $C \leqq 1$, whereas Theorem 5.1 and inequality (5.1) are best possible in a nontrivial sense. Whether rank C in (5.2) can be replaced by a constant is an open question; certainly the constant 1 is too small, as can be seen from

$$X = \begin{pmatrix} 3 & -3 \\ -3 & 1 \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}, \quad \delta = 1,$$

$$\delta \|X\|_1 = 2 + \sqrt{10} = 5.16 \cdots > \|AX - XB\|_1 = 3\sqrt{2} = 4.24 \cdots .$$

Another variation upon the theme of Theorem 5.1 concerns unbounded operators. Although that theorem was stated for bounded operators B and X, its statement and proof encompass the case where A is an unbounded operator with domain dense in $\mathscr{Y}$; for example, A could be the inverse of a compact operator with dense range (so that $AA^{-1} = 1$). Here is a further variation which allows B to be unbounded too.

THEOREM 5.2. *Let $\mathscr{X}$ and $\mathscr{Y}$ be Hilbert spaces; let A on $\mathscr{Y}$ and B on $\mathscr{X}$ be semi-bounded self-adjoint operators satisfying*

$$A \geqq \gamma + \delta > \gamma \geqq B$$

for some scalars γ and δ. Assume $AX = XB + C$, where X and C are bounded operators from $\mathscr{X}$ to $\mathscr{Y}$. Then

$$\|C\| \geqq \delta \|X\|$$

for every unitary-invariant norm.

Proof. Write the spectral resolution [23, Section 120] of B thus:

$$-B = \int_{-\gamma}^{+\infty} \lambda \, d\Omega(\lambda),$$

where $\Omega(\lambda)$ is a spectral family of projections with the property, among others, that $\Omega(\lambda)x \to x$ as $\lambda \to +\infty$ for every x in $\mathscr{X}$. For every $\tau > -\gamma$ we may define $B_\tau \equiv B\Omega(\tau) + (\tau - \gamma)/2$, $A_\tau \equiv A + (\tau - \gamma)/2$ and $\alpha \equiv (\tau + \gamma)/2$; then

$$A_\tau \geqq \delta + \alpha > \alpha \geqq B_\tau \geqq -\alpha,$$

so B_τ is a bounded self-adjoint operator and $0 < A_\tau^{-1} \leqq (\delta + \alpha)^{-1}$. Post-multiplying the given equation $AX = XB + C$ by $\Omega(\tau)$ yields, after minor modification, an equation

$$A_\tau X\Omega(\tau) = X\Omega(\tau) \cdot B_\tau + C\Omega(\tau)$$

in which all but A_τ are bounded operators defined over the whole of their respective spaces. Now apply Theorem 5.1 to infer that

$$\|C\Omega(\tau)\| \geqq \delta \|X\Omega(\tau)\|$$

for any unitary-invariant norm and all $\tau > -\gamma$. The final step in the proof is the invocation of the following lemma.

LEMMA 5.1. *Let $\Omega(\tau)$ be a family of projectors such that $\Omega(\tau) \to 1$ strongly as $\tau \to \infty$; let κ_ν and $\kappa_\nu(\tau)$ be the ν-th singular values of K and $K\Omega(\tau)$ respectively. Then $\kappa_\nu(\tau) \to \kappa_\nu$ also.*

Proof. Since (1.10) implies $\kappa_\nu \geqq \kappa_\nu(\tau) \geqq 0$, the result we want will be proved if we can show that, for every $\varepsilon > 0$, the inequality

$$\sum_1^\nu \kappa_j(\tau)^2 > \sum_1^\nu \kappa_j^2 - \varepsilon$$

or, equivalently,

$$\|\Omega(\tau)K^*K\Omega(\tau)\|_\nu > \|K^*K\|_\nu - \varepsilon$$

is satisfied whenever τ is sufficiently large. Now consider (1.13); it implies the existence of ν orthonormal vectors u_j and a ν-projector $\Upsilon \equiv \sum_1^\nu u_j u_j^*$ for which $\|\Upsilon K^*K\Upsilon\|_\nu > \|K^*K\|_\nu - \varepsilon$. Furthermore, our hypothesis upon $\Omega(\tau)$ ensures that $\Omega(\tau)u_j \to u_j$ in norm as $\tau \to \infty$, so $K\Omega(\tau)\Upsilon \to K\Upsilon$ in norm too, and hence

$$\|\Omega(\tau)K^*K\Omega(\tau)\|_\nu \geqq \|\Upsilon\Omega(\tau)K^*K\Omega(\tau)\Upsilon\|_\nu \to \|\Upsilon K^*K\Upsilon\|_\nu > \|K^*K\|_\nu - \varepsilon$$

as desired. So ends the proof.

6. Proof of the single-angle theorems. We begin with two simple lemmas on norm inequalities which will be used in this and the next section.

LEMMA 6.1. *Let Ω and Υ be projectors. If $\|\Omega K\Upsilon\| \leqq \|\Omega L\Upsilon\|$ and $\|\tilde{\Omega}K\tilde{\Upsilon}\| \leqq \|\tilde{\Omega}L\tilde{\Upsilon}\|$ for all unitary-invariant norms, then $\|\Omega K\Upsilon + \tilde{\Omega}K\tilde{\Upsilon}\| \leqq \|\Omega L\Upsilon + \tilde{\Omega}L\tilde{\Upsilon}\|$ for all unitary-invariant norms. The converse holds whenever $\Omega K\Upsilon$ has the same singular values as $\tilde{\Omega}K\tilde{\Upsilon}$ and $\Omega L\Upsilon$ has the same singular values as $\tilde{\Omega}L\tilde{\Upsilon}$.*

Both proofs are immediate once the problem has been reduced, via the theorem of Ky Fan, to consideration of the ν-norms.

LEMMA 6.2. *Let Ω and Υ be projectors. Then $\|\Omega K\Upsilon + \tilde{\Omega}K\tilde{\Upsilon}\| \leqq \|K\|$ for all unitary-invariant norms.*

Proof.

$$\begin{aligned} 2\|\Omega K\Upsilon + \tilde{\Omega}K\tilde{\Upsilon}\| &= \|K + (\Omega - \tilde{\Omega})K(\Upsilon - \tilde{\Upsilon})\| \\ &\leqq \|K\| + \|(\Omega - \tilde{\Omega})K(\Upsilon - \tilde{\Upsilon})\| = 2\|K\| \end{aligned}$$

because $\Omega - \tilde{\Omega}$ and $\Upsilon - \tilde{\Upsilon}$ are unitary.

Proof of the $\sin\theta$ *theorem.* To begin with, we may add a multiple of the identity operator to A, translating the spectra of A_0 and Λ_1 without affecting R. Accordingly, assume without loss of generality that $0 \leqq \alpha = -\beta$ in the hypotheses of the theorem.

By (1.8), $R = HE_0 = (A + H)E_0 - E_0A_0$. Because F_1 has bound norm 1, we have by the compatibility property $\|R\| = \|R^*\| \geqq \|R^*F_1\|$. Now using the second expression (1.3) and the properties of the E_j and F_j, $R^*F_1 = E_0^*F_1\Lambda_1 - A_0E_0^*F_1$. This is in the form to which Theorem 5.1 applies, giving the conclusion

$$\|E_0^*HF_1\| = \|R^*F_1\| \geqq \delta\|E_0^*F_1\| \tag{6.1}$$

for every unitary-invariant norm. Recall from (1.7) that $E_0^*F_1$ has the same singular values as S_1—the same, therefore, as $\sin\Theta_0$. Combining these relations gives $\|R\| \geqq \delta\|\sin\Theta_0\|$ as desired.

Note that the hypotheses do not suffice for the conclusion $\delta\|\sin\Theta\| \leqq \|H\|$ (unless we speak only of the bound norm: $\delta\|\sin\Theta\|_1 = \delta\|\sin\Theta_0\|_1 \leqq \|R\|_1 \leqq \|H\|_1$). For a counterexample, take $A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, $H = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$, $\Lambda = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}$. Then $\delta = 2$ is the gap between $A_0 = 0$ and $\Lambda_1 = 2$. We compute $\theta_1 = \pi/4$ and $\delta\|\sin\Theta\|_{\mathrm{sq}} = 2 \nleqq \sqrt{3} = \|H\|_{\mathrm{sq}}$. This example is so constructed that the gap between the spectra of A_1 and Λ_0 is less than δ. Excluding this eventuality, we can state the following proposition.

PROPOSITION 6.1 (Symmetric $\sin\theta$ theorem). *For given $\delta > 0$, assume that the spectra of A_0 and Λ_1 are separated as in the hypotheses of the* $\sin\theta$ *theorem, and assume that the spectra of A_1 and Λ_0 are also separated as in the hypotheses of the* $\sin\theta$ *theorem. Then for every unitary-invariant norm, $\delta\|\sin\Theta\| \leqq \|H\|$.*

Proof. Applying the $\sin\theta$ theorem (or strictly speaking, inequality (6.1)) to A_0 and Λ_1 gives $\delta\|P\tilde{Q}\| = \delta\|\sin\Theta_0\| = \delta\|E_0^*F_1\| \leqq \|E_0^*HF_1\| = \|PH\tilde{Q}\|$. Applying the same inequality to A_1 and Λ_0 gives

$$\delta\|\tilde{P}Q\| = \delta\|\sin\Theta_1\| = \delta\|E_1^*F_0\| \leqq \|E_1^*HF_0\| = \|\tilde{P}HQ\|.$$

Combine the two inequalities by Lemmas 6.1 and 6.2, and the proposition is proved.

The proof of the $\sin\theta$ theorem has used very little of the special properties of norms, or of angles between subspaces. Consequently the theorem is valid more generally. We state the generalized form as Theorem 6.1 (this theorem and Theorems 6.2 and 6.3 are not needed for the rest of § 6–§ 8). *Warning*: some notations whose usage has been fixed throughout are here slightly re-interpreted.

THEOREM 6.1 (Generalized $\sin\theta$ theorem). *Assume the Hermitian operator $A + H$ satisfies* (1.3) *and R is given by* (1.8); *assume as before that F_0 and F_1 are isometries with $F_0F_0^* + F_1F_1^* = 1$, but assume regarding E_0 only that $E_0^*E_0 \geqq \varepsilon^2$ for some $\varepsilon > 0$. Let P and Q be the projectors onto $\mathscr{R}(E_0)$ and $\mathscr{R}(F_0)$ as before, but without any hypothesis upon the dimensionality of these subspaces. Let $\sin\Theta_0$ be any operator with the same singular values as $P\tilde{Q}$. Assume there is an interval $[\beta, \alpha]$ and a $\delta > 0$ such that the spectrum of A_0 lies entirely in $[\beta, \alpha]$ while that of Λ_1 lies entirely outside of $]\beta - \delta, \alpha + \delta[$ (or such that the spectrum of Λ_1 lies entirely in $[\beta, \alpha]$ while that of A_0 lies entirely outside of $]\beta - \delta, \alpha + \delta[$). Then for every unitary-invariant norm, $\delta\varepsilon\|\sin\Theta_0\| \leqq \|R\|$.*

In this formulation two generalizations have been made, both important in practice. First, E_0 is no longer required to be an isometry. In the numerical-analytic formulation of § 1, this means our putative eigenvectors are not required to be exactly orthonormal. Presumably they are almost orthonormal, so that ε above is almost 1 and $\|E_0\|_1$ is not much bigger. Then Theorem 6.1 gives an estimate on $\|\sin\Theta_0\|$ which uses the actual computed R, and which falls short of the precision which perfect orthonormality would permit only insofar as the ε occurring falls below $\|E_0\|_1$.

Second, an eigenspace of $A + H$ may be compared to an eigenspace of A of different dimensionality. This freedom will be used in one of the numerical illustrations in § 9. It somewhat spoils the geometric description given in § 1 and § 3, but not altogether. Even there, the subspaces $\mathscr{N}_P = P\mathscr{H} \cap \tilde{Q}\mathscr{H}$ and $\mathscr{N}_Q = Q\mathscr{H} \cap \tilde{P}\mathscr{H}$ complicated the discussion. But in general, $P\mathscr{H} \ominus \mathscr{N}_P$ and $Q\mathscr{H} \ominus \mathscr{N}_Q$ are in the acute case (Definition 3.2). We shall want to apply Theorem 6.1 when R is small, hence $P\tilde{Q}$ small, hence surely $\mathscr{N}_P = \{0\}$; that is, when we may have taken too few columns in E_0 for the true dimensionality of the space $Q\mathscr{H}$ being approximated. The singular values of our $\sin\Theta_0$ are the sines of the angles between $P\mathscr{H}$ and that part of $Q\mathscr{H}$ to which $P\mathscr{H}$ is close, namely, $Q\mathscr{H} \ominus \mathscr{N}_Q$.

Proof of Theorem 6.1. As in the proof of the original $\sin\theta$ theorem, we have $R^*F_1 = E_0^*F_1\Lambda_1 - A_0E_0^*F_1$, and we deduce by Theorem 5.1 that $\|R\| \geqq \delta\|E_0^*F_1\|$ for any unitary-invariant norm. It remains to relate $\|E_0^*F_1\|$ to $\|P\tilde{Q}\| = \|\sin\Theta_0\|$. Now $\tilde{Q}$, the projector onto $\mathscr{R}(F_1)$, is still equal to $F_1F_1^*$. But with E_0 no longer isometric, we must first observe that $P = E_0(E_0^*E_0)^{-1}E_0^*$. Then

$$\begin{aligned}\|P\tilde{Q}\| &= \|E_0(E_0^*E_0)^{-1}E_0^*F_1F_1^*\|\\ &\leqq \|E_0(E_0^*E_0)^{-1}\|_1\|E_0^*F_1\|\,\|F_1^*\|_1\\ &\leqq \varepsilon^{-1}\times\|E_0^*F_1\|\times 1,\end{aligned}$$

which is precisely the inequality we need to complete the proof.

For some applications, the hypothesis in Theorem 6.1 concerning the spectra of A_0 and Λ_1 is too restrictive. We may weaken this hypothesis provided we weaken the conclusion as in the following theorem.

THEOREM 6.2 (Second generalized $\sin\theta$ theorem). *Assume the same as in Theorem* 6.1 *except that the only restriction on the spectra is that* $|\lambda - \alpha| \geqq \delta > 0$ *for all* λ *in the spectrum of* Λ_1 *and* α *in the spectrum of* A_0. *Then*

$$\delta\varepsilon\|\sin\Theta_0\|_{\mathrm{sq}} \leqq \|R\|_{\mathrm{sq}}.$$

Proof. The proof is the same as for Theorem 6.1 except that the appeal to Theorem 5.1 is replaced by one to inequality (5.1). If we use (5.2) instead, we find

$$\delta\varepsilon\|\sin\Theta_0\|_1 \leqq \|R\|_1\sqrt{\operatorname{rank} R}.$$

The foregoing results are slightly sharper than Stewart's [28] generalization of Swanson's [30]. A weaker version of Theorem 6.2 has been given by Varah [31, Theorem 2.1] for non-Hermitian problems.

In the remaining major theorems, the argument is more delicate and does seem to require the particular background assumed in § 1 and § 2. Accordingly we restore the hypotheses and notation which were in force there.

We use the direct rotation

$$U \simeq \begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix} = \begin{pmatrix} \cos\Theta_0 & -J_0^*\sin\Theta_1 \\ J_0\sin\Theta_0 & \cos\Theta_1 \end{pmatrix}, \tag{6.2}$$

$$J_0\Theta_0 = \Theta_1 J_0, \quad C_j \geqq 0;$$

in terms of it we write this alternate form of (1.3):

$$\begin{pmatrix} A_0 + H_0 & B^* \\ B & A_1 + H_1 \end{pmatrix}\begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix} = \begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix}\begin{pmatrix} \Lambda_0 & 0 \\ 0 & \Lambda_1 \end{pmatrix}, \tag{6.3}$$

and, in particular,

$$(A_0 + H_0)(-S_0^*) + B^*C_1 = -\,S_0^*\Lambda_1. \tag{6.4}$$

Proof of the $\tan\theta$ *theorem.* To the foregoing equations are added the particular hypotheses $\beta \leqq A_0 \leqq \alpha < \alpha + \delta \leqq \Lambda_1$ and $H_0 = 0$. The last equation simplifies two things. First from (1.8),

$$\|R\| = \left\|\begin{pmatrix} H_0 \\ B \end{pmatrix}\right\| = \|B\|$$

for every unitary-invariant norm. Secondly, (6.4) transposed is

$$C_1 B = S_0 A_0 - \Lambda_1 S_0. \tag{6.5}$$

As a further simplification, let us assume temporarily that all operators are bounded and that S_0 is compact; a more general proof, modelled upon this simplified one, will be given at the end of the section in an Appendix.

We shall use (1.13) to estimate $\|B\|_\nu$ for integers ν exceeding neither $\dim \mathscr{K}(E_0)$ nor $\dim \mathscr{K}(E_1)$. (If either dimension is finite, larger values of ν can contribute nothing to $\|B\|_\nu$ because $B = E_1^* H E_0$.) First choose orthonormal eigenvectors $x_{01}, \cdots, x_{0\nu}$ of $S_0^* S_0$ belonging respectively to its eigenvalues $\sin^2 \theta_1, \cdots, \sin^2 \theta_\nu$. Then orthonormal vectors $y_{11}, \cdots, y_{1\nu}$ are defined by $y_{1j} = -S_0 x_{0j} \div \sin \theta_j$ for those $\theta_j \neq 0$; and for those $\theta_j = 0$ choose corresponding y_{1j}'s to form an orthonormal set drawn from $\mathscr{N}(S_0^*)$. In any case, $S_0^* y_{1j} = -\sin \theta_j x_{0j}$ and, since $C_1 = (1 - S_0 S_0^*)^{1/2}$, $C_1 y_{1j} = \cos \theta_j y_{1j}$. From (6.5),

$$\begin{aligned} \cos \theta_j y_{1j}^* B x_{0j} &= y_{1j}^* C_1 B x_{0j} = y_{1j}^*(S_0 A_0 - \Lambda_1 S_0) x_{0j} \\ &= \sin \theta_j (y_{1j}^* \Lambda_1 y_{1j} - x_{0j}^* A_0 x_{0j}) \\ &\geqq \sin \theta_j (\alpha + \delta - \alpha) = \delta \sin \theta_j \end{aligned} \tag{6.6}$$

because $\Lambda_1 \geqq \alpha + \delta$ and $\alpha \geqq A_0$. The inequality shows that $\cos \theta_j > 0$, so divide by it and sum over j. Finally, appeal to (1.13) to deduce that

$$\|R\|_\nu = \|B\|_\nu \geqq \delta \sum_1^\nu \tan \theta_j = \delta \|\tan \Theta_0\|_\nu$$

and to Ky Fan's theorem to conclude that $\|R\| \geqq \delta \|\tan \Theta_0\|$ for all unitary-invariant norms.

To conclude further that $\|H\| \geqq \delta \|\tan \Theta\|$, observe first that

$$\|\tan \Theta\| = \left\|\begin{pmatrix} 0 & -J_0^* \tan \Theta_1 \\ J_0 \tan \Theta_0 & 0 \end{pmatrix}\right\|$$

and

$$\|J_0 \tan \Theta_0\| = \|J_0^* \tan \Theta_1\| = \|\tan \Theta_0\| \leqq \|B\|/\delta.$$

Therefore Lemmas 6.1 and 6.2 imply in turn

$$\delta \|\tan \Theta\| \leqq \left\|\begin{pmatrix} 0 & B^* \\ B & 0 \end{pmatrix}\right\| \leqq \left\|\begin{pmatrix} 0 & B^* \\ B & H_1 \end{pmatrix}\right\| = \|H\|.$$

It might be thought that only the proof method obliged us to assume $\Lambda_1 \geqq \alpha + \delta$. Why can the tan θ theorem not hold when Λ_1 has spectrum both above and below A_0, as the sin θ theorem does? Here is why.

Example 6.1. Take $A_0 = H_0 = 0$, $B^* = (0 \quad 1/\sqrt{2})$, and $A_1 = A_1 + H_1 = \begin{pmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{pmatrix}$. Then the direct rotation is obtained by setting $C_0 = 1/\sqrt{2}$, $S_0^* = (-1/\sqrt{2} \quad 0)$, $C_1 = \operatorname{diag}(1/\sqrt{2}, 1)$. The "diagonalized" form of $A + H$ is then given by $\Lambda_0 = 0$, $\Lambda_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. The reader should verify that (6.3) holds. All the hypotheses of the $\tan\theta$ theorem hold except that the spectrum of Λ_1 lies both above and below that of A_0. We may take $\alpha = 0$, $\delta = 1$. The conclusion of the theorem fails emphatically; $\delta\|\tan\Theta_0\| = 1 > 1/\sqrt{2} = \|R\|$ for every unitary-invariant norm.

A more general $\tan\theta$ theorem, analogous to the first generalized $\sin\theta$ theorem, permits a given eigenspace of A to be compared with a higher-dimensional eigenspace of $A + H$ thus.

THEOREM 6.3 (Generalized $\tan\theta$ theorem). *Assume the Hermitian operator $A + H$ satisfies* (1.3), *and R is given by* (1.8) *with $A_0 = E_0^*(A + H)E_0$; assume as in* § 1 *that E_0, E_1, F_0 and F_1 are isometries, satisfying $E_0E_0^* + E_1E_1^* = F_0F_0^* + F_1F_1^* = 1$, whose ranges $\mathscr{R}(E_i)$ and $\mathscr{R}(F_i)$ are invariant subspaces of A and $A + H$ respectively, but assume that* $\dim \mathscr{H}(E_0) < \dim \mathscr{H}(F_0)$ *instead of* (1.5). *Let $\sin\Theta_0$ be any operator whose singular values are the same as those of $E_0^*F_1$. Also assume that there is a gap of width $\delta > 0$ between some interval $[\beta, \alpha]$ containing A_0's spectrum and an interval $[\alpha + \delta, \infty[$ containing the spectrum of $\Lambda_1 = F_1^*(A + H)F_1$. Then for every unitary-invariant norm,*

$$\delta\|\tan\Theta_0\| \leqq \|R\|.$$

Proof. In view of the discussions around (1.8) and after Theorem 6.1, we see that the singular values $\sin\theta_k$ of $E_0^*F_1$ are just the sines of the angles θ_k between $\mathscr{R}(E_0)$ and that part of $\mathscr{R}(F_0)$ approximated by $\mathscr{R}(E_0)$; and from (1.3) and (1.8) we find that (6.4) is satisfied with $H_0 = 0$ (so $\|R\| = \|B\|$ as before) provided we first substitute $S_0^* = -E_0^*F_1$ and $C_1 = E_1^*F_1$. However we no longer have $C_1^* = C_1 = (1 - S_0S_0^*)^{1/2} \geqq 0$; instead we have a weaker relation

$$C_1^*C_1 = F_1^*(1 - E_0E_0^*)F_1 = 1 - S_0S_0^*$$

which complicates the previous proof (q.v.) slightly, starting with (6.5). The eigenvectors $x_{01}, \cdots, x_{0\nu}$ can be introduced again; but there might be only μ orthonormal vectors $y_{1j}, \cdots, y_{1\mu}$ satisfying $S_0x_{0j} = -\sin\theta_jy_{1j}$ and $S_0^*y_{1j} = -\sin\theta_jx_{0j}$ for some integer $\mu \leqq \nu$, because we must have $\mu \leqq \dim\mathscr{H}(F_1) \leqq \dim\mathscr{H}(E_1)$. This will not be serious, because if $\mu < \nu$ then $\theta_{\mu+1} = \cdots = \theta_\nu = 0$. Also $C_1y_{1j} \neq \cos\theta_jy_{1j}$ in general; but we can easily obtain ν orthonormal vectors $z_{11}, \cdots, z_{1\nu}$ in $\mathscr{H}(E_1)$ satisfying $C_1y_{1j} = \cos\theta_jz_{1j}$ for $1 \leqq j \leqq \mu$, even if some $\theta_j = \pi/2$. Then (6.6) must be replaced for $1 \leqq j \leqq \mu$ by

$$\begin{aligned} \cos\theta_jx_{0j}^*B^*z_{1j} &= x_{0j}^*B^*C_1y_{1j} = x_{0j}^*(A_0S_0^* - S_0^*\Lambda_1)y_{1j} \\ &= \sin\theta_j(y_{1j}^*\Lambda_1y_{1j} - x_{0j}^*A_0x_{0j}) \geqq \delta\sin\theta_j. \end{aligned}$$

Evidently these $\theta_j < \pi/2$, so $x_{0j}^*B^*z_{1j} \geqq \delta\tan\theta_j$; if necessary this inequality can be asserted for $\mu < j \leqq \nu$ too because then the sign of z_{1j} is at our disposal and $\theta_j = 0$. The proof concludes in the same way as before.

While proving Theorem 6.3, we had to revoke again some of the hypotheses and notation of § 1 and § 3 and now we must reinstate them again.

6. Appendix. Unbounded operators. The $\sin\theta$ theorem as stated admits unbounded Λ_1 (or A_0, but not both). It remains valid under the following more general hypothesis:

Assume there is an interval which contains the spectrum of A_0, while the spectrum of Λ_1 lies entirely distant at least δ from that interval.

If the interval is finite then the conclusion $\delta\|\sin\Theta_0\| \leqq \|R\|$ has been deduced from Theorem 5.1. If the interval is infinite, say $]-\infty, \alpha]$, then there is no conclusion at which to aim unless R is bounded; therefore we assume $(A + H)E_0$ and E_0A_0 have common dense domain, on which R as defined by (1.8) is bounded, and extend R by continuity. Now Theorem 5.2 may be applied just as Theorem 5.1 was before, yielding $\delta\|\sin\Theta_0\| \leqq \|R\|$.

The hypotheses of Proposition 6.1 and of Theorem 6.1 can be relaxed in a similar way.

The $\tan\theta$ theorem must be considered more carefully, because we must both use the technique of Theorem 5.2 and allow for noncompact Θ. Accordingly we give its proof in the general case.

As before, $A_0 \leqq \alpha$ and $\Lambda_1 \geqq \alpha + \delta$, but now both operators may be unbounded. We still have $\|R\| = \|B\|$, and only the case where this is finite interests us. This means that (6.5) holds on the common dense domain of S_0A_0 and Λ_1S_0.

Take any $\nu = 1, 2, \cdots$, and small $\varepsilon > 0$. We shall choose a ν-projector Υ on $\mathscr{K}(E_0)$ such that the singular values $\sin\phi_1 \geqq \sin\phi_2 \geqq \cdots$ of $S_0\Upsilon$ satisfy both

$$\sum_{k=1}^{\nu} \tan\phi_k > \sum_{k=1}^{\nu} \tan\theta_k - \varepsilon \tag{6.7}$$

and

$$\sum_{k=1}^{\nu} \sin^2\phi_k > \sum_{k=1}^{\nu} \sin^2\theta_k - \varepsilon^2; \tag{6.8}$$

and we shall prove that $\|B\Upsilon\|_\nu \geqq \delta\sum_1^\nu \tan\phi_k - \gamma_\varepsilon$, where γ_ε goes to 0 with ε. This will imply that $\sup\|B\Upsilon\|_\nu \geqq \delta\sum_1^\nu \tan\theta_k$, the supremum being over all ν-projectors Υ; and this in turn, by (1.12) and the theorem of Ky Fan, will give us the desired conclusion $\|B\| \geqq \delta\|\tan\Theta_0\|$.

Now, it is not hard to show from (1.13), as was done to prove Lemma 5.1, that there must be *some* ν-projector Υ which gives us (6.8). Tentatively choose any such, and denote it by Π.

For the spectral resolution of A_0 write

$$-A_0 = \int_{-\alpha}^{\infty} \lambda\, d\Omega(\lambda).$$

Consider $\Omega(\tau)\Pi$ as $\tau \to \infty$. Because $\|\tilde{\Omega}(\tau)\Pi\|$ approaches 0, the subspace

$\Omega(\tau)\Pi\mathscr{K}(E_0)$ is ultimately ν-dimensional and approaches $\Pi\mathscr{K}(E_0)$. Let Υ_τ denote the ν-projector onto it.

The singular values of $S_0\Upsilon_\tau$ depend continuously on Υ_τ, so they approach those of $S_0\Pi$, so for sufficiently large τ they too will satisfy (6.8). Assign such a large value to τ (it depends in an unknown way upon ε). Our new choice of ν-projector, Υ_τ, has this advantage over Π: because $\Upsilon_\tau = \Omega(\tau)\Upsilon_\tau$, $A_0\Upsilon_\tau = \Omega(\tau)A_0\Omega(\tau)\Upsilon_\tau$; we prefer to consider this because $\Omega(\tau)A_0\Omega(\tau)$ is an everywhere defined self-adjoint operator with spectrum in $[-\tau, \alpha]$. (Without loss of generality $|\alpha| \leqq \tau = \|\Omega(\tau)A_0\Omega(\tau)\|$.) Our choice of ν-projector is still not final, but the ν-projector now to be chosen will retain all the advantages enjoyed by Υ_τ.

Since the singular values of $S_0\Upsilon_\tau$ satisfy (6.8), so must the singular values of $S_0\Omega(\tau)$, which we denote by $\sin\psi_1 \geqq \sin\psi_2 \geqq \cdots$.

$$\sum_1^\nu \sin^2\psi_k - \sum_1^\nu \sin^2\theta_k + \varepsilon^2 > 0.$$

Take for η a positive number so small that η^2 is less than the left-hand member. Now apply (1.13) once more; obtain a ν-projector $\Upsilon = \Omega(\tau)\Upsilon$ such that the singular values $\sin\phi_k$ of $S_0\Upsilon = S_0\Omega(\tau)\Upsilon$ satisfy

$$\sum_1^\nu \sin^2\phi_k > \sum_1^\nu \sin^2\psi_k - \eta^2 \tag{6.9}$$

Then by the choice of η they also satisfy (6.8).

Next we imitate the proof of the tan θ theorem in the earlier special case, using the properties provided for Υ to make the needed estimates.

Choose an orthonormal basis $\{x_{01}, \cdots, x_{0\nu}\}$ of $\Upsilon\mathscr{K}(E_0)$ consisting of eigenvectors of $\Upsilon S_0^* S_0\Upsilon$, where x_{0k} belongs to the eigenvalue $\sin^2\phi_k$. Let $y_{11}, \cdots, y_{1\nu}$ be orthonormal vectors satisfying $S_0 x_{0k} = -\sin\phi_k y_{1k}$; this determines them uniquely unless some of the ϕ_k are zero, in which case we prescribe further that the corresponding y_{1k} lie in $\mathscr{N}(\Upsilon S_0^*)$. In any case, $\Upsilon S_0^* y_{1k} = -\sin\phi_k x_{0k}$. Let Γ denote the projector $\sum_1^\nu y_{1k}y_{1k}^*$, and observe that $S_0\Upsilon = \Gamma S_0\Upsilon$.

Now operate on (6.5) from the left by Γ and from the right by Υ. The result may be written

$$-\Gamma C_1 B\Upsilon + \Gamma S_0(\Omega(\tau)A_0\Omega(\tau))\Upsilon = (\Gamma\Lambda_1\Gamma)\Gamma S_0\Upsilon. \tag{6.10}$$

The left-hand member represents an everywhere defined bounded operator; hence so does the right-hand member. Therefore $\Gamma\Lambda_1\Gamma$ is an everywhere defined bounded operator, and its restriction to $\Gamma\mathscr{K}(E_1)$ has spectrum lying in $[\alpha + \delta, \infty[$.

In treating the two terms on the left, we shall use the following simple fact.

LEMMA 6.3. *Let K be an operator with singular values $\kappa_1 \geqq \kappa_2 \geqq \cdots$; let Γ and Ψ be ν-projectors such that $K\Psi = \Gamma K\Psi$; and let $\eta > 0$. Assume that the singular values $\mu_1 \geqq \mu_2 \geqq \cdots$ of $K\Psi$ satisfy*

$$\sum_{k=1}^\nu \mu_k^2 > \sum_{k=1}^\nu \kappa_k^2 - \eta^2.$$

Then $\|\Gamma K\tilde{\Psi}\|_1 \leqq \eta$.

Proof. $\|\Gamma K\tilde{\Psi}\|_1 = \sup\|\Gamma Kx\|$, the supremum being over unit vectors $x \in \mathscr{R}(\tilde{\Psi})$. But for any such x,

$$\sum_1^v \kappa_k^2 \geqq \operatorname{tr}(\Gamma KK^*\Gamma) \geqq \operatorname{tr}(\Gamma K(\Psi + xx^*)K^*\Gamma)$$

$$= \sum_1^v \mu_k^2 + \|\Gamma Kx\|^2,$$

so that by the hypothesis, $\|\Gamma Kx\|^2 < \eta^2$. The lemma is proved.

Our first application is to the second term in (6.10), which may be broken down into

$$\Gamma S_0(\Omega(\tau)A_0\Omega(\tau))\Upsilon = \Gamma S_0\Upsilon(\Upsilon A_0\Upsilon) + (\Gamma S_0\tilde{\Upsilon}\Omega(\tau))(\Omega(\tau)A_0\Omega(\tau)).$$

Call the second term on the right F. We shall show that it is small. By (6.9), we may apply Lemma 6.3 to the operator $S_0\Omega(\tau)$, with the conclusion $\|\Gamma S_0\tilde{\Upsilon}\Omega(\tau)\|_1 \leqq \eta$. Therefore $\|F\|_1 \leqq \eta\tau$. But η can be taken as small as we like without altering ε or τ; let us say $\eta\tau \leqq \varepsilon$.

The term $\Gamma S_0\Upsilon(\Upsilon A_0\Upsilon)$, on the other hand, is $\Gamma S_0\Upsilon$ times a self-adjoint operator which, on its range, is $\leqq \alpha$. We are ready to apply y_{1k}^* to (6.10) on the left and x_{0k} on the right. There ensues, exactly as in (6.6),

$$y_{1k}^*C_1Bx_{0k} + y_{1k}^*Fx_{0k} \geqq \delta \sin \phi_k. \tag{6.11}$$

We know that $|y_{1k}^*Fx_{0k}| \leqq \varepsilon$. Also we shall prove shortly that the $\cos \phi_k$ have a positive lower bound. Now if $y_{1k}^*C_1Bx_{0k}$ were simply $(\cos \phi_k)\, z_{1k}^*Bx_{0k}$ for some orthonormal set $\{z_{11}, \cdots, z_{1v}\}$, then we would divide by $\cos \phi_k$ and sum from 1 to v, and the rest of the way would be clear. But this is not quite so; let us see how close it comes.

The Gram matrix of the vectors $C_1y_{11}, \cdots, C_1y_{1v}$ has as entries

$$y_{1j}^*C_1^2y_{1k} = y_{1j}^*(1 - S_0S_0^*)y_{1k} = y_{1j}^*(1 - S_0\Upsilon S_0^*)y_{1k} - y_{1j}^*S_0\tilde{\Upsilon}S_0^*y_{1k}.$$

The first term on the right is $\delta_{jk}\cos^2 \phi_k$. The second term is small. Indeed, (6.8) entitles us to apply Lemma 6.3 to the operator S_0, with the conclusion $\|\Gamma S_0\tilde{\Upsilon}\|_1 \leqq \varepsilon$, and hence the second term is smaller than ε^2.

Returning to (6.11), we first extract the crude estimate

$$\delta \sin \phi_k \leqq \|B\|_1\|C_1y_{1k}\| + \varepsilon \leqq \|B\|_1(\cos \phi_k + \varepsilon) + \varepsilon.$$

Letting $\varepsilon \to 0$ here proves the theorem for the bound norm and, for the general proof, provides assurance that there is a positive lower bound under all the $\cos \phi_k$, independent of ε. We conclude first that the vectors $(\sec \phi_k)C_1y_{1k}$ can be approximated by an orthonormal set within an error going to 0 with ε, and secondly that (6.7) will be satisfied too if ε is small enough. By our previous remarks, this suffices to complete the proof of the $\tan \theta$ theorem for unbounded operators. A similar proof allows Theorem 6.3 to be applied to unbounded operators too.

7. Proof of the double-angle theorems. The new idea which enters here is the symmetric perturbation. We shall use the same notations as in (6.2) and (6.3) and ask the reader also to recall the definitions $X = P - \tilde{P}$ and $Q = XQX$, and some of the discussion of them in § 3. Now we shall consider $A + H$ along with the symmetric perturbation

$$A + XHX \simeq \begin{pmatrix} A_0 + H_0 & -B^* \\ -B & A_1 + H_1 \end{pmatrix}. \tag{7.1}$$

Since it is obtained from $A + H$ by a unitary similarity it must have the same "diagonal form," and indeed we have, corresponding to (6.3),

$$\begin{pmatrix} A_0 + H_0 & -B^* \\ -B & A_1 + H_1 \end{pmatrix}\begin{pmatrix} C_0 & S_0^* \\ -S_0 & C_1 \end{pmatrix} = \begin{pmatrix} C_0 & S_0^* \\ -S_0 & C_1 \end{pmatrix}\begin{pmatrix} \Lambda_0 & 0 \\ 0 & \Lambda_1 \end{pmatrix}. \tag{7.2}$$

The unitary that does the trick is actually the inverse of the one in (6.2) and (6.3); this slight simplification comes from using the direct rotations.

Combining (6.3) and (7.2) we obtain

$$\begin{aligned} &\begin{pmatrix} A_0 + H_0 & B^* \\ B & A_1 + H_1 \end{pmatrix}\begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix}^2 \\ &\qquad = \begin{pmatrix} C_0 & -S_0^* \\ S_0 & C_1 \end{pmatrix}^2 \begin{pmatrix} A_0 + H_0 & -B^* \\ -B & A_1 + H_1 \end{pmatrix}, \end{aligned} \tag{7.3}$$

or simply $(A + H)U^2 = U^2(A + XHX)$. The unitary here is

$$U^2 \simeq \begin{pmatrix} 2C_0^2 - 1 & -2C_0S_0^* \\ 2S_0C_0 & 2C_1^2 - 1 \end{pmatrix} = \begin{pmatrix} \cos 2\Theta_0 & -J_0^* \sin 2\Theta_1 \\ J_0 \sin 2\Theta_0 & \cos 2\Theta_1 \end{pmatrix} \tag{7.4}$$

(cf. (6.2)). Recall from Proposition 3.4 that this unitary, though it may not be the direct rotation of $Q_-\mathscr{H}$ to $Q\mathscr{H}$, does have the property $U^2Q_- = QU^2$.

We now obtain the $\sin 2\theta$ theorem by regarding $A + H$ as a perturbation, not of A, but of $A + XHX$. Then the perturbation is $H - XHX$ instead of H. We still treat the parts of $A + H$ on $Q\mathscr{H}$ and $\tilde{Q}\mathscr{H}$, represented by Λ_0 and Λ_1 respectively:

$$\Lambda_j = F_j^*(A + H)F_j.$$

But now we let the roles of A_0 and A_1 be taken by the parts of $A + XHX$ on $Q_-\mathscr{H}$ and $\tilde{Q}_-\mathscr{H}$ respectively; and of course in a different coordinate system these are represented by Λ_0 and Λ_1 also:

$$\Lambda_j = (XF_j)^*(A + XHX)XF_j.$$

Thus the hypotheses put upon the spectra of Λ_0 and Λ_1 in the $\sin 2\theta$ theorem allow us to invoke Proposition 6.1. In place of $E_0^*F_1$ we examine $(XF_0)^*F_1 = 2(F_0^*E_0)(E_0^*F_1)$, from which it is easy to see that, for purposes of evaluating norms, the role of $\sin \Theta_0$ can now be played by $\sin 2\Theta_0$. Thus Proposition 6.1 yields

$$\delta\|\sin 2\Theta\| \leqq \|H - XHX\| \leqq \|H\| + \|XHX\| = 2\|H\| \tag{7.5}$$

for all unitary-invariant norms, and this is one of the conclusions of the $\sin 2\theta$ theorem.

To get the other conclusion, we rewrite the first inequality in (7.5) in the form

$$\delta\left\|\begin{pmatrix} 0 & -\sin 2\Theta_0 J_0^* \\ J_0 \sin 2\Theta_0 & 0 \end{pmatrix}\right\| \leqq \left\|\begin{pmatrix} 0 & B^* \\ B & 0 \end{pmatrix}\right\|$$

and invoke Lemma 6.1; $\delta\|\sin 2\Theta_0\| \leqq \|B\| \leqq \|R\|$. This completes the proof.

Notice that the inference $\delta\|\sin 2\Theta\| \leqq 2\|H\|$ can also be drawn from one or two gaps of width δ in the spectrum of A instead of Λ; merely interchange the roles of A and $A + H$. But the inference $\delta\|\sin 2\Theta_0\| \leqq 2\|R\|$ is valid only when δ pertains to gaps in the spectrum of Λ; no such inference could be drawn from hypotheses upon a gap in the spectrum of A. For if $A \simeq \begin{pmatrix} 0 & 0 \\ 0 & \delta \end{pmatrix}$ and $H \simeq \begin{pmatrix} 0 & 1 \\ 1 & -\delta \end{pmatrix}$, then surely $2\|R\| = 2$, whereas $\delta\|\sin 2\Theta_0\| = \delta$ can be as large as you like.

Proof of the $\tan 2\theta$ *theorem.* Although the motivation is the same as above, the proof goes not by applying a version of a single-angle theorem, but by imitating the proof of the $\tan\theta$ theorem. We give the details only for the case of bounded operators and compact S_0; the extension to the general case resembles that for the $\tan\theta$ theorem.

The hypotheses are now $H_0 = 0$, $H_1 = 0$, $A_0 \leqq \alpha$, $\alpha + \delta \leqq A_1$. We obtain from (1.7)

$$F_0^*(A + H)F_1 = (C_0 \quad S_0^*)\begin{pmatrix} A_0 & B^* \\ B & A_1 \end{pmatrix}\begin{pmatrix} -S_0^* \\ C_1 \end{pmatrix} = 0;$$

i.e.,

$$-C_0B^*C_1 + S_0^*BS_0^* = S_0^*A_1C_1 - C_0A_0S_0^*. \tag{7.6}$$

Next let $x_{01}, \cdots, x_{0\nu}$ and $y_{11}, \cdots, y_{1\nu}$ be orthonormal sets of eigenvectors of $S_0^*S_0$ and $S_0S_0^*$ respectively, constructed so as to satisfy $S_0x_{0j} = \mp \sin\theta_j y_{1j}$ and $S_0^*y_{1j} = \mp \sin\theta_j x_{0j}$. The sign will be chosen in a moment. These vectors are applied to (7.6) to yield

$$\begin{aligned} \pm(\cos^2\theta_j x_{0j}^*B^*y_{1j} - \sin^2\theta_j y_{1j}^*Bx_{0j}) &= \pm x_{0j}^*(C_0B^*C_1 - S_0^*BS_0^*)y_{1j} \\ &= \sin\theta_j\cos\theta_j(y_{1j}^*A_1y_{1j} - x_{0j}^*A_0x_{0j}) \\ &\geqq \delta\sin\theta_j\cos\theta_j; \\ \pm 2\cos 2\theta_j \operatorname{Re}(y_{1j}^*Bx_{0j}) &\geqq \delta\sin 2\theta_j. \end{aligned}$$

This shows that $\cos 2\theta_j \neq 0$; by properly choosing the sign which was left free until now, we can write $2\operatorname{Re}(y_{1j}^*Bx_{0j}) \geqq \delta\|\tan 2\theta_j\|$, so $2\|B\|_\nu \geqq \delta\|\tan 2\Theta_0\|_\nu$. As before, we can drop the subscript ν and replace $\|B\|$ by $\|R\|$ to obtain the first conclusion of the theorem; the second conclusion requires merely an application of Lemma 6.1.

8. Interpretation of the double-angle theorems. The force of all four of our main theorems is to bound Θ. In the case of the single-angle theorems, the situation is straightforward; Θ is asserted to be close to 0. For example, if the hypotheses of the $\sin\theta$ theorem are satisfied with $\|R\|_1 = 1$ and $\delta = 2$, then the conclusion is $\|\sin\Theta_0\|_1 \leqq 1/2$, which means exactly that $\Theta \leqq \pi/6$.

The conclusions of the double-angle theorems allow angles θ_k close to $\pi/2$ instead of close to 0. There can even be some close to $\pi/2$ *and* some close to 0, but this requires explanation. Assume Θ_0 has just two eigenvalues, θ_1 close to $\pi/2$ and θ_2 close to 0. Let $x_1 \simeq \begin{pmatrix} x_{0k} \\ 0 \end{pmatrix}$ and $x_2 \simeq \begin{pmatrix} x_{02} \\ 0 \end{pmatrix}$ be corresponding eigenvectors: $\Theta_0 x_{0k} = \theta_k x_{0k}$. Then there will, to be sure, be vectors of $P\mathscr{H}$ which are rotated through intermediate angles by U. For instance, if $x = x_1 + x_2$ then one computes that $\cos \angle(x, Ux)$ is close to 1/2. This does not prevent $\sin 2\Theta_0$ or $\tan 2\Theta_0$ from having small norm, because the $\sin 2\theta_k$ are both small.

Thus there is no contradiction, but is there not an anomaly? Indeed, does this not violate our intent of showing that rotation is small if Θ is small (§ 3 and § 4) and Θ is small if the perturbation is small (§ 6 and § 7)?

There is an explanation, and we give it in this section. The point is that in the double-angle theorems there was no need to make any special assumption about the reducing subspace $Q\mathscr{H}$ of $A + H$, so we left it arbitrary! In past treatments of this subject it has been customary to compare a spectral subspace of the unperturbed operator with "the right" spectral subspace of $A + H$, that spectral subspace belonging to nearby spectral values. In proving the double-angle theorems without such a hypothesis, we of course left open the possibility that part of $Q\mathscr{H}$ could be reached from $P\mathscr{H}$ only by very large rotations (near $\pi/2$), for this might be so even for $H = 0$.

In the off-diagonal case there always is a "right" choice of $Q\mathscr{H}$. In the following theorem we fix A, P and H, but let Q (hence also Λ_0 and Λ_1) vary, and we look for conditions under which Θ as well as $\tan 2\Theta$ will be small.

THEOREM 8.1. *Assume the hypotheses of the* $\tan 2\theta$ *theorem. We have* $\Theta \leqq \pi/4$ *if and only if* $\Lambda_1 \geqq \alpha + \delta$ *and* $\Lambda_0 \leqq \alpha$. *For given* A, P *and* H, *there always exists a reducing projector* Q *such that* $\Lambda_1 \geqq \alpha + \delta$ *and* $\Lambda_0 \leqq \alpha$; *and for this* Q, *stronger inequalities hold*:

(i) $A_1 - \alpha \leqq C_1(\Lambda_1 - \alpha)C_1$, *and a similar relation for* Λ_0.

(ii) *In the finite-dimensional case, the eigenvalues* $\lambda_1 \leqq \lambda_2 \leqq \cdots$ *of* Λ_1 *are farther away from the gap than the eigenvalues* $\alpha_1 \leqq \alpha_2 \leqq \cdots$ *of* A_1, *by the relation*

$$\alpha_k - \alpha \leqq \|C_1\|_1^2(\lambda_k - \alpha);$$

a similar relation for Λ_0, *and natural extensions to the infinite-dimensional case.*

(iii) *In the finite-dimensional case, the* $\lambda_k - \alpha_k$ *may also be bounded below by*

$$\Phi(\alpha_1 - \alpha, \cdots, \alpha_n - \alpha) \leqq \Phi[(\lambda_1 - \alpha)\cos^2\theta_1, \cdots, (\lambda_n - \alpha)\cos^2\theta_n]$$

for any symmetric gauge function Φ; *a similar relation for* Λ_0.

(On symmetric gauge functions, see [12, Chap. III, Section 3], [25].)

We begin by proving the existence of Q which preserves the gap. This part of the theorem is familiar, especially in the finite-dimensional case, but the other parts are new.

P is the spectral projector of A belonging to $]-\infty, \alpha]$; choose Q to be the spectral projector of $A + H$ belonging to the same interval. Suppose if possible that $P\mathscr{H} \cap \tilde{Q}\mathscr{H}$ contains a unit vector x. Because $x \in P\mathscr{H}$, $x^*Ax \leqq \alpha$; because $x \in \tilde{Q}\mathscr{H}$, $x^*(A + H)x > \alpha$. On the other hand, off-diagonality means $PHP = 0$, so $x^*(A + H)x = x^*P(A + H)Px = x^*Ax$. A similar contradiction arises from supposing $\tilde{P}\mathscr{H} \cap Q\mathscr{H}$ contains a unit vector. We have proved we are in the acute case in the sense of Definition 3.2, and we may proceed to use the direct rotation. The construction has guaranteed $\Lambda_0 \leqq \alpha$; to prove $\Lambda_1 \geqq \alpha + \delta$ we prove (i), from which it follows.

It is easy to see from (6.3) that $A_1 = S_0\Lambda_0S_0^* + C_1\Lambda_1C_1$. With our present choice of Q, the first term on the right is $\leqq S_0\alpha S_0^* = \alpha - C_1\alpha C_1$. This yields (i).

From this (ii) follows by Weyl's theorem on monotonicity of eigenvalues [12, Chap. II, Lemma 1.1], [23, Section 96].

Again by Weyl's theorem, (i) implies for the ν-norms that $\|A_1 - \alpha\|_\nu \leqq \|C_1(\Lambda_1 - \alpha)C_1\|_\nu$; from this we shall deduce (iii). Let M_1 denote an operator unitary-equivalent to Λ_1 but such that its eigenvalue λ_k has the same corresponding eigenvector(s) as the eigenvalue θ_k of Θ_1. Our notation indexes the eigenvalues $\lambda_k - \alpha$ of $\Lambda_1 - \alpha$ and the eigenvalues $\cos\theta_k$ of C_1 both in increasing order. By a generalization [12, Chap. II, Equation 4.11] of a theorem of von Neumann [22], $\|C_1(\Lambda_1 - \alpha)C_1\|_\nu \leqq \|C_1(M_1 - \alpha)C_1\|_\nu$. By the theorem of Ky Fan, the inequality $\|A_1 - \alpha\| \leqq \|C_1(M_1 - \alpha)C_1\|$ holds for all unitary-invariant norms. Since the singular values of $A_1 - \alpha$ are the $\alpha_k - \alpha$ and the singular values of $C_1(M_1 - \alpha)C_1$ are the $(\lambda_k - \alpha)\cos^2\theta_k$, this gives (iii).

So there is always some Q with $\Lambda_1 \geqq \alpha + \delta$ and $\Lambda_0 \leqq \alpha$ (and of course it is unique). It is more difficult to prove from this that $\Theta \leqq \pi/4$. We revert to a method used in [5], [6].

One derives from (6.3) that

$$\Lambda_0 = C_0^{-1}A_0C_0 + C_0^{-1}B^*S_0 = S_0^{-1}BC_0 + S_0^{-1}A_1S_0$$

(at least on the orthogonal complement of $\mathscr{N}(S_0)$). Let x_0 be a unit vector such that $\Theta_0x_0 = \theta x_0$, and $y_1 = J_0x_0$. Then

$$\begin{aligned} x_0^*\Lambda_0x_0 &= x_0^*A_0x_0 + \tan\theta\, x_0^*B^*y_1 \\ &= \cot\theta\, y_1^*Bx_0 + y_1^*A_1y_1. \end{aligned} \tag{8.1}$$

This shows at once that $x_0^*B^*y_1$ is real, hence equal to $y_1^*Bx_0$. The second equality of (8.1) now gives

$$x_0^*B^*y_1(\tan\theta - \cot\theta) = y_1^*A_1y_1 - x_0^*A_0x_0 \geqq \delta > 0. \tag{8.2}$$

This shows incidentally that $\theta \neq \pi/4$; indeed (B being bounded) it bounds θ away from $\pi/4$. Now suppose if possible that $\theta > \pi/4$; then (8.2) would imply $x_0^*B^*y_1 > 0$. Using (8.1) once more, $x_0^*\Lambda_0x_0 \geqq y_1^*A_1y_1$; whereas we know that $y_1^*A_1y_1 - x_0^*A_0x_0 \geqq \delta$. This proves that Θ has no eigenvalue $\geqq \pi/4$. In the infinite-dimensional case, we still require an approximation argument such as [6, Theorem 6.1, Step 1].

Instead of the computation involving (8.1), we could have shown $\Theta < \pi/4$ by a continuity argument using the Rellich theory [23, Sections 135–136]; cf. the proof of Theorem 8.2 below.

For the converse, it is enough by symmetry to show that any reducing subspace $\mathcal{M}$ of $A + H$ consisting entirely of vectors at an angle $\leqq \pi/4$ with $P\mathcal{H}$ must also consist entirely of vectors x with $x^*(A + H)x \leqq \alpha x^*x$. Suppose not. Then letting Q still denote that Q found above, $\mathcal{M}$ reduces Q but $\mathcal{M} \nsubseteq Q\mathcal{H}$; therefore there exists a unit vector $x \in \tilde{Q}\mathcal{H} \cap \mathcal{M}$. Such a vector makes an angle $\leqq \pi/4$ with $P\mathcal{H}$ because it is in $\mathcal{M}$, but by the first part of the proof it makes an angle $< \pi/4$ with $\tilde{P}\mathcal{H}$. This contradiction completes the proof.

We interject a remark on conditions (ii), (iii) of Theorem 8.1. They are an addition to the meager information on the relation between change in eigenvalues and change in eigenvectors caused by the same perturbation. Whereas [5, Theorem 3.2] says a perturbation which changes eigenvectors a lot cannot also change eigenvalues too much, conditions (ii) and (iii) go in the other direction; they say that an off-diagonal perturbation which changes all eigenvectors a lot ($\|C_1\|_1$ well below 1) is obliged to change eigenvalues a certain amount too.

THEOREM 8.2. *To the hypotheses of the* sin 2θ *theorem add these*: $\|H\|_1 < \delta/2$ *or* $\|R\|_1 < \delta/2$, *and the spectrum of* A_0 *lies in* $[\beta - \delta/2, \alpha + \delta/2]$. *Then beside* $\delta\|\sin 2\Theta\| \leqq 2\|H\|$ *or* $\delta\|\sin 2\Theta_0\| \leqq 2\|R\|$, *we also have* $\Theta < \pi/4$.

Proof. Let $\gamma = \|H\|_1$ $(< \delta/2)$. We consider the family of perturbed operators $A(\sigma) = A + H - \sigma H$ for σ going from 0 to 1, and argue by continuity. From the given fact that the spectrum of $A(0) = A + H$ is disjoint from $]\beta - \delta, \beta[$, we can see that every $A(\sigma)$ (being obtained from $A(0)$ by a perturbation σH of bound norm at most γ) has spectrum disjoint from $]\beta - \delta + \gamma, \beta - \gamma[$. Similarly, $A(\sigma)$ has spectrum disjoint from $]\alpha + \gamma, \alpha + \delta - \gamma[$. Consider $Q(\sigma)$, the spectral projector of $A(\sigma)$ belonging to the interval $[\beta - \delta/2, \alpha + \delta/2]$. By [23, Section 135], $Q(\sigma)$ as a function of σ is continuous in the norm topology. But this in turn means that $\theta(\sigma)$, which we define as $\theta(\sigma) = \arcsin\|Q(\sigma) - Q(0)\|_1$, is continuous. Obviously $\theta(0) = 0$; and because the hypothesis $\beta \leqq A_0 \leqq \alpha$ implies $P = PQ(1)$, we have also $\theta(1) \geqq \Theta$. We aim to prove $\theta(1) < \pi/4$, and this will prove the theorem.

By a *close* σ let us denote a $\sigma \in [0, 1[$ such that $\theta(\sigma) \leqq \pi/4$. For a close σ, we compare by the sin 2θ theorem the reducing subspaces $Q(\sigma)$ of $A(\sigma)$ and $Q(0)$ of $A(0)$, and really get acute angles. For close σ, accordingly, we must have

$$\theta(\sigma) \leqq \tfrac{1}{2} \arcsin (2\|\sigma H\|_1/\delta) = \tfrac{1}{2} \arcsin (2\sigma\gamma/\delta)$$

$$\leqq \frac{\pi}{2}\frac{\sigma\gamma}{\delta} < \frac{\pi}{2}\frac{\gamma}{\delta} < \frac{\pi}{4}.$$

By continuity, there is some larger value of σ which is close. But $\sigma = 0$ is close. Therefore all σ are close, and the conclusion follows.

We used here the hypothesis $\|H\|_1 < \delta/2$. If we were given instead that $\|R\|_1 < \delta/2$, we would reason as follows. Without changing $A_1 + H_1$ or R or the Λ_j, we can change H_1. But by a theorem of Kreĭn [23, Section 125], [15] there is some choice of H_1 making $\|H\|_1 = \|R\|_1$. Thus this hypothesis also suffices.

The sin 2θ theorem can be extended to cope with the possibility that dim $\mathcal{K}(E_0) <$ dim $\mathcal{K}(F_0)$. This extension is so similar to Theorems 6.1 and 6.3 that we shall not discuss it further here. However, no such extension of the tan 2θ theorem is known.

9. A numerical example. The following example was used by H. F. Weinberger [34] to illustrate his eigenvector estimates. It will serve here to illustrate our notation and theorems, and to compare bounds obtainable by the different procedures, as to their nature and their precision.

The problem. Let $\mathscr{H}$ be real $\mathscr{L}_2(0, 1)$. We write $u, v, \cdots$ for its elements $u(t), v(t), \cdots$, so that $u^*v = \int_0^1 u(t)v(t)\,dt$. The operator equal to $(d/dt)^4$ acting on those $u \in \mathscr{H}$ satisfying

$$u''(0) = u'''(0) = u''(1) = u'''(1) = 0$$

has self-adjoint closure [9, Chap. XIII] which we denote by A. Let H denote the bounded Hermitian operator of multiplication by εt for some small constant ε satisfying $0 < \varepsilon < 100$.

We want to study the lowest two eigenvalues of $A + H$ and their eigenvectors. In the notation of differential equations this eigenproblem would be written

$$u^{iv} + \varepsilon t u = \lambda u,$$

$$u''(0) = u'''(0) = u''(1) = u'''(1) = 0.$$

We compare it with the eigenproblem for A, namely,

$$w^{iv} = \alpha w,$$

$$w''(0) = w'''(0) = w''(1) = w'''(1) = 0.$$

The eigenvalues of the operator A are $\alpha_1 = 0 = \alpha_2 < \alpha_3 < \cdots$, where the α_k for $k > 2$ are the positive roots of

$$\cos \alpha^{1/4} \cosh \alpha^{1/4} = 1,$$

all of which exceed 500. As eigenfunctions belonging to α_1 and α_2 we need two orthonormal linear functions; Weinberger would have chosen

$$w_k(t) = (1 + (-1)^k\sqrt{3}(2t - 1))/\sqrt{2}, \qquad k = 1, 2,$$

but for some arithmetic oversight in his paper [34, p. 223]. We choose $e_k = w_k$ for $k = 1$ and 2 to conform with the notation of § 1, and we further write $E_0 = (e_1 \quad e_2)$, an operator from $\mathbf{R}^2$ to $\mathscr{H}$.

Similarly, let $\lambda_1 \leqq \lambda_2 \leqq \cdots$ be the eigenvalues of $A + H$; let $f_1, f_2, \cdots$ be corresponding orthonormal eigenfunctions and write $F_0 = (f_1 \quad f_2)$. Broadly, the problem is to bound the difference between the 2-subspaces $E_0\mathbf{R}^2$ and $F_0\mathbf{R}^2$ of $\mathscr{H}$.

For both Weinberger's method and ours, we need estimates of some eigenvalues of $A + H$. Since in this case $H \geqq 0$, we have immediately $\lambda_3 \geqq \alpha_3 > 500$; in our notation, $\Lambda_1 > 500$.

As we pointed out in § 1, we have an option as to what we use as comparison matrix. The straightforward choice, as the problem is posed, is $A_0 = E_0^* A E_0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$. This gives the residual

$$R \equiv (A + H)E_0 - E_0 \cdot 0 = HE_0 = (r_1 \quad r_2).$$

This is of course again an operator from $\mathscr{K}(E_0) = \mathbf{R}^2$ to $\mathscr{H}$, so we have written it as a row of elements of $\mathscr{H}$. Namely,

$$r_k(t) = \varepsilon t e_k(t) = \varepsilon t(1 + (-1)^k\sqrt{3}(2t - 1))/\sqrt{2}.$$

From this we compute

$$R^*R = \frac{\varepsilon^2}{30}\begin{pmatrix} 11 - \sqrt{75} & -1 \\ -1 & 11 + \sqrt{75} \end{pmatrix}$$

and its eigenvalues $\varepsilon^2(11 \pm \sqrt{76})/30$.

Now the sin θ theorem applies; since $A_0 = 0$, the gap is $\delta = 500$, and we have $\|\sin \Theta_0\| < \|R\|/500$ for every unitary-invariant norm. For the bound norm in particular, $\|\sin \Theta_0\|_1 = \sin \theta_1$, and θ_1 is the usual angle between the spectral subspaces $E_0\mathbf{R}^2$ and $F_0\mathbf{R}^2$. The value so obtained is

$$\sin \theta_1 < 0.001622\varepsilon. \tag{9.1}$$

Note that we could have saved ourselves computing $\|R\|_1$ by using the sin 2θ theorem instead: A_1, like Λ_1, is greater than 500, so we can again take $\delta = 500$. The second version of the theorem (with A and $A + H$ interchanged) then says $\|\sin 2\Theta\| < 2\|H\|/500$. All the singular values of H equal ε, so this is very easy to apply. For the bound norm it gives

$$\sin 2\theta_1 < 0.004\varepsilon, \tag{9.2}$$

not quite so good as (9.1).

We want to illustrate computation of other norms too, and we choose the simplest conceptually (not computationally), $\|\cdot\|_2$, the sum of the top two singular values. We know the singular values of R and H so we can give the results corresponding to (9.1) and (9.2):

$$\sin \theta_1 + \sin \theta_2 < 0.00218\varepsilon, \tag{9.3}$$

$$\sin 2\theta_1 + \sin 2\theta_2 < 0.008\varepsilon. \tag{9.4}$$

This time the advantage of the sin θ theorem is more pronounced.

A refinement mentioned in § 1 is the choice of A_0 in such a way that H_0 will be zero. We do not change any subspaces; we just use the generalized Rayleigh–Ritz quotient

$$\hat{A}_0 \equiv E_0^*(A + H)E_0 = \tfrac{1}{2}\varepsilon\begin{pmatrix} 1 - 1/\sqrt{3} & 0 \\ 0 & 1 + 1/\sqrt{3} \end{pmatrix}$$

in place of the A_0 above. This gives the residual

$$\hat{R} \equiv (A + H)E_0 - E_0\hat{A}_0 = R - E_0\hat{A}_0 \equiv (\hat{r}_1 \quad \hat{r}_2);$$

and then, because $E_0^*\hat{R} = 0$,

$$\hat{R}^*\hat{R} = R^*R - \hat{A}_0^2 = \frac{1}{30}\varepsilon^2\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},$$

so that $\|\hat{R}\|_1 = \|\hat{R}\|_2 = \varepsilon/\sqrt{15} = .2582\varepsilon$.

To apply the $\tan\theta$ theorem with this off-diagonal perturbation, we have again the estimate $\Lambda_1 > 500$, but now we have to modify the estimate at the bottom of the gap. Denote the eigenvalues of $\hat{A}_0$ by $\hat{\alpha}_1 < \hat{\alpha}_2$. We saw above that

$$\hat{\alpha}_k = \tfrac{1}{2}\varepsilon(1 + (-1)^k/\sqrt{3}), \tag{9.5}$$

so that $\hat{A}_0 < .7887\varepsilon$ and we can take in the theorem $\delta = 500 - .7887\varepsilon$. Now the $\tan\theta$ theorem for bound norm gives

$$\tan\theta_1 < \frac{0.0005164\varepsilon}{1 - 0.0015774\varepsilon}; \tag{9.6}$$

and for the 2-norm, it gives exactly the same bound for $\tan\theta_1 + \tan\theta_2$. To apply the $\tan 2\theta$ theorem we have to use, not the straightforward choice of A_1 but again a choice such that our perturbation will be off-diagonal: $\hat{A}_1 \equiv E_1^*(A + H)E_1$. Fortunately $\hat{A}_1 - A_1 = E_1^*HE_1 \geqq 0$ so we have still the estimate $\hat{A}_1 > 500$. The results improve on (9.6): for the bound norm,

$$\tan 2\theta_1 < \frac{0.0010328\varepsilon}{1 - 0.0015774\varepsilon}; \tag{9.7}$$

and for the 2-norm, exactly the same bound upon $\tan 2\theta_1 + \tan 2\theta_2$.

So much for the estimates which flow most naturally out of our approach; let us compare them now with Weinberger's [34]. He needs the Rayleigh–Ritz values $\hat{\alpha}_1$ and $\hat{\alpha}_2$ of (9.5) as upper bounds for λ_1 and λ_2 respectively, and he also needs respective lower bounds $\check{\alpha}_1$ and $\check{\alpha}_2$, and the fact that $\hat{\alpha}_2 < 500 < \lambda_3$. Then his Theorem 2 yields bounds

$$\sin^2\phi_k \leqq (\hat{\alpha}_k - \check{\alpha}_k)/(500 - \check{\alpha}_k), \qquad k = 1, 2,$$

for the angles ϕ_k between e_k and the subspace $F_0\mathbf{R}^2$ spanned by the two eigenvectors f_k of $A + H$ belonging to λ_1 and λ_2. He used lower bounds $\check{\alpha}_k = \alpha_k = 0$ in his paper, but these are too crude to exhibit the power of his theorem. The best bounds $\check{\alpha}_k$ that can be deduced from $\hat{A}_0$, $\hat{R}^*\hat{R}$ and the fact that $\hat{A}_1 > 500$ are the two lower eigenvalues of

$$\begin{pmatrix} \hat{\alpha}_1 & 0 & \varepsilon/\sqrt{30} \\ 0 & \hat{\alpha}_2 & \varepsilon/\sqrt{30} \\ \varepsilon/\sqrt{30} & \varepsilon/\sqrt{30} & 500 \end{pmatrix};$$

the process of deduction follows Weinberger [33] and Lehmann [19], and will not be described here. It turns out that

$$\frac{\varepsilon^2/30}{500 - \hat{\alpha}_k} > \hat{\alpha}_k - \check{\alpha}_k = \frac{\varepsilon^2/30}{500 - \hat{\alpha}_k} - O(\varepsilon^4)$$

for the small values of ε that we are considering $(0 < \varepsilon < 100)$, whence follow

$$\begin{aligned} &\tan \phi_1 < 0.0005164\varepsilon/(1 - 0.0004227\varepsilon), \\ &\tan \phi_2 < 0.0005164\varepsilon/(1 - 0.0015774\varepsilon). \end{aligned} \tag{9.8}$$

These bounds closely resemble our (9.6) and (9.7), but the resemblance is deceptive because his results and ours answer different questions. Our θ_1 is the largest angle that *any* vector e in $E_0\mathbf{R}^2$ can make with the invariant subspace $F_0\mathbf{R}^2$, whereas the ϕ_k are the angles that *specific* vectors e_k in $E_0\mathbf{R}^2$ make with $F_0\mathbf{R}^2$. Therefore $\theta_1 \geqq \phi_k$, although ϕ_1 and ϕ_2 cannot both be much smaller than θ_1 because $\sin^2 \phi_1 + \sin^2 \phi_2 = \sin^2 \theta_1 + \sin^2 \theta_2$.

To compare the methods more directly, let us obtain bounds for the ϕ_k from our tan θ theorem. Since the ϕ_k are angles between subspaces of different dimensionality, our Theorem 6.3 will be used, this time taking $E_0 = e_k$, $A_0 = \hat{\alpha}_k = e_k^*(A + H)e_k$, and $R = (A + H)e_k - e_k\hat{\alpha}_k = \hat{r}_k$, which appeared above as one of the "columns" of $\hat{R}$. We shall define Λ_0 implicitly by requiring $\Lambda_1 > 500$, whence $F_0\mathbf{R}^2$ remains as before that invariant subspace of $A + H$ belonging to the two smallest eigenvalues; now the gap is $\delta = 500 - \hat{\alpha}_k$. Consequently we find

$$\tan \phi_1 < \frac{\varepsilon/\sqrt{30}}{500 - \hat{\alpha}_1} = 0.0003652\varepsilon/(1 - 0.0004227\varepsilon),$$

$$\tan \phi_2 < \frac{\varepsilon/\sqrt{30}}{500 - \hat{\alpha}_2} = 0.0003652\varepsilon/(1 - 0.0015774\varepsilon),$$

which are sharper than (9.8).

Although our results appear here to be sharper, they cannot supplant Weinberger's. Our results are inferences from the norm of a residual R or a perturbation H and from a gap δ between appropriate spectra; the smaller the norm relative to the gap, the smaller are our bounds. Weinberger's results are inferences from certain Rayleigh–Ritz upper bounds $\hat{\alpha}_k$ as well as lower bounds $\check{\alpha}_k$ (including here $\check{\alpha}_3 = 500$); the smaller the differences $\hat{\alpha}_k - \check{\alpha}_k$ relative to the gaps $500 - \hat{\alpha}_k$, the smaller are his bounds. Weinberger's results can be used to get bounds that resemble ours in that they proceed from a norm and a gap, but only by first inferring lower bounds $\check{\alpha}_k$ from the norm; this link is the weakest in the chain of inference, and causes Weinberger's results to appear weaker than ours. If, however, one has another source of information giving lower bounds $\check{\alpha}_k$, Weinberger's method can put them to use in improving eigenvector bounds while ours cannot.

For example, suppose that for some small positive constant $\mu \ll 0.6$ we let $e \equiv (1, \mu, \mu^2, \cdots, \mu^n, \cdots)^* \in l_2$ and $A + H \equiv \operatorname{diag}(1, \mu^{-1}, \mu^{-2}, \cdots, \mu^{-n}, \cdots)$.

Strictly speaking, e is not in the domain of $A + H$ because $(A + H)e = (1, 1, 1, \cdots, 1, \cdots)^*$ has infinite norm, but an arbitrarily small change in e would remedy this defect so let us ignore it. We can compute $\hat{\alpha}_1 \equiv e^*(A + H)e/e^*e = 1 + \mu$, but $\hat{r} \equiv (A + H)e - e\hat{\alpha}_1$ has $\|r\| = \infty$, so none of our theorems can be used. On the other hand, if we knew lower bounds $\check{\alpha}_1 \leqq \lambda_1 = 1$ and $\check{\alpha}_2 \leqq \lambda_2 = \mu^{-1}$, and provided $\check{\alpha}_2 > \hat{\alpha}_1$, we could obtain from Weinberger's Theorem 1

$$\sin^2 \theta \leqq (1 + \mu - \check{\alpha}_1)/(\check{\alpha}_2 - \check{\alpha}_1)$$

as a bound for the angle $\theta = \arcsin \mu$ between e and the first eigenvector $f = (1, 0, 0, \cdots, 0, \cdots)^*$. The best such bound (when $\check{\alpha}_1 = 1$ and $\check{\alpha}_2 = \mu^{-1}$) is

$$(\mu =) \sin \theta \leqq \mu/\sqrt{1 - \mu}.$$

Therefore neither Weinberger's approach nor ours can supplant the other.

So far, neither approach has been used to discern separately the eigenvectors f_k which span that eigenspace of $A + H$ belonging to some cluster of nearly indistinguishable eigenvalues. To do so is difficult, as we suggested in the discussion preceding (1.8); but the reader should not infer that it is always too difficult to reward analysis. We turn again to Weinberger's example for illustration.

We had orthonormal vectors e_1, e_2 spanning the approximate eigenspace $\mathscr{R}(E_0)$, and orthonormal eigenvectors f_1, f_2 spanning $\mathscr{R}(F_0)$. We estimated the angles θ_1, θ_2 between the two subspaces; we also estimated the angles ϕ_i between the e_i and $\mathscr{R}(F_0)$. We are now trying to estimate ω_k, the angle between the 1-subspace $[e_k]$ and the 1-subspace $[f_k]$.

Let g_k be that unit vector of $\mathscr{R}(E_0)$ which is closest to f_k, and let $\eta_k = \arccos g_k^* f_k$, so that $Pf_k = (\cos \eta_k) g_k$. Further let ψ_k denote the angle between the 1-subspaces $[g_k]$ and $[e_k]$ of $\mathscr{R}(E_0)$. Then $\cos \omega_k = \cos \eta_k \cos \psi_k$, or, less precisely, $\omega_k^2 \leqq \psi_k^2 + \eta_k^2$; so the desired bounds upon the ω_k can be obtained from bounds upon the ψ_k and the η_k.

First consider ψ_k. Let us write (in notation slightly modified from § 1) $e_k \simeq \begin{pmatrix} u_k \\ 0 \end{pmatrix}$ and $f_k \simeq \begin{pmatrix} x_k \\ y_k \end{pmatrix}$, with $u_k, x_k \in \mathscr{K}(E_0) = \mathbf{R}^2$, so that

$$\begin{pmatrix} \hat{A}_0 & B^* \\ B & \hat{A}_1 \end{pmatrix} \begin{pmatrix} x_k \\ y_k \end{pmatrix} = \lambda_k \begin{pmatrix} x_k \\ y_k \end{pmatrix} \tag{9.9}$$

and $(\cos \eta_k) g_k = \begin{pmatrix} x_k \\ 0 \end{pmatrix}$. Here $B^*B = \hat{R}^*\hat{R}$ is a 2×2 matrix which has been computed above, along with $\hat{A}_0 \equiv E_0^*(A + H)E_0 = \operatorname{diag}(\hat{\alpha}_1, \hat{\alpha}_2)$. We know that $\hat{A}_1 \equiv E_1^*(A + H)E_1 \geqq E_1^* A E_1 > 500$. But the eigenvalues λ_1, λ_2 which we seek are < 500. This entitles us to write, from (9.9),

$$y_k = (\lambda_k - \hat{A}_1)^{-1} B x_k, \tag{9.10}$$

$$[\hat{A}_0 + B^*(\lambda_k - \hat{A}_1)^{-1} B] x_k = \lambda_k x_k. \tag{9.11}$$

Thus λ_k is an eigenvalue and x_k the corresponding eigenvector of the eigenproblem

(9.11) in 2-space. The matrix $\hat{A}_0 + B^*(\lambda_k - \hat{A}_1)^{-1}B$ occurring here is the sum of a diagonal matrix $\hat{A}_0 - \varepsilon^2/(30\gamma_k)$ and an off-diagonal perturbation $\hat{H} \equiv \varepsilon^2\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\Big/(30\gamma_k)$ for some $\gamma_k > 500 - \lambda_k$; these relations follow by writing

$$0 \leqq \varepsilon^2/(30\gamma_k) - \hat{H} \equiv B^*(\hat{A}_1 - \lambda_k)^{-1}B \leqq B^*B/(500 - \lambda_k),$$

and recalling that $B^*B = \hat{R}^*\hat{R}$ is of rank 1.

In this subspace, ψ_k appears as the angle between the 1-dimensional eigenspace $[x_k]$ and the eigenspace $[u_k]$ of $\hat{A}_0 - \varepsilon^2/(30\gamma_k)$; this diagonal matrix has eigenvectors $u_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $u_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ belonging to eigenvalues $\hat{\alpha}_1 - \varepsilon^2/(30\gamma_k)$ and $\hat{\alpha}_2 - \varepsilon^2/(30\gamma_k)$ respectively, where $\hat{\alpha}_l$ are given by (9.5). The tan 2θ theorem now gives us $(\hat{\alpha}_2 - \hat{\alpha}_1)\tan 2\psi_k \leqq 2\|\hat{H}\|_1 < \varepsilon^2/[15(500 - \lambda_k)]$. Provided we take $0 < \varepsilon < 100$, we can also assert by Theorem 8.1 that $0 \leqq \psi_k < \pi/4$ (i.e., that $[x_k]$ is the nearest eigenspace to $[u_k]$), by virtue of the bounds

$$\hat{\alpha}_k - \varepsilon^2/(15000 - 30\hat{\alpha}_k) < \check{\alpha}_k \leqq \lambda_k \leqq \hat{\alpha}_k,$$

discussed earlier. We conclude that

$$2\psi_k < \arctan\left(\frac{\varepsilon}{\sqrt{75}(500 - \hat{\alpha}_k)}\right).$$

As to η_k, it is the angle between $f_k \in \mathscr{R}(F_0)$ and $g_k \in \mathscr{R}(E_0)$, so of course it is less than θ_1, for which we have the bound (9.7). Though this bound (the same for both values of k) is fairly sharp, we prefer a bound of the tan θ type because it simplifies the subsequent computation. Namely, from (9.10),

$$\tan \eta_k = \|y_k\|/\|x_k\| < \|B\|_1/(500 - \lambda_k) \leqq \frac{\varepsilon}{\sqrt{15}(500 - \alpha_k)}.$$

Combining the estimates by means of

$$\omega_k^2 \leqq \psi_k^2 + \eta_k^2 < (\tfrac{1}{2}\tan 2\psi_k)^2 + \tan^2 \eta_k,$$

we find that

$$\omega_1 < 0.00053\varepsilon/(1 - 0.00043\varepsilon), \quad \omega_2 < 0.00053\varepsilon/(1 - 0.0016\varepsilon).$$

These bounds, surprisingly small considering how close together are the eigenvalues ($\alpha_2 - \alpha_1 = 0$ and $\lambda_2 - \lambda_1 < 0.58\varepsilon + O(\varepsilon^2)$) compared with the given perturbation H ($\|H\|_1 = \varepsilon$), provide added incentive, if any more be needed, to use Rayleigh–Ritz approximations wherever possible.

However, the foregoing bounds upon ω_k can be improved. The best possible bound upon ω_k for $k = 1$ and 2 turns out to be the angle between the kth coordinate vector and the kth eigenvector of

$$\begin{pmatrix} \hat{\alpha}_1 & 0 & \varepsilon/\sqrt{30} \\ 0 & \hat{\alpha}_2 & \varepsilon/\sqrt{30} \\ \varepsilon/\sqrt{30} & \varepsilon/\sqrt{30} & 500 \end{pmatrix},$$

but the proof of this claim must be deferred to a time when Question 10.2 of the next section is investigated.

10. Some open questions.

Question 10.1. If it is known of the spectra of A_0 and Λ_1 only that the distance between them is at least δ, how well can we bound Θ_0 in terms of R? Compare the discussions after Theorems 5.1 and 6.2.

Question 10.2. Generalizing the set-up in § 1, let E_0, E_1, E_2 be isometric mappings into $\mathscr{H}$ such that $E_0E_0^* + E_1E_1^* + E_2E_2^* = 1$, and F_0, F_1, F_2 similarly. We may measure difference between the decompositions of the space by the size (in some norm) of the off-diagonal entries of

$$\begin{pmatrix} E_0^*F_0 & E_0^*F_1 & E_0^*F_2 \\ E_1^*F_0 & E_1^*F_1 & E_1^*F_2 \\ E_2^*F_0 & E_2^*F_1 & E_2^*F_2 \end{pmatrix},$$

analogously to the way (1.7) figured in this paper. If the decompositions of the space were associated with reducing subspaces of two nearby operators, could we then find estimates parallel to those in this paper?

Question 10.3. Pursuing the remark following Theorem 8.1, we should seek best possible bounds on expressions involving both changes in eigenvalues and changes in eigenvectors.

Question 10.4. The spectral decomposition $A = \int_{-\infty}^{\infty} \lambda \, d\Omega(\lambda)$ affords a definition of $f(A) = \int_{-\infty}^{\infty} f(\lambda) \, d\Omega(\lambda)$ for various real functions f. The algebraic and topological properties of this functional calculus (for fixed A and varying f) are satisfactory and well known. But still little is known about bounds upon $f(A + H) - f(A)$ in terms of H. Our paper sheds some light upon this subject for special functions f; for example, if $f(\xi) = 1$ for $\xi \leqq \alpha$ while $f(\xi) = 0$ for $\alpha + \delta \leqq \xi$, and if the hypotheses of the tan 2θ theorem are satisfied, then $f(A) = P$, $f(A + H) = Q$ and $f(A_0) = 1$, so

$$\|f(A + H) - f(A)\| = \|Q - P\| = \|\sin \Theta\|,$$

where

$$\delta\|\tan 2\Theta\| \leqq 2\|H\|,$$

and

$$\|(f(A + H) - f(A))E_0\| = \|f(A + H)E_0 - E_0 f(A_0)\| = \|\tilde{Q}E_0\| = \|\sin \Theta_0\|,$$

where

$$\delta\|\tan 2\Theta_0\| \leqq 2\|R\|.$$

Analogous bounds upon more general functions f would be valuable. Some work in this area has been done by Davis [4] and others he cites therein.

Added in proof. In the bibliographical note which concludes § 3, we should also mention the notion of angle operator K introduced independently by R. S. Phillips and Ju. P. Ginzburg. See, e.g., M. G. Kreĭn, *Introduction to the theory of indefinite J-spaces and operator theory in these spaces*, Second Mathematical Summer School, vol. I, Naukova Dumka, Kiev, 1965, pp. 15–92, especially pp. 23–24 (in Russian). This notion is related to (and can be expressed in terms of) our J_0.

In connection with Question 10.4, an important additional reference is M. G. Kreĭn, *Some new studies of perturbation theory of self-adjoint operators*, First Mathematical Summer School, Naukova Dumka, Kiev, 1964 (in Russian).

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