

ON THE NUMBER OF CROSSINGS
IN THE SPECTRUM OF A HERMITIAN MATRIX
WHICH DEPENDS ON A REAL PARAMETER

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Synopsis

Intersection of the eigenvalues $\varepsilon_i(h)$ of an n -dimensional hermitian matrix $A + hB$ (h being a real parameter) is discussed. An upper limit for the number of intersections is derived in terms of the rank of the Gramian of the symmetrized products of order 0, 1, ..., $n - 1$ of A and B .

1. *Introduction.* Consider an n -dimensional hermitian matrix \mathcal{H} , defined by

$$\mathcal{H} \stackrel{\text{def}}{=} A + hB; \quad (1.1)$$

A and B are hermitian matrices, the eigenvalues of B all being different; h is a real scalar; without loss of generality we assume B diagonal.

In general \mathcal{H} has n different eigenvalues, $\varepsilon_i(h)$, which are functions of h . On account of the non-degeneracy of the spectrum of B , all $\varepsilon_i(h)$ are different for sufficiently large values of $|h|$. Values $h = h'$, however, may exist, where some, say k , functions $\varepsilon_i(h)$ intersect; this will be called a k -fold level crossing[†]. Caspers¹⁾ has proved that the number of level crossings does not exceed $\frac{1}{2}n(n - 1)$, more precisely that

$$\sum_{k=2}^n c_k \frac{1}{2}k(k - 1) \leq \frac{1}{2}n(n - 1), \quad (1.2)$$

where c_k gives the number of k -fold level crossings.

The aim of this paper is to find a relation between the number and the kind of level crossings at one hand and properties of A and B at the other.

Section 2 is devoted to the formulation of a necessary and, in general, sufficient condition for the occurrence of level crossing.

[†] The case that two or more functions $\varepsilon_i(h)$ are tangent, has to be considered as the limiting case of two or more coinciding intersections.

In section 3 it is shown that the upper limit for the left-hand member of (1.2) can be made smaller:

$$\sum_{k=2}^n c_k \frac{1}{2}k(k-1) \leq q_s; \quad (1.3)$$

in this inequality q_s denotes the number of independent linear relations between the symmetrized products of A and B of order $0, 1, 2, \dots, n-1$ †.

This research is a preparation for the study of quantum-mechanical systems of which the hamiltonian depends on an external parameter (*e.g.* a spin system with internal interaction placed in a slowly varying magnetic field).

A survey of studies, devoted to the present subject, is given in ref. 1.

2. *A necessary and, in general, sufficient condition for level crossing.* Consider the set of symmetrized products of order $0, 1, 2, \dots, n-1$ of A and B , and denote the elements by s_i . The s_i are hermitian matrices and the set $\{s_i\}$, which we call S , contains $\frac{1}{2}n(n+1)$ elements. The collection of all n -dimensional square matrices forms an n^2 -dimensional vectorspace over the field of the complex numbers; an inner product, obeying the usual axioms, can be defined by

$$(P, Q) = \text{Tr}(P^\dagger Q), \quad (2.1)$$

where P^\dagger is the hermitian conjugate of P .

Now we define a square matrix C of dimension $\frac{1}{2}n(n+1)$

$$[C]_{ij} = (s_i, s_j), \quad i, j = 1, \dots, \frac{1}{2}n(n+1). \quad (2.2)$$

This matrix is usually called the matrix of Gram or the Gramian and we can prove the following theorem.

Theorem 1. A necessary condition for the occurrence of level crossing in the spectrum of $A + hB$ is given by

$$\det C = 0. \quad (2.3)$$

Proof. If for some value $h = h'$, $\mathcal{H} = A + h'B$ has some coincident eigenvalues, the degree of the minimal polynomial of $\mathcal{H}(h')$ is smaller than the degree of its characteristic polynomial; for this and other questions of linear algebra we are dealing with, we refer to Gantmacher²).

† If k and l are non-negative integers and $l \leq k$, $\binom{k}{l}$ products of $k-l$ factors A and l factors B can be formed, which differ by the permutation of the factors. The sum of all these different products is called a symmetrized product of order k and is denoted by $\{A^{k-l}B^l\}$.

This means that there exist numbers c_i , not all equal to zero, so that the following equality is true

$$\sum_{i=0}^{n-1} c_i \mathcal{H}^i(h') = 0. \tag{2.4}$$

From the relation

$$\mathcal{H}^i = \sum_{j=0}^i \{A^{i-j}B^j\} h^j, \tag{2.5}$$

where $\{A^{i-j}B^j\}$ denotes a symmetrized product, it then follows that there exists a linear relation between the elements of S . Linear algebra tells us, that $\det C = 0$ is a necessary and sufficient condition for such a linear relation. □ †

Example. If $n = 2$, C has the form

$$C = \begin{pmatrix} 2 & \text{Tr } A & \text{Tr } B \\ \text{Tr } A & \text{Tr } A^2 & \text{Tr } AB \\ \text{Tr } B & \text{Tr } BA & \text{Tr } B^2 \end{pmatrix}.$$

Then

$$\det C = 2 |A_{12}|^2 (B_{11} - B_{22})^2, \tag{2.6}$$

and so $A_{12} = 0$ is a necessary condition for degeneracy, the eigenvalues of B being different.

Now we shall investigate the question under what circumstances theorem 1 gives a sufficient condition for level crossing.

First we look at the sets of commutators $\{[s_i, B]\}$ and $\{[A, s_i]\}$, about which two lemmas shall be proved.

Lemma 1.

$$[A, \{A^{k-j}B^j\}] = [\{A^{k-j+1}B^{j-1}\}, B], \quad \begin{matrix} k = 1, 2, \dots, \dots; \\ j = 1, \dots, k. \end{matrix} \tag{2.7}$$

Proof. With $[A + hB, \mathcal{H}^k] = 0$ it follows

$$[A, \mathcal{H}^k] = h[\mathcal{H}^k, B]. \tag{2.8}$$

Substitution of (2.5) into (2.8) results in

$$[A, \sum_{j=0}^k h^j \{A^{k-j}B^j\}] = [\sum_{j=0}^k h^{j+1} \{A^{k-j}B^j\}, B] \tag{2.9}$$

† Here and in the following sections we use the symbol □ to indicate the end of a proof.

or

$$\sum_{j=1}^k h^j [A, \{A^{k-j} B^j\}] = \sum_{j=1}^k h^j [\{A^{k-j+1} B^{j-1}\}, B]. \quad (2.10)$$

(2.10) expresses that two matrix polynomials are identical and so the coefficients of equal powers of h on both sides of (2.10) have to be equal; this is just the statement of this theorem.

From lemma 1 it follows immediately that the two sets of commutators $\{[A, s_i]\}$ and $\{[s_i, B]\}$ are identical. Each set contains $\frac{1}{2}n(n+1)$ elements, n of them, however, being trivially equal to zero, namely the elements corresponding with respectively A^j and B^j ($j = 0, 1, \dots, n-1$). There are $\frac{1}{2}n(n-1)$ commutators $[s_i, B]$, respectively $[A, s_i]$, which are not trivially equal to zero; the collection of these commutators will be called K ; its elements will be denoted by k_i . Between the elements of the collection of symmetrized products S and the elements of K there exists a relation, which is expressed in the following lemma.

Lemma 2. The number of independent linear relations between the elements of K equals the number of independent linear relations between the elements of S .

Proof. Say, there exist q_k independent linear relations between elements k_i

$$\sum_{k=1}^{n-1} \sum_{j=0}^{k-1} \alpha_{lkj} [\{A^{k-j} B^j\}, B] = 0, \quad l = 1, 2, \dots, q_k. \quad (2.11)$$

This implies, because the spectrum of B is non-degenerate, q_k linear relations between the symmetrized products s_i

$$\sum_{k=1}^{n-1} \sum_{j=0}^{k-1} \alpha_{lkj} \{A^{k-j} B^j\} = \sum_{m=0}^{n-1} \beta_{lm} B^m. \quad (2.12)$$

Because the relations (2.11) are independent, the same holds for the relations (2.12); so, if q_s gives the number of independent linear relations between the elements of S , we may conclude

$$q_s \geq q_k. \quad (2.13)$$

Now we take the case that there exist q_s independent linear relations of the type (2.12); then one finds, commuting (2.12) with B , q_s relations of the type (2.11). With the coefficients α_{lkj} in these relations, q_s column vectors $\text{col}(\alpha_{lkj})$ ($k = 1, \dots, n-1$; $j = 0, \dots, k-1$) can be formed. These vectors are linearly independent, otherwise it should be possible, with (2.12), to form relations as

$$\sum_{m=0}^{n-1} \gamma_m B^m = 0, \quad (2.14)$$

with not all γ_m equal to zero; this, however, is excluded by the non-degeneracy of the spectrum of B . So we conclude that the q_s relations (2.11) are independent and

$$q_k \geq q_s. \tag{2.15}$$

Eqs. (2.13) and (2.15) together, give the required result.

Now we are able to indicate a case for which theorem 1 gives a sufficient condition for level crossing.

Theorem 2. If the rank of matrix C equals $\frac{1}{2}n(n + 1) - 1$ then the spectrum of $\mathcal{H} = A + hB$ is degenerate for one and only one value of h ; this degeneracy is a two-fold one.

Proof. With the theory of linear algebra²⁾ it can be proved that the rank of matrix C , r_c , is given by

$$r_c = \frac{1}{2}n(n + 1) - q_s. \tag{2.16}$$

Then it follows from the assumption in this theorem, that there exists one and only one non-trivial linear relation

$$\sum_{i=0}^{n-1} \sum_{j=0}^i \alpha_{ij} \{A^{i-j} B^j\} = 0. \tag{2.17}$$

Commuting (2.17) with respectively A and B one gets two relations

$$\sum_{i=1}^{n-1} \sum_{j=1}^i \alpha_{ij} [A, \{A^{i-j} B^j\}] = 0, \tag{2.18}$$

$$\sum_{i=1}^{n-1} \sum_{j=0}^{i-1} \alpha_{ij} [\{A^{i-j} B^j\}, B] = 0. \tag{2.19}$$

With lemma 1, (2.18) turns into

$$\sum_{i=1}^{n-1} \sum_{j=1}^i \alpha_{ij} [\{A^{i-j+1} B^{j-1}\}, B] = \sum_{i=1}^{n-1} \sum_{j=0}^{i-1} \alpha_{i,j+1} [\{A^{i-j} B^j\}, B] = 0. \tag{2.20}$$

Because there is only one linear relation between the s_i , this is also true for the commutators $[\{A^{k-j} B^j\}, B]$ (lemma 2), and so the coefficients of the left-hand members of (2.20) and (2.19) differ only by a constant factor, or

$$\alpha_{i,j+1} / \alpha_{ij} = \alpha_{11} / \alpha_{10} \stackrel{\text{def}}{=} \lambda; \tag{2.21}$$

from (2.21) it follows

$$\alpha_{ij} = \alpha_{i0} \lambda^j. \tag{2.22}$$

With (2.17) and (2.5) we can write

$$\sum_{i=0}^{n-1} \alpha_{i0} (A + \lambda B)^i = 0. \tag{2.23}$$

The last expression shows that there is a level crossing for $h = \lambda$. That this level crossing for $h = \lambda$ is a two-fold one and that it is the only one, follows immediately from theorem 3, proved in section 3 of this paper.

Theorem 1 is only useful if $\det C$ is not identically equal to zero, and so we shall study now $\det C$ in more detail. $\det C$ is a rational function of $n^2 + n$ real variables (n^2 from A and n from B) which can be considered as independent. This rational expression is not identical to zero, as can be shown with the following counter-example:

$$\begin{aligned} A_{ij} &= 0, & |i - j| > 1, \\ A_{ij} &\neq 0, & |i - j| = 1. \end{aligned} \quad (2.24)$$

The explicit proof that for this case $\det C$ does not equal zero is not interesting and omitted here. So it holds in general that $\det C \neq 0$.

A similar problem rises by the interpretation of theorem 2, which is only useful if there are cases for which the condition $r_c = \frac{1}{2}n(n+1) - 1$ is fulfilled. It can be shown that the following pair of matrices A and B satisfies this condition

$$B = SA'S^{-1}, \quad A = SB'S^{-1};$$

A' is a matrix subjected to the condition (2.24), S is the diagonalizing matrix of A' , and B' is a diagonal matrix for which only the following two elements are equal: $B_{11} = B_{22}$.

3. *On the number of level crossings.* Consider the set of matrix polynomials $\{(e_i(h))\}$ given by

$$e_i(h) \stackrel{\text{def}}{=} \mathcal{H}^{i-1}, \quad i = 1, \dots, n. \quad (3.1)$$

If a matrix D is defined by

$$[D]_{ij} \stackrel{\text{def}}{=} (e_i, e_j) = \text{Tr } \mathcal{H}^{i+j-2} = \sum_{k=1}^n \varepsilon_k^{i+j-2}, \quad i, j = 1, \dots, n \quad (3.2)$$

(ε_k are eigenvalues of \mathcal{H}), a necessary and sufficient condition for degeneracy of the spectrum of \mathcal{H} is (*cf.* the proof of theorem 1)

$$\det D = 0. \quad (3.3)$$

From (3.2) it follows

$$\det D = \prod_{\substack{i,j=1 \\ i>j}}^n (\varepsilon_i - \varepsilon_j)^2, \quad (3.4)$$

and so $\det D$ equals the square of Vandermonde's determinant (*cf.* ref. 1). From (3.4) we see that $\det D$ is a positive semi-definite expression and that a k -fold level crossing corresponds with a $k(k-1)$ -fold zero of $\det D$.

We shall prove a property of a set of n n -dimensional square matrix polynomials $g_i(h)$ of degree k_i

$$g_i(h) = \sum_{j=0}^{k_i} A_{ij}h^j. \tag{3.5}$$

Lemma 3. If q equals the number of independent linear relations between the matrix coefficients A_{ij} in the polynomials $g_i(h)$ (3.5), then the largest number (t) of linearly independent matrices $y_m = \sum_{i=1}^n \beta_{mi}g_i(h_m)$, which can be found by suitable choices of β_{mi} and h_m , is given by

$$t = n + \sum_{i=1}^n k_i - q. \tag{3.6}$$

Proof. First we define by suitable choices of β_{mi} and h_m a non-singular square matrix Q with dimension and rank $r_q = n + \sum_{i=1}^n k_i$

$$[Q]_{ij,m} \stackrel{\text{def}}{=} \beta_{mi}h_m^j, \quad i = 1, \dots, n; j = 0, \dots, k_i; \tag{3.7}$$

$$m = 1, \dots, r_q.$$

Now note, that the collection of n -dimensional square matrices forms an n^2 -dimensional vectorspacc. F being an element of this space and the set $\{d_i\}$ being a basis, it can be written $F = \sum_{i=1}^{n^2} \alpha_i d_i$; $\text{col } F$ then means the n^2 -dimensional column vector $\text{col}(\alpha_1, \alpha_2, \dots, \alpha_{n^2})$. With the aid of this notation we define matrices P and R of dimension $n^2 \times r_q$

$$[P]_{k,m} \stackrel{\text{def}}{=} (\text{col } y_m)_k, \quad m = 1, \dots, r_q;$$

$$[R]_{k,ij} \stackrel{\text{def}}{=} (\text{col } A_{ij})_k, \quad i = 1, \dots, n; j = 0, \dots, k_i; \tag{3.8}$$

$$k = 1, \dots, n^2.$$

Then $P = RQ$ and for the rank of $P(r_p)$ it follows with Silvesters inequality²⁾ (r_r being the rank of R)

$$r_r + r_q - r_q \leq r_p \leq \min(r_r, r_q). \tag{3.9}$$

With $r_r = r_q - q$ it follows from (3.9) $r_p = r_r = n + \sum_{i=1}^n k_i - q$. From the definition of P we see that $r_p = t$ and so the proof of (3.6) is given. \square

Now the main theorem of this paper will be formulated and proved.

Theorem 3. If c_k denotes the number of k -fold level crossings, and r_c denotes the rank of C (2.2), then it holds

$$\sum_{k=2}^n c_k \frac{1}{2}k(k-1) \leq \frac{1}{2}n(n+1) - r_c. \tag{3.10}$$

Proof. The set $\{e_i(h)\}$ (3.1) forms a basis for the space of matrix polynomials in h that commute with \mathcal{H} . If the number of real zeros of $\det D$

(3.4) equals $2s$, then

$$\sum_{k=2}^n c_k \frac{1}{2}k(k-1) = s. \tag{3.11}$$

Furthermore, in that case the basis $\{e_i(h)\}$ may be replaced by another one, $\{e'_i(h)\}$, where $e'_i(h)$ is a polynomial in h of degree not larger than that of $e_i(h)$ and where the sum of the degrees of all elements $e'_i(h)$ equals $\frac{1}{2}n(n-1) - s$; this is proved by Caspers¹). If q_s equals the number of independent linear relations between the symmetrized products s_i , then for the maximum numbers $t(t')$ of linearly independent vectors $\sum_{i=1}^n \beta_{mi}e_i(h_m)$ ($\sum_{i=1}^n \beta'_{mi}e'_i(h'_m)$) which can be formed by choosing suitable sets $\{\beta_{mi}, h_m\}$ ($\{\beta'_{mi}h'_m\}$) one has, with (3.6),

$$t = n + \frac{1}{2}n(n-1) - q_s, \tag{3.12}$$

$$t' \leq n + \sum_{i=1}^n \text{degree } e'_i(h) = n + \frac{1}{2}n(n-1) - s.$$

On account of the equivalence of $\{e_i(h)\}$ and $\{e'_i(h)\}$, t equals t' and so it follows $q_s \geq s$. Then, with $r_c = \frac{1}{2}n(n+1) - q_s$ and (3.11), (3.10) is proved.

One may ask whether or not the equality sign in (3.10) ever applies, as in the special case $r_c = \frac{1}{2}n(n+1) - 1$ (*cf.* theorem 2); an example, however, for which the inequality holds, is found in an easy way.

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