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# 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 $0, 1, \ldots, n-1$ of $A$ and $B$.

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

$$\mathscr{H} \underset{\text{def}}{=} A + hB; \tag{1.1}$$

$A$ 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 $\mathscr{H}$ 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†. Caspers[1]) has proved that the number of level crossings does not exceed $\frac{1}{2}n(n-1)$, more precisely that

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

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:

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

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 ..., $n-1$†.

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, ..., $n-1$ 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

$$(P, Q) = \mathrm{Tr}(P^\dagger Q), \tag{2.1}$$

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

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

$$[C]_{ij} = (s_i, s_j), \qquad i, j = 1, \ldots, \tfrac{1}{2}n(n+1). \tag{2.2}$$

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

$$\det C = 0. \tag{2.3}$$

Proof. If for some value $h = h'$, $\mathscr{H} = A + h'B$ has some coincident eigenvalues, the degree of the minimal polynomial of $\mathscr{H}(h')$ is smaller than the degree of its characteristic polynomial; for this and other questions of linear algebra we are dealing with, we refer to Gantmacher[2]).

† 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

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

From the relation

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

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

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

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.

$$[A, \{A^{k-j}B^j\}] = [\{A^{k-j+1}B^{j-1}\}, B], \qquad k = 1, 2, \ldots, \ldots; \quad j = 1, \ldots, k. \tag{2.7}$$

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

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

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

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

(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 $B^j$ ($j = 0, 1, \ldots, n-1$). 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 $k_i$

$$\sum_{k=1}^{n-1} \sum_{j=0}^{k-1} \alpha_{lkj}[\{A^{k-j}B^j\}, B] = 0, \qquad l = 1, 2, \ldots, q_K. \tag{2.11}$$

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

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

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

$$q_S \geq q_K. \tag{2.13}$$

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 $\alpha_{lkj}$ in these relations, $q_S$ column vectors $\mathrm{col}(\alpha_{lkj})(k = 1, \ldots, n-1;\ j = 0, \ldots, k-1)$ can be formed. These vectors are linearly independent, otherwise it should be possible, with (2.12), to form relations as

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

with not all $\gamma_m$ 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 $\mathscr{H} = A + hB$ is degenerate for one and only one value of $h$; this degeneracy is a two-fold one.

Proof. With the theory of linear algebra[2]) it can be proved that the rank of matrix $C$, $r_c$, is given by

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

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

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

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:

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

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

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

$A'$ 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

$$e_i(h) \underset{\text{def}}{=} \mathscr{H}^{i-1}, \qquad i = 1, \ldots, n. \tag{3.1}$$

If a matrix $D$ is defined by

$$[D]_{ij} \underset{\text{def}}{=} (e_i, e_j) = \operatorname{Tr} \mathscr{H}^{i+j-2} = \sum_{k=1}^{n} \varepsilon_k{}^{i+j-2}, \qquad i, j = 1, \ldots, n \tag{3.2}$$

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

$$\det D = 0. \tag{3.3}$$

From (3.2) it follows

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

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 choises of $\beta_{mi}$ 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 $\beta_{mi}$ and $h_m$ a non-singular square matrix $Q$ with dimension and rank $r_q = n + \sum_{i=1}^n k_i$

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

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

$$[P]_{k,m} \underset{\text{def}}{=} (\text{col}\, y_m)_k, \qquad m = 1, \ldots, r_q;$$
$$[R]_{k,ij} \underset{\text{def}}{=} (\text{col}\, A_{ij})_k, \qquad i = 1, \ldots, n;\ j = 0, \ldots, k_i; \quad k = 1, \ldots, n^2. \tag{3.8}$$

Then $P = RQ$ and for the rank of $P(r_p)$ it follows with Silvesters inequality[2]) ($r_r$ 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. □

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

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

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

(3.4) equals $2s$, then

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

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 Caspers[1]). 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),

$$\begin{aligned} t &= n + \tfrac{1}{2}n(n-1) - q_s, \\ t' &\leq n + \sum_{i=1}^{n} \text{degree } e_i'(h) = n + \tfrac{1}{2}n(n-1) - s. \end{aligned} \tag{3.12}$$

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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