Physica **63** (1973) 113–138 © *North-Holland Publishing Co.*

LEVEL CROSSING AND THE SPACE OF OPERATORS COMMUTING WITH THE HAMILTONIAN

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Received 12 April 1972

Synopsis

The space of n-dimensional hermitean matrices that commute with a given hermitean matrix $A + hB$, h being a real parameter, is discussed. In particular a basis in this space is constructed consisting of polynomials in h of the lowest possible total degree. The sum of the degrees of the elements of this minimal basis equals $\frac{1}{2}n\,(n-1) - q$, q being the number of linearly independent linear relations between the symmetrized products of A and B of order $0, \ldots, n-1$. These linear relations determine the values of h for which crossing occurs, the total number of crossings for each value, and in some cases the order of the different crossings. A discussion of the noncrossing rule concludes this paper.

1. *Introduction.* This paper is devoted to the study of a hermitean matrix H of the form

$$H = A + hB. \tag{1.1}$$

A and B are n-dimensional hermitean matrices over the field of the complex numbers and h is a real scalar; the n eigenvalues of H, $\varepsilon_i(h)$, are supposed to be different for almost all values of h.

The elements of H are elements of the field of rational expressions in h with complex coefficients. This field is called $C(h)$. The set of n-dimensional hermitean matrices over $C(h)$ that commute with $H(h)$, constitutes a vector space of dimension n over the field of rational expressions in h with real coefficients. This field is called $R(h)$. The set $\{H(h)^{k-1} \mid k = 1, \ldots, n\}$ is a basis in this space; the elements of this basis are matrix polynomials. The sum of the degrees of these polynomials equals $\frac{1}{2}n\,(n-1)$.

Section 2 of this paper is devoted to the construction of a basic set, consisting of matrix polynomials for which the sum of the degrees is minimal. Such a basis will be called a basis of minimal degree or, shortly, a minimal basis. The sum of the degrees of the elements will be called the degree of a basis. In ref. 1 the first step was made toward this construction: a method was developed for constructing a basic set for which the degree equals $\frac{1}{2}n(n-1)$ minus the total number of level crossings in the spectrum of $H(h)$. Here it is shown that the degree of the minimal basis equals $\frac{1}{2}n(n-1)-q$, if q gives the number of linearly independent linear relations in the set of hermitean matrices $\{G_{kj}|\, k=1,\ldots,n;\, j=0,\ldots,k-1\}$, G_{kj} being defined by $H^{k-1}=\sum_{j=0}^{k-1} G_{kj}h^j$.

The relation between level crossing and reduction of the degree of a basis is emphasized in ref. 2: in that paper it is shown that the number of level crossings does not exceed q. In the third section of this paper, this relation is made clearer. The linear relations between the matrices G_{kj} are shown to give information about the total number of level crossings, the values of h for which they occur and, partially, the order of the level crossings. It will be clarified in section 3 what is meant by the order of a crossing and by the total number of crossings. The above-mentioned results lead to a discussion of the existence of a nontrivial constant operator that commutes with $H(h)$ and its relation with level crossing. This discussion is given in section 4. Appendix A contains an example.

The noncrossing property of the spectrum of the hamiltonian of a magnetic system in a magnetic field, played a fundamental role in the examination of the difference between the isolated and adiabatic susceptibilities of a system[3,4,5]). This examination and also papers of Von Neumann and Wigner[6]) and Hund[7]) have given rise to the present study.

2. *A basis of minimal degree.* Consider a set of matrix polynomials $\{L_k(h)|\, k=1,\ldots,n\}$, that is a basis for the vector space of matrices that commute with $H(h)$. The elements of this set have the general form

$$L_k(h)=\sum_{i=0}^{m_k} G_{ki}h^i \qquad (k=1,\ldots,n). \tag{2.1}$$

The coefficients G_{ki} are hermitean matrices over the complex number field. The set $\{L_k(h)\}$ is ordered, *i.e.* $m_k \leqslant m_{k+1}$. The set $\{G_{km_k}|\, k=1,\ldots,n\}$ is supposed to be linearly independent.

We shall use the concept of linear relation for a set of hermitean, respectively antihermitean, matrices. This is allowed, because the collection of all n-dimensional hermitean matrices and that of all n-dimensional antihermitean matrices over some complex field, both form a vector space of dimension n^2 over the corresponding real subfield. An inner product and consequently norm and metric, can be defined by

$$(A,B)\underset{\text{def}}{=}\operatorname{Tr} A^+B, \qquad \|A\|\underset{\text{def}}{=}(\operatorname{Tr} A^+A)^{\frac{1}{2}}, \qquad \mathrm{d}\,(A,B)\underset{\text{def}}{=}\|A-B\|. \tag{2.2}$$

A^+ denotes the hermitean conjugate of A. The first theorem provides a lower bound for the degree of some arbitrary polynomial basis $\{L_k'(h)\}$, given a basic set $\{L_k(h)\}$ and the number of linear relations between the corresponding matrices G_{ki}.

Theorem 2–1. If the sets of matrix polynomials $\{L_k(h)|\ k = 1, \dots, n\}$ and $\{L'_k(h)|\ k = 1, \dots, n\}$ are both basic sets for the vector space of matrices that commute with $H(h)$, and if q gives the number of linearly independent linear relations in the set $\{G_{ki}|\ k = 1, \dots, n;\ i = 0, \dots, m_k\}$ [*cf.* eq. (2.1)], then:

$$\sum_{k=1}^{n} [\text{degree } L_k(h) - \text{degree } L'_k(h)] \leqslant q. \tag{2.3}$$

Proof. The largest number of linearly independent matrices $T_k = \sum_{i=1}^{n} a_{ik} L_i(h_k)$ that can be constructed by suitable choice of sets of real numbers $\{a_{ik}, h_k|\ i = 1, \dots, n\}$ is denoted by t. According to lemma 3 in ref. 2,

$$t = \sum_{i=1}^{n} (m_i + 1) - q. \tag{2.4}$$

The vector space that is spanned by such a set of hermitean matrices is called V_t. In the same way a vector space $V'_{t'}$ can be found, with the aid of the set $\{L'_k(h)\}$. A primed symbol will always refer to the set $\{L'_k(h)\}$.

If we suppose $t > t'$, then there is a set $\{a_{ik}, h_k|\ i = 1, \dots, n\}$ so that the corresponding matrix T_k is not an element of $V'_{t'}$. For all the values of h in a sufficiently small neighbourhood of h_k, say $|h - h_k| \leqslant \varepsilon$, the matrices $\sum_{i=1}^{n} a_{ik} L_i(h)$, $(|h - h_k| \leqslant \varepsilon)$, also do not belong to $V'_{t'}$. Now one can write, because $L'_k(h)$ is a basis,

$$\sum_{i=1}^{n} a_{ik} L_i(h) = \sum_{i=1}^{n} \alpha_i(h)\, L'_i(h), \tag{2.5}$$

where the coefficients $\alpha_i(h)$ are elements of the field $R(h)$, defined in the introduction. Surely there is a value $h = h_0$, with $|h_0 - h_k| \leqslant \varepsilon$, such that all the $\alpha_i(h_0)$ $(i = 1, \dots, n)$ are finite. Then the matrix $\sum_{i=1}^{n} \alpha_i(h_0)\, L'_i(h_0)$ is not an element of $V'_{t'}$. However, according to the definition of $V'_{t'}$ it has to be, and so our assumption $t > t'$ is wrong and consequently $t \leqslant t'$. In the same way it can be proved that $t' \leqslant t$, so that t equals t'. With eq. (2.4) it then follows that

$$\sum_{i=1}^{n} (m_i - m'_i) = q - q'. \tag{2.6}$$

q' is a non-negative number and thus the theorem is proved, *q.e.d.*

Theorem 2–1 provides a lower bound for the degree of the minimal basis in terms of properties of the set $\{L_k(h)\}$. The following step is to construct, starting from a given set $\{L_k(h)\}$, a basic set $\{L'_k(h)\}$ for which the equality in theorem 2–1 holds. Provisionally it is assumed that the spectrum of B [*cf.* eq. (1.1)] is non-degenerate. This restriction will be dropped in theorem 2–3 and the following. First some auxiliary concepts will be developed.

A set of antihermitean matrices K_{kj} is defined as follows:

$$K_{kj} \underset{\text{def}}{=} [B, G_{kj}] \qquad (k = 1, \ldots, n, m_k \neq 0; \; j = 0, \ldots, m_k - 1). \tag{2.7}$$

In this way a number of $\sum_{i=1}^{n} m_i$ matrices K_{kj} are defined. Because $L_k(h)$ commutes with $H(h)$,

$$[G_{k0}, A] = [B, G_{km_k}] = 0 \qquad (k = 1, \ldots, n),$$

$$[G_{k,j+1}, A] = [B, G_{kj}] \qquad (k = 1, \ldots, n, m_k \neq 0; j = 0, \ldots, m_k - 1). \tag{2.8}$$

From eqs. (2.8) it will immediately be clear, that the set $\{K_{kj} | \; k = 1, \ldots, n, m_k \neq 0; j = 0, \ldots, m_k - 1\}$ can be generated in two ways: commuting the matrices G_{kj} from the right with A or from the left with B, where the trivial zero elements, respectively $[G_{k0}, A]$ and $[B, G_{km_k}]$ $(k = 1, \ldots, n)$ are omitted.

We shall now discuss linear relations with real coefficients, in respectively the sets $\{G_{kj}\}$ and $\{K_{kj}\}$.

Lemma 2–1. If there exist q and no more then q linearly independent linear relations in the set $\{G_{kj}\}$

$$\sum_{k=1}^{n} \sum_{j=0}^{m_k} a_{kj}^i G_{kj} = 0 \qquad (i = 1, \ldots, q), \tag{2.9}$$

then there exist q and no more then q linearly independent linear relations in the set $\{K_{kj}\}$. These linear relations can be represented with the coefficients of eq. (2.9)

$$\sum_{\substack{k=1 \\ m_k \neq 0}}^{n} \sum_{j=0}^{m_k - 1} a_{kj}^i K_{kj} = 0 \qquad (i = 1, \ldots, q). \tag{2.10}$$

Proof. Commuting the set (2.9) from the left with B, we get immediately the set (2.10). We shall prove first, that this last set is a linearly independent set and secondly that, if a $(q + 1)$th relation is added to the set (2.10), this new set of $q + 1$ relations is a linearly dependent set. Then the lemma is proved.

Let $[a_{kj}^i]$ denote the coefficient matrix of the set (2.10). This matrix is of dimension $q \times \sum_{i=1}^{n} m_i$. If there exists a linear combination of the rows of this matrix that vanishes, then the corresponding linear combination of eqs. (2.9) provides an equation $\sum_{k=1}^{n} b_{km_k} G_{km_k} = 0$. Not all coefficients b_{km_k} equal zero, because the set (2.9) is linearly independent. Thus we have constructed a linear relation between the matrices G_{km_k} and this is not in accordance with the conditions formulated at the beginning of this section. So the rank of $[a_{kj}^i]$ equals q and the relations (2.10) are linearly independent.

If there exists a $(q + 1)$th relation

$$\sum_{\substack{k=1\\ m_k\neq 0}}^{n} \sum_{j=1}^{m_k-1} a_{kj}^{q+1} K_{kj} = 0, \tag{2.11}$$

that is linearly independent of the relations (2.10), then the rank of the coefficient matrix $[a_{kj}^{i}]'$ of this new set of $q + 1$ equations equals $q + 1$. From eq. (2.11) and the definition of K_{kj} it follows that

$$\left[\sum_{\substack{k=1\\ m_k\neq 0}}^{n} \sum_{j=0}^{m_k-1} a_{kj}^{q+1} G_{kj}, B\right] = 0. \tag{2.12}$$

Because the spectrum of B is nondegenerate, the linear combination of the G_{kj} in eq. (2.12), is a linear combination of the first n powers of B. From the equation $[B, G_{km_k}] = 0$ and the linear independence of the set $\{G_{km_k}\}$ it then follows that

$$\sum_{\substack{k=1\\ m_k\neq 0}}^{n} \sum_{j=0}^{m_k-1} a_{kj}^{q+1} G_{kj} = -\sum_{k=1}^{n} a_{km_k}^{q+1} G_{km_k}, \tag{2.13}$$

where the coefficients $a_{km_k}^{q+1}$ are real numbers. Because the coefficient matrix $[a_{kj}^{i}]'$ has rank $q + 1$, the relation (2.13) together with (2.9) forms a linearly independent set; this, however, is in contradiction with the assumption in the theorem that there are only q linearly independent linear relations in the set $\{G_{kj}\}$. So eq. (2.11) is a linear combination of eqs. (2.10), *q.e.d.*

If a linear relation between matrices G_{kj} is commuted with A or B, in general the result will be a linear relation between the matrices K_{kj}. This procedure can simply be described by the following formalism. Let the number s be equal to $\sum_{i=1}^{n} (m_i + 1)$ and consider the complex euclidean vector spaces C_s and C_{s-n}. The components of vectors $v \in C_s$ and $w \in C_{s-n}$ will be labelled with two subscripts as follows

$$v = \mathrm{col}\,(v_{kj} |\, k = 1, \ldots, n;\ j = 0, \ldots, m_k),$$

$$w = \mathrm{col}\,(w_{kj} |\, k = 1, \ldots, n, m_k \neq 0; j = 0, \ldots, m_k - 1). \tag{2.14}$$

Two linear operators, $\hat{O}_A$ and $\hat{O}_B$ that map C_s onto C_{s-n} are defined as follows:

$$(\hat{O}_A v)_{kj} \underset{\text{def}}{=} v_{k,j+1}, \qquad (\hat{O}_B v)_{kj} \underset{\text{def}}{=} v_{kj},$$

$$(k = 1, \ldots, n, m_k \neq 0;\ j = 0, \ldots, m_k - 1). \tag{2.15}$$

We suppose again the existence of q and no more then q linearly independent linear relations between the matrices G_{kj}. These relations have the general form of eqs. (2.9). From these equations we now construct an equivalent set in which the coefficients satisfy certain relations [eqs. (2.22)]. The latter are fundamental in the proof of theorem 2–2. With the coefficients of eq. (2.9), q linearly independent vectors $\boldsymbol{a}^i$ are defined, that are elements of C_s,

$$\boldsymbol{a}^i \underset{\text{def}}{=} \text{col}\,(a^i_{kj} |\, k = 1, \ldots, n;\ j = 0, \ldots, m_k) \qquad (i = 1, \ldots, q). \tag{2.16}$$

Commuting the set (2.9) respectively with A and with B and making use of eqs. (2.7), (2.8) and (2.15), we get two sets of linear relations between the matrices K_{kj}

$$\sum_{\substack{k=1 \\ m_k \neq 0}}^{n} \sum_{j=0}^{m_k - 1} (\hat{O}_A \boldsymbol{a}^i)_{kj}\, K_{kj} = 0 \qquad (i = 1, \ldots, q), \tag{2.17}$$

$$\sum_{\substack{k=1 \\ m_k \neq 0}}^{n} \sum_{j=0}^{m_k - 1} (\hat{O}_B \boldsymbol{a}^i)_{kj}\, K_{kj} = 0 \qquad (i = 1, \ldots, q). \tag{2.18}$$

The set (2.18) is the same as the set (2.10). With lemma 2–1 it then follows that each relation of eqs. (2.17) is a linear combination of the relations (2.18). This implies q relations for the vectors $\boldsymbol{a}^i$:

$$\hat{O}_A \boldsymbol{a}^i = \sum_{j=1}^{q} s_{ji} \hat{O}_B \boldsymbol{a}^j \qquad (i = 1, \ldots, q), \tag{2.19}$$

where the coefficients s_{ji} are real numbers, which define a real $q \times q$ matrix S: $[S]_{ij} = s_{ij}$.

Let P be the Jordan normal form of S. Then P is a matrix that is partitioned into blocks

$$P = \begin{pmatrix} P_1 & 0 & \cdot & 0 \\ 0 & P_2 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & P_t \end{pmatrix}. \tag{2.20}$$

The submatrices P_i are square matrices. Their number equals, say, t and their respective dimensions are d_i. P is said to be the direct sum of the matrices P_i. P_i has the general form

$$P_i = \begin{pmatrix} p_i & 1 & 0 & \cdot & \cdot & 0 & 0 \\ 0 & p_i & 1 & \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & p_i & 1 \\ 0 & 0 & 0 & \cdot & \cdot & 0 & p_i \end{pmatrix}. \tag{2.21}$$

A matrix of this form is called a Jordan block. Generally p_i is a complex number. Because S is real, the complex conjugate of P, P^*, is also a Jordan normal form of S. That means that if p_j is complex, one of the P_i equals P_j^*. The asterisk denotes complex conjugation.

Let T be the nonsingular transforming matrix of S so that $S = TPT^{-1}$ and let a set of vectors $\{\boldsymbol{b}^l\}$ be defined by $\{\boldsymbol{b}^l \underset{\text{def}}{=} \sum_{j=1}^{q} \boldsymbol{a}^j [T]_{jl} | \, l = 1, \ldots, q\}$, then eq. (2.19) transforms into

$$\hat{O}_A \boldsymbol{b}^{ik} = \sum_{j=1}^{d_i} [P_i]_{jk} \, \hat{O}_B \boldsymbol{b}^{ij} \qquad (i = 1, \ldots, t; \; k = 1, \ldots, d_i). \tag{2.22}$$

For convenience the superscript of the vectors $\boldsymbol{b}^i$ is changed. The first index now refers to a particular P_i. Generally the vectors $\boldsymbol{b}^{ik}$ are complex. Because each $\boldsymbol{b}^{ik}$ is a linear combination of the set $\{\boldsymbol{a}^i | \, i = 1, \ldots, q\}$ with coefficients equal to the elements of the columns of the nonsingular matrix T, we have, equivalent to the set (2.9),

$$\sum_{k=1}^{n} \sum_{j=0}^{m_k} b_{kj}^{im} G_{kj} = 0 \qquad (i = 1, \ldots, t; \; m = 1, \ldots, d_i). \tag{2.23}$$

If the spectrum of B is still supposed to be nondegenerate, the following theorem applies.

Theorem 2–2. If the number q of linearly independent linear relations in the set $\{G_{kj} | \, k = 1, \ldots, n; \; j = 0, \ldots, m_k\}$ does not equal zero, then there exists a set of hermitean matrix polynomials $\{L_k'(h)\}$, which is, as the set $\{L_k(h)\}$, a basis for the vector space of matrices that commute with $H(h)$, with the following properties: a) the degree of the set $\{L_k'(h)\}$ is one lower than the degree of the set $\{L_k(h)\}$; b) the number of linearly independent linear relations in the set $\{G_{kj}' | \, k = 1, \ldots, n; \; j = 0, \ldots, m_k'\}$ equals $q - 1$; c) the set $\{G_{km_k}' | \, k = 1, \ldots, n\}$ is a linearly independent one; d) $m_k' \leqslant m_{k+1}'$.

Proof. q linearly independent linear relations can be chosen in such a way that their coefficient vectors satisfy eqs. (2.22). If both indices i and k in eq. (2.23) are taken to be 1, then for the vector $\boldsymbol{b}^{11}$ we get the relation $\hat{O}_A \boldsymbol{b}^{11} = p_1 \hat{O}_B \boldsymbol{b}^{11}$. This equation reads in components $(\hat{O}_A \boldsymbol{b}^{11})_{kj} = p_1 \, (\hat{O}_B \boldsymbol{b}^{11})_{kj}$, so that with eq. (2.15), $b_{k,j+1}^{11} = p_1 b_{kj}^{11}$. Immediately it follows that

$$b_{kj}^{11} = p_1^j b_{k0}^{11} \qquad (k = 1, \ldots, n; \; j = 0, \ldots, m_k). \tag{2.24}$$

As a consequence the first of the eqs. (2.23) can be written as

$$\sum_{k=1}^{n} b_{k0} L_k(p) = 0, \tag{2.25}$$

where the indices 1 are omitted.

If r is the largest value of k for which $b_{k0} \neq 0$, then it follows from eq. (2.25) that

$$\sum_{k=1}^{r} b_{k0} L_k(h) = (h - p) \sum_{j=0}^{m_r - 1} F_j h^j, \tag{2.26}$$

where F_j ($j = 0, \ldots, m_r - 1$) are matrices over the complex numbers. If a hermitean polynomial $M(h)$ is defined by

$$M(h) \underset{\text{def}}{=} \sum_{j=0}^{m_r - 1} \tfrac{1}{2} (F_j + F_j^+) h^j, \tag{2.27}$$

then

$$M(h) = \sum_{k=1}^{r} \operatorname{Re} [b_{k0}/(h - p)] L_k(h). \tag{2.28}$$

The coefficient of the highest power in $M(h)$ is given by [cf. eq. (2.26)]

$$\tfrac{1}{2} (F_{m_r - 1} + F_{m_r - 1}^+) = \sum_{k=1}^{r} \delta_{m_r m_k} \operatorname{Re}(b_{k0}) G_{km_k}. \tag{2.29}$$

Without restrictions b_{r0} may be supposed to equal 1, so that not all coefficients of G_{km_k} in the right-hand part of eq. (2.29) equal zero. On account of the linear independence of the set $\{G_{km_k}\}$, the right-hand member of eq. (2.29) does not equal zero so that $M(h)$ is of degree $m_r - 1$.

Let a set of matrix polynomials $L_k'(h)$ be given by

$$\begin{aligned} L_k'(h) &\underset{\text{def}}{=} L_k(h) \qquad (k = 1, \ldots, n;\ k \neq r), \\ L_r'(h) &\underset{\text{def}}{=} M(h) = \sum_{j=1}^{r} \operatorname{Re} [b_{j0}/(h - p)] L_j(h). \end{aligned} \tag{2.30}$$

The coefficient matrix that describes the transformation of the set $\{L_k(h)\}$ into the set $\{L_k'(h)\}$, is a matrix over the field $R(h)$. Furthermore it is a nonsingular matrix, so that the set $\{L_k'(h)\}$ is, just as the set $\{L_k(h)\}$, a basis in the space of matrices that commute with $H(h)$.

Now it is immediately clear that property a) is true. So it is true that $\sum_{i=1}^{n} (m_i - m_i') = 1$, which in combination with eq. (2.6) results in b). c) is proved by eq. (2.29) and $G_{km_k} = G'_{km_k'}$ ($k = 1, \ldots, n$; $k \neq r$). Property d) can always be reached by rearranging the elements of $\{L_k'(h)\}$, *q.e.d.*

The set of matrix polynomials $\{H^{k-1} | k = 1, \ldots, n\}$ is, as has already been mentioned in the introduction, a basic set for the space of hermitean matrices over $C(h)$ that commute with $H(h)$. $H^{k-1}(h)$ is a polynomial in h of degree $k - 1$. The matrix coefficients of H^{k-1} are called symmetrized products of order $k - 1$ of A

and B (*cf.* refs. 1 and 2). Usually the symmetrized products are indicated by braces and one may write

$$H^{k-1}(h) = \sum_{i=0}^{k-1} \{A^{k-i-1}B^i\}\, h^i \qquad (k = 1, \ldots). \tag{2.31}$$

If A and B do not commute, eq. (2.31) serves as a definition of symmetrized products. Clearly the set $\{H^{k-1} | \, k = 1, \ldots, n\}$ satisfies the restrictions that are imposed on the set $\{L_k(h)\}$ [eq. (2.1) and the following]. We shall prove now the main theorem of this section, whereby the condition of the nondegeneracy of the spectrum of B is dropped.

Theorem 2–3. If there exist q and no more than q linearly independent linear relations between the symmetrized products of A and B of order $0, \ldots, n-1$, the space of hermitean matrices over $C(h)$ that commute with $H(h)$ has a basis of matrix polynomials $L_k'(h)$ with a degree that equals $\frac{1}{2}n\,(n-1) - q$. This is a basis of minimal degree.

Proof. First we prove the theorem for the case that the spectrum of B is nondegenerate. Starting with the basic set $\{H^{k-1} | \; k = 1, \ldots, n\}$, we apply theorem 2–2 q times alltogether. The degree of the basic set $\{L_k'(h)\}$ at which we then arrive equals $\frac{1}{2}n\,(n-1) - q$. Furthermore there are no linear relations in the set $\{G_{kj}'\}$ and so it is a basis of minimal degree (*cf.* theorem 2–1).

If the spectrum of B is degenerate, we study, instead of $H(h)$, the matrix $\bar{H}(g)$, defined as follows:

$$\bar{H} \underset{\text{def}}{=} \bar{A} + g\bar{B}, \;\; \bar{A} \underset{\text{def}}{=} B, \;\; \bar{B} \underset{\text{def}}{=} A + h_0 B, \;\; g \underset{\text{def}}{=} (h - h_0)^{-1}. \tag{2.32}$$

The real constant h_0 is chosen so that the spectrum of $\bar{B}$ is nondegenerate. This is possible, because we have excluded matrices for which two or more eigenvalues $\varepsilon_i(h)$ are identically equal. In appendix B it is shown that the number of linear relations between the symmetrized products of A and B on one hand and those between the products of $\bar{A}$ and $\bar{B}$ on the other are equal, *i.e.*, $q = \bar{q}$. A symbol with a bar always refers to $\bar{H}(g)$. The minimal basis $\{\bar{L}_k'(g)\}$ belonging to $\bar{H}$ can then be constructed on the basis of the foregoing. The degree of this basis equals $\frac{1}{2}n\,(n-1) - q$. The set $\{L_k'(h)\}$, defined by

$$L_k'(h) = (h - h_0)^{\bar{m}_k}\, \bar{L}_k'\,((h - h_0)^{-1}) \qquad (k = 1, \ldots, n), \tag{2.33}$$

is simply shown to be a minimal basis, with degree $\frac{1}{2}n\,(n-1) - q$, for the space of matrices that commute with $H(h)$, *q.e.d.*

From the above discussion a corollary follows immediately, which we state without explicit proof.

Corollary. If and only if the set of matrix polynomials $\{L'_k(h)|\ k = 1, \ldots, n\}$ is a minimal basis, then there are no linear relations in the set $\{G'_{kj}|\ k = 1, \ldots, n;\ j = 0, \ldots, m'_k\}$, *q.e.d.*

A minimal basis is trivially not unique. A theorem about this question concludes this section.

Theorem 2–4. Let $\{L'_k(h)\}$ as well as $\{L''_k(h)\}$ be minimal bases for the vector space of matrices that commute with $H(h)$. If both sets are ordered according to increasing degree,

$$\text{degree}\, L'_k(h) = \text{degree}\, L''_k(h) \qquad (k = 1, \ldots, n). \tag{2.34}$$

Proof. $L'_i(h)$ is a linear combination of the matrices $L''_k(h)$: $L'_i(h) = \sum_{k=1}^{n} \beta_{ki}(h) \times L''_k(h)$. The coefficients $\beta_{ki}(h)$ are elements of $R(h)$. They should be polynomials, otherwise linear relations between the matrices G''_{kj} could be constructed. The same reasoning leads to $\beta_{ki}(h) = 0$ for fixed i and every k for which $m''_k > m'_i$. So the elements of the set $\{L'_j(h)|\ j = 1, \ldots, i\}$ are linear combinations of the elements of the set $\{L''_k(h)|\ k = 1, \ldots, n;\ m''_k \leqslant m'_i\}$. Because the set $\{L'_j|\ j = 1, \ldots, i\}$ is a linearly independent set, the set $\{L''_k|\ k = 1, \ldots, n, m''_k \leqslant m'_i\}$ contains at least i elements. So, because of the ordering according to increasing degree of the set $\{L''_i(h)\}$, it contains L''_i and so $m''_i \leqslant m'_i$. In the same way it can be proved that $m'_i \leqslant m''_i$, and so $m'_i = m''_i$, *q.e.d.*

3. *Level crossing.* The number of linearly independent linear relations between symmetrized products of A and B of order $0, \ldots, n - 1$ has been shown to give an upper bound for the total number of level crossings in the spectrum of $H = A + hB^2$). This result has been achieved under the restriction that the spectrum of B be non-degenerate. In this section it becomes clear that this is not an essential restriction. The foregoing section offers the possibility to clarify the relation between the linear relations mentioned and level crossing. First, however, four lemmas are proved.

Let the set of matrix polynomials $\{L_k(h)|\ k = 1, \ldots, n\}$ be a basis for the vector space of hermitean matrices over $C(h)$ that commute with $H(h)$. This basic set is subjected to the conditions that are mentioned at the beginning of section 2 [*cf.* eq. (2.1) and what follows]. Define an $n \times n$ matrix D as follows

$$[D]_{ij} \underset{\text{def}}{=} \operatorname{Tr} L_i L_j \qquad (i, j = 1, \ldots, n). \tag{3.1}$$

Trivially, the determinant of D, which we denote by $|D|$, is a polynomial in h with real coefficients. Because the matrices $L_k(h)$ are elements of a real vector space, with inner products defined by eq. (2.2), $|D|$ is the gramian (*cf.* ref. 8) of the set $\{L_k(h)\}$. In this way it is a positive semidefinite expression. The following lemma expresses two important properties of $|D|$.

Lemma 3–1. a) If $|D(h_0)| = 0$ for real h_0, then there is a linear relation in the set $\{L_k(h_0)|\ k = 1, \ldots, n\}$. b) If the set $\{G_{km_k}|\ k = 1, \ldots, n\}$ is linearly independent, then the degree of $|D|$ equals $2(\sum_{i=1}^{n} m_i)$.

Proof. $|D(h_0)|$ is the gramian of the set $\{L_k(h_0)\}$ and so a) immediately follows. The degree of $|D|$ trivially does not exceed $2s = 2\sum_{i=1}^{n} m_i$. Let a set of matrices $\bar{L}_k(g)$ be defined by $\{\bar{L}_k(g) \doteq g^{m_k} L_k(g^{-1})\}$. If $|\bar{D}(g)|$ denotes the gramian of the set $\{\bar{L}_k(g)\}$, then $|\bar{D}(g)| = g^{2s}\,|D(g^{-1})|$. If the degree of $|D(h)|$ is less then $2s$, then $|\bar{D}(g)|$ has a zero for $g = 0$. So, by a), there is a linear relation in the set $\{\bar{L}_k(0)\}$. However, $\bar{L}_k(0) = G_{km_k}$ and so b) is proved, *q.e.d.*

Let $\{L'_k(h)\}$ be another basic set subjected to the same conditions as the set $\{L_k(h)\}$. $L_k(h)$ can be expressed in terms of the set $\{L'_k(h)\}$

$$L_k(h) = \sum_{i=1}^{n} L'_i(h)\,\beta_{ik}(h) \qquad (k = 1, \ldots, n), \tag{3.2}$$

where $\beta_{ij}(h)$ are elements of $R(h)$. These coefficients define a matrix M

$$[M]_{ij} \underset{\text{def}}{=} \beta_{ij}(h) \qquad (i, j = 1, \ldots, n). \tag{3.3}$$

The gramian of the set $\{L'_k(h)\}$ will be denoted by $|D'|$. Between the determinants $|D|$, $|D'|$ and $|M|$ a simple relation exists.

Lemma 3–2.

$$|D| = |M|^2\,|D'|. \tag{3.4}$$

Proof. The hermitean matrices $L_k(h)$ are elements of a vector space of dimension n^2 over $R(h)$ with inner product [*cf.* eq. (2.2)]. Let the set $\{K_i|\ i = 1, \ldots, n^2\}$ be an orthonormal basis in that space. It then holds that $L_k(h) = \sum_{i=1}^{n^2} \alpha_{ik}(h)\,K_i$, $\alpha_{ik}(h) \in R(h)$. If a matrix G is defined by $[G]_{ik} = \alpha_{ik}(h)$, $(i = 1, \ldots, n^2; k = 1, \ldots, n)$, then [*cf.* eq. (3.1)]

$$D = G^+G, \qquad G' = GM, \tag{3.5}$$

where G' is the analogue of G for the set $L'_k(h)$. With eq. (3.5) the lemma is immediately proved, *q.e.d.*

Lemma 3–3. Let there exist a relation of the type

$$\sum_{i=1}^{n} L_i(h)\,\lambda_i(h) = (h - h_0)^m\,P(h), \tag{3.6}$$

where the coefficients $\lambda_i(h)$ are scalar polynomials in h, not all divisible by $h - h_0$, $P(h)$ being a matrix polynomial. The relation (3.6) results in m linear relations in the set $\{G_{kj} |\, k = 1, \ldots, n; j = 0, \ldots, m_k\}$. These relations are linearly independent if the set $\{G_{km_k}\}$ is a linearly independent set. The set of vectors $\{\boldsymbol{a}^i |\, i = 1, \ldots, m\}$ that can be defined with the coefficients in these relations [*cf.* eqs. (2.9) and (2.16)] satisfies

$$\hat{O}_A \boldsymbol{a}^i = h_0 \hat{O}_B \boldsymbol{a}^i + \hat{O}_B \boldsymbol{a}^{i-1}, \qquad \boldsymbol{a}^0 = \boldsymbol{0}, \qquad (i = 1, \ldots, m). \tag{3.7}$$

Proof. The $(i - 1)$th derivative of the left-hand part of eq. (3.6) is given by the expression

$$\sum_{k=1}^{n} \sum_{p=0}^{i-1} \sum_{j=0}^{m_k} G_{kj} h^{j-p} p! \binom{j}{p} \binom{i-1}{p} \left(\frac{\mathrm{d}}{\mathrm{d}h}\right)^{i-1-p} \lambda_k \qquad (i = 1, \ldots). \tag{3.8}$$

Recall that $\binom{j}{p} = 0$ if $p > j$. If h_0 is substituted in the expressions (3.8) they should equal zero for $i = 1, \ldots, m$. We then have m linear relations among the matrices G_{kj}. The coefficients a^i_{kj} [*cf.* eq. (2.9)] are given by

$$a^i_{kj} = \sum_{p=0}^{i-1} h_0^{j-p} \binom{j}{p} a^{i-p}_{k0},$$

$$a^{i-p}_{k0} = [(i - 1 - p)!]^{-1} \left[\left(\frac{\mathrm{d}}{\mathrm{d}h}\right)^{i-1-p} \lambda_k\right]_{h_0} \tag{3.9}$$

$$(i = 1, \ldots, m;\ k = 1, \ldots, n,\ j = 0, \ldots, m_k).$$

If we use the definitions of $\hat{O}_A$ and $\hat{O}_B$ [eq. (2.15)], eq. (3.7) can be rewritten as a recurrence relation for the a^i_{kj}

$$a^i_{k,j+1} = h_0 a^i_{kj} + a^{i-1}_{kj}$$

$$(i = 1, \ldots, m;\ k = 1, \ldots, n;\ m_k \neq 0;\ j = 0, \ldots, m_k - 1), \tag{3.10}$$

which is obeyed by the coefficients a^i_{kj} as given in eq. (3.9), as a consequence of the well-known relation of binomial coefficients $\binom{s+1}{t} = \binom{s}{t} + \binom{s}{t-1}$.

Now we shall prove that the set $\{\boldsymbol{a}^i\}$ is linearly independent. Suppose that there exist l and no more than l linearly independent linear relations between the vectors $\boldsymbol{a}^i$:

$$\sum_{j=1}^{m} c^k_j \boldsymbol{a}^j = \boldsymbol{0} \qquad (k = 1, \ldots, l). \tag{3.11}$$

Let the matrix T be a Jordan block of dimension m [eq. (2.21)] with diagonal elements equal to h_0. The relations (3.7) can be written in the form

$$\hat{O}_A a^i = \sum_{j=1}^{m} \hat{O}_B a^j [T]_{ji} \qquad (i, \dots, m). \tag{3.12}$$

From eqs. (3.11) and (3.12) it follows that

$$\hat{O}_B \sum_{j=1}^{m} a^j \sum_{i=1}^{m} [T]_{ji} c_i^k = 0 \qquad (k = 1, \dots, l). \tag{3.13}$$

The vectors $d^k \underset{\text{def}}{=} \sum_{j=1}^{m} a^j \sum_{i=1}^{m} [T]_{ji} c_i^k$ are linear combinations of the vectors a^j and so the components of d^k are coefficients in a linear relation between matrices G_{kj}. Eq. (3.13) implies $(d^k)_{ij} = 0$ $(i = 1, \dots, n;\ j \neq m_i)$ [*cf.* eq. (2.15)] so that $\sum_{k=1}^{n} G_{km_k}(d^i)_{km_k} = 0$ $(i = 1, \dots, l)$. This relation, however, implies that the coefficients $(d^i)_{km_k}$ $(i = 1, \dots, l)$ equal zero, because there does not exist a linear relation between the matrices G_{km_k}. Thus, eq. (3.13) implies:

$$\sum_{j=1}^{m} a^j \sum_{i=1}^{m} [T]_{ji} c_i^k = 0 \qquad (k = 1, \dots, l). \tag{3.14}$$

Eq. (3.11) describes fully the linear relations between the vectors a^j and so each relation of (3.14) is a linear combination of the relations (3.11). This can be expressed as follows:

$$Tc^k = \sum_{j=1}^{l} c^j s_{jk} \qquad (k = 1, \dots, l), \tag{3.15}$$

where the set of vectors c^k is defined by

$$\{c^k \underset{\text{def}}{=} \text{col}\,(c_i^k |\ i = 1, \dots, m);\ k = 1, \dots, l\},$$

and the s_{jk} are complex numbers. T can be considered as an operator in the m-dimensional complex Euclidean space C_m. Because T is a Jordan block [*cf.* eq. (2.21)], the vector $(1, 0, \dots, 0)$ is, apart from a constant, the only eigenvector of T. From eq. (3.15) it follows that the set $\{c^k |\ k = 1, \dots, l\}$ spans an invariant subspace of C_m. This subspace cannot be the space spanned by the zero vector and so, because every invariant subspace contains an eigenvector, $(1, 0, \dots, 0)$ is a linear combination of the vectors c^k. As a consequence there are numbers g_i such that (δ_{ij} is the Kronecker symbol)

$$\sum_{i=1}^{l} g_i c_j^i = \delta_{j1}. \tag{3.16}$$

Then, with eq. (3.11) it follows that

$$\sum_{i=1}^{l} g_i \left(\sum_{j=1}^{m} c_j^i \boldsymbol{a}^i \right) = \boldsymbol{a}^1 = \boldsymbol{0}. \tag{3.17}$$

Specifically the components a_{k0}^1 of $\boldsymbol{a}^1$ equal zero, and so, with eq. (3.9), $\lambda_k(h_0) = 0$ for $k = 1, \ldots, n$. This, however, is excluded by hypothesis and so the set $\{\boldsymbol{a}^i\}$ is a linearly independent set, *q.e.d.*

The last lemma 3–4 shall be proved under the restriction that the coefficients β_{ij} in eq. (3.2) are polynomials. Then M is a matrix of rank n over the ring of polynomials in h with real coefficients, $R[h]$. Such a matrix is equivalent over this ring to a diagonal matrix, *i.e.*, there exist V and W such that

$$VMW = \text{diag}\,(\delta_i(h)|\; i = 1, \ldots, n). \tag{3.18}$$

V and W are nonsingular matrices over $R[h]$, and $\delta_i(h)$ is an element of $R[h]$, which does not equal zero as a consequence of M having rank n. V and W can be chosen so that

$$|V| = |W| = 1, \qquad |M| = \prod_{i=1}^{n} \delta_i(h). \tag{3.19}$$

Clearly V^{-1} and W^{-1} exist; both are again matrices over $R[h]$. All these results follow from the theory of matrices (*cf. e.g.* ref. 9, in particular ch. 7, theorem 7.1).

With the equivalence relation (3.18), eq. (3.2) gives

$$\sum_{k=1}^{n} L_k(h)\, [W]_{ki} = \delta_i(h) \sum_{k=1}^{n} L_k'[V^{-1}]_{ki} \qquad (i = 1, \ldots, n). \tag{3.20}$$

Let $\delta_i(h)$ have t_i different zeros, say for $h = h_{ij}$ ($j = 1, \ldots, t_i$), each zero being of order d_{ij}; then eq. (3.20) leads to a set of equations

$$\sum_{k=1}^{n} L_k(h)\, [W]_{ki} = (h - h_{ij})^{d_{ij}}\, P_{ij}(h) \qquad (i = 1, \ldots, n;\; j = 1, \ldots, t_i), \tag{3.21}$$

where P_{ij} is a matrix polynomial. Each relation of (3.21) is of the type (3.6) appearing in lemma 3–3, and so there exist a number of linear relations among the matrices G_{kj}. For each relation of (3.21) a set of d_{ij} vectors can be defined $\{\boldsymbol{a}^{ijk}|\; k = 1, \ldots, d_{ij}\}$, the components of which are coefficients in the linear relations

$$\sum_{l=1}^{n} \sum_{m=1}^{m_k} G_{lm} a_{lm}^{ijk} = 0 \qquad (i = 1, \ldots, n;\; j = 1, \ldots, t_i;\; k = 1, \ldots, d_{ij}). \tag{3.22}$$

According to lemma 3–3

$$\hat{O}_A \boldsymbol{a}^{ijk} = h_{ij} \hat{O}_B \boldsymbol{a}^{ijk} + \hat{O}_B \boldsymbol{a}^{ij,k-1}, \qquad \boldsymbol{a}^{ij0} = 0 \qquad (i = 1, \ldots, n;\; j = 1, \ldots, t_i). \tag{3.23}$$

The total number of vectors a^{ijk} constructed in this way is given by the sum of all d_{ij}. The relation

$$\sum_{i=1}^{n} \sum_{j=1}^{t_i} d_{ij} = \sum_{i=1}^{n} (m_i - m_i'), \tag{3.24}$$

holds, which follows from lemmas 3–1 and 3–2 and eq. (3.19).

Lemma 3–4. The set of $\sum_{i=1}^{n} (m_i - m_i')$ vectors $\{a^{ijk} | \, i = 1, \ldots, n; j = 1, \ldots, t_i; k = 1, \ldots, d_{ij}\}$ that is constructed in the foregoing [*cf.* eqs. (3.22) and (3.23)] is a linearly independent set.

Proof. Define Jordan blocks T_{ij} of dimension d_{ij} as in eq. (2.21) with diagonal elements h_{ij}. Let the matrix T be the direct sum [*cf.* eq. (2.20)] of all T_{ij}

$$T \underset{\text{def}}{=} \sum_{i=1}^{n} \sum_{j=1}^{t_i} \oplus T_{ij}. \tag{3.25}$$

The symbol $\oplus$ is used to denote the direct sum.

Suppose there exists a set of l and no more than l linearly independent linear relations between the vectors a^{ijk}

$$\sum_{i=1}^{n} \sum_{j=1}^{t_i} \sum_{k=1}^{d_{ij}} a^{ijk} c_{ijk}^{m} \qquad (m = 1, \ldots, l). \tag{3.26}$$

With the reasoning which is used in the proof of lemma 3–3 it can be shown that a set of coefficients s_{jk} exists such that for the set of vectors

$$\{c^m \underset{\text{def}}{=} \text{col}\,(c_{ijk}^m | \, i = 1, \ldots, n; \; j = 1, \ldots, t_i; \; k = 1, \ldots, d_{ij}); \; m = 1, \ldots, l\}$$

eq. (3.15) holds.

Consider T as an operator in the euclidean space C_t, t being the dimension of T. The spectrum of T is given by the set $\{h_{ij} | \, i = 1, \ldots, n; \; j = 1, \ldots, t_i\}$. T being a Jordan form, there are certain restrictions on the components of the eigenvectors. Consider an eigenvector belonging to h_{11}. Let the Jordan blocks T_{ij} be ordered so that, if for some i there is a j such that $h_{ij} = h_{11}$, this j equals 1. It must be remarked that $h_{ij} \neq h_{ik}$ if $j \neq k$. If d is an eigenvector belonging to the eigenvalue h_{11}, then for its components

$$d_{ijk} = 0, \qquad \text{unless} \qquad h_{i1} = h_{11} \qquad \text{and} \qquad k = 1. \tag{3.27}$$

Eq. (3.27) follows immediately from the relation $(T - h_{11} I)\, d = 0$, where I denotes the identity.

Eq. (3.15) shows that the set $\{c^k | \, k = 1, \ldots, l\}$ spans an invariant subspace of C_t. This subspace contains an eigenvector. Without loss of generality the corresponding eigenvalue may be assumed to be h_{11}, so that for the components of the eigenvector eq. (3.27) holds. This eigenvector is a linear combination of the vectors $\boldsymbol{c}^k$, and so from eq. (3.26) one can derive

$$\sum_{i=1}^{n} \boldsymbol{a}^{i11} d_{i11} = 0 \qquad (d_{i11} = 0 \quad \text{if} \quad h_{i1} \neq h_{11}). \tag{3.28}$$

For the components of $\boldsymbol{a}^{i11}$ we have [eqs. (3.9) and (3.21)]

$$a_{kj}^{i11} = h_{i1}^{j} \, [W(h_{11})]_{ki} \qquad (k = 1, \ldots, n; \; j = 0, \ldots, m_k). \tag{3.29}$$

Eqs. (3.28) and (3.29) imply a linear relation between the vectors

$$\{\boldsymbol{v}^i \underset{\text{def}}{=} \text{col}\,([W(h_{11})]_{ki} |\, k = 1, \ldots, n); \; i = 1, \ldots, n\}.$$

This, however, is excluded because $|W(h_{11})| = 1$ [eq. (3.19)] and so the assumption of eq. (3.26) is wrong, *q.e.d.*

We are now able to discuss level crossing of $H(h)$ in connection with linear relations between symmetrized products of A and B. Let us identify the set $\{L_k(h)\}$ with the set $\{H^{k-1} |\, k = 1, \ldots, n\}$. Then $[D]_{ij} = \text{Tr}\, H^{i+j-2}$ and so (*cf.* refs. 1 and 2)

$$|D| = \prod_{i,j=1\, i>j}^{n} (\varepsilon_i - \varepsilon_j)^2 . \tag{3.30}$$

If for a real value of h a number, say k, of functions $\varepsilon_i(h)$ have the same value, then in general, *i.e.*, if the derivatives are all different, there is a zero of $|D|$ of order $k\,(k-1)$. The functions $\varepsilon_i(h)$ are analytic for real h, *cf.*, *e.g.*, ref. 10, p. 120. Such an intersection of the levels is called a k-fold level crossing, or equivalently, a crossing of order k. If in such a case some levels are tangent to one another, then clearly the zero of $|D|$ is of higher order than $k\,(k-1)$. This case can be considered as the limiting case of two or more "normal" crossings. If $|D|$ has a zero for real h_0 of order $2s$, then it is said that the total number of crossings for $h = h_0$ equals s. Consequently, half of the sum of the orders of all real zeros of $|D|$ gives the total number of level crossings in the spectrum of $H(h)$. If the spectrum of B is nondegenerate, the degree of $|D|$ is $n\,(n-1)$ (*cf.* lemma 3–1). This spectrum being degenerate, the degree equals $n\,(n-1) - 2s$, where s is a positive integer. This can be interpreted as a zero of order $2s$ at infinity, so that the total number of level crossings at infinity equals s. This is more precisely formulated in theorem 3–1.

The meaning of a complex zero of $|D|$ is more complicated. If k functions $\varepsilon_i(h)$ have the same value for some complex value of h, and if they are all analytic at that point, there is no difference with the real case, apart from h being complex. However, also branchpoints of $\varepsilon_i(h)$ lead to zeros of $|D|$. So generally a complex zero of

$|D|$ is caused by a set of functions $\varepsilon_i(h)$ that have the same value, but it is not necessary that all functions be analytic at that point.

Now we apply the results that have been reached so far on the basic sets $\{L_k = H^{k-1}\}$ and $\{L'_k\}$, the latter being minimal. The coefficients $\beta_{ik}(h)$ [eq. (3.2)] are polynomials in this case. If they were not, a linear relation between the matrix coefficients G'_{kj} of this minimal basis would exist, and that is not possible for a minimal basis. If the spectrum of B is nondegenerate then the set $\{G_{km_k}\}$ is a linearly independent one, and so the lemmas 3–1, 3–3 and 3–4 can be applied. If there are q linearly independent linear relations in the set $\{\{A^{k-j-1}B^j\} | k = 1, \ldots, n; j = 0, \ldots, k\}$, then $|M(h)|$ is of degree q (lemmas 3–1 and 3–2, theorem 2–3). The matrix T [*cf.* eq. (3.25)] is of dimension q. Then [*cf.* eq. (3.19)]

$$|M(h)| = a\,|hI - T|, \tag{3.31}$$

where a is a real constant and I the identity matrix. Apart from the order of the blocks, P [*cf.* eq. (2.20)] equals T. The q linear relations can be written in such a way that for the coefficient vectors $\boldsymbol{a}^{ijk}$ [*cf.* eq. (3.23)]

$$\hat{O}_A \boldsymbol{a}^{ijk} = \sum_{l=1}^{d_{ij}} \hat{O}_B \boldsymbol{a}^{ijl} [T_{ij}]_{lk} \qquad (i = 1, \ldots, n;\ j = 1, \ldots, t_i;\ k = 1, \ldots, d_{ij}). \tag{3.32}$$

If the spectrum of B is degenerate, both eq. (3.31) and the special form of the linear relations between the symmetrized products do not follow immediately and have to be derived anew. We make use of the matrix $\bar{H}(g)$ [eq. (2.32)], for which the spectrum of $\bar{B}$ is nondegenerate, so that the above results can be used. We have

$$H^{k-1}(h) = (h - h_0)^{k-1}\,\bar{H}((h - h_0)^{-1}) \qquad (k = 1, \ldots, n), \tag{3.33}$$

so that, with eqs. (2.33) and (3.2),

$$\beta_{ik}(h) = (h - h_0)^{k-1-\bar{m}_i}\,\bar{\beta}_{ik}((h - h_0)^{-1}),$$

$$|M(h)| = (h - h_0)^q\,|\bar{M}((h - h_0)^{-1})|. \tag{3.34}$$

The number of linearly independent linear relations in the sets $\{\{\bar{A}^{k-1-j}\bar{B}^j\}\}$ and $\{\{A^{k-1-j}B^j\}\}$ both equal q (*cf.* appendix B), so that $|\bar{M}(g)|$ is of degree q. The spectrum of $\bar{H}(g)$ is degenerate for $g = 0$. Thus from the first part of theorem 3–1, formulated below, it follows that $|\bar{M}(g)|$ has a zero for $g = 0$, say of order s. Then clearly $|M(h)|$ is a polynomial of degree $q - s$.

Consider the blocks $\bar{T}_{ij}$ of $\bar{T}$ with nonzero diagonal elements g_{ij} and define for each such $\bar{T}_{ij}$ a Jordan block T_{ij} of dimension $\bar{d}_{ij}$, with diagonal elements h_{ij}:

$$h_{ij} = h_0 + g_{ij}^{-1}. \tag{3.35}$$

Let T be the direct sum of these blocks T_{ij}. The dimension of T then equals $q - s$. With $|\bar{M}(g)| = a\,|gI - \bar{T}|$ and eq. (3.34), it then follows that eq. (3.31) holds.

If one starts from the $q - s$ vectors $\bar{a}^{ijk}$ that correspond to blocks $\bar{T}_{ij}$ with non-zero diagonal elements, $q - s$ vectors a^{ijk} can be found that satisfy eqs. (3.32) and that form the coefficient vectors of $q - s$ linearly independent linear relations between the symmetrized products of A and B. This is shown in appendix B.

Now we shall prove two theorems that express the relation between level crossing and linear relations between symmetrized products.

Theorem 3–1. If there exist q and no more than q linearly independent linear relations between the symmetrized products of A and B of order $0, \ldots, n - 1$, then

$$\prod_{i,j=1\ i>j}^{n} (\varepsilon_i - \varepsilon_j)^2 = b\,|hI - T|^2\,|D'|. \tag{3.36}$$

$|D'|$ is a polynomial in h with real coefficients of degree $n(n - 1) - 2q$, which has no real zeros. b is a real constant.

T is a matrix in Jordan normal form. The diagonal elements of a block of T, T_{ij}, may be complex. In that case another block equals T_{ij}^*.

If the spectrum of B is nondegenerate, the dimension of T equals q. The q linear relations between the symmetrized products of A and B can be written in such a way that the coefficient vectors satisfy eqs. (3.32).

If the spectrum of B is degenerate, the dimension of T equals $q - s$, where s can be interpreted as the total number of level crossings of the spectrum of $H(h)$ for $|h| \to \infty$. $q - s$ linearly independent linear relations can be written in such a way that the coefficient vectors satisfy eqs. (3.32).

Proof. Eq. (3.36) follows from lemma 3–2 and eqs. (3.30) and (3.31). $|D'|$ is the gramian of the minimal basis $\{L_k'(h)\}$. Its properties follow from lemma 3–1. The properties of T and eqs. (3.32) are discussed above. The number s equals the total number of level crossings in the spectrum of $\bar{H}(g)$ for $g = 0$. Thus it can be interpreted as the total number of level crossings in the spectrum of $H(h)$ for $|h| \to \infty$, as follows from $\varepsilon_i(h) = (h - h_0)\,\bar{\varepsilon}_i\,((h - h_0)^{-1})$. The last statement is proved in appendix B, *q.e.d.*

This theorem shows that the linear relations contain information about the values of h for which the crossings occur and about the total number of level crossings for each value. The set of matrices $\{T_{ij}\}$, however, contains more information.

Theorem 3–2. If the spectrum of $H(h)$ contains a level crossing for $h = h_0$, then the total number of different eigenvalues of $H(h_0)$ equals $n - r$ where r equals the number of matrices T_{ij} with diagonal elements h_0.

Proof. If there are r matrices T_{ij} with diagonal elements h_0, then there are at least r linearly independent linear relations between the matrices $H^k(h_0)$ ($k = 0, \ldots, n - 1$). There are no more than r such linear relations, because this should give rise to more than r matrices T_{ij} with diagonal elements equal to h_0. Because $H(h_0)$ is hermitean the number of different eigenvalues equals $n - r$, *q.e.d.*

One may ask if the dimension of the matrices T_{ij} contains information about the order of the level crossing. In fact it does; the information, however, does not fully describe the problem. We discuss shortly a simple case. Let q be equal to three and let $\prod_{i>j} (\varepsilon_i - \varepsilon_j)^2$ have a sixfold root for real $h = h_0$.

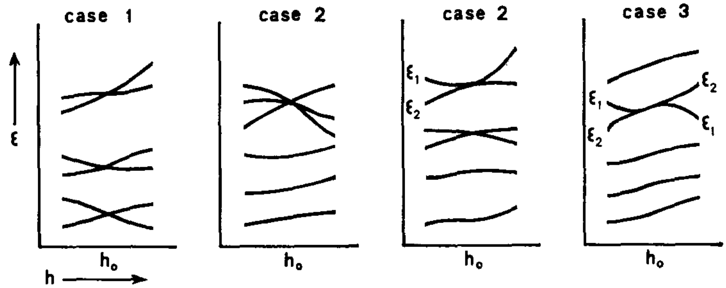

Fig. 1. Typical parts of the spectrum of H for $n = 6$ with T given by eq. (3.37).

Then for the matrix T there are three possibilities, as follows:

$$1)\begin{pmatrix} h_0 & 0 & 0 \\ 0 & h_0 & 0 \\ 0 & 0 & h_0 \end{pmatrix} \qquad 2)\begin{pmatrix} h_0 & 1 & 0 \\ 0 & h_0 & 0 \\ 0 & 0 & h_0 \end{pmatrix} \qquad 3)\begin{pmatrix} h_0 & 1 & 0 \\ 0 & h_0 & 1 \\ 0 & 0 & h_0 \end{pmatrix}. \tag{3.37}$$

In the first case there are $n - 3$ different eigenvalues of $H(h_0)$ so that there are three twofold level crossings. In the second case there are $n - 2$ different eigenvalues. This, however, can be realized in two ways: one threefold crossing or two twofold crossings, one of them being the limit of two twofold crossings with

$$(\mathrm{d}\varepsilon_1/\mathrm{d}h)_{h_0} = (\mathrm{d}\varepsilon_2/\mathrm{d}h)_{h_0}.$$

In the third case there are $n - 1$ different eigenvalues and this results in one twofold crossing, that can be considered as the limiting case of three twofold crossings with

$$(\mathrm{d}\varepsilon_1/\mathrm{d}h)_{h_0} = (\mathrm{d}\varepsilon_2/\mathrm{d}h)_{h_0}, \qquad (\mathrm{d}^2\varepsilon_1/\mathrm{d}h^2)_{h_0} = (\mathrm{d}^2\varepsilon_2/\mathrm{d}h^2)_{h_0}.$$

4. *The noncrossing rule.* The results of the foregoing sections allow a short discussion of the noncrossing rule, of course only for the case of a finite-dimensional hamiltonian that has the parameter dependence of eq. (1.1). The noncrossing rule was formulated, as a hypothesis, by Hund[7]. He stated that level crossing only occurs "if it is required by symmetry in the particles or by a separable coordinate". In other words, it can be said that, if level crossing occurs, there is an operator that

does not depend on the parameter, and that commutes with the hamiltonian for all values of the parameter.

Suppose that there exists a set of p and no more than p linearly independent constant hermitean operators, that commute with $\hat{H}(h)$. The identity is included in this set. The restriction to hermitean operators is not essential. The set of constant operators that commute with $\hat{H}(h)$ constitutes a vector space over the complex numbers. It is always possible to choose a basis, the elements of which are hermitean. Because p equals the maximum number of linearly independent hermitean operators, the above-mentioned set is a basic set. Then the space in which $\hat{H}$ acts can be split up into p orthogonal subspaces V_i that are invariant for $\hat{H}(h)$, *i.e.*, if ψ is an element of such a subspace, the same is true for $\hat{H}(h)\,\psi$ for all values of h. The dimension of the ith subspace equals n_i.

$\hat{H}$ is the sum of p operators $\hat{H}_i$

$$\hat{H} = \sum_{i=1}^{p} \hat{H}_i, \qquad \hat{H}_i \underset{\text{def}}{=} \hat{H}\hat{P}_i. \tag{4.1}$$

In eq. (4.1) $\hat{P}_i$ is the projection operator on V_i. The set

$$\{\hat{I}_1, \ldots, \hat{H}_1^{n_1-1}, \hat{I}_2, \ldots, \ldots, \hat{H}_p^{n_p-1}\}$$

is a basis for the space of operators commuting with $\hat{H}(h)$. The degree of this basis equals $\frac{1}{2}n(n-1) - \sum_{i>j} n_i n_j$. Levels belonging to different $\hat{H}_i$ may cross in general.

A number of examples for which there are level crossings without constant commuting operator are easily found. If two systems 1 and 2 with their respective hamiltonians $\hat{H}_{1,2} = \hat{A}_{1,2} + h\hat{B}_{1,2}$ are coupled to the same external field, then in the spectrum of the hamiltonian $\hat{H} = \hat{H}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{H}_2$, which describes both systems together, a lot of crossings may occur, without the consequence of the existence of a constant commuting operator. This example is already mentioned implicitly by Hund[7]). A more extensive discussion is found in ref. 1. The Hubbard hamiltonian for benzene, which was studied by Heilman and Lieb[11]) and also case c) in appendix A of this paper, provides a counter example for this rule. Finally we mention a case that cannot be directly interpreted as the hamiltonian of some physical system. A hermitean matrix $A + hB$ of general dimension n can easily be constructed for which there exists only one linear relation between the symmetrized products of A and B, so that there is one twofold level crossing. For $n > 2$ there is no constant commuting matrix, because the degree of the minimal basis equals $\frac{1}{2}n(n-1) - 1$.

The number of crossings contains information about the existence of a constant commuting operator only in extreme cases, as is stated in the following theorem.

Theorem 4–1. If the total number of crossings in the spectrum of an n-dimensional hermitean matrix $H = A + hB$ that has no identical levels exceeds $\frac{1}{2}(n-1) \times (n-2)$, then there is a constant nontrivial matrix that commutes with H.

Proof. Under the conditions mentioned in the theorem, the degree of the minimal basis is less than $\frac{1}{2}n(n-1) - \frac{1}{2}(n-1)(n-2) = n-1$. So the minimal basis contains, apart from the identity, a constant matrix, *q.e.d.*

Theorem 4–1 is not a trivial one as is demonstrated by the following example. If the matrices A and B are restricted to

$$A = \text{diag}\,(1, 1, \ldots, 1, a_{nn}), \qquad a_{nn} \neq 1,$$

$$[B]_{ij} = 0, \quad [B]_{ii} \neq [B]_{jj}, \quad [B]_{in} \neq 0 \quad (i, j = 1, \ldots, n-1, i \neq j), \tag{4.2}$$

then the spectrum of H has an $(n-1)$-fold crossing for $h = 0$. The total number of crossings then equals $\frac{1}{2}(n-1)(n-2)$. It is easy to show, that there is no constant matrix that commutes with A and B and hence with $H(h)$.

Generally on account of the existence of level crossing, only the following statement about commuting operators can be made.

Theorem 4–2. If there is a level crossing, say for $h = h_0$, in the spectrum of a hermitean matrix $H = A + hB$, then there is a hermitean matrix polynomial $P(h)$, that commutes with $H(h)$, that is not a linear combination of the set $\{H^0, \ldots, H^{n-1}\}$ with scalar polynomial coefficients.

Proof. If there is a level crossing, say for $h = h_0$, then there exists a linear relation $\sum_{i=1}^{n} a_i H^{i-1}(h_0)$, where the coefficients a_i are real numbers. Then there is a hermitean polynomial $P(h)$ that satisfies $(h - h_0)\,P(h) = \sum_{i=1}^{n} a_i H^{i-1}(h)$. $P(h)$ commutes with $H(h)$ and is a linear combination of the powers of H with coefficients $a_i\,(h - h_0)^{-1}$. Note that these coefficients are unique for a given $P(h)$, *q.e.d.*

APPENDIX A

Consider the spin hamiltonian $\hat{H}_s$

$$\hat{H}_s = d\,[\hat{S}_z^2 - \tfrac{1}{3}s\,(s+1)\,\hat{I}] + e\,[\hat{S}_x^2 - \hat{S}_y^2] + g\beta_0\,(\boldsymbol{H} \cdot \hat{\boldsymbol{S}}), \tag{A.1}$$

in which d and e are real constants, g is a gyromagnetic ratio, β_0 the Bohr magneton. The spin quantum number s is taken to be one. This hamiltonian is used in the description of paramagnetic resonance spectra of salts for which the lowest orbital level is nondegenerate[12]) (*e.g.*, for the iron group). The quadratic terms in $\hat{H}_s$ describe the combined effect of spin–orbit coupling and the interaction with the crystalline field. The spectrum of this hamiltonian was also discussed in ref. 1, however, in a different way than we do it here.

Instead of $\hat{H}_s$ we discuss the operator $\hat{H}$ that equals $\hat{H}_s$ apart from the identity term. With

$$r = d + e, \qquad t = d - e, \qquad h = g\beta_0\,|\boldsymbol{H}|, \qquad \boldsymbol{u} = (a, b, c),$$
$$a = \sin\theta\cos\phi, \qquad b = \sin\theta\sin\phi, \qquad c = \cos\theta, \tag{A.2}$$

θ and ϕ being the angles that characterize the direction of $\boldsymbol{H}$, we get

$$\hat{H} = \hat{A} + h\hat{B},$$
$$\hat{A} = \tfrac{1}{2}(r + t)\,\hat{S}_z^2 + \tfrac{1}{2}(r - t)(\hat{S}_x^2 - \hat{S}_y^2), \qquad \hat{B} = \hat{S}_u = (\boldsymbol{u}\cdot\hat{\boldsymbol{S}}). \tag{A.3}$$

If for the operators $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$ the following representation is chosen

$$S_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \qquad S_y = \begin{pmatrix} 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix}, \qquad S_z = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{A.4}$$

then for the matrices of $\hat{A}$ and $\hat{B}$ we have

$$A = \begin{pmatrix} t & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & -\mathrm{i}c & \mathrm{i}b \\ \mathrm{i}c & 0 & -\mathrm{i}a \\ -\mathrm{i}b & \mathrm{i}a & 0 \end{pmatrix}. \tag{A.5}$$

The three symmetrized products of second order are given by

$$A^2 = \begin{pmatrix} t^2 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \{AB\} = \begin{pmatrix} 0 & -\mathrm{i}c\,(r + t) & \mathrm{i}bt \\ \mathrm{i}c\,(r + t) & 0 & -\mathrm{i}ar \\ -\mathrm{i}bt & \mathrm{i}ar & 0 \end{pmatrix},$$

$$B^2 = \begin{pmatrix} c^2 + b^2 & -ab & -ac \\ -ab & a^2 + c^2 & -bc \\ -ac & -bc & a^2 + b^2 \end{pmatrix}. \tag{A.6}$$

We want to know the number of linear relations between the six symmetrized products for different values of a, b, c, d, e. The spectrum of B being nondegenerate, we study equivalently (*cf.* lemma 2–1), linear relations between the three following commutators:

$$[A, B] = \begin{pmatrix} 0 & & \\ -\mathrm{i}c\,(t - r) & 0 & \\ \mathrm{i}bt & -\mathrm{i}ar & 0 \end{pmatrix},$$

$$[A^2, B] = \begin{pmatrix} 0 & & \\ -ic(t^2 - r^2) & 0 & \\ ibt^2 & -iar^2 & 0 \end{pmatrix},$$
$$[\{AB\}, B] = \begin{pmatrix} 0 & & \\ ab(t - r) & 0 & \\ act & bcr & 0 \end{pmatrix}. \qquad (A.7)$$

These commutators being elements of a real vector space, the number of linearly independent linear relations between them equals three minus the rank of the following matrix G

$$G \underset{\text{def}}{=} \begin{pmatrix} -c(t-r) & bt & -ar & 0 & 0 & 0 \\ -c(t^2 - r^2) & bt^2 & -ar^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & ab(t-r) & act & bcr \end{pmatrix}. \qquad (A.8)$$

We shall discuss three typical cases for which level crossing occurs and for which the degree of the minimal basis for $\hat{H}$ is less than three.

a) If $t = r$ and if the magnetic field is in the direction of the z axis ($a = b = 0$, $c = 1$), the rank of G, denoted by r_G, equals zero.

There are three linearly independent linear relations, such that the degree of the minimal basis equals zero. Then $\hat{H} = t\hat{S}_z^2 + h\hat{S}_z$ and the set $\{I, \hat{S}_z, \hat{S}_z^2\}$ is a minimal basis. Three twofold level crossings occur, respectively for $h = \pm t$, $h = 0$.

b) If $t \neq r$ and again $a = b = 0$, $c = 1$, r_G equals one. Then there are two linearly independent linear relations between the symmetrized products,

$$-B(t + r) + \{AB\} = 0, \qquad (t + r)A - A^2 - trB^2 = 0. \qquad (A.9)$$

With the coefficients in these two relations two vectors $\boldsymbol{a}^i$ are formed [*cf.* eqs. (2.16) and (2.9), $G_{kj} = \{A^{k-j-1}B^i\}$]

$$\boldsymbol{a}^1 = \text{col}(0, 0, -(t + r), 0, 1, 0), \qquad \boldsymbol{a}^2 = \text{col}(0, t + r, 0, -1, 0, -tr). \qquad (A.10)$$

Eqs. (2.19) then read in matrix form

$$\begin{pmatrix} -(t+r) & 0 \\ 1 & 0 \\ 0 & -tr \end{pmatrix} = \begin{pmatrix} 0 & t+r \\ 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -tr \\ -1 & 0 \end{pmatrix}. \qquad (A.11)$$

The Jordan form of the matrix $S = \begin{pmatrix} 0 & -tr \\ -1 & 0 \end{pmatrix}$ is given by

$$\begin{pmatrix} (tr)^{\frac{1}{2}} & 0 \\ 0 & -(tr)^{\frac{1}{2}} \end{pmatrix} \quad (tr \neq 0), \quad \text{or} \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad (tr = 0). \qquad (A.12)$$

The degree of the minimal basis equals 1, and so there is a constant operator commuting with $\hat{H}$. Then $[\{AB\}, B] = [A, B^2]$ so that with $a = b = 0$ and eq. (A.7) we have $[A, B^2] = 0$. Because also $[B, B^2] = 0$, a minimal basis is given by the set $\{\hat{I}, \hat{S}_z^2, \hat{H}\}$. If $tr > 0$ there are two twofold level crossings, respectively, for $h = \pm(tr)^{\frac{1}{2}}$. If $tr = 0$ there is a twofold level crossing for $h = 0$, the levels, however, are tangent. If $tr < 0$ there is no level crossing.
c) If $t = r$ and $t \neq 0$, then r_G equals 2 for nonzero a, b and c. There is only one linear relation between the symmetrized products

$$-tA + A^2 = 0, \tag{A.13}$$

corresponding with a twofold level crossing for $h = 0$. On account of eq. (A.13)

$$-tH + H^2 = h(P + hQ), \qquad Q = B^2, \qquad P = -tB + \{AB\}. \tag{A.14}$$

In this case $\hat{H} = \hat{S}_z^2 + h\hat{S}_u$, so that the set $\{\hat{I}, \hat{H}, -t\hat{S}_u + \hat{S}_z^2\hat{S}_u + \hat{S}_u\hat{S}_z^2 + h\hat{S}_u^2\}$ is a minimal basis.

APPENDIX B

Let there be q linearly independent linear relations in the set $\{\{A^{k-j-1}B^j\} | k = 1, \ldots, n;\ j = 0, \ldots, k-1\}$. If the spectrum of B is degenerate, the coefficient vectors of these linear relations cannot immediately be written in such a way as to satisfy eqs. (3.32). Making use of the matrix $\bar{H}(g)$ [eq. (2.32)], we shall show that $q - s$ linearly independent relations can be written so that eqs. (3.32) hold where s can be interpreted as the total number of level crossings in the spectrum of $H(h)$ at infinity.

First we shall write the matrices $\{\bar{A}^{k-1-j}\bar{B}^j\}$ as a linear combination of the matrices $\{A^{k-1-j}B^j\}$. Then [*cf.* eq. (3.33)]

$$\bar{H}^{k-1}(g) = g^{k-1}H^{k-1}(h_0 + g^{-1}). \tag{B.1}$$

Both sides of this equation can be written as a sum of powers of g. Equating equal powers we get

$$\{\bar{A}^{k-1-j}\bar{B}^j\} = \sum_{i=k-j-1}^{k-1} \binom{i}{k-j-1} h_0^{i+j-k+1}\{A^{k-i-1}B^i\}$$

$$(j = 0, \ldots, k-1). \tag{B.2}$$

With the coefficients in eq. (B.2), square matrices Q_k ($k = 1, \ldots, n$) of dimension k may be defined such that $\{\bar{A}^{k-1-j}\bar{B}^j\} = \sum_{p=0}^{k-1} [Q_k]_{p+1,j+1}\{A^{k-1-p}B^p\}$

$$[Q_k]_{pj} = \binom{p-1}{k-j} h_0^{j+p-k-1} \qquad (p, j = 1, \ldots, k). \tag{B.3}$$

Define the matrix Q by $Q \underset{\text{def}}{=} \sum_{k=1}^{n} \oplus Q_k$. Q_k is a nonsingular matrix and so is Q. Thus the number of linearly independent linear relations in both sets $\{\{\bar{A}^{k-1-j}\bar{B}^j\}$ and $\{A^{k-1-j}B^j\}\}$ are equal.

The q linear relations between the matrices $\{\bar{A}^{k-1-j}\bar{B}^j\}$ can be written so that eqs. (3.32) are satisfied by their coefficient vectors $\bar{\boldsymbol{a}}^{ijk}$. Considering these vectors as columns, the vectors $Q\bar{\boldsymbol{a}}^{ijk}$ are linearly independent, and they are the coefficient vectors of the linear relations in the set $\{A^{k-j-1}B^j\}$. We shall prove now the following relation

$$\hat{O}_A\,(Q\bar{\boldsymbol{a}}^{ijk}) = \sum_{l=1}^{\bar{d}_{ij}} \hat{O}_B\,(Q\bar{\boldsymbol{a}}^{ijl}\,[\bar{T}_{ij}^{-1} + h_0 I]_{lk}), \tag{B.4}$$

provided that the diagonal elements of $\bar{T}_{ij}$, g_{ij}, do not equal zero. It has to be noted, that the matrices $\bar{T}_{ij}$ are Jordan blocks. The Jordan normal form of $\bar{T}_{ij}^{-1} + h_0 I$ is easily shown to be a Jordan block of dimension $\bar{d}_{ij}$ and with diagonal elements $h_{ij} = h_0 + g_{ij}^{-1}$ [*cf.* eq. (3.35)]. From the discussion in section 3 [especially eq. (3.31)] it follows that the number of vectors $Q\bar{\boldsymbol{a}}^{ijk}$ that appear in eq. (B.4) equals $q - s$, where s is the order of the zero of $|\bar{M}(g)|$ for $g = 0$. So the aim of this appendix is reached.

In order to prove eq. (B.4), we claim that this equation is true if and only if the following relation holds

$$\hat{O}_A\left(\sum_{l=1}^{\bar{d}} Q\bar{\boldsymbol{a}}^l\,[\bar{T}]_{lk}\right) = \hat{O}_B\left(\sum_{l=1}^{\bar{d}} Q\bar{\boldsymbol{a}}^l\,[I + h_0\bar{T}]_{lk}\right) \qquad (k = 1, \ldots, \bar{d}), \tag{B.5}$$

because $\bar{T}$ is nonsingular. The indices i, j are omitted and the diagonal elements of $\bar{T}$ are denoted by g_0. Eq. (B.5) is equivalent with [*cf.* eqs. (2.15) and (3.7)]

$$(Q\,(g_0\bar{\boldsymbol{a}}^l + \bar{\boldsymbol{a}}^{l-1}))_{k,j+1} = (Q\,[\bar{\boldsymbol{a}}^l + h_0\,(g_0\bar{\boldsymbol{a}}^l + \bar{\boldsymbol{a}}^{l-1})])_{kj}, \tag{B.6}$$

$$\bar{\boldsymbol{a}}^0 = \boldsymbol{0} \qquad (l = 1, \ldots, \bar{d};\; k = 2, \ldots, n;\; j = 0, \ldots, k-2).$$

Further:

$$(Q\bar{\boldsymbol{a}}^l)_{kj} = \sum_{p=1}^{k} \binom{j}{k-p} h_0^{p+j-k}\bar{a}^l_{k,p-1} \qquad (k = 2, \ldots, n;\; j = 0, \ldots, k-1), \tag{B.7}$$

and [*cf.* eqs. (2.15) and (3.7)]:

$$\bar{a}^l_{k,p+1} = g_0\bar{a}^l_{kp} + \bar{a}^{l-1}_{kp} \qquad (p = 0, \ldots, k-2). \tag{B.8}$$

Substitution of eq. (B.7) into eq. (B.6) gives

$$\sum_{p=1}^{k}\left\{\binom{j+1}{k-p} - \binom{j}{k-p}\right\} h_0^{p+j+1-k}(g_0\bar{a}^l_{k,p-1} + \bar{a}^{l-1}_{k,p-1})$$

$$= \sum_{p=0}^{k-1}\binom{j}{k-p-1} h_0^{p+j+1-k}\bar{a}^l_{kp} \qquad (j = 0, \ldots, k-2). \tag{B.9}$$

If the terms for respectively $p = 0$ and $p = k$ are taken apart and if eq. (B.8) is substituted, eq. (B.9) is seen to be true on the basis of properties of binomial coefficients.

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