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Some simple results following from Löwdin's partitioning technique

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It is shown that several simple theorems follow from Löwdin's partitioning technique. Our results concern the properties of matrices whose eigenvectors have linearly dependent parts. It is also demonstrated that the solutions of most energy eigenvalue problems satisfy a non-trivial manifold of quadratic equations in energy.

KEY WORDS: partitioning technique, eigenvector, matrix rank

1. Introduction

Throughout this communication, all our equations are written in a finite-dimensional, matrix-vector form. Löwdin's partitioning technique [1–4], which we briefly outline below, is an important tool in the development of quantum chemical formalisms and is actively applied in contemporary research [5–10]. The variation of the Rayleigh–Ritz functional

$$E = \langle C|H|C\rangle / \langle C|C\rangle \tag{1}$$

written in terms of the discrete variational configuration interaction coefficients C_i results in the well-known eigenvalue equation, which for the purpose of partitioning is written in the following block matrix form

$$\left(\begin{array}{c|c} H^{QQ} & H^{QR} \\ \hline H^{RQ} & H^{RR} \end{array}\right) \left(\begin{array}{c} C^{Q} \\ \hline C^{R} \end{array}\right) = E \left(\begin{array}{c} C^{Q} \\ \hline C^{R} \end{array}\right) \tag{2}$$

or, multiplying the blocks,

$$H^{QQ}|C^{Q}\rangle + H^{QR}|C^{R}\rangle = E|C^{Q}\rangle, \tag{3}$$

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$$H^{RQ}|C^Q\rangle + H^{RR}|C^R\rangle = E|C^R\rangle. \tag{4}$$

The superscripts in these equations have the meaning of the dimension of the corresponding quantities. The total dimension of the system (2) is $N = Q + R$. To arrive at the effective eigenvalue problem, which is the central equation of the partitioning technique, we use the second of these equations to express C^R through C^Q

$$|C^R\rangle = (E - H^{RR})^{-1} H^{RQ}|C^Q\rangle, \tag{5}$$

we eliminate C^R and arrive at the representation

$$\left[H^{QQ} + H^{RQ}(E - H^{RR})^{-1}H^{RQ}\right]|C^Q\rangle = E|C^Q\rangle, \tag{6}$$

which is equivalent to (2). The partitioning technique may be used for a direct solution of the eigenvalue problem. Various expansion techniques [1] allow us to write the energy E contained in this non-linear equation as an infinite series of terms. It is possible to derive in such a way, for example, the Brillouin–Wigner and Rayleigh–Schrödinger perturbation formulas. When E and C^Q have been determined from (6), the remaining component C^R is calculated from (5). Assuming that $(E - H^{RR})^{-1}$ exists and the perturbation series used to calculate E converges, equation (2) is solved. Although in practice the perturbation series is terminated at the second or third order and E and C are determined with an error, it is important to observe that this approach in principle provides the exact solution of (2).

2. Discussion

The usefulness of the partitioning technique rests on its ability to find C and E, which are the solutions of the eigenvalue problem (2). If, however, we assume that C and E are already known, a few interesting mathematical results follow from equation (2). In what follows we prove some results concerning the spectral properties of matrices with eigenvectors whose parts are linearly dependent.

Surprisingly, it is possible to write the formal solution of the eigenvalue equations in a closed form. Multiplying (4) by H^{QR} from the left (so that the matrix acting on C^Q becomes square) and then expressing C^Q through E as in

$$|C^Q\rangle = W^{QR}\left(E - H^{RR}\right)|C^R\rangle, \tag{7}$$

$$W^{QR} = (H^{QR}H^{RQ})^{-1}H^{QR}, \tag{8}$$

we rewrite (3) as a quadratic equation in E:

$$E^2|a\rangle + E|b\rangle + |c\rangle = 0, \tag{9}$$

where the vectors $|a\rangle$, $|b\rangle$, and $|c\rangle$ are defined as

$$|a\rangle = -W^{QR}|C^R\rangle, \tag{10}$$

$$|b\rangle = H^{QQ}W^{QR}|C^R\rangle - W^{QR}|U^R\rangle, \tag{11}$$

$$|c\rangle = H^{QQ}W^{QR}|U^R\rangle - |U^Q\rangle \tag{12}$$

and the following abbreviations are used

$$|U^Q\rangle = -H^{QR}|C^R\rangle, \tag{13}$$

$$|U^R\rangle = -H^{RR}|C^R\rangle. \tag{14}$$

The assumption that the inverse of $H^{QR}H^{RQ}$ exists leads us to the necessary condition $Q \leqslant R$ (which will be adhered to in the rest of the paper, unless indicated otherwise). For convenience of discussion, the Q equations which constitute (9) may also be 'averaged' by means of a contraction with an arbitrary non-zero vector $\langle X^Q|$:

$$\langle X^Q|a\rangle E^2 + \langle X^Q|b\rangle E + \langle X^Q|c\rangle = 0. \tag{15}$$

Clearly, when C^R is exact, the root E of the projected equation (15), which is at the same time the root of (2), does not depend on the particular choice of $\langle X^Q|$. Note that for a two-by-two matrix H equation (9) is a scalar one and is identical to the characteristic equation of H.

Suppose we choose such an eigenvector C_i of H that has a unique C^R. In other words, no other eigenvector of H shares the part C^R with our chosen eigenvector. The eigenvalue corresponding to this eigenvector is E_i. Then the projected equation (15) constructed from this C^R will have two roots, one of which is guaranteed to be E_i. Another root does not have to satisfy the eigenvalue equations and in the general case depends on the projection $\langle X^Q|$. The independence of projection may allow us to distinguish the true solution of (2) from the spurious one. The spurious root has its origin in the act of projection by $\langle X^Q|$ and its existence is explained by the fact that the scalar equations which constitute (9) are satisfied by the actual eigenvalue of (2) only. Assume now that we have two eigenvectors C_i and C_j with two distinct eigenvalues E_i and E_j and two identical parts C^R. In this case the individual scalar equations in (9) may be satisfied by two different roots, and the projected equation (15) will have two solutions, E_i and E_j which do not depend on the projection.

Now we would like to make a comment that will be used in the proof of the results below. It is well-known that two eigenvectors $|d_1\rangle$ and $|d_2\rangle$ of $N \times N$ matrix A that correspond to the same eigenvalue E may be added together with arbitrary coefficients α_1 and α_2, and the vector $|d_3\rangle$ resulting from this linear combination will also be an eigenvector of A with the same eigenvalue E. Suppose that we want to take two linear combinations of $|d_1\rangle$ and $|d_2\rangle$ in such a way that two resulting eigenvectors $|d_1'\rangle$ and $|d_2'\rangle$ are partly coincident:

$$|d_1'\rangle - |d_2'\rangle = \{d_{11}' - d_{21}', d_{12}' - d_{22}', \ldots, d_{1k}' - d_{2k}', 0, 0, \ldots, 0, \\ d_{1l}' - d_{2l}', d_{1l+1}' - d_{2l+1}', \ldots, d_{1N}' - d_{2N}'\}. \tag{16}$$

In this formula, d_{1k}' is the kth component of the vector $|d_1'\rangle$. Obviously, this is possible only when $l-k-1$ corresponding components of $|d_1\rangle$ and $|d_2\rangle$ constitute linearly dependent vectors, i.e. if at least one of these vectors is zero or

$$\{d_{1,k+1}, d_{1,k+2}, \ldots, d_{1,l-1}\} = \alpha\{d_{2,k+1}, d_{2,k+2}, \ldots, d_{2,l-1}\}, \tag{17}$$

where $\alpha \neq 0$. If the $l-k-1$ components of $|d_1\rangle$ and $|d_2\rangle$ constitute linearly independent vectors, two different vectors $|d_1'\rangle$ and $|d_2'\rangle$, which satisfy (16) cannot be constructed because a vector has unique coordinates in the basis of $|d_1\rangle$ and $|d_2\rangle$. So, it appears that if two eigenvectors $|d_1\rangle$ and $|d_2\rangle$ have linearly dependent parts, we may always convert them into the eigenvectors $|d_1'\rangle$ and $|d_2'\rangle$, which have the coincident parts, so that $|d_1'\rangle$ and $|d_2'\rangle$ remain eigenvectors with the eigenvalues of $|d_1\rangle$ and $|d_2\rangle$, respectively.

Theorem 1. If an arbitrary square matrix H separated into blocks in the manner of that in equation (2) (so that $R \geqslant Q$) possesses two eigenvectors C_1, C_2 with the same eigenvalue and with linearly dependent parts C_1^R, C_2^R, then $\mathrm{rank}(H^{QR}) < Q$.

Proof. Suppose $\mathrm{rank}(H^{QR}) = Q$, then $H^{QR}H^{RQ}$ is invertible and expression (7) can be constructed. Further, C_1 and C_2 may be converted into the eigenvectors C_1' and C_2' by two suitable linear combinations so that $C_1'^R = C_2'^R \equiv C^R$. Then (by equation (7)) C^Q is a linear, deterministic function of E and C^R. This contradicts the fact that different vectors C^Q may correspond to one eigenvalue E and one vector C^R. Thus, our supposition is not true and $\mathrm{rank}(H^{QR}) < Q$.

As an important corollary used in the proof of the next theorem, we note that if an arbitrary square matrix H separated into blocks in the manner of that in equation (2) (so that $R \geqslant Q$) possesses two eigenvectors C_1 and C_2 with linearly dependent parts C_1^R, C_2^R and $\mathrm{rank}(H^{QR}) = Q$, then two eigenvalues corresponding to C_1 and C_2 are non-degenerate. Indeed, under the conditions of theorem 1, if the two eigenvalues are degenerate, then $\mathrm{rank}(H^{QR}) < Q$. If they are not degenerate, $\mathrm{rank}(H^{QR})$ may be either Q or less than Q. So, we conclude that the equality $\text{rank}(H^{QR}) = Q$ may correspond only to the situation in which the two eigenvalues are non-degenerate.

Now we prove another theorem related to the possibility of having three eigenvectors with identical parts C^R which further explains some properties of equation (9).

Theorem 2. If an arbitrary square matrix H separated into blocks in the manner of that in equation (2) (so that $R \geqslant Q$) possesses three eigenvectors C_1, C_2, C_3 with linearly dependent parts C^R, then $\text{rank}(H^{QR}) < Q$.

Proof. Suppose $\text{rank}(H^{QR}) = Q$. Then $H^{QR}H^{RQ}$ is invertible and (9–15) can be constructed. By theorem 1, three eigenvalues corresponding to the three eigenvectors C_1, C_2, C_3, are distinct. By suitable multiplications we may convert C_1, C_2, C_3 into the eigenvectors C_1', C_2', C_3' with $C_1'^R = C_2'^R = C_3'^R \equiv C^R$. The projected quadratic equation (15) is satisfied with all possible eigenvalues of H that correspond to C_1, C_2, C_3. However, since the equation is quadratic, it cannot be satisfied with three distinct values of E. Hence, we arrive at the contradiction and $\text{rank}(H^{QR}) < Q$.

Another simple conclusion follows directly from equation (5).

Theorem 3. If an arbitrary square matrix H separated into blocks in the manner of that in equation (2) possesses two eigenvectors C_1 and C_2 with linearly dependent parts C_1^Q and C_2^Q (Q is arbitrary) and identical eigenvalues E, then E is also an eigenvalue of the matrix H^{RR}.

Proof. Suppose $(E - H^{RR})^{-1}$ exists. The vectors C_1^Q and C_2^Q may be equated ($C_1^Q = C_2^Q \equiv C^Q$) by two suitable linear combinations. Then C^R is a linear, deterministic function of E and C^Q. This contradicts the fact that C_1^R, C_2^R correspond to only one vector C^Q and one value E. The only way to resolve this contradiction is to assume that (5) cannot be constructed because $(E - H^{RR})^{-1}$ does not exist. Consequently, E is the eigenvalue of H^{RR}.

Note that using this theorem for the case when $Q = 1$ we arrive at the corollary which also follows from the separation theorem by MacDonald [11] if the matrix $||H_{ij}||_{1 \leqslant i,j \leqslant N}$ possesses degenerate eigenvalue E the matrix $||H_{ij}||_{1 \leqslant i,j \leqslant N-1}$ possesses this eigenvalue too.

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