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Abstract

Full Text

Physics

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On the Reduction to Cell-Diagonal Form of Matrices of Operators Commuting with a Group of Symmetry Operators

(Presented by Academician I. V. Obreimov, 31 X 1964)

Let Q be a unitary space of dimension n , whose elements are vectors

$$\mathbf{q} = q_1 \mathbf{e}_1 + q_2 \mathbf{e}_2 + \dots + q_n \mathbf{e}_n = \sum_{i=1}^n q_i \mathbf{e}_i; \quad (1)$$

here q_i are the natural coordinates defined in the sense of (1).

Let, further, G be a group of unitary symmetry operators $\hat{S}^{(1)}, \hat{S}^{(2)}, \dots, \hat{S}^{(l)}$ (see (2)), satisfying the condition $\hat{S}^* = \hat{S}^{-1}$ (\hat{S}^* is the operator adjoint with respect to \hat{S}) and transforming each vector \mathbf{q} of the space Q into some vector \mathbf{q}' of the same space

$$\mathbf{q}' = \hat{S} \mathbf{q}. \quad (2)$$

Suppose that the space of natural coordinates Q decomposes into subspaces of equivalent coordinates $^{(1)} Q_1, Q_2, \dots, Q_k$, whose dimensions are respectively r_1, r_2, \dots, r_k ($n = r_1 + r_2 + \dots + r_k$).

From the definition of equivalence of coordinates it follows that each Q_j is invariant with respect to all symmetry operators. Then, in the basis $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$, the symmetry operators $\hat{S}^{(i)}$ correspond to matrices $S^{(i)}$ having a stepwise structure

$$S^{(i)} = \left\| \begin{array}{c|c|c|c} S_1^{(i)} & 0 & \dots & 0 \\ \hline 0 & S_2^{(i)} & \dots & 0 \\ \hline \vdots & \vdots & & \vdots \\ \hline 0 & 0 & \dots & S_k^{(i)} \end{array} \right\| \quad (i = 1, 2, \dots, l), \quad (3)$$

where on the diagonal stand square matrices of orders r_1, r_2, \dots, r_k , respectively.

Let us now consider a Hermitian operator \hat{A}^* which, in the orthonormal basis of the displacement space $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$, has the matrix $A = \|a_{ik}\|$, satisfying the invariance condition

$$S^{(i)-1}AS^{(i)} = A, \quad (4)$$

where $i = 1, 2, \dots, l$.

Among all possible matrices satisfying condition (4), below we consider matrices possessing the least symmetry, i.e. the greatest possible number of essentially distinct elements a_{ik} .

* Here by \hat{A} is meant one of the following operators: \hat{T} –the kinetic-energy operator, \hat{V} –the potential-energy operator.

In accordance with the decomposition of the space Q into subspaces of equivalent coordinates, the matrix $\|a_{ik}\|$ can be represented in block form:

$$A = \left\| \begin{array}{c|c|c|c} A_1 & A_{12} & \dots & A_{1k} \\ \hline A_{21} & A_2 & \dots & A_{2k} \\ \hline \vdots & \vdots & \dots & \vdots \\ \hline A_{k1} & A_{k2} & \dots & A_k \end{array} \right\|, \quad \begin{array}{l} \}r_1 \\ \}r_2 \\ \vdots \\ \}r_k \end{array} \quad (5)$$

where, from the self-adjointness of the operator \hat{A} , it follows that

$$A_{ik}^* = A_{ki}.$$

We shall now formulate the main proposition of the present work: if in each of the subspaces Q_j ($j = 1, 2, \dots, k$) one chooses, as a basis, the eigenvectors of the corresponding matrices A_j , and then forms a basis of the space Q as the direct sum of the linear subspaces Q_j (see (3)), then in this new basis the matrix of the operator \hat{A} , after a suitable permutation of rows and columns, will have block-diagonal form.

A justification of this proposition can be given as follows. Performing operations on the block matrices (3) and (5), we obtain, on the basis of (4),

$$S_j^{(i)-1}A_jS_j = A_j \quad (i = 1, 2, \dots, l; j = 1, 2, \dots, k),$$

whence

$$A_j S_j^{(i)} = S_j^{(i)} A_j. \quad (7)$$

Let us note that the collection $S_j^{(1)}, S_j^{(2)}, \dots, S_j^{(l)}$ forms a representation G_j of the point symmetry group in the subspace of equivalent coordinates Q_j .

We now construct the fundamental matrix (4) C_j , whose columns are the eigenvectors of the operator \hat{A}_j . Owing to the Hermitian nature of \hat{A}_j , there always exists an orthonormal system of eigenvectors ⁽⁵⁾. Then the similarity transformation brings the matrix A_j to diagonal form:

$$C_j^{-1} A_j C_j = \|\lambda_s^{(j)} \delta_{st}\| = A'_j. \quad (8)$$

Suppose that among the λ_s there is an eigenvalue λ_p of multiplicity m ; to this eigenvalue there corresponds an m -dimensional eigensubspace L_p . Then in the diagonal matrix A'_j one can distinguish a scalar submatrix $A_p = \lambda_p E$ of order m .

Thus the subspace of equivalent coordinates Q_j decomposes into the direct sum of the linear subspaces L_p , whose dimensions are equal to the multiplicities of the corresponding eigenvalues λ_p .

From the commutativity of A_j with all $S_j^{(i)}$ it follows from (6) that the similarity transformation (8), performed on $S_j^{(i)}$, leads to the decomposition of the representation G_j

$$G_j = \sum_p \Gamma_p^{(j)}, \quad (9)$$

where Γ_p are the representations according to which the subspaces L_p transform, since the eigensubspaces of the operator \hat{A}_j are invariant subspaces of each $S_j^{(i)}$. This follows from the fact that \hat{A}_j has a common complete system of eigenvectors with each of the $S_j^{(i)}$ (4). For different i these will, generally speaking, be different systems.

Thus, the dimension of the representation Γ_p is equal to the multiplicity of the corresponding eigenvalue λ_p .

Let us now show that the representations Γ_p are irreducible. This is obvious for the case of a one-dimensional eigensubspace L_p ($m = 1$), which will be an irreducible subspace in the sense of (7). Let us note in passing that the subspace Q'_j itself will be irreducible if its dimension is equal to one. Let us also note that if, on the right-hand side of (8), all eigenvalues are simple, then all Γ_p will be one-dimensional and irreducible and, consequently, the group G_j is abelian.

Consider the case when G_j is nonabelian and A'_j has at least one eigenvalue λ_p whose multiplicity is $m \neq 1$. Suppose that the corresponding representation Γ_p is reducible. Then, in accordance with (6), there must exist a nonscalar submatrix B_p of order m , commuting with Γ_p . Now construct a matrix B'_j which differs from A'_j only in that, in place of the scalar matrix A'_p , the matrix B_p stands. It is obvious that, by construction, B'_j commutes with all $S_j^{(i)'} -$ the matrices of the reduced representation G'_j . If, further, we carry out the transformation inverse to the transformation (8) on the matrix B'_j , we obtain

$$B_j = C_j B'_j C_j^{-1}, \quad (10)$$

where B_j must satisfy a condition analogous to (6), i.e.

$$S_j^{(i)-1} B_j S_j^{(i)} = B_j. \quad (11)$$

From comparison of (11) and (6) it is clear that B_j must satisfy the condition of invariance with respect to the same group of matrices $S_j^{(i)}$ as A_j . But the matrix B_j must possess less symmetry than A_j , in the sense that the number of essentially distinct elements of the matrix B_j must be greater than that of A_j (otherwise B_j would be reducible to diagonal form,* on the diagonal of which there would stand no more distinct eigenvalues than for A'_j). Thus we arrive at a contradiction with the choice of the matrix A_j as a matrix of least symmetry satisfying relation (6).

Thus, all eigensubspaces L_p of the operator \hat{A}_j are irreducible subspaces transforming according to irreducible representations Γ_p .

Let us now construct the matrix C .**

$$C = \left\| \begin{array}{cccc} C_1 & 0 & \cdots & 0 \\ 0 & C_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & C_k \end{array} \right\| \begin{array}{l} \} r_1 \\ \} r_2 \\ \\ \} r_k \end{array} \quad \underbrace{\quad}_{r_1} \quad \underbrace{\quad}_{r_2} \quad \cdots \quad \underbrace{\quad}_{r_k}, \quad (12)$$

in which each submatrix C_j ($j = 1, 2, \dots, k$) is fundamental for the submatrix A_j (4). The columns of the matrix (12) constitute the coordinates of the vectors $\mathbf{e}'_1, \mathbf{e}'_2, \dots, \mathbf{e}'_n$ (in the basis $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$), which, as is clear from the preceding discussion, form a basis of the completely reduced representation G .

If we then perform the similarity transformation

$$C^{-1} A C = A', \quad (13)$$

* From the commutativity $A_p B_p = B_p A_p$ (A_p is scalar) it follows that $A'_j B'_j = B'_j A'_j$ (by construction) and $A_j B_j = B_j A_j$. Hence A_j and B_j have a complete common system of eigenvectors. Consequently, the transformation C'_j (not coinciding, generally speaking, with C_j) which brings B_j to diagonal form diagonalizes A_j to A'_j .

** In forming the matrix C one must take into account the “orientation effect” (8).

then the matrix A' , after a suitable permutation of rows and columns, is brought to block-diagonal form. The proof that the matrix of the operator \hat{A} in the basis in which G decomposes completely into irreducible representations is transformed to block-diagonal form can be carried out analogously to the way this was done in (2) for the vibration operator \hat{W} .

In this case the coordinates of the vector \mathbf{q} (see (1)) are transformed in accordance with the equality

$$\xi = C^{-1}q, \quad (14)$$

where q is the column matrix of the coordinates of the vector \mathbf{q} in the basis e_1, e_2, \dots, e_n , and ξ is the column matrix of the coordinates of the same vector in the basis e'_1, e'_2, \dots, e'_n ; ξ_i are the symmetry coordinates ^(1,2,8).

On the basis of what has been set forth, one may give the following definition: symmetry coordinates are the coordinates of the vector \mathbf{q} in a basis composed of eigenvectors of submatrices of equivalent coordinates.

Thus, the matrix C can be obtained directly from the properties of the matrix A , without invoking the theory of representations of symmetry groups. However, on the basis of the results obtained it is easy to find the irreducible representations of the symmetry group; for this it suffices to write the matrices of the operators $S^{(i)}$ in the new basis.

In conclusion, let us note that the vibration operator $\hat{W} = \hat{T}^{-1}\hat{V}$, which is not Hermitian, is reduced, by symmetry, by the same transformation as \hat{A} (see (1)).

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