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The rotational invariance means that a matrix A whose elements depend on the selected basis, $|\chi\rangle$, transforms consistently with the transformation of the basis. More specifically, the condition of the rotational invariance can be expressed as:

$$UA(\chi')U^T = A(\chi), \qquad (1)$$

where $A(*)$ is the matrix A with its elements expressed in the given basis *,

$U : U^T = U^{-1}$ is the unitary transformation matrix, and

$$|\chi\rangle = U|\chi'\rangle. \qquad (2)$$

Examples:

1) Overlap matrix:

The overlap matrix can be expressed in terms of the scalar product of the basis vectors, so:

$$S(\chi) = \chi\chi^T, \qquad (3)$$

Now, using Eq. 2, we get:

$$S(\chi) = \chi\chi^T = U\chi'\chi'^T U^T = US(\chi')U^T, \qquad (4)$$

which satisfies Eq. 1. Thus, the overlap matrix is rotationally-invariant.

2) Density matrix:

The density matrix is defined as:

$$P = COC^T, \qquad (5)$$

where O – is the diagonal occupation matrix in MO basis, C – is the matrix of MO-LCAO coefficients such that:

$$\psi^T = (\psi_1 \quad \cdots \quad \psi_N) = (\chi_1 \quad \cdots \quad \chi_N)\begin{pmatrix} C_{11} & \cdots & C_{N1} \\ \cdots & \cdots & \cdots \\ C_{N1} & \cdots & C_{NN} \end{pmatrix} = \chi^T C \Leftrightarrow \psi = C^T \chi. \qquad (6)$$

So:

$$\psi = C^T \chi = C^T U\chi' = C'^T \chi', \qquad (7)$$

meaning that the MO-LCAO coefficients transform according to:

$$C' = U^T C \Leftrightarrow C = UC'. \qquad (8)$$

So Eq. 5 transforms:

$$P(\chi) = COC^T = UC'OC'^T U^T = UC'O'C'^T U^T = UP(\chi')U^T. \qquad (9)$$

Hence, the density matrix is also rotationally-invariant.

3) Products of any powers of density and overlap matrices

Indeed, since $P(\chi) = UP(\chi')U^T$ and $S(\chi) = US(\chi')U^T$, we get:

$$P^n(\chi) = UP(\chi')U^T \cdots UP(\chi')U^T = UP^n(\chi')U^T, \qquad (10a)$$

and

$$S^m(\chi) = US(\chi')U^T \cdots US(\chi')U^T = US^m(\chi')U^T, \qquad (10b)$$

and

$$P^n(\chi)S^m(\chi) = UP^n(\chi')U^T US^m(\chi')U^T = UP^n(\chi')S^m(\chi')U^T. \qquad (10c)$$

Now, lets show that the extended Hückel theory (EHT) Hamiltonian is not rotationally-invariant.
The matrix elements of the Hamiltonian can be represented as:
$H_{ij} = K_{ij} S_{ij}$
The elements of the transformed Hamiltonian are:
$$\left(UH'U^T\right)_{ij} = \sum_{k,l} u_{ik} H_{kl} u_{lj}^T = \sum_{k,l} u_{ik} K_{kl} S'_{kl} u_{jl} = \sum_{k,l} u_{ik} u_{jl} K_{kl} S'_{kl}, \quad \text{(11a)}$$
The elements depending on transformed orbitals:
$$H_{ij} = K_{ij} S_{ij} = K_{ij} \left(US'U^T\right)_{ij} = K_{ij} \sum_{k,l} u_{ik} u_{jl} S'_{kl} = \sum_{k,l} u_{ik} u_{jl} K_{ij} S'_{kl}. \quad \text{(11b)}$$

One of the ways to satisfy the rotational invariance is via:
$K_{ij} = K_{kl}, \forall i, j, k, l$
In other words, the coefficient must be constant.

In the weaker rotationally-invariant version, when the matrix U is composed of blocks acting only on the atomic-centered orbitals – independently for each atoms – the coefficient K is allowed to depend on atom type (or pair of atom types).