Program IrrepMain

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Program Irrep

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IrrepMain is a Matlab-version of the previous Irrep, written in FORTRAN. The algorithm has been extended to handle irreducible representations with no non-degenerate eigenvalue, e.g. the fourth order irreducible representation of the product group $\mathbf{C_{4v}xC_{4v}}$, according to ref. [1] and [2].

1 IrrepMain

The script IrrepMain calculates the irreducible characters and the irreducible representations of an algebraic group. The group is input as a square matrix, **multab**. The group order, **G**, is read. The irreducible characters are calculated; calling several functions by **IrrepMain**. The functions called are pictured in figure 1. You will have to update the IrrepMain statements:

load xx.dat;
G = xx; where xx shall be name of your input file, containing the group order and

load yy.dat;
multab = yy; where yy shall be name of your file, containing the GxG multiplication table of your group.

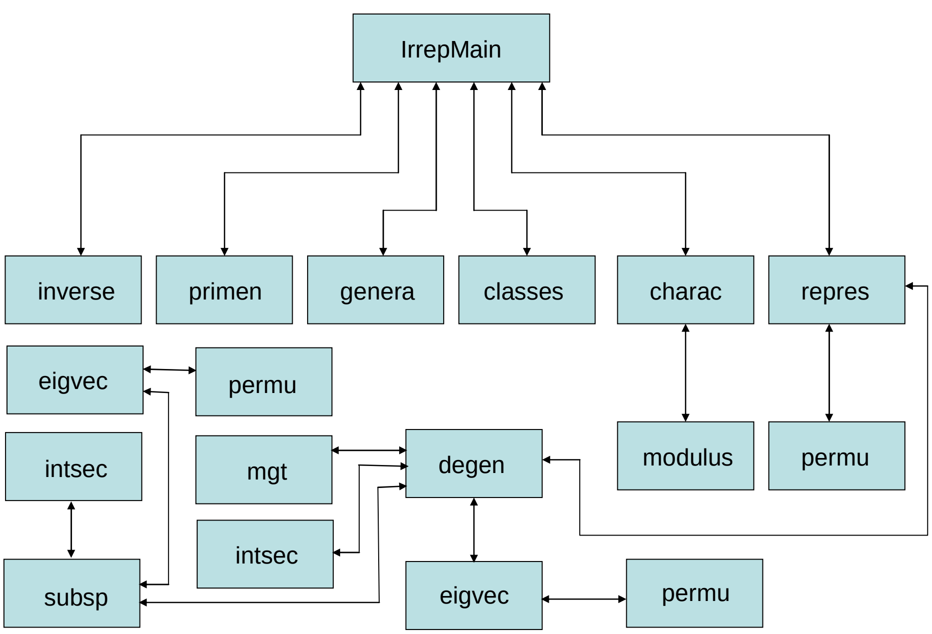

Figure 1: Functions called by IrrepMain

Table 1: Conventions for input data steer

I	If **steer(I)** ~= 0	If **steer(I)** == 0
1	The multiplication table of the group will be printed.	No print
2	Calculate for this group the irreducible representation matrices (not only the irreducible characters).	Calculate only the irreducible characters.
3	Print the inverse group elements (function **inverse**)	No print.
4	Print the number of generators **nmberg**, the group indices of the generators **ngen(I)**, the map **map(1:G,1:2)** by which each group element can be constructed as a product of generators (function **genera**). Print loop structure (function **permu**) of the group element with a unique eigenvalue (function **repres**).	No print.
5	Print the number of classes and the group elements in each class (function **classes**).	No print.
6	Print the table of primes (function **primen**). Print the exponent **ex** of the group, the prime **P** used in the calculations of the present group, **Zprim**, the used primitive root of unity modulus **P**, the characters as sums of roots of unity (function **charac**).	No print.
7	Print the dimensions **lj(1:ncl)** of the irreducible representations and the irreducible characters **ch(1:ncl,1:ncl)** (function **charac**).	No print
8	Print the one-dimensional group representation (function **repres**).	No print.
9	Print the irreducible representations of the group of dimension higher than one (function **repres**).	No print.
10	Not used.	No print.
11	In the input, steer(11) should always be “true”. This means that no error has occurred so far for this group. The program may change the value of the **steer(11)** if it detects an error.	Stop execution for the present group and continue with the next group.
12-20	No effect. These parameters can be neglected or used for own purposes.	No effect.

2 Functions called by IrrepMain

2.1 Inverse

The function **inverse** calculates the inverse of each group element and stores the inverses in **inverse(1:G)**. **inverse(I)** is the inverse group element of element **I**.

2.2 Primen

Function **primen** calculates one hundred prime numbers and stores these numbers in **primen(1:100)**. The algorithm of Euclides is used in the calculation.

Genera

A set of generating elements of the group is calculated and stored in **ngen(1:nmberg)**, where **nmberg** is the number of generating elements of the group. **map(L,2)** is zero if **L** is a generating element of the group. If **map(L,2)** is not equal to zero, **map(L,1)*map(L,2)** equals group element **L**.

2.3 Classes

The group elements are collected into the different conjugate classes of the group. The group elements of the **ncl** classes are ordered in **classl(1:G)**, such that **classl(nfirst(I))** contains the first element in class **I** and **classl(nfirst(I)+h(I)-1)** contains the last element of class number **I**. **nfirst(I)** is the index of the first group element of class **I** in **classl(1:G)**. **h(I)** is the order of the **Ith** class.

2.4 Charac

The irreducible characters of the group are calculated according to Dixon's method, see ref [3].

The class index of each group element is calculated and stored as **cind(N) = I** if group element **N** belongs to class **I**. The order **norder(1:ncl)**, and the powers **npow(I,K)**, of the elements in each class **I** are found. That is, the index of the class to which group element $\mathbf{Q}^{\mathbf{K}}$ belongs, if **Q** belongs to class **I**.

An exponent **ex** is found as the least common multiple of the orders **norder(1:ncl)** using the method of Euclides.

A conjugate class whose elements have the lowest possible degeneracy is registered for each irreducible representation, in case there are no non-degenerate eigenvalues.

2.5 Modulus

Function modulus calculates an integer **I** modulus an integer **P** and stores the resulting integer **J**, using the relation **J = modulus(I,P)**.

2.6 Repres

Function **repres** calculates the irreducible representations of the group elements in case there is at least one non-degenerate eigenvalue for at least one group element. The calculation starts with determining the loop structure of the group elements using function **permu**. In case all eigenvalues for all group elements are degenerate, function **degen** is called.

An eigenvector to group element **IN** with the non-degenerate eigenvalue **lab** is calculated in the regular representation. This eigenvector is projected on the **Jth** irreducible subspace using the projection operator $\mathbf{S_j}$. The resulting vector is stored in **fi(1:G,1)**. **fi(1:G,1)** is operated on, using group elements other than powers of **IN** in order to create an orthonormal set of **LJ1** vectors **fi(1:G,1:LJ1)**. The regular representation of each generator of the group is transformed to the irreducible representation using the orthonormal set **fi(1:G,1:LJ1)**. The irreducible representation of each group element is calculated by multiplying the irreducible representations of the appropriate generators. For one-dimensional irreps, the representations are obvious from the corresponding characters.

2.7 Degen

In case there is no non-degenerate eigenvalue for any group element in the irreducible representation, function **repres** calls on function **degen**.

The eigenvectors of group element **IN**, corresponding to eigenvalue **lab** in the regular representation are calculated using function **eigvec**. A set of mutual independent, commuting group elements to element **IN** is calculated and stored in **ntry1(1:I3)**. Group elements from the set **ntry1(1:I3)** are successively taken and the eigenvectors corresponding to possible eigenvalues of the group element. Function **intsec** is called where the intersection of the subspaces spanned by the eigenvectors of IN and a group element belonging to the set **ntry1(1:I3)**. If this intersection spanned by an orthonormal basis has the dimension **LJ1**, an othonormal basis which transforms irreducibly is formed by operating on the vectors with group elements not belonging to the loop of **IN**. A set of orthonormal columns is no formed, which will transform the regular representation to the irreducible one when returned to function **repres**.

2.8 Permu

The loop of each group element, i.e. the successive powers of each group element is calculated. The loop length of each loop is stored in **loopl(1:numl)**, where **numl** is the number of loops. The group elements are ordered in the vector **lpstr(1:G)** as successive loops.

2.9 Eigvec

The eigenvectors of group element **IN**, with eigenvalue **lab** are calculated. Function **permu** is called to create eigenvectors, using the loop structure of element **IN**. The eigenvectors are projected on the **Jth** irreducible eigenspace, using the projection operator $\mathbf{S_j}$. The resulting eigenvectors are orthonormalized to each other. If no eigenvector corresponding to eigenvalue **lab** is found, **nvec** is set equal to 0.

2.10 Intsec

The intersection of the spaces spanned by **fi(1:G,1:nvr2)** and **dfi(1:nvr1,1:G)** in the sum of the two spaces ($fi \oplus dfi$) is found. The normals to the two space are calculated and stored in the vectors **dfin(1:G,1:K5)** and **fin(1:K6,1:G)**. The intersection of **fi** and **dfi** is spanned by an orthonormal basis which is simultaneously orthogonal to the vectors **dfin** and **fin**.

2.11 Subsp

In case the degeneracy is not split using group elements of the maximal abelian subgroup stored in **kelem(1:nvct)**, but for **dfi(1:nvr1,1:G)** also constitute an invariant set of columns. Then it might be possible to remove the degeneracy, using this subspace of the irreducible space. The group elements except those stored in **kelem(1:nvct)** for which **dfi(1:nvr1,1:G)** constitute an invariant space are stored in **ninv(1:N)**. The group elements stored in **ninv(1:N)** are diagonalized in the representation spanned by **dfi(1:nvr1,1:G)**. If the corresponding eigenvalues are not fully degenerate the degeneracy is at least partly removed. If it is possible to fully remove the degeneracy within function **subsp**, the control is returned to function **degen** and then to function **repres**; otherwise a call is made to function **mgt**.

2.12 Mgt

If the degeneracy is neither removed in function **degen** nor in function **subsp**, a call is made for function **mgt**. In **mgt** the degeneracy is split by forming a matrix **subm(1:G,1:G,1:ntry(J1))**, as a result of linear combination of matrix representatives of the group elements. We use the set of columns stored in **dfi(1:nvr,1:G)** to form a basis for a matrix representation which contains the irreducible representation **dprim** times. **dprim** is the residual degeneracy after executing functions **degen** and **subsp**. **D** is the original degeneracy. This basis of columns is stored in **fi(1:G,1:nvr)**. The regular representation is then transformed into a new one containing the irreducible one **dprim** times, where the degenerate eigenvalue **lab** of group element **IN** appears in the first **D*dprim** diagonal places. A block diagonal matrix is created by a linear combination of matrix representatives. This matrix is stored in **subm(1:G,1:G,1:ntry(J1))**. The submatrix made up from the first **D*dprim**-dimensional block is diagonalized and all the matrix representatives are transformed to the same basis. An eigencolumn of the **L1*L1**-dimensional (**L1**=**D*dprim**) submatrix of **subm(1:G,1:G,1:ntry(J1))** is used for creating an irreducible basis. The projection onto the irreducible space of the matrix representation is equivalent to the one used in **repres**.

Note, subfunction **mgt** has not been fully tested, as no group has been found where **mgt** necessarily is executed.

3 References

[1] S Flodmark and P-O Jansson, Lecture Notes in Physics **94**, 73 (1979)

[2] S Flodmark and P-O Jansson in "Proc. Of the 10th Int. Colloquium on Group-Theoretical Methods in Physics", North-Holland Amsterdam, 485-492 (reprint from Physica **114A**, Nos. 1-3)

[3] J.D. Dixon, Numer. Math. **10**, 446 (1967)

[4] S Flodmark, J. Comp. Phys. **25**, 314 (1977)

[5] S Flodmark and E Blokker in "Group Theory and its Applications 2", Acad. Press NY, 1971

[6] S Flodmark and E Blokker, Int. J. Quantum Chem. **1S**, 703 (1967), **4**, 463 (1971), **5**, 569 (1971), **6**, 925 (1972)