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USING SOFTWARE MATHEMATICA AND GAP IN DETECTING CALCULATION ERRORS ON A COMPLEX MATHEMATICAL PROOF

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ABSTRACT
In this paper we will present how the software Mathematica and Gap assist in eliminating calculation errors, when computing the zeta and normal zeta functions for crystallographic group whose point group is isomorphic to the cyclic group of order 2.
Keywords: subgroups of finite index, zeta and normal zeta function, crystallographic groups

1. INTRODUCTION

The zeta function of a group G is defined as Dirichlet series $\zeta_G(s)=\sum_{n\in} a_n(G)n^{-s}$, where $a_n(G)$ denote the number of subgroup of index n in G. Similary, we define the normal zeta function of a group G to be $\zeta^{\triangleleft}_G(s)=\sum_{n\in} c_n(G)n^{-s}$, where $c_n(G)$ is the number of normal subgroup of index n in G. John J. McDermott, in [4], described method for calculating the number of subgroups of any given index in a group G having abelian normal subgroup T of finite index. This method could be applied to any polycyclic group or to any poly-(infinite) cyclic-by-finite group.

Space group, in *crystallography*, represent a description of the symmetry of the crystal, and the knowledge of the zeta function of these groups could be useful.

Zeta and normal zeta function for the fifth crystallographic group *C2* were calculated in [1] using the method described in [4]. Using the software GAP and Mathematica, we have checked the accuracy of the first 30 coefficients obtained Dirichlet series. Here we describe how we are using the software GAP to get the number of subgroups of the final index, and using Mathematica, we are taking the normal subgroups in a separate list. Also, we are using Mathematica to determine coefficients of obtained Dirichlet's series and compare the results. The possibly disagreements can help in the detection of computational errors arising in the calculation of the zeta and normal zeta function of the group. Of course, in this example, we get completely matching the above list.

2. ALGORITHM

$C2$ is a finite extension of a free abelian group T of rank 3. When writing a space group in an abstract form, we follow the descriptions of these groups given in [2] i [3]. So, we get: $G = C2 = \langle x, y, z, c \mid [x,y],[x,z],[y,z],c^2, x^c = xy, y^c = y^{-1}, z^c = z^{-1} \rangle$

$C2$ is a *finitely presented group.* So to create a finitely presented group in GAP, we first have to generate a free group. Then a list of relators is constructed as words in the generators of the free group and is factored out to obtain the finitely presented group. Its generators *are* the images of the free generators. We can use the following commands:

```
f:=FreeGroup(4);
x:=f.1; y:=f.2; z:=f.3;c:=f.4;
G:=f/[x*y*x^-1*y^-1,x*z*x^(-1)*z^(-1),y*z*y^-1*z^-1,c^2,c*x*c*y^-1*x^-1,c*y*c*y,c*z*c*z];
S:= LowIndexSubgroupsFpGroup(G, TrivialSubgroup(G),30);
```

LowIndexSubgroupsFpGroup returns a list of the representatives of those conjugation class, whose elements are subgroups of finite index, where the index does not exceed the specified index. In this case, the specified index is 30. The time required to do this depends, of course, on the presentation of *G*, but in general it will grow exponentially with the value of index.

```
lista1=List( S, H -> Index( G, H ) );
       # the indices of the subgroups

lista2= List(S, H -> Index( G, Normalizer( G, H ) ) );
# the lengths of the conjugacy classes
```

The result of the following code is the list of ordered pairs (lista4), where the first entry is index subgroups, and the second entry is the number of subgroups of given index in the group $C2$.

```
lista3=SplitBy[Sort[Table[{lista[[i]],lista2[[i]]},{i,1,Length[lista]}]],First];
lista4=Table[{0,0},{i,1,Length[lista3]}];
For[i=1,i<=Length[lista3],i++,
  lista4[[i,1]]=lista3[[i,1,1]];
  For[j=1,j<=Length[lista3[[i]]],j++,
    lista4[[i,2]]=lista4[[i,2]]+lista3[[i,j,2]]]];
lista4
{{1,1},{2,7},{3,13},{4,43},{5,31},{6,91},{7,57},{8,211},{9,130},{10,217},{11,133},{12,559},{13,
183},{14,399},{15,403},{16,931},{17,307},{18,910},{19,381},{20,1333},{21,741},{22,931},{23,55
3},{24,2743},{25,806},{26,1281},{27,1210},{28,2451},{29,871},{30,2821}}
```

The result of the following code is the list of ordered pairs, where the first entry is index subgroups, and the second entry is the number of normal subgroups of given index in the group $C2$.

```
lista5=Table[{0,0},{i,1,Length[lista3]}];
For[i=1,i<=Length[lista3],i++,
  lista5[[i,1]]=lista3[[i,1,1]];
  For[j=1,j<=Length[lista3[[i]]],j++,
   If[lista3[[i,j,2]]=1,
    lista5[[i,2]]=lista5[[i,2]]+lista3[[i,j,2]]]]]];
lista5
{{1,1},{2,7},{3,1},{4,11},{5,1},{6,11},{7,1},{8,19},{9,1},{10,13},{11,1},{12,23},{13,1},{14,15},{
15,1},{16,39},{17,1},{18,24},{19,1},{20,29},{21,1},{22,19},{23,1},{24,63},{25,1},{26,21},{27,1},
{28,35},{29,1},{30,41}}
```

Zeta and normal zeta functions of $C2$ are $\zeta_{C2}(s)=(1+2^{-2s+3})\zeta(s)\zeta(s-1)\zeta(s-2)$ and $\zeta_{C2}^{\lhd}(s)=(2\cdot 2^{-2s}+5\cdot 2^{-s}+1)\zeta(s)+2^{-s}\cdot(1-2^{-s}+4\cdot 2^{-2s})\zeta(s)\zeta(s)\zeta(s-1)$, where $\zeta(s)=\sum_{s=1}^{\infty}\frac{1}{n^s}$, $\operatorname{Re} s>1$ is Riemann zeta function. These functions are given in [1].

From the equation of the zeta (normal zeta) function group of $C2$ and product of two Dirichlet series, it follows the formula for the exact number of subgroups (resp. normal subgroups) of finite index in the group $C2$ for any positive integer n. These results are given in the form of the following propositions. These propositions are taken from [1].

Proposition 1: The number of all subgroups of index n in the group $C2$ is:

$$a_n=\begin{cases}\sum_{l\mid n} l\cdot\sigma(l),\ (n\equiv 1\vee n\equiv 2\vee n\equiv 3)(\operatorname{mod}4)\\ \sum_{l\mid n} l\cdot\sigma(l)+8\cdot\sum_{l\mid\left(\frac{n}{4}\right)} l\cdot\sigma(l)n\equiv 0(\operatorname{mod}4)\end{cases},$$

In particular, if p is an odd prime, then $a_p=p^2+p+1$.

Proposition 2: The number of all normal subgroups of index n in the group $C2$ is:

a) If n is even, then

$$c_n=\begin{cases}6+\sum_{l\mid\left(\frac{n}{2}\right)}\sigma(l), n\equiv 2(\operatorname{mod}8)\vee n\equiv 6(\operatorname{mod}8)\\ 8-\sum_{l\mid\left(\frac{n}{4}\right)}\sigma(l)+\sum_{l\mid\left(\frac{n}{2}\right)}\sigma(l), n\equiv 4(\operatorname{mod}8)\\ 8+4\cdot\sum_{l\mid\left(\frac{n}{8}\right)}\sigma(l)-\sum_{l\mid\left(\frac{n}{4}\right)}\sigma(l)+\sum_{l\mid\left(\frac{n}{2}\right)}\sigma(l), n\equiv 0(\operatorname{mod}8)\end{cases}$$

b) If n is odd, then $c_n=1$.

We make the code in Mathematica, based on these propositions, and then compare the resulting list with the lists we got above.

```
a[n_]:=Module[{},numberSubgroup=0;
  divis=Divisors[n];
  For[i=1,i≤Length[divis],i++,
    numberSubgroup=numberSubgroup+divis[[i]]*DivisorSigma[1,divis[[i]]]]
   If[Mod[n,4]   0,
    divis2=Divisors[n/4];
    For[i=1,i≤Length[divis2],i++,
     umberSubgroup=numberSubgroup+8*divis2[[i]]*DivisorSigma[1,divis2[[i]]]]];numberSubgroup];
```

```
Table[{n,a[n]},{n,1,30}]
```

{{1,1},{2,7},{3,13},{4,43},{5,31},{6,91},{7,57},{8,211},{9,130},{10,217},{11,133},{12,559},
{13,183},{14,399},{15,403},{16,931},{17,307},{18,910},{19,381},{20,1333},{21,741},{22,931},
{23,553},{24,2743},{25,806},{26,1281},{27,1210},{28,2451},{29,871},{30,2821}}

```
c[n_]:=Module[{},numberSubgroup=0;
divis=Divisors[n/4];divis2=Divisors[n/2];divis3=Divisors[n/8];
  If[Mod[n,8]   4,numberSubgroup=8;
   For[i=1,i≤Length[divis],i++,
    numberSubgroup=numberSubgroup-DivisorSigma[1,divis[[i]]]];
   For[i=1,i≤Length[divis2],i++,
    numberSubgroup=numberSubgroup+DivisorSigma[1,divis2[[i]]]]];
  If[Mod[n,8]   2||Mod[n,8]   6,numberSubgroup=6;
   For[i=1,i≤Length[divis2],i++,
    numberSubgroup=numberSubgroup+DivisorSigma[1,divis2[[i]]]
    ]];
  If[Mod[n,8]   0,numberSubgroup=8;
   For[i=1,i≤Length[divis2],i++,
    numberSubgroup=numberSubgroup+DivisorSigma[1,divis2[[i]]]];
   For[i=1,i≤Length[divis],i++,
    numberSubgroup=numberSubgroup-DivisorSigma[1,divis[[i]]]];
   For[i=1,i≤Length[divis3],i++,
    numberSubgroup=numberSubgroup+4*DivisorSigma[1,divis3[[i]]]
   ]];If[Mod[n,8]   1||Mod[n,8]   3||Mod[n,8]   5||Mod[n,8]   7,numberSubgroup=1];numberSubgroup];
```

```
Table[{n,c[n]},{n,1,30}]
```

{{1,1},{2,7},{3,1},{4,11},{5,1},{6,11},{7,1},{8,19},{9,1},{10,13},{11,1},{12,23},{13,1},{14,15},
{15,1},{16,39},{17,1},{18,24},{19,1},{20,29},{21,1},{22,19},{23,1},{24,63},{25,1},{26,21},
{27,1},{28,35},{29,1},{30,41}}

3. REFERENCES

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