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Thimm

Email exchange

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From: thimm@idiap.ch (Georg Thimm)
Message-Id: <9409220944.AA13324@idiap.ch>
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In-Reply-To: <9409220132.AA12575@idiap.ch> (njas@research.att.com)
Subject: Sequences
Cc: thimm@idiap.ch
Status: O

Hello Neil!

I am working on growth sequences in crystals, where growth sequence means: select on and count all atoms which are reachable by a path over i atom bindings, but not more or less. This gives a sequence of atom counts n(i), which may differ for non-symmetric atoms.

In our research (I'm working with E.W. Klee), we found out, that for some crystals the second difference of this sequences may be decomposed in polynomials of degree two:

let p be the period of the crystals (or the number of polynomials).

Then

```
n(i*p+p0)'' = a0 * i^2 + b0 * i + c0
n(i*p+p1)'' = a1 * i^2 + b1 * i + c1
....
```

except for the first few numbers of a sequence.

Example:
Feldspar has two different growth sequences:

```
   4     10     20     38     58     80    112    144    180    226
     270    320    380    436    500    574    642    720    808    888
     980   1082   1174   1280   1396   1500   1620   1750   1866   2000
    2144   2272   2420   2578   2718   2880   3052   3204   3380   3566
    3730   3920   4120   4296   4500   4714   4902   5120   5348   5548
-------------------------------------------------------------------------
       4     10     22     38     56     82    112    142    182    226
     268    322    380    434    502    574    640    722    808    886
     982   1082   1172   1282   1396   1498   1622   1750   1864   2002
    2144   2270   2422   2578   2716   2882   3052   3202   3382   3566
    3728   3922   4120   4294   4502   4714   4900   5122   5348   5546
```

which gives the second differences:

2

```
   4     8     2     2    10     0     4    10    -2     6
  10    -4     8    10    -6    10    10    -8    12    10
 -10    14    10   -12    16    10   -14    18    10   -16
  20    10   -18    22    10   -20    24    10   -22    26
  10   -24    28    10   -26    30    10   -28
-------------------------------------------------------------------------
   6     4     2     8     4     0    10     4    -2    12
   4    -4    14     4    -6    16     4    -8    18     4
 -10    20     4   -12    22     4   -14    24     4   -16
  26     4   -18    28     4   -20    30     4   -22    32
   4   -24    34     4   -26    36     4   -28
```

with the following characteristic polynomials for the first sequence:

```
 3.333333 -0.666667 x +0.000000 x^2
 0.000000 +0.666667 x +0.000000 x^2
10.000000 +0.000000 x +0.000000 x^2
```

The problem: we have no idea, whether this sequences are necessarily decomposable in this way, nor the maximal size of p.

And now or problem: coesite, which we were not able to analyze.

```
   4    10    22    47    83   125   171   215   288   349
 415   518   591   674   816   904  1002  1177  1271  1388
1617  1710  1840  2112  2204  2358  2684  2769  2939  3314
3391  3581  4023  4084  4287  4791  4833  5054  5633  5655
5893  6533  6526  6788  7513  7479  7751  8545  8478  8773
9664  9557  9862 10831 10680 11015 12086 11886 12229 13386
13142 13507 14773 14476 14851 16211 15853 16255 17736 17315
17728 19307 18818 19258 20967 20412 20858 22670 22040 22515
24471 23761 24238 26308 25517 26027 28241 27363 27880 30212
29247 29794 32282 31221 31771 34392 33231 33810 36596 35334
35920 38837 37467 38086 41179 39702 40320 43552 41962 42614
46032 44323 44975 48540 46707 47399 51157 49194 49885 53799
51711 52434 56547 54327 55049 59327 56966 57724 62213 59709
60469 65125 62474 63271 68146 65349 66142 71191 68238 69071
74354 71240 72065 77532 74258 75125 80827 77386 78249 84139
80531 81435 87570 83787 84684 91021 87058 87994 94587 90442
91376 98170 93836 94813 101873 97353 98318 105588 100875 101883
109429 104517 105516 113278 108163 109212 117256 111931 112969 121240
115709 116790 125350 119606 120676 129471 123507 124622 133719 127532
128638 137972 131558 132712 142354 135715 136855 146740 139865 141055
151265 144148 145321 155785 148427 149652 160441 152837 154047 165095
157244 158504 169887 161781 163025 174679 166314 167607 179606 170979
172260 184531 175634 176969 189596 180432 181745 194652 185216 186581
```

```
   4    10    23    47    83   127   174   221   276   356
 428   494   603   698   781   912  1035  1131  1289  1435
1542  1735  1903  2014  2245  2435  2556  2817  3032  3160
3459  3694  3824  4166  4426  4551  4937  5222  5345  5771
6083  6204  6675  7004  7125  7645  7997  8107  8677  9056
9155  9775 10179 10265 10943 11364 11440 12174 12619 12677
```

3

```
 13468  13941  13980  14826  15326  15347  16256  16772  16775  17751
 18290  18265  19309  19872  19822  20931  21520  21443  22620  23231
 23126  24376  25012  24869  26197  26856  26682  28081  28763  28559
 30034  30736  30495  32052  32780  32492  34136  34887  34557  36282
 37059  36688  38496  39293  38880  40777  41598  41133  43121  43967
 43454  45530  46401  45836  48009  48898  48281  50553  51464  50789
 53159  54097  53364  55827  56795  56002  58568  59553  58701  61375
 62381  61464  64244  65274  64293  67177  68234  67184  70179  71256
 70138  73247  74348  73153  76378  77505  76237  79573  80724  79385
 82838  84007  82594  86167  87362  85863  89562  90781  89198  93021
 94264  92600  96547  97809  96064 100138 101427  99588 103793 105108
103180 107514 108852 106835 111304 112660 110552 115159 116538 114330
119078 120482 118176 123058 124491 122086 127109 128562 126056 131227
132702 130090 135408 136905 134192 139652 141176 138355 143965 145510
142579 148346 149913 146865 152789 154381 151221 157294 158913 155640
161870 163508 160120 166511 168173 164662 171217 172903 169269 175987
177698 173941 180826 182554 178676 185729 187483 183472 190694 192477
```

Would you mind to feed a complete sequence into superseeker?
Unfortunately, this sequences are too long to pass the mail system,
which cuts lines to 256 character chunks, and your system seems to
insist that the sequence is on one line.

Greetings,
Georg Thimm

P.S. I wrote a small program which tries to decompose a sequence into
polynomials - it needs probably some work to fit into your system, but
if you send me the specifications...

```
From idiap.ch!thimm Thu Sep 22 14:03:03 +0200 1994
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From: thimm@idiap.ch (Georg Thimm)
Message-Id: <9409221203.AA13476@idiap.ch>
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To: njas@research.att.com
In-Reply-To: <9409221136.AA13431@idiap.ch> (njas@research.att.com)
Subject: Re: Sequences
Status: O

#  just to make things simple, suppose the crystal was a simple cubic lattice.
#  then your growth sequence would be
#  1, 6, ...
  6     18     38     66    102    146    198    258    326    402
486    578    678    786    902   1026   1158   1298   1446   1602

#
#
#  no, stop, let me ask you if this is correct:
```
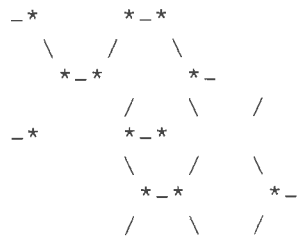

4

```
#  take the simple hexagonal lattice in 2 dimensions.
#  then the growth sequence is 1, 6, 12, 18, 24, 30, ... - is
#  tht correct?  just to make sure
#  we are talking the same language!
 3      6      9     12     15     18     21     24     27     30
33     36     39     42     45     48     51     54     57     60
```

is the correct sequence, supposed you mean the lattice



Atoms, which are reachable by several path of the same length
are only counted once!

Georg Thimm

s = count 1

018 = Δs

019 = Δ²s

020 = Δ³s → 024

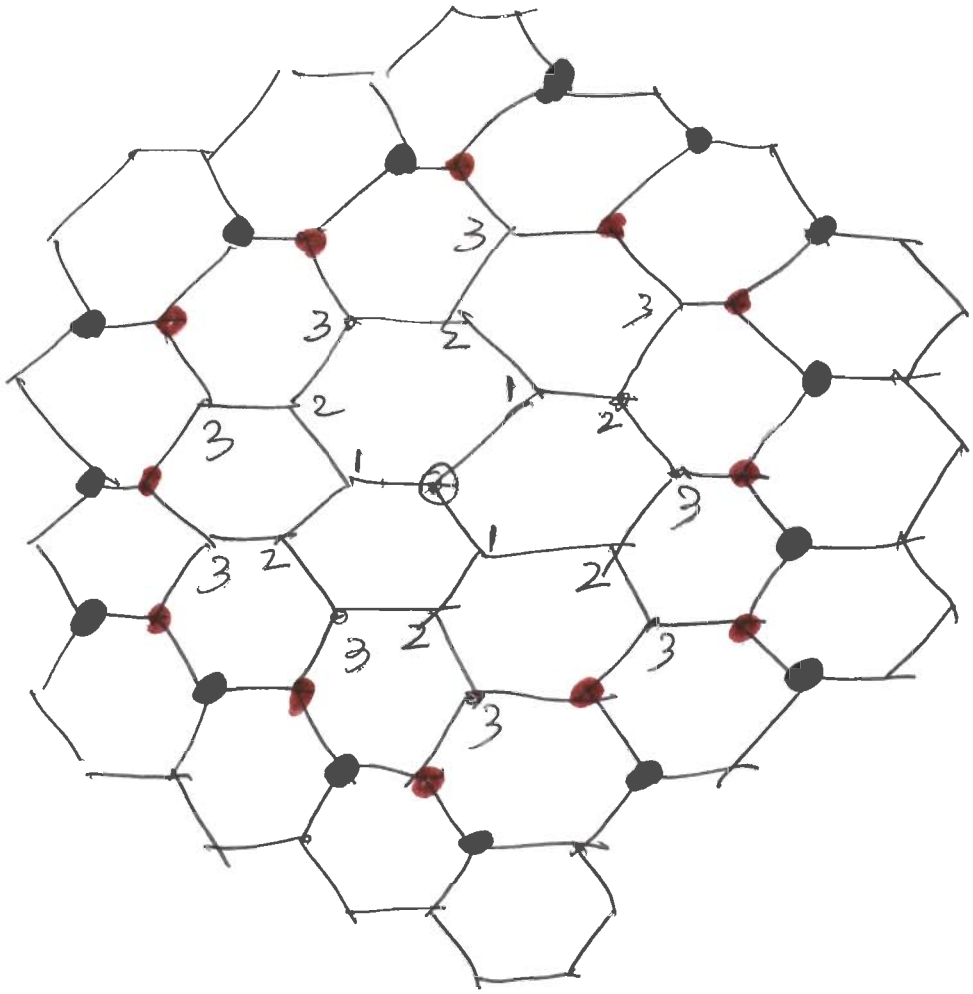
... 32 49 ~~64~~

⇒ 025

01 = s1

02 = Δ²s1

03 = trisect(0)



i	a_i
0	1
1	3
2	6
3	9
4	12
5	15

7

~~000~~	1	
100	6	
200	6	18
110	12	
~~300~~	6	38
210	24	
111	8	

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To: njas@research.att.com
In-Reply-To: <9409270557.AA21008@idiap.ch> (njas@research.att.com)
Status: RO

Hello!

i have been looking at your coesite sequences. it would be
helpful
if i knew what the coordinates of the points were.
#
not just the sequences:
#
4, 10, 22, 47, 83, 125, 171, 215, 288, 349, 415,...
but the actual points

I don't think, the coordinates are helpful for you, as the generation
of the sequences is based (and simplified) by data structure / description
method, which Mr. Klee and I call quotient graph.

A simple example is the diamant, which has 2 classes of C Atoms.
All atoms in a class are equivalent under translation. This means that
if you shift the crystal in a way, that one atom of a class is located
on the place of another atom of the same class, you can't see any difference.

Now you choose a coordinate system, which fits to the translation
mentioned above and choose in each class of atoms one with zero coordinates.
>From this one you follow every atom binding and note the class name of the
the other atom and the coordinates:

(c-0, c-1; 1 0 0)
(c-0, c-1; 0 1 0)
(c-0, c-1; 0 0 1)
(c-0, c-1; 0 0 0)

Where occurrences like (c-1, c-0; -1 0 0) are removed, as they are
redundant.

To produce the growth sequences for the class of atoms c-0, you create a
list:

[c-0(0 0 0)]

Now you 'apply' every edge (and its inverse) in the quotient graph to every
atom in the list, which gives:
[c-1(1 0 0), c-1(0 1 0), c-1(0 0 1), c-1(0 0 0)]

and the next:
```
[c-0(0 0 0),  c-0(1 -1 0), c-0(1 0 -1), c-0(1 0 0),
 c-0(-1 1 0), c-0(0 0 0),  c-0(0 1 -1), c-0(0 1 0),
 c-0(-1 0 1), c-0(0 -1 1), c-0(0 0 0),  c-0(0 0 1),
 c-0(-1 0 0), c-0(0 -1 0), c-0(0 0 -1), c-0(0 0 0)]
```

now you remove double entries, and those which are already present in
other lists:
```
[             c-0(1 -1 0), c-0(1 0 -1), c-0(1 0 0),
 c-0(-1 1 0),              c-0(0 1 -1), c-0(0 1 0),
 c-0(-1 0 1), c-0(0 -1 1),              c-0(0 0 1),
 c-0(-1 0 0), c-0(0 -1 0), c-0(0 0 -1)             ]
```
and count the remaining entries, which gives for diamant the first three
elements of the growth sequence: (1, 4, 12)
Where the first entry is always 1 and therefore usually omitted.

BTW.: the sequence for c-1 is identical to the one of c-0, as the atoms
in both classes are are equivalent under rotation.

For Coesite the quotient graph is:
```
( e , a ; 0 0 0)
( a , b ; -1 -1 -1)
( a , g ; 0 0 -1)
( a , h ; -1 0 -1)
( e , g ; 0 0 0)
( b , f ; 0 0 0)
( b , g ; 1 0 0)
( b , h ; 0 0 0)
( f , h ; 0 0 -1)
( c , d ; 1 1 0)
( c , e ; 0 0 0)
( c , f ; 0 1 0)
( c , g ; 0 0 -1)
( d , e ; 0 -1 0)
( d , f ; 0 0 0)
( d , h ; 0 0 0)
```

where 2 different sequences exist.

# of course i don't promise anything!

Sure.

If you want a more detailed explanation of the quotient graph,
let me know. If you want to 'play' with quotient graphs and
try to produce some growth sequences, I wrote a program to do so.

Greetings,
        Georg