Symmetry Implementation for Pair Distribution Function

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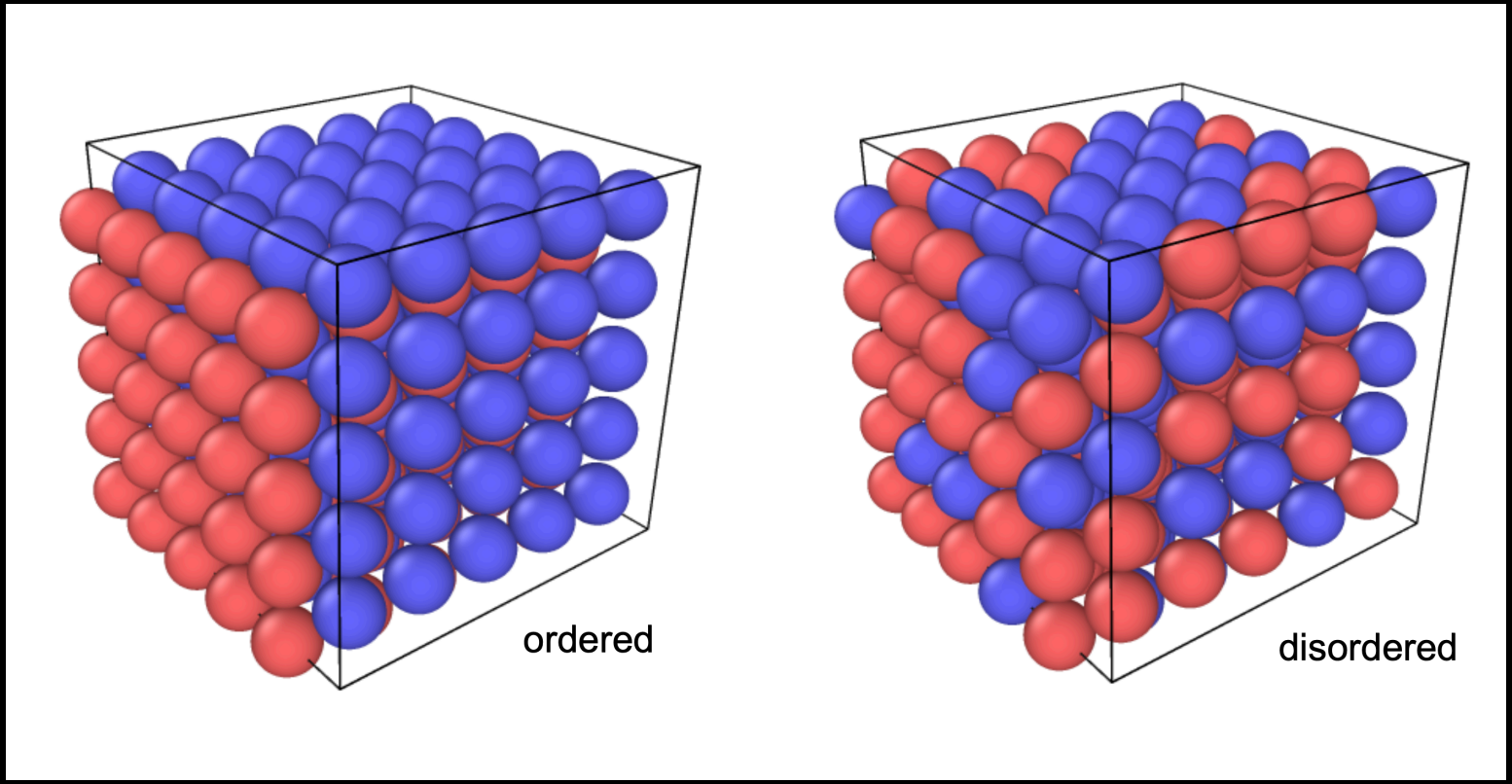
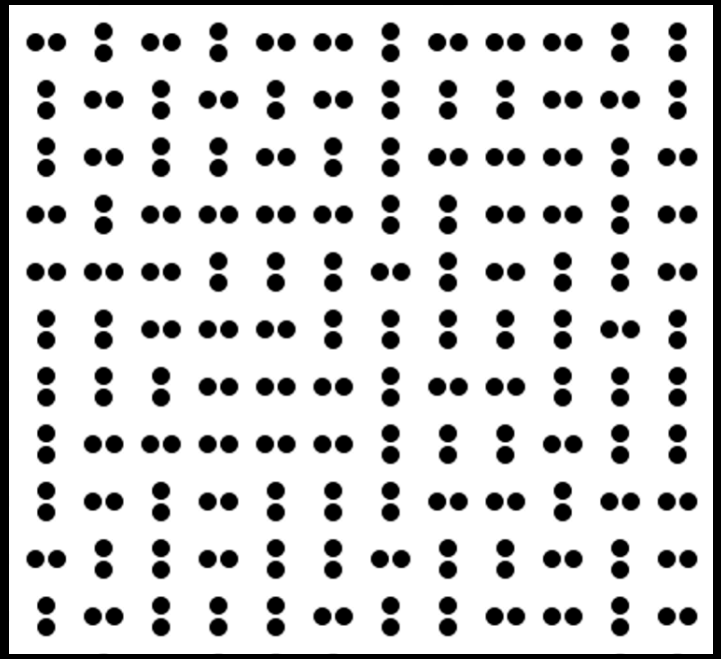
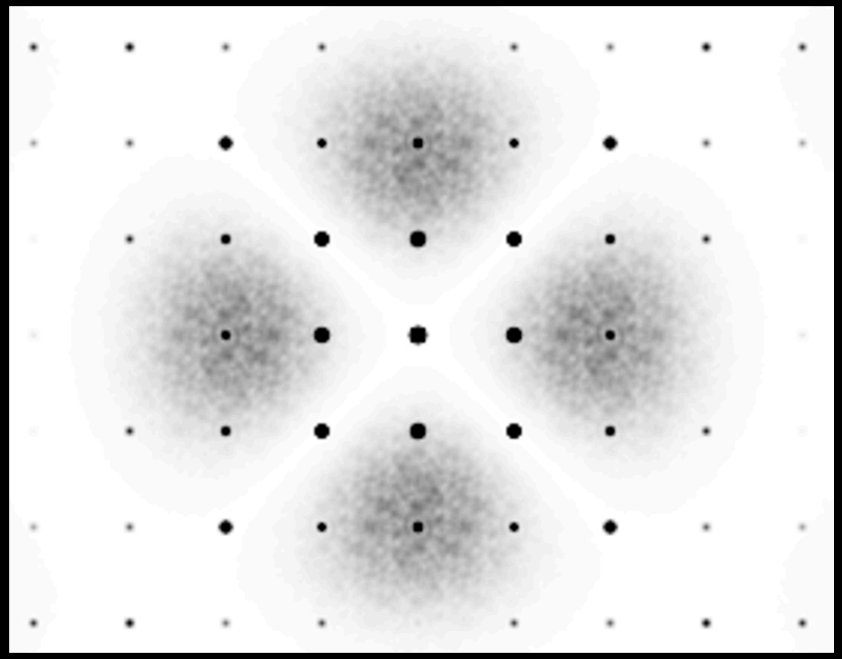
Disordered Crystals



Diffraction



Structure



Diffraction Pattern

Pair Distribution Function

$$\mathrm{PDF}(\vec{x}) = \int_{\mathbb{R}^3} \rho\left(\vec{\xi}\right)\rho\left(\vec{\xi} - \vec{x}\right)d\vec{\xi}$$

Pair Distribution Function

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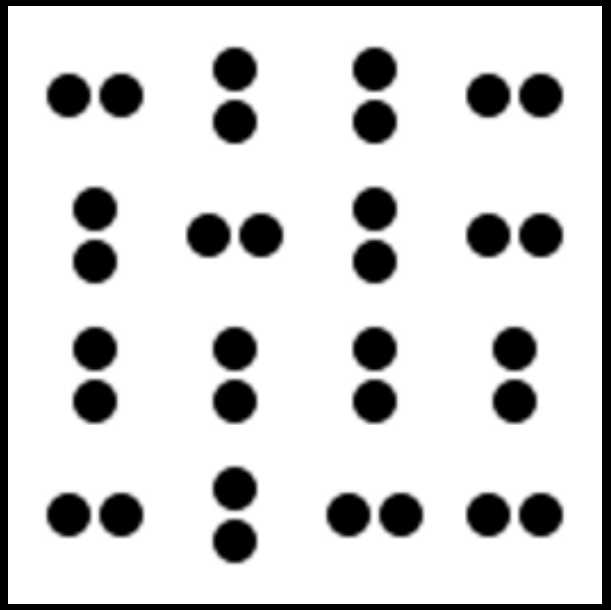
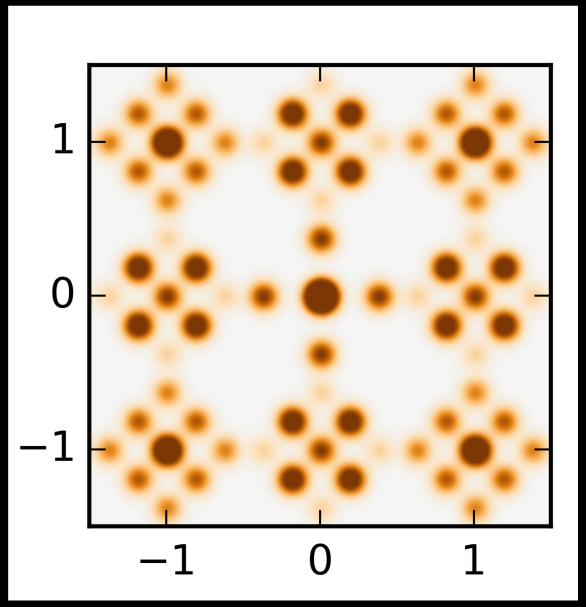
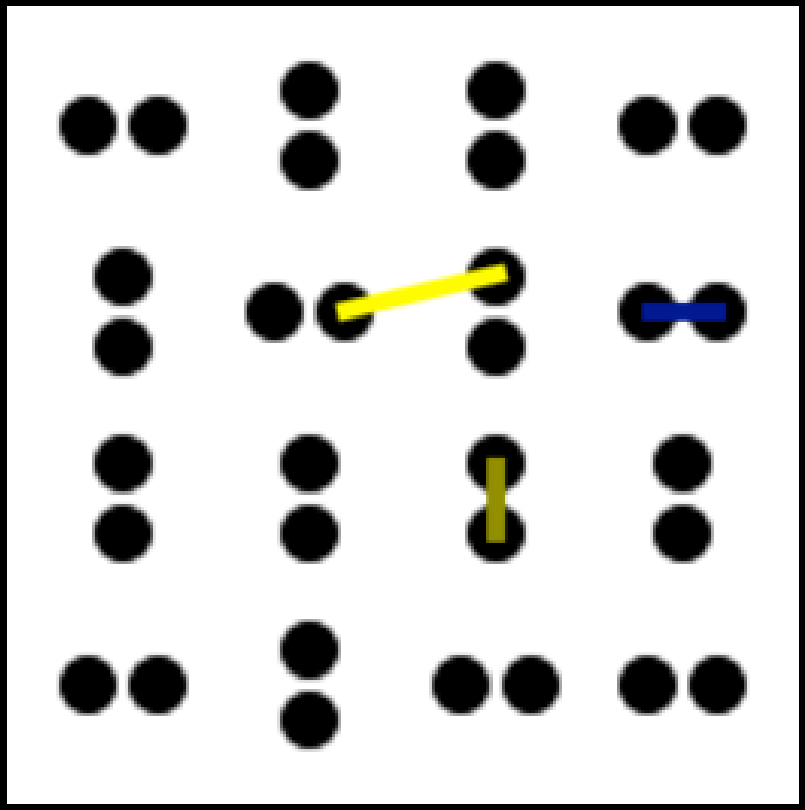
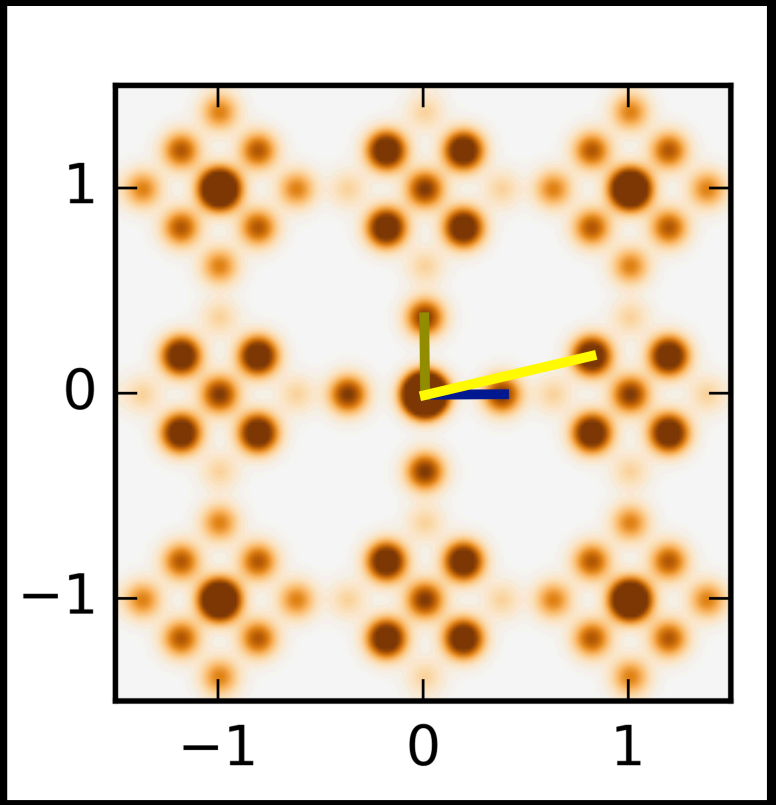


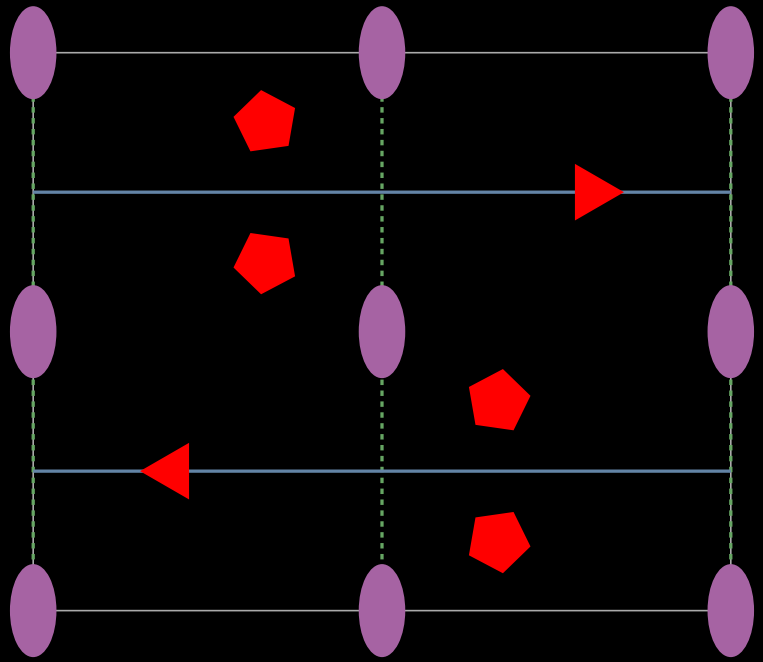


Pair Distribution Function





Wyckoff Positions

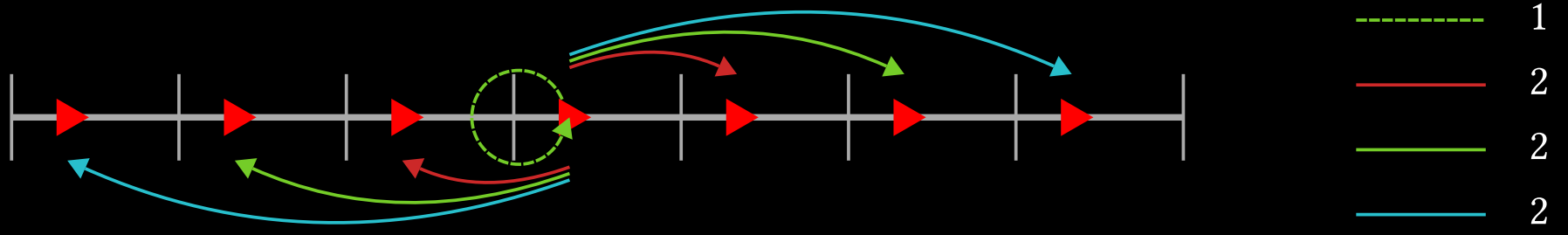


Wallpaper Group p2mg

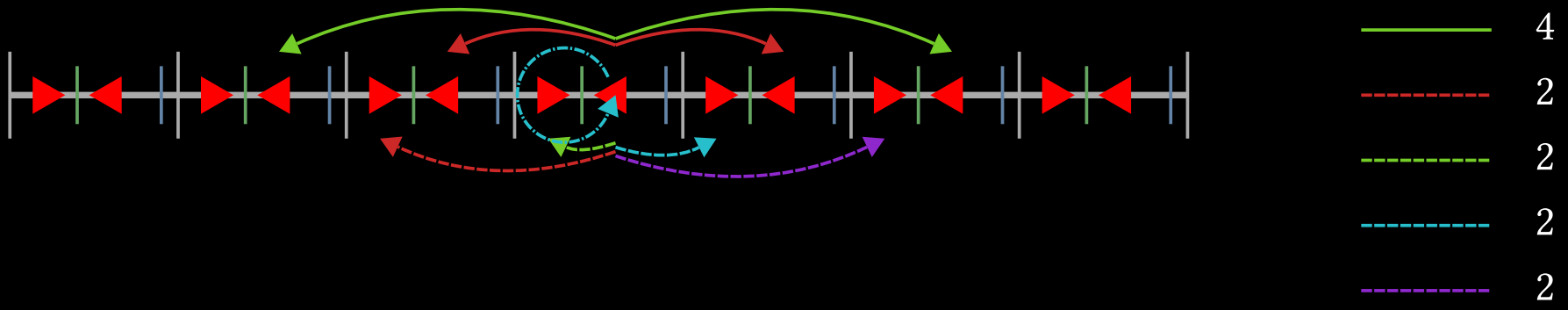
Examples

- Line Group p1
- Line Group p1m
- Wallpaper Group p2mg
- Space Group $Pm\bar{3}m$

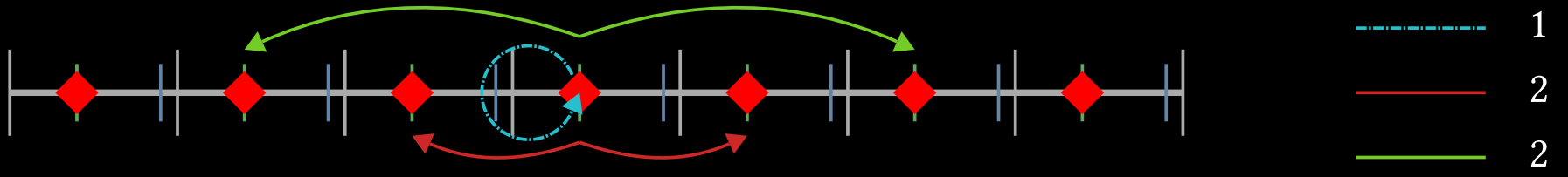
Line Group p1

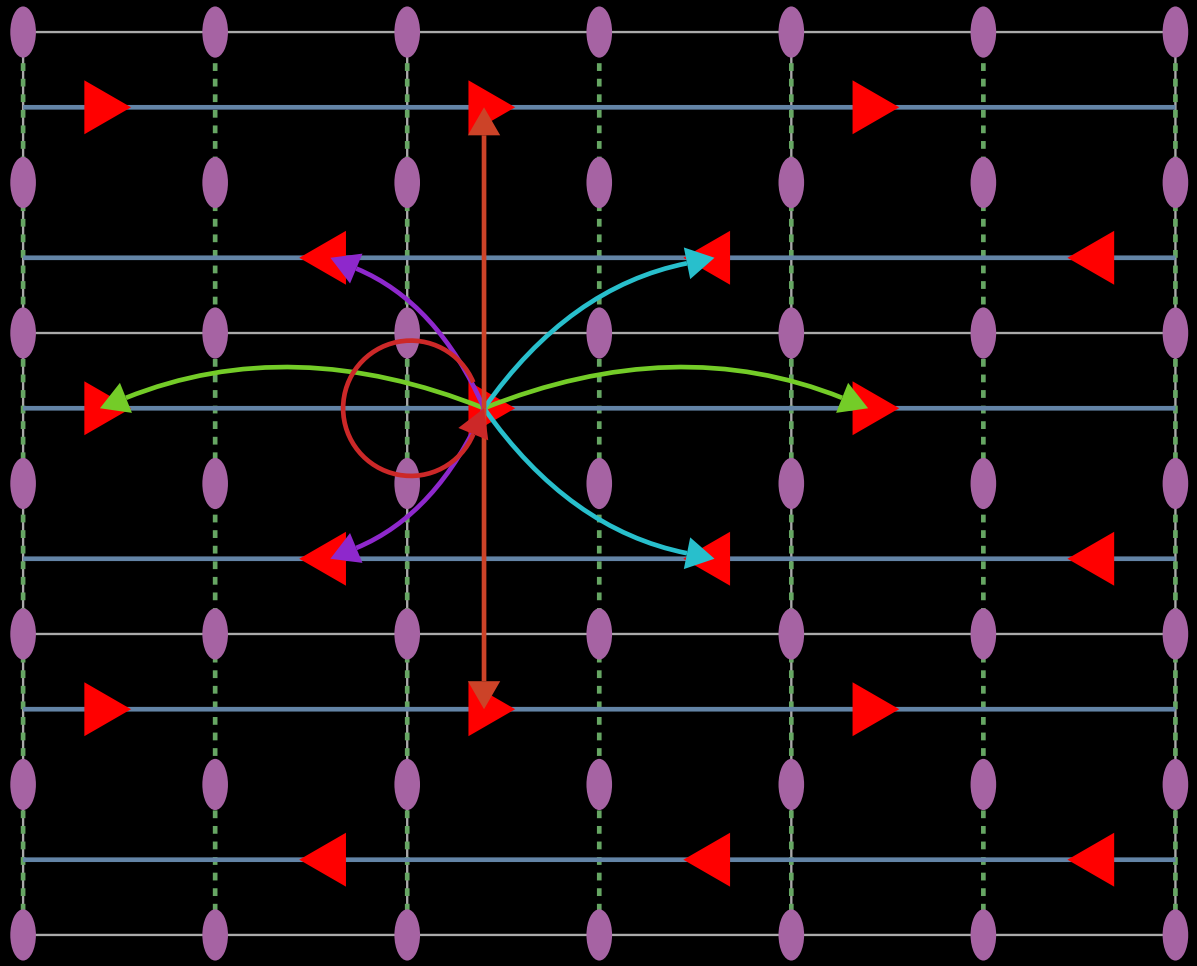


Line Group p1m General Position



Line Group p1m Special Position

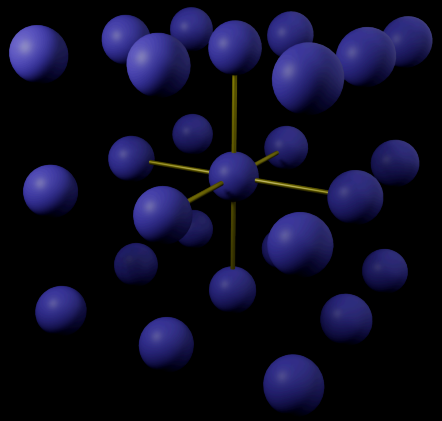




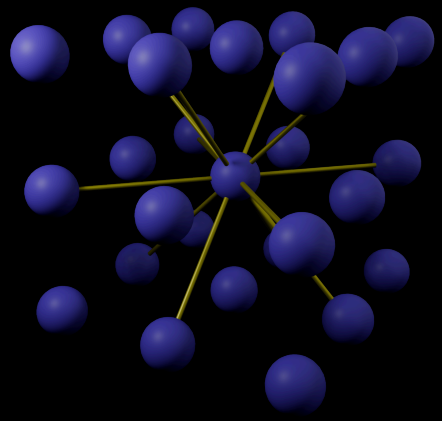
Wallpaper Group p2mg

2
4
4
4
4

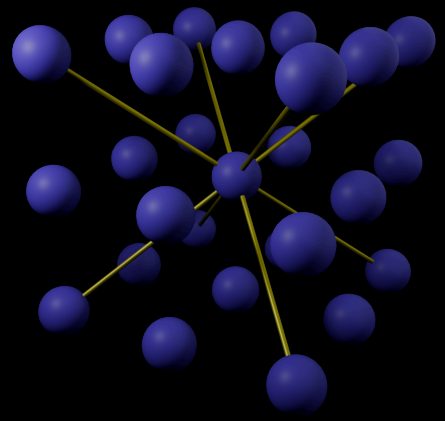
Space Group $Pm\bar{3}m$



$\langle 100 \rangle : 6$



$\langle 110 \rangle : 12$



$\langle 111 \rangle : 8$

Example Yell Input

```
[
  [(0,0,0)
  Multiplicity 1
  SubstitutionalCorrelation(Var,Var,0.67)

  ADPCorrelation(MnCN_x, MnCN_x,zerocorr)
  ADPCorrelation(MnCN_y, MnCN_y,zerocorr)
  ADPCorrelation(MnCN_z, MnCN_z,zerocorr)
  #ADPCorrelation(Mn2_x,  Mn2_x, zerocorr)
  #ADPCorrelation(Mn2_y,  Mn2_y, zerocorr)
  #ADPCorrelation(Mn2_z,  Mn2_z, zerocorr)
  ]

  [(0,0,0)
  #NB this is a vector 0.5 0 0
  #And it also connects different things
  #thus multiplicity is:
  Multiplicity 2*6
  ADPCorrelation(MnCN_x, Mn2_x, first_corrx1)
  ADPCorrelation(MnCN_y, Mn2_y, first_corrz1)
  ADPCorrelation(MnCN_z, Mn2_z, first_corrz1)
  SizeEffect(MnCN, Mn2_x, se_x1)
  ]

  [(1/2,1/2,0)
  Multiplicity 12
  SubstitutionalCorrelation(Var,Var,4/9+sc_hh0)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrx2)
  ADPCorrelation(MnCN_y, MnCN_y,first_corrx2)
  ADPCorrelation(MnCN_x, MnCN_y,first_corrxy2)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxy2)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrz2)
  ADPCorrelation(Mn2_x, Mn2_x, first_corrx2)
  ADPCorrelation(Mn2_y, Mn2_y, first_corrx2)
  ADPCorrelation(Mn2_x, Mn2_y, first_corrxy2)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxy2)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrz2)

  SizeEffect(MnCN,MnCN_x,se2)
  SizeEffect(MnCN,MnCN_y,se2)
  ]

  [(0,1/2,1/2)
  Multiplicity 2*8
  ADPCorrelation(MnCN_x, Mn2_x,first_corrx3)
  ADPCorrelation(MnCN_y, Mn2_y,first_corrx3)
  ADPCorrelation(MnCN_z, Mn2_z,first_corrx3)

  ADPCorrelation(MnCN_x, Mn2_y,first_corrxy3)
  ADPCorrelation(MnCN_x, Mn2_z,first_corrxy3)
  ADPCorrelation(MnCN_y, Mn2_x,first_corrxy3)
  ADPCorrelation(MnCN_y, Mn2_z,first_corrxy3)
  ADPCorrelation(MnCN_z, Mn2_x,first_corrxy3)
  ADPCorrelation(MnCN_z, Mn2_y,first_corrxy3)

  SizeEffect(MnCN,Mn2_x,se3)
  SizeEffect(MnCN,Mn2_y,se3)
  SizeEffect(MnCN,Mn2_z,se3)
  ]

  [(1,0,0)
  Multiplicity 6
  SubstitutionalCorrelation(Var,Var,4/9+sc_l00)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrx4)
  ADPCorrelation(MnCN_y, MnCN_y,first_corrz4)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrz4)
  ADPCorrelation(Mn2_x, Mn2_x, first_corrx4)
  ADPCorrelation(Mn2_y, Mn2_y, first_corrz4)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrz4)

  SizeEffect(MnCN,MnCN_x,se4)
  ]

  [(1/2,1/2,0)
  Multiplicity 2*24
  ADPCorrelation(MnCN_x, Mn2_x,corrx5)
  ADPCorrelation(MnCN_y, Mn2_y,corry5)
  ADPCorrelation(MnCN_x, Mn2_y,corrxy5)
  ADPCorrelation(MnCN_y, Mn2_x,corrxy5)
  ADPCorrelation(MnCN_z, Mn2_z,corrz5)

  SizeEffect(MnCN,Mn2_x,se5)
  SizeEffect(MnCN,Mn2_y,se5)
  ]

  [(1,1/2,1/2)
  Multiplicity 24
  SubstitutionalCorrelation(Var,Var,4/9+sc_1hh)
  ADPCorrelation(MnCN_x, MnCN_x, first_corrx6)
  ADPCorrelation(MnCN_y, MnCN_y, first_corry6)
  ADPCorrelation(MnCN_z, MnCN_z, first_corry6)

  ADPCorrelation(MnCN_y, MnCN_z, first_coryz6)
  ADPCorrelation(MnCN_z, MnCN_y, first_coryz6)

  ADPCorrelation(Mn2_x, Mn2_x, first_corrx6)
  ADPCorrelation(Mn2_y, Mn2_y, first_corry6)
  ADPCorrelation(Mn2_z, Mn2_z, first_corry6)

  ADPCorrelation(Mn2_y, Mn2_z, first_coryz6)
  ADPCorrelation(Mn2_z, Mn2_y, first_coryz6)

  SizeEffect(MnCN,MnCN_x,se_x6)
  SizeEffect(MnCN,MnCN_y,se_y6)
  SizeEffect(MnCN,MnCN_z,se_y6)
  ]

  [(1,1,0)
  Multiplicity 12
  SubstitutionalCorrelation(Var,Var,4/9+sc_l10)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrx7)
  ADPCorrelation(MnCN_y, MnCN_y,first_corrx7)
  ADPCorrelation(MnCN_x, MnCN_y,first_corrxy7)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxy7)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrz7)
  ADPCorrelation(Mn2_x, Mn2_x, first_corrx7)
  ADPCorrelation(Mn2_y, Mn2_y, first_corrx7)
  ADPCorrelation(Mn2_x, Mn2_y, first_corrxy7)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxy7)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrz7)

  SizeEffect(MnCN,MnCN_x,se7)
  SizeEffect(MnCN,MnCN_y,se7)
  ]

  [(1/2,1,1/2)
  Multiplicity 2*24
  ADPCorrelation(MnCN_x, Mn2_x,corrx8)
  ADPCorrelation(MnCN_y, Mn2_y,corrx8)
  ADPCorrelation(MnCN_x, Mn2_y,corrxy8)
  ADPCorrelation(MnCN_y, Mn2_x,corrxy8)
  ADPCorrelation(MnCN_z, Mn2_z,corrz8)

  ADPCorrelation(MnCN_x, Mn2_z,corrxz8)
  ADPCorrelation(MnCN_y, Mn2_z,corrxz8)
  ADPCorrelation(MnCN_z, Mn2_x,corrxz8)
  ADPCorrelation(MnCN_z, Mn2_y,corrxz8)

  SizeEffect(MnCN,Mn2_x,se_x8)
  SizeEffect(MnCN,Mn2_y,se_x8)
  SizeEffect(MnCN,Mn2_z,se_z8)
  ]

  [(1,1,1)
  Multiplicity 8
  SubstitutionalCorrelation(Var,Var,4/9+sc_111)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrx9)
  ADPCorrelation(MnCN_y, MnCN_y,first_corrx9)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrx9)

  ADPCorrelation(MnCN_x, MnCN_y,first_corrxy9)
  ADPCorrelation(MnCN_x, MnCN_z,first_corrxy9)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxy9)
  ADPCorrelation(MnCN_y, MnCN_z,first_corrxy9)
  ADPCorrelation(MnCN_z, MnCN_x,first_corrxy9)
  ADPCorrelation(MnCN_z, MnCN_y,first_corrxy9)

  ADPCorrelation(Mn2_x, Mn2_x, first_corrx9)
  ADPCorrelation(Mn2_x, Mn2_x, first_corrx9)
  ADPCorrelation(Mn2_x, Mn2_x, first_corrx9)

  ADPCorrelation(Mn2_x, Mn2_y, first_corrxy9)
  ADPCorrelation(Mn2_x, Mn2_z, first_corrxy9)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxy9)
  ADPCorrelation(Mn2_y, Mn2_z, first_corrxy9)
  ADPCorrelation(Mn2_z, Mn2_x, first_corrxy9)
  ADPCorrelation(Mn2_z, Mn2_y, first_corrxy9)

  SizeEffect(MnCN,MnCN_x,se9)
  SizeEffect(MnCN,MnCN_y,se9)
  SizeEffect(MnCN,MnCN_z,se9)
  ]

  [(1,0,0)
  Multiplicity 2*6
  ADPCorrelation(MnCN_x, Mn2_x,corrx10)
  ADPCorrelation(MnCN_y, Mn2_y,corrz10)
  ADPCorrelation(MnCN_z, Mn2_z,corrz10)
  SizeEffect(MnCN,Mn2_x,se_x10)
  ]

  [(3/2,1/2,0)
  Multiplicity 24
  SubstitutionalCorrelation(Var,Var,4/9+sc_uh0)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrxl1)
  ADPCorrelation(MnCN_y, MnCN_y,first_corryl1)
  ADPCorrelation(MnCN_x, MnCN_y,first_corrxyl1)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxyl1)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrz11)

  ADPCorrelation(Mn2_x, Mn2_x, first_corrx11)
  ADPCorrelation(Mn2_y, Mn2_y, first_corry11)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrz11)

  ADPCorrelation(Mn2_x, Mn2_y, first_corrxyl1)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxyl1)

  SizeEffect(MnCN,MnCN_x,se_x11)
  SizeEffect(MnCN,MnCN_y,se_y11)
  ]

  [(1,1/2,1/2)
  Multiplicity 2*24

  ADPCorrelation(MnCN_x, Mn2_x,corrx12)
  ADPCorrelation(MnCN_y, Mn2_y,corry12)
  ADPCorrelation(MnCN_z, Mn2_z,corryl2)

  ADPCorrelation(MnCN_y, Mn2_z,corryz12)
  ADPCorrelation(MnCN_z, Mn2_y,corryz12)

  ADPCorrelation(MnCN_x, Mn2_y,corrxy12)
  ADPCorrelation(MnCN_x, Mn2_z,corrxy12)
  ADPCorrelation(MnCN_y, Mn2_x,corrxy12)
  ADPCorrelation(MnCN_z, Mn2_x,corrxy12)

  SizeEffect(MnCN,Mn2_x, se_x12)
  SizeEffect(MnCN,Mn2_y, se_y12)
  SizeEffect(MnCN,Mn2_z, se_y12)
  ]

  [(1,1,0)
  Multiplicity 2*32
  ADPCorrelation(MnCN_x, Mn2_x,corrx13)
  ADPCorrelation(MnCN_y, Mn2_y,corry13)
  ADPCorrelation(MnCN_z, Mn2_z,corrz13)

  ADPCorrelation(MnCN_x, Mn2_y,corrxy13)
  ADPCorrelation(MnCN_y, Mn2_x,corrxy13)

  SizeEffect(MnCN,Mn2_x,se_x13)
  SizeEffect(MnCN,Mn2_y,se_y13)
  ]

  [(3/2,1,1/2)
  Multiplicity 48
  SubstitutionalCorrelation(Var,Var,4/9+sc_u1h)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrxl4)
  ADPCorrelation(MnCN_y, MnCN_y,first_corryl4)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrzl4)

  ADPCorrelation(MnCN_x, MnCN_y,first_corrxyl4)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxyl4)
  ADPCorrelation(MnCN_y, MnCN_z,first_corryzl4)
  ADPCorrelation(MnCN_z, MnCN_y,first_corryzl4)
  ADPCorrelation(MnCN_x, MnCN_z,first_corrxzl4)
  ADPCorrelation(MnCN_z, MnCN_x,first_corrxzl4)

  ADPCorrelation(Mn2_x, Mn2_x, first_corrxl4)
  ADPCorrelation(Mn2_y, Mn2_y, first_corryl4)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrzl4)

  ADPCorrelation(Mn2_x, Mn2_y, first_corrxyl4)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxyl4)
  ADPCorrelation(Mn2_y, Mn2_z, first_corryzl4)
  ADPCorrelation(Mn2_z, Mn2_y, first_corryzl4)
  ADPCorrelation(Mn2_x, Mn2_z, first_corrxzl4)
  ADPCorrelation(Mn2_z, Mn2_x, first_corrxzl4)

  SizeEffect(MnCN,MnCN_x,se_x14)
  SizeEffect(MnCN,MnCN_y,se_y14)
  SizeEffect(MnCN,MnCN_z,se_z14)
  ]

  [(1,1,1)
  Multiplicity 2*24
  ADPCorrelation(MnCN_x, Mn2_x,corrx15)
  ADPCorrelation(MnCN_y, Mn2_y,corry15)
  ADPCorrelation(MnCN_z, Mn2_z,corry15)

  ADPCorrelation(MnCN_x, Mn2_y,corrxy15)
  ADPCorrelation(MnCN_y, Mn2_x,corrxy15)
  ADPCorrelation(MnCN_x, Mn2_z,corrxy15)
  ADPCorrelation(MnCN_z, Mn2_x,corrxy15)
  ADPCorrelation(MnCN_y, Mn2_z,corryz15)
  ADPCorrelation(MnCN_z, Mn2_y,corryz15)

  SizeEffect(MnCN,Mn2_x,se_x15)
  SizeEffect(MnCN,Mn2_y,se_y15)
  SizeEffect(MnCN,Mn2_z,se_y15)
  ]

  [(3/2,3/2,0)
  Multiplicity 12
  SubstitutionalCorrelation(Var,Var,4/9+sc_uu0)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrx16)
  ADPCorrelation(MnCN_y, MnCN_y,first_corrx16)
  ADPCorrelation(MnCN_x, MnCN_y,first_corrxy16)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxy16)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrz16)
  ADPCorrelation(Mn2_x, Mn2_x, first_corrx16)
  ADPCorrelation(Mn2_y, Mn2_y, first_corrx16)
  ADPCorrelation(Mn2_x, Mn2_y, first_corrxy16)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxy16)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrz16)

  SizeEffect(MnCN,MnCN_x,se16)
  SizeEffect(MnCN,MnCN_y,se16)
  ]

  [(1,3/2,1/2)
  Multiplicity 2*24
  ADPCorrelation(MnCN_x, Mn2_x,corrx17)
  ADPCorrelation(MnCN_y, Mn2_y,corrx17)
  ADPCorrelation(MnCN_z, Mn2_z,corrz17)

  ADPCorrelation(MnCN_y, Mn2_z,corryz17)
  ADPCorrelation(MnCN_z, Mn2_y,corryz17)
  ADPCorrelation(MnCN_x, Mn2_z,corryz17)
  ADPCorrelation(MnCN_z, Mn2_x,corryz17)

  ADPCorrelation(MnCN_x, Mn2_y,corrxy17)
  ADPCorrelation(MnCN_y, Mn2_x,corrxy17)

  SizeEffect(MnCN,Mn2_x, se_x17)
  SizeEffect(MnCN,Mn2_y, se_x17)
  SizeEffect(MnCN,Mn2_z, se_z17)

  ]

  [(3/2,3/2,1)
  Multiplicity 24
  SubstitutionalCorrelation(Var,Var,4/9+sc_uu1)
  ADPCorrelation(MnCN_x, MnCN_x,first_corrx18)
  ADPCorrelation(MnCN_y, MnCN_y,first_corrx18)
  ADPCorrelation(MnCN_x, MnCN_y,first_corrxy18)
  ADPCorrelation(MnCN_y, MnCN_x,first_corrxy18)
  ADPCorrelation(MnCN_z, MnCN_z,first_corrz18)

  ADPCorrelation(MnCN_x, MnCN_z,first_corrxz18)
  ADPCorrelation(MnCN_y, MnCN_z,first_corryz18)
  ADPCorrelation(MnCN_z, MnCN_y,first_corryz18)
  ADPCorrelation(MnCN_z, MnCN_x,first_corrxz18)

  ADPCorrelation(Mn2_x, Mn2_x, first_corrx18)
  ADPCorrelation(Mn2_y, Mn2_y, first_corrx18)
  ADPCorrelation(Mn2_x, Mn2_y, first_corrxy18)
  ADPCorrelation(Mn2_y, Mn2_x, first_corrxy18)
  ADPCorrelation(Mn2_z, Mn2_z, first_corrz18)

  ADPCorrelation(Mn2_z, Mn2_x, first_corrxz18)
  ADPCorrelation(Mn2_z, Mn2_y, first_corryz18)
  ADPCorrelation(Mn2_x, Mn2_z, first_corrxz18)
  ADPCorrelation(Mn2_y, Mn2_z, first_corryz18)

  SizeEffect(MnCN,MnCN_x,se18)
  SizeEffect(MnCN,MnCN_y,se18)
  SizeEffect(MnCN,MnCN_z,se_z18)
  ]

  [(1,3/2,3/2)
  Multiplicity 2*8

  ADPCorrelation(MnCN_x, Mn2_x,first_corrx19)
  ADPCorrelation(MnCN_y, Mn2_y,first_corrx19)
  ADPCorrelation(MnCN_z, Mn2_z,first_corrx19)

  ADPCorrelation(MnCN_x, Mn2_y,first_corrxy19)
  ADPCorrelation(MnCN_x, Mn2_z,first_corrxy19)
  ADPCorrelation(MnCN_y, Mn2_x,first_corrxy19)
  ADPCorrelation(MnCN_y, Mn2_z,first_corryz19)
  ADPCorrelation(MnCN_z, Mn2_x,first_corrxy19)
  ADPCorrelation(MnCN_z, Mn2_y,first_corrxy19)

  SizeEffect(MnCN,Mn2_x,se19)
  SizeEffect(MnCN,Mn2_y,se19)
  SizeEffect(MnCN,Mn2_z,se19)
  ]
]
```

The Algorithms and their Implementation

- Isometries
- Space Groups
- Bounds
- Wyckoff Positions
- Pair Expansions
- Main Algorithm

Isometry Implementation

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- Rational Numbers $\frac{p}{q}$

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$$\widetilde{X} = \mathcal{A}X = \boldsymbol{A}X + \boldsymbol{a}$$

- Isometries

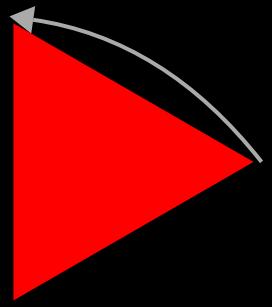
  special affine transformation which preserve distances and angles

Space Groups

Generators

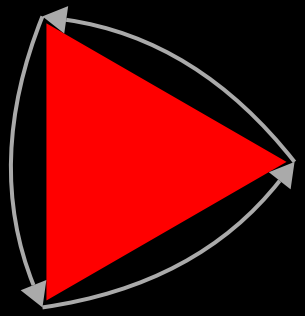
Space Groups

Generators



Space Groups

Generators



Space Groups

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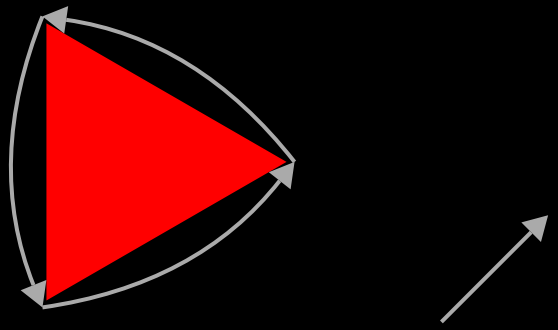

Space Groups

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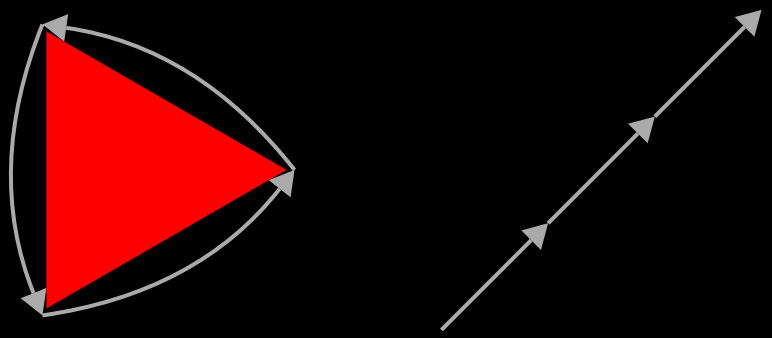
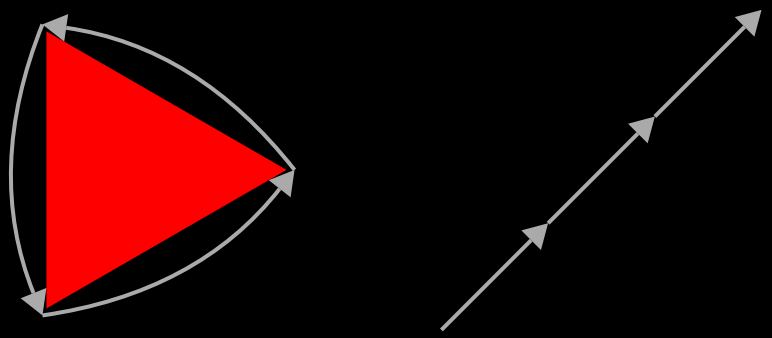


Space Groups

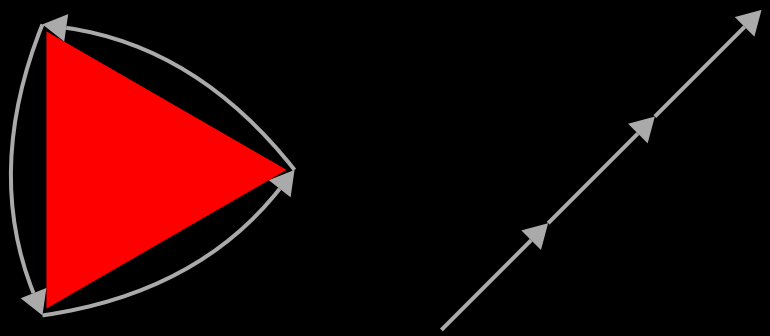
Generators



Space groups are infinite!
What should we do?

Space Groups

Generators



Space groups are infinite!
What should we do?

Bounds

- act on positions, vectors, and affine transformations
- allow finite representation of space group
- for unitcell and space group bound to $[1, 1, 1]$

Wyckoff Positions

```
fn site_new(position, group) -> Site {
  bounds = Bounds3(1, 1, 1);
  position = position % bounds;
  orbit = [position];
  stabilizer = [];

  for sym in group.get_symmetries() {
    new_pos = sym * position;
    if new_pos % bounds == position {
      stabilizer.push(symmetry_from_translation(position - new_pos) * sym);
    } else if new_pos % bounds not in orbit {
      orbit.push(new_pos % bounds);
    }
  }

  return Site { position, orbit };
}
```

Pair Expansions

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Main Algorithm

- generates the space group
- determines the Wyckoff position of the sites
- determines all possble pairs between these position

Pair Expansions

- represents all equivalent pairs starting at a certain position
- generated in a similar fashion to the orbit wyckoff positions
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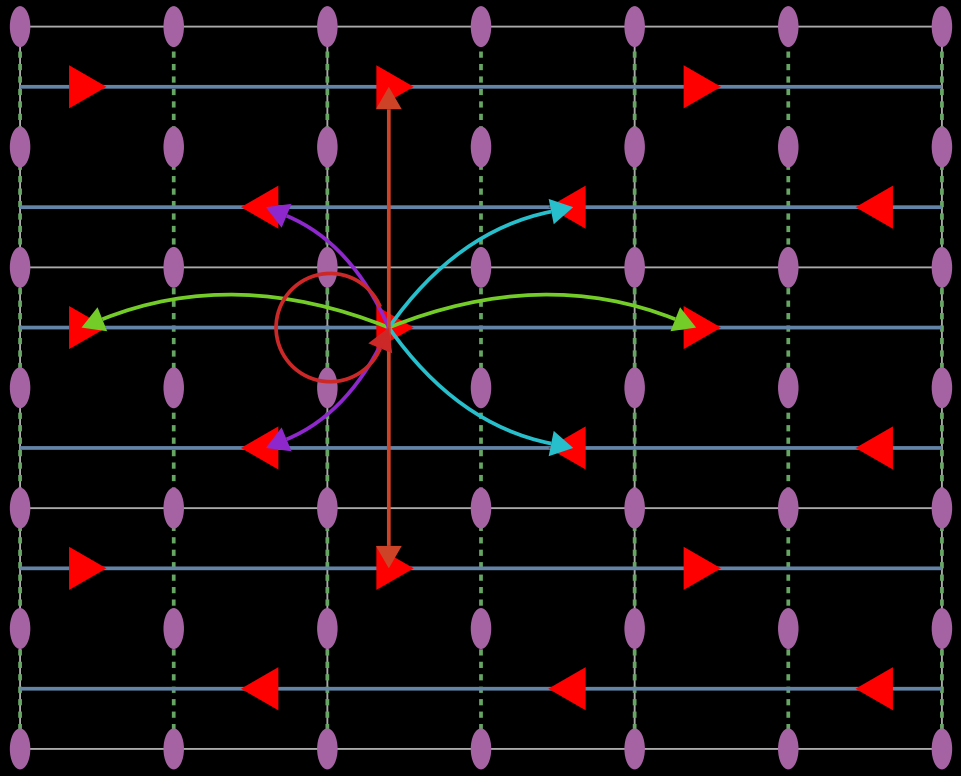
Main Algorithm

- generates the space group
- determines the Wyckoff position of the sites
- determines all possble pairs between these position
- calculates the pair multiplicity

Website



Thank you for your Attention!