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# Multidimensional Necklaces:

## Enumeration, Generation, Ranking and Unranking

**Duncan Adamson**, Argyrios Deligkas, Vladimir V. Gusev and Igor Potapov
University of Liverpool, Department of Computer Science

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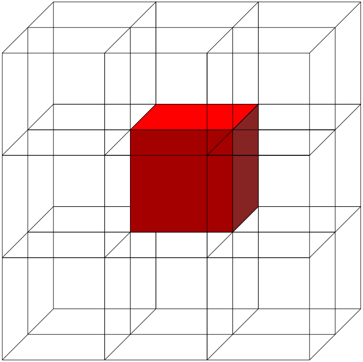
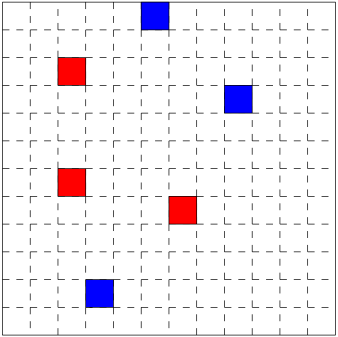
diamond Hartree Centre Imperial College London ICNS King Abdullah University of Science and Technology University of Southampton

# Crystals

Crystals are a fundamental material structure defined by an infinitely repeating unit cell.



# Unit Cells



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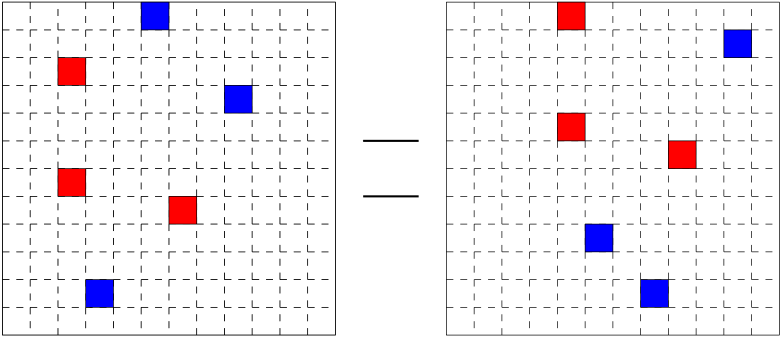

# The Problem

- Given a unit cell in $d$ dimensions of size $N_1 \times N_2 \times \ldots \times N_d$, and $k-1$ types of ions, how many ways of arraigning ions in the cell are there up to translational equivalence?
- We assume that the space is discrete and there is no limits on how many of each type of ion can be placed.

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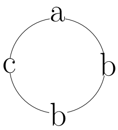
- We assume that the space is discrete and there is no limits on how many of each type of ion can be placed.
- **Idea:** Represent each unit cell as a multidimensional string.
- Represent each ion as a character plus one for blank space.
  - This gives an alphabet of size $k$.

# Necklaces

- In one dimension, counting the number of arraignments corresponds to counting the number of **Necklaces** of size $N_1$ over an alphabet of size $k$.
  - A **necklace** is the lexicographically smallest representation of a cyclic string.
  - This means every necklace is unique under cyclic rotation.




**abbc**
bbca
bcab
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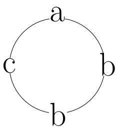


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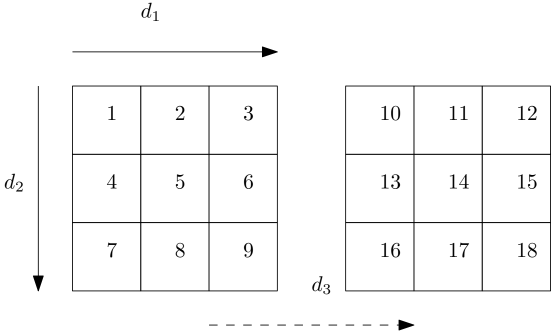
- **Problem**
  - Crystals are not 1d.
  - How can we generalise the concept of necklaces to multiple dimensions?

# What is known about necklaces?

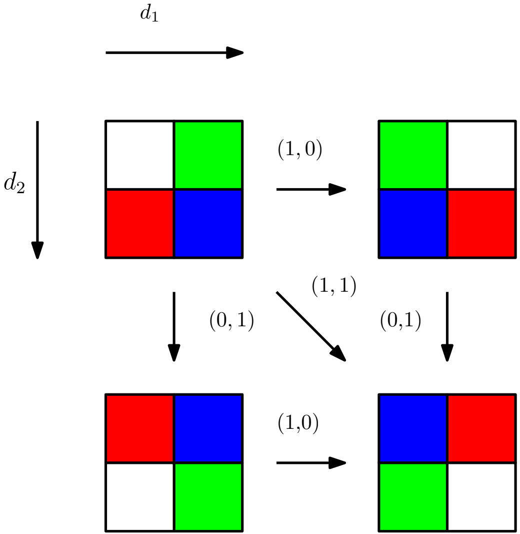
- Necklaces are a heavily studied combinatorial object, the main results are:
  - **Enumeration**: How many necklaces are there for a given alphabet?
  - **Generation**: How can we quickly generate all necklaces in order?
  - **Ranking**: How many necklaces are there smaller than a given necklace?
  - **Unranking**: How can we generate the necklace corresponding to a given rank?

# Multidimensional Necklaces

- A multidimensional cyclic string is the generalisation of a cyclic string into more than 1 dimension.
- Here we may rotate along one or more dimension.
- A multidimensional necklace is the lexicographically smallest rotation of a cyclic string.
  - The lexicographical ordering will be "book" style.



# Multidimensional Necklaces



# Multidimensional Necklaces

- Each necklace will be defined over some alphabet $\Sigma$ of length $k$.
- The largest dimension will be denoted $d$.
- The length of the necklace in dimension $i$ will be $N_i$.
  - This gives the total size as $N_1 \times N_2 \times \ldots \times N_d$.
  - We will use $m$ to denote the total number of positions, i.e. $m = N_1 \times N_2 \times \ldots \times N_d$.
- The set of necklaces of size $N_1 \times N_2 \times \ldots \times N_d$ over alphabet $k$ will be denoted $N_k^{N_1, N_2, \ldots, N_d}$.

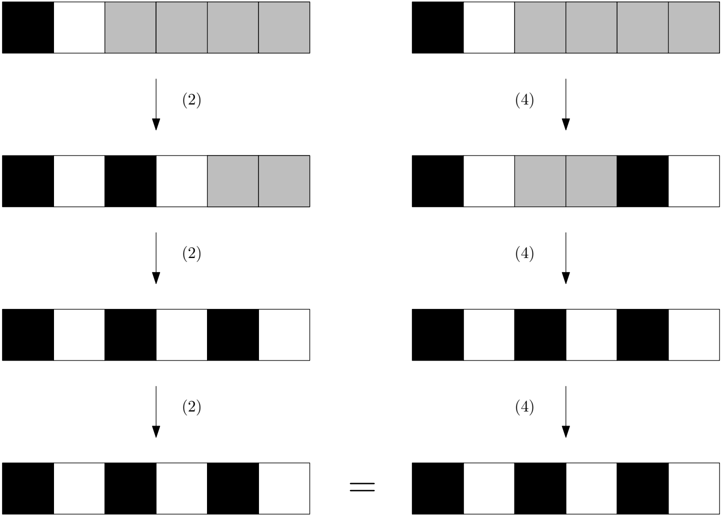
# Enumeration

- The symmetry of this space may be captured by the direct product of the cyclic groups $\mathbf{Z}_{N_i}$ for each $i$ from 1 to $d$.
  - $G = \times_{i=1}^{d} \mathbf{Z}_{N_i}$
- This can be used with the Pólya ennumeration theorem to giving:

$$\left| N_k^{N_1, N_2, \dots, N_d} \right| = \frac{1}{|G|} \sum_{g \in G} k^{c(g)}$$

- Here $c(g)$ returns the number of cycles of group operation $g$.
- Note also that $|G| = m$ by definition.

# Example



# $c(g)$

- Given an action $g \in G$ with a rotation by $g_i$ in dimension $i$, what is $c(g)$?
- Let $l_i$ be the length of the cycles in dimension $i$.
- In one dimension, we want the smallest $l_i$ such that $l_i \cdot g_i \bmod N_i \equiv 0$.
- This is given by $l_i = \frac{N_i}{GCD(N_i, g_i)}$.
- As all cycles will have the same length under translation, this gives (for one dimension):

$$c(i) = \frac{N_i}{l_i} = GCD(N_i, g_i)$$

# $c(g)$ in multiple dimensions

- Observe that the rotation in each dimension acts independently.
- For the cycle to be complete, we need the smallest $j$ such that, for each $i$ from 1 to $d$, $j \cdot g_i \bmod N_i \equiv 0$.
- Note that each $l_i$ must be a factor of $j$ so that $j \cdot g_i \bmod N_i \equiv 0$.
- Therefore the smallest $j$ will be the least common multiple of $l_1, l_2, \ldots, l_d$.
- Thus:

$$c(g) = \frac{m}{j} = \frac{m}{LCM(GCD(N_1, g_1), \ldots, GCD(N_d, g_d))}$$

# Enumeration - Can we do better

- If we can work out quickly how many times each value of $c(g)$ occurs, we remove a large amount of computation.
- In the $1d$ case, this is quite straight forward:
    - Given two rotations, by $i$ and $j$, $c(i) = c(j)$ iff $GCD(N_1, i) = GCD(N_1, j)$.
    - This means we only need to consider factors of $N_1$, as for any rotation by $i$, $GCD(N_1, i)$ must be a factor of $N_1$.
- Given $GCD(N_1, i) = l$, the number of groups where $c(g) = l$ is given by $\phi\left(\frac{N_1}{l}\right)$.
- Putting these observations together gives:

$$\left|N_k^{N_1}\right| = \frac{1}{N_1} \sum_{f|N_1} \phi\left(\frac{N_1}{f}\right) k^f$$

# Number of cycles in multiple dimensions

- As in one dimension, in multiple we only care about factors of each dimension.
  - Again the number of times each factor $f$ occurs will be $\phi(f)$.
- As each dimension is independent of each other, the number of times each combination occurs will be $\phi(f_1) \times \phi(f_2) \times \ldots \times \phi(f_d)$.
- Therefore the number of necklaces will be:

$$N_k^{N_1,N_2,\ldots,N_d} = \frac{1}{m} \sum_{f_1 | N_1} \phi\left(\frac{N_1}{f_1}\right) \sum_{f_2 | N_2} \phi\left(\frac{N_2}{f_2}\right) \cdots \sum_{f_d | N_d} \left(\frac{N_d}{f_d}\right) k^{c(g)}$$

# Generation

- The generation of necklaces is a well studied problem.
- Despite the exponential number of necklaces, this can be done relatively efficiently.
    - One notable result is a constant amortized time algorithm [1].
- We have extend this to an algorithm with an average time of $O(d)$ to generate each necklace.

# Ranking

- Ranking (also known as indexing) necklaces is the problem of determining how many necklaces there are smaller than some given string.
- The idea of ranking necklaces comes originates from the problem of ranking de Bruijn Sequences [2].
- In one dimension it is possible to rank necklaces is $O(m^2)$ [3].
- Our generalisation of this to higher dimensions require $O(d^3m^4)$ time.

| Necklace | Rank | Necklace | Rank | Necklace | Rank |
|---|---|---|---|---|---|
| aaa | 1 | abc | 5 | bbc | 9 |
| aab | 2 | acb | 6 | bcc | 10 |
| aac | 3 | acc | 7 | ccc | 11 |
| abb | 4 | bbb | 8 | | |

# Unranking

- Unranking is the complimentary process to ranking, taking a rank and finding the corresponding necklace.
- A binary search based algorithm can be used in combination with the ranking algorithm to solve this in $O(m^3 \log(k))$ time [3].
- The same algorithm can be adapted to the multidimensional case to do unranking in $O(d^3 m^6 \log(k))$

# Fixed Content necklaces

- One notable generalisation of necklaces is when the number of occurrences of each character is fixed.
- This known as a **fixed** content necklaces.
- There exists variations on our existing algorithms for the enumeration, generation, ranking and unranking of fixed content multi-dimensional necklaces, requiring at most a factor of $O(k)$ longer.

# Next Steps

- **Concerning Rotations**: Beyond just translational symmetry, we would want to consider rotational and reflective symmetry.
- This is a much harder problem, even in 1 dimension, it is not known how to rank when taking into account reflective symmetry.

# Thank you for listening

Feel free to email any questions to
duncan.adamson@liverpool.ac.uk

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