

Mathematical Recipes for Never-repeating Quasicrystals

Dr Priya Subramanian is supported by the L'Oréal UK and Ireland Fellowship for Women in Science. The annual Fellowships programme provides £15,000 of flexible financial support for outstanding female postdoctoral researchers to continue research in their fields, as part of a wider L'Oréal-UNESCO programme aimed at supporting and increasing the number of women working in STEM professions in the UK, where 85% of jobs are held by men. To find out more about the L'Oréal-UNESCO programme see www.womeninscience.co.uk

Priya Subramanian is a mathematician researching mathematical recipes for never-repeating quasicrystals. Repeating patterns of tiles and crystals occur throughout the natural world, but never-repeating patterns are special because they possess order without repeatability. Such never-repeating arrangements of atoms and molecules – called quasicrystals – are thought to require less energy to assemble, and could offer advantages in manufacturing, insulation and photonic devices. In this article, Priya gives an introduction to her award-winning research.

What are quasicrystals?

The dynamics of many physical systems often evolve to asymptotic states that exhibit spatial and temporal variations in their properties such as density, temperature, etc. Among all possible arrangements of such spatio-temporal patterns, regular crystalline arrangements are often preferred in nature because they are associated with the least amount of energy required to assemble. Regular patterns such as graph paper and honeycombs look the same when moved by a basic unit and/or rotated by certain special angles. They possess both translational and rotational symmetries giving rise to discrete spatial Fourier transforms.

In contrast, an aperiodic quasicrystal displays long range order despite having no periodicity. Such quasicrystals lack the lattice symmetries of regular crystals, yet they still have discrete Fourier



Dr Priya Subramanian speaking at the L'Oréal-UNESCO award ceremony at the Royal Society on 4 May 2017.

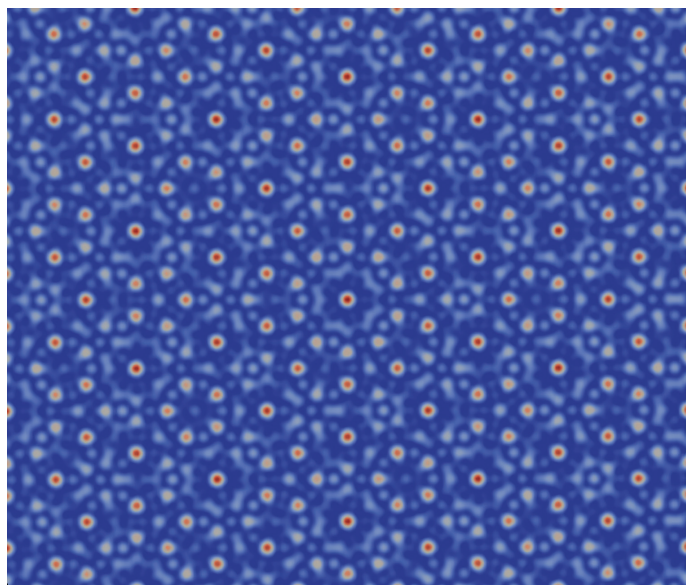


Figure 1: Section through a 3D quasicrystal in a periodic cubic domain with icosahedral symmetry showing variation of the scalar density field. The 10 lines of symmetry about the central peak indicate icosahedral symmetry.

spectra. Figure 1 shows the density variation along a section through a 3D quasicrystal. Note the 10 lines of symmetry about the central peak, which is indicative of icosahedral symmetry.

Why are they important?

The vast majority of the quasicrystals discovered so far are metallic alloys but recently quasicrystals have been found in soft-matter systems such as polymers. Metallic quasicrystals (3D quasicrystals in bulk) are excellent heat insulators and also have low friction and high corrosion resistance which are advantageous in prosthesis manufacture, while polymeric quasicrystals (2D quasicrystals on surfaces) might be useful in photonic devices to manipulate light. Considering the difference in scale between metallic and polymeric quasicrystals, there is a need for mathematical models that explore the unifying mechanisms that generate quasicrystals independent of the microscopic structure. Together with collaborators at Loughborough University and University of California, Berkeley, we at University of Leeds have been investigating the minimal mechanism required to promote the formation of both 2D and 3D polymeric quasicrystals using a single model.

How are they formed?

Patterns formed by interlinked polymeric molecules are investigated in terms of the soft potential between their centres of masses in density functional theory (DFT). This can be simplified by expanding densities and gradients around the homogeneous liquid state in a phase field crystal (PFC) approach.

We describe the evolution of density differences (U) of a scalar from a mean value by a partial differential equation (PDE) as given below, which is related to the Swift-Hohenberg equation (one of the standard PDEs used in investigating pattern formation).

$$\frac{\partial U}{\partial t} = -\nabla^2 (LU + QU^2 - U^3).$$

Here the linear operator L is as defined in [1] and allows for independent periodic density modulations in two length scales, while the value of parameter Q sets the relative importance of second-order non-linear interactions in the system. This evolution equation describes a linearly unstable system that is stabilised non-linearly by the cubic term. In soft matter systems, the two wavelengths can be associated with the core and corona of the polymer micelles, which are determined by the polymer architecture.

Results using this model indicate that the same requirements for promoting the formation of dynamically stable two-dimensional QCs; periodic density modulations with two wavelengths (within a factor of two) and strong resonant non-linear interactions, remain extant in the formation of three-dimensional icosahedral QCs [1]. By changing the ratio of the two length scales, we are able to obtain both 2D 12-fold and 3D icosahedral quasicrystals in a phase field crystal model for soft matter as shown in Figure 2.

Recent results and future outlook

Regular icosahedral quasicrystals are obtained as the global minimum of this model system in a range where both the interacting wavelengths are marginally stable. Simple structures such as lamellae, columnar hexagons and body-centred cubic crystals at each of the two length scales are the other globally minimal energy structures for other parameter values. Weakly non-linear approximations of the pattern amplitudes and other more complicated patterns are obtained by solving the appropriate amplitude equations.

We employ the method of homotopy continuation (computational algebraic geometry) to solve the coupled set of algebraic equations to determine all the real solutions of the amplitude equations [2]. The availability of the full set of solutions makes it possible to calculate the

global minima of free energy among all pattern types and to also identify new solutions corresponding to different symmetry subspaces of the icosahedral symmetry superset.

With the support of the L'Oréal-UNESCO Women in Science Fellowship, I will be involved in extensions to the PFC model to connect it to DFT model for polymers. Along with this, I plan to develop tools to characterise their properties using topological data analysis methods and analyse their growth and stability using numerical continuation and equivariant bifurcation methods.

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REFERENCES

- 1 Subramanian, P., Archer, A.J., Knobloch, E. and Rucklidge, A.M. (2016) Three-Dimensional Icosahedral Phase Field Quasicrystal, *Physical Review Letters*, vol. 117, p.075501.
- 2 Bates, D.J., Hauenstein, J.D., Sommese, A.J. and Wampler, C.W. (2013) Bertini: Software for Numerical Algebraic Geometry. Available at: <https://bertini.nd.edu>

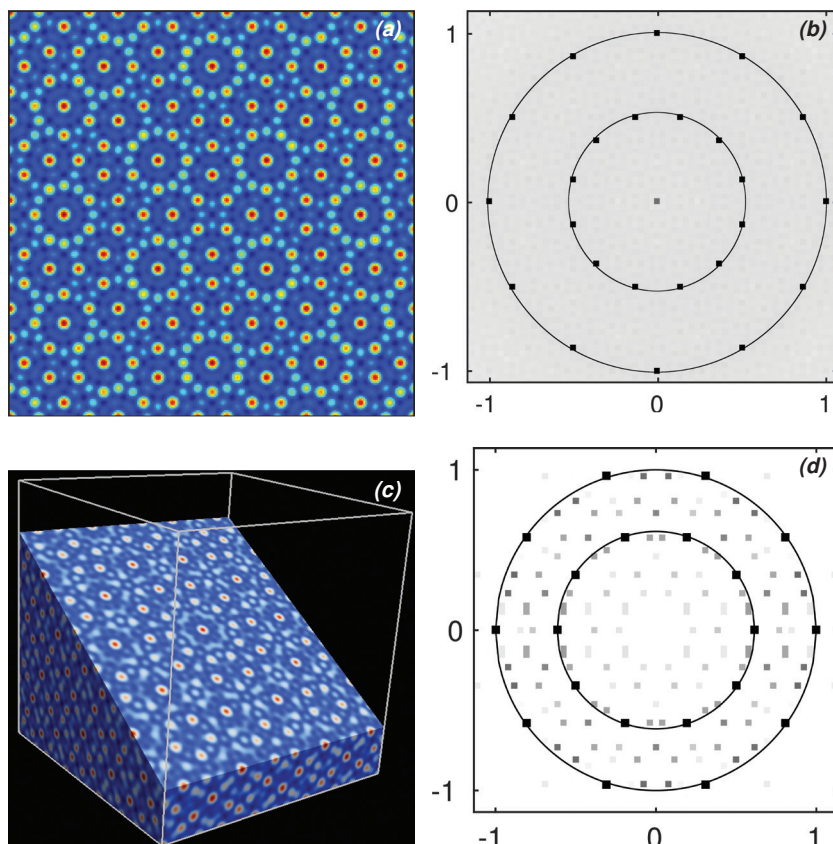


Figure 2: Simulation results for the PFC model in periodic domains. (a) 2D quasicrystals with 12-fold symmetry. (b) Diffraction pattern of the 2D quasicrystals in Fourier space. The 12-fold rotation symmetry of the diffraction pattern is indicated by the 12 peaks observed on each circle. (c) 3D quasicrystal with icosahedral symmetry. The box has had a slice cut away, chosen to reveal the 10-fold rotation symmetry. (d) Diffraction pattern taken in a plane parallel to the slice in (c) shown in Fourier space. The 10-fold rotation symmetry of the diffraction pattern is indicated by the 10 peaks observed on each circle. The two circles (b,d) indicate the two interacting length scales.