Numerical Mathematics of Quasicrystals

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Quasicrystals with non-crystallographic rotational symmetry and no translational symmetry, are one kind of fascinatingly ordered materials between periodic structures and disordered phases. The discovery of Quasicrystals changes the traditional concept of classifying structures into: crystals and non-crystals, and gives a strong impact on materials science, solid state chemistry, condensed matter physics and soft matters. The mathematics of quasicrystals has been studied earlier by mathematician, Quasicrystals can be characterized by a remarkable Diophantine approximation property.

Penrose discovered an aperiodic tilling, a five-fold symmetric quasicrystal; Meyer proposed a model set (cut-and-project) to construct discrete quasi-lattices, this model sets anticipated Penrose tiling and the physical quasicrystals.

Due to lack of periodicity, quasicrystals are space-filling structures which can be hardly restricted into a finite region to calculate numerically. There have been several numerical algorithms to compute quasicrystals approximately. However, all of these approaches have their own deficiency. Recently, we developed a high-precision projection method which considers quasicrystals as a projection of higher-dimensional space. The projection method connects quasi-lattices in reciprocal space and almost periodic functions. Numerical results demonstrate the excellent performance in studying the emergence and thermodynamic stability in physics. We hope that the projection method can build a bridge between mathematical and physical quasicrystals.