Numerical Methods of Quasicrystals

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Quasicrystals (QCs), with long-range order and non-crystallographic symmetry, is one kind of fascinatingly ordered structures between period structures (crystals) and disordered structures. The discovery of QCs 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 matter, both on basic experimental and theoretical tools. This concept of QCs also promotes the development of several branches of mathematics, such as number theory, geometry, group theory and applied mathematics.

The first observation of QCs was done in April 1982 by D. Shechtman. He observed that a rapid cooled Al-Mn alloy exhibit 5 fold non-crystallographic symmetry. Since the original discovery of D. Shechtman, hundreds of QCs have been reported and confirmed in metallic alloys with 5, 8, 10, 12 fold orientational symmetry. Shechtman also received the Nobel Prize in Chemistry in 2011 for the discovery of QCs. Two decades after the first discovery of QCs in metallic alloys, soft-matter QCs were found in nature. Since then a number of materials successively joined the family of soft QCs, including liquid crystals, polymers, nonoparticles, colloids and mesoporous silica.

There exist several difficult problems in the theoretical research on QCs: how to building mathematical models which make the QCs exist and thermodynamical stability; how to design general numerical methods to capture QCs; how to compare the theoretical results with physical experiments quantitatively. Here, we focus on the development of numerical methods. QCs are a kind of whole-spatial structures. Traditionally the same dimensional numerical methods need period structures to approximate QCs. However, these methods can just compute few kinds of QCs, such as 12-fold QCs, because of the limitation of Simultaneous Diophantine Approximation. We provide a systematic numerical method to calculate all QCs where QCs could be treated as projections of a higher-dimensional space. We also present how to compute the energy density exactly without boundary effect. Finally, we take Lifshitz-Petrich model as an example to demonstrate our methods and show some numerical results.