How to determine thermodynamically stable soft matter quasicrystals efficiently?

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Matter does not normally self-organise into quasicrystals (QCs). Regular crystalline packings are much more common in nature and some specific ingredients are required for QC formation, which is why the first QCs were not identified until 1982, in certain metallic alloys. Subsequently, the seminal work in Refs. [1, 2] showed that normally a crucial element in QC formation, at least in soft matter, is the presence of two prominent wave numbers in the linear response behaviour to periodic modulations of the particle density distribution. This is equivalent to having two prominent peaks in the static structure factor or in the dispersion relation.

Some of our understanding of how and why QCs can form has come from studies of particle based computer simulation models – see for example [3-5]. Another source of important insights has been continuum theories for the density distribution, consisting of both the generalised Landau-type order-parameter theories [1, 2] and more recently classical density functional theory (DFT). In the first half of the talk, we demonstrate how the crucial pair of prominent wave numbers are connected to the length and energy scales present in the pair potentials. Whilst the ratio between the two length scales is important, we show here that for thermodynamically stable soft matter quasicrystals, the ratio of these wave numbers should be close to certain special values. We identify features in the particle pair interaction potentials which can suppress or encourage density modes with wave numbers associated with one of the regular crystalline orderings that compete with quasicrystals, enabling either the enhancement or suppression of quasicrystals.

In the second half of the talk we look how to compute phase diagrams for a given interaction potential in an efficient manner. In order to do this, we focus on the representation of the density distribution in soft matter systems. The form of the average (probability) density distribution in solids is often represented as a sum of Gaussian peaks (or similar functions) centred on lattice sites or via a Fourier sum. Here, we argue that representing instead the logarithm of the density distribution via a Fourier sum is better. The advantage of this representation is that it excels both deep in the crystalline region of the phase diagram and also close to melting. Additionally, we show how a strongly nonlinear theory (SNLT) enables efficient computation of the phase diagram for a three-dimensional quasicrystal-forming system using an accurate nonlocal density functional theory. In the figure, we show the icosahedral QC determined at a point far from melting. Initial conditions created using SNLT are then fed into Picard iterations to converge to the above profiles. Results in this talk are based on two publications [6, 7].
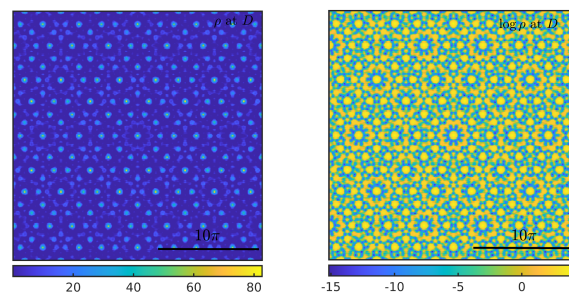
Figure 1. The density profiles and the corresponding logarithm for the IQC phase for a modified BEL potential in 3D. These are plotted in the plane normal to the vector $(0, -1, 2\cos(\pi/5))$.

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