Phase transitions in a two-dimensional system of core-softened particles

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We use computer simulation techniques to study systems of classical particles that interact according to a purely repulsive effective potential and with two characteristic length scales, represented by $V(r) \sim \exp(-r^4) + C/r^6$. These two characteristic scales, determined according to the C parameter, imply the formation of spatial patterns with specific symmetries due to the competitive interaction between the two factors.

In the regime of high densities and for small values of the C parameter, the formation of 2D patterns such as bubbles, stripes and inverted bubbles is noted [1]. In the area of soft-matter, this characteristic is normally called self-assembly and plays an important role in the physical properties of the system, especially in relation to the elastic properties and melting [2] — which is defined here as the succession of transitions that take the system from the solid state to the liquid state.

We focus on a statistical mechanics perspective to study this system. Defining specific order parameters, we determine how they scale with the size of the system, in order to describe the correlations present in the system during melting. According to the leading theory of melting in two dimensions, known as BKTHNY, two continuous transitions in sequence must occur in two-dimensional materials (which present continuous symmetries): the first from a solid state to an intermediate phase — known as the hexatic phase — and the second from the hexatic phase to an isotropic liquid phase.

Little has been explored in the literature on the melting of two-dimensional systems that present the formation of patterns with non-trivial symmetries, as in this case. We hope to explore this system in order to understand how the symmetry of the configurations can affect the critical properties. We focus in the phases that have a low occupation number per site, mainly 1 and 2 particles per unit cell.

References

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