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Percolating transition from order to disorder in two-dimensional Yukawa system

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Percolation is a phenomenon in which a network is formed by connecting active or inactive sites, and it is commonly observed in various non-equilibrium systems that are influenced by different control parameters. Percolation of liquids through porous material, the failure of power grids, the spread of forest fires and epidemics, and the transition to turbulence in hydrodynamic and nonlinear wave systems are a few good macroscopic systems exhibiting percolation transition [1].

In passive coupled many-body systems in the microscopic discrete level, such as cold liquids and solids, there is a dynamic interplay between the emergence of order through mutual coupling and the disruptive effects of thermal agitation. This interplay gives rise to the formation and dissolution of local ordered (disordered) microstructures and motion. Recent researches have shown that phenomena such as the clustering of cooled liquids into gels [2], the yielding of glasses under external stress [3], and the layering of liquids induced by confinement [4], exhibit similar transition behaviors that can be explained by percolation theory. These findings highlight the presence of generic transition phenomena in these systems.

Melting of a crystal in two dimensions (2D) is associated with the dissociation of topological defects. These topological defects destroy the order of crystals. The KTHNY-theory predicts two continuous phase transitions from the crystalline to the liquid phase, through the intermediate hexatic phase, associated with the loss of the translational order, followed by the loss of the orientational order [5]. However, with increasing temperature, how localized disordered sites emerge, spread and aggregate into a lager disordered domain, still remains an unexplored question.

In this work, the above issues are numerically addressed in a 2D Yukawa system, through Langevin-type molecular dynamic simulation with periodic boundary condition. Localized ordered sites (LOSs) and disordered sites (LDSs) are identified based on the local bond orientational order. It is found that with increasing temperature, the transition from the solid to the liquid phase through the hexatic phase are associated with the sporadic emergence, spreading, and termination of LDSs in the form of multiscale clusters in the *xyt* space. The area fraction of LOSs also exhibits a transition from the gradual rise to a smooth rapid rise at the solid-hexatic transition, followed by a transition to a smooth slow rise at the hexatic-liquid transition. The defect cluster percolates in the *xyt* space at the hexatic-liquid transition.

References

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