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Percolation of defect and hopping clusters in the melting transition of two-dimensional Yukawa solids

Jun-Zhong Wen, Wei-Shuo Lo, Yi-Cheng Zhao, and Lin I
Department of Physics and Center for Complex Systems,
National Central University, Jhongli 32001, Taiwan
e-mail (speaker): junzhong1211@gmail.com

The melting transition in two-dimensional (2D) systems has long been a fundamental problem in condensed matter and soft matter physics. It is governed by a delicate interplay between disorder by stochastic thermal fluctuations and order through mutual particle interactions. With increasing temperatures, particles can exhibit small amplitude rattling in cages formed by surrounding nearest neighbor particles, or exhibit cooperative hopping out of caging wells after accumulating sufficient constructive perturbation, which induces structural rearrangement. It consequently leads to the sporadic emergence of hopping strings and topological defects, including dislocations and disclinations, in the form of multiscale clusters. [1-3]. The solid-hexatic phase transition with a continuous deterioration of the long-range translational order, followed by the hexatic-liquid transition with diminishing long-range orientational order as temperature increases has been widely observed in various 2D systems with soft-core interactions [1-3].

In the general direct percolating transition theory for nonequilibrium extended media, local sites can be binarized into active and inactive sites. With the increase of a certain control parameter, active sites can form clusters exhibiting power law cluster size distribution in the spatiotemporal space until formation of the largest percolating cluster spanning over the spatial as well as temporal spaces [4-6].

In this study, we explore the melting transition in a two-dimensional Yukawa system using Langevin-type molecular dynamics simulations under periodic boundary conditions, from the perspective of direct percolating (DP) transition for a nonequilibrium extended system [5,6]. We address the structural as well as dynamical transitions, by classifying local sites into active sites with poor structural order (SPSOs) and inactive sites with good structural order for the former; and into active sites exhibiting hopping over a certain distance over a finite time interval (SHs) and inactive site exhibiting caged rattling, for the latter. It is found that both SPSOs and SHs intermittently form multiscale clusters in the *xyt* space exhibiting power law size distributions, whose characteristic sizes increase with temperature. With increasing temperature, these clusters expand and eventually merge to form system-spanning percolating clusters in the spatiotemporal space at the hexatic-liquid transition. The fractions of SPSOs and SHs both grow gradually during the solid-hexatic transition, followed by steep increases near the hexatic-liquid transition. They then slowly saturate as the system enters the fully disordered liquid phase.

The observed formation of multiscale clusters exhibiting power law size distribution and formation of percolating clusters, associated with sharp increases of the fractions of SPSOs and SHs are akin to the finding in various nonequilibrium systems governed by the DP theory, regardless of the difference of the equations of motions [5,6]. The difference between the scaling exponents of the SPSO (SHs) clusters and those according to the DP transition theory might be caused by the local structural network which has some memory effect, instead of the randomly excited active sites in the DP theory.

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