Collapse transition of polymers modeled as trails on a lattice

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In a solvent, polymer chains may change from an extended (coil) to a collapsed (globule) configuration as, for example, the temperature is changed. In one of the models to study this transitions, the chains are represented by self-avoiding walks on a lattice, with attractive interactions between monomers on first-neighbor sites which are not consecutive along a chain. The collapse transition (theta point) in this model was recognized by De Gennes to be a tricritical point, and the collapse arises from the competition between the ecluded volume interaction and the monomer-monomer attraction. In an alternative model, the chains are represented by trails on a lattice, which are walks which may visit a site more than once but ar constrained to pass only one through each lattice edge. In these models the attractive interactions are on site. The nature of the collapse transition in such models is still not clear. On Bethe and Husimi lattices, in general we find rich phase diagrams with several multicritical points, for four coordinated lattices the collapse transition is a bicritical point (1). If the chains are semi-flexible, a nematic phase appears inside the polymerized phase in the phase diagram. The transition between these phases has a rather unusual discontinuous critical nature (2).

(1) T. J. Oliveira e J. F. Stilck, Physical Review E v. 93, 012502 (2016).
(2) W. G. Dantas, T. J. Oliveira, J. F. Stilck e T. Prellberg, Phys. Rev. E (aceito) (2017).