What is the Shape of a Polymer Chain near the Theta Point?

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What is the Shape of a Polymer Chain near the Theta Point?

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We address the question of the conformation of a polymer near the θ point. To this end, we present an argument that the statistics of polymer rings at the θ point in two dimensions is exactly given by the statistics of the external perimeter ("hull") of a percolation cluster. As a consequence, the fractal dimension $d_f(\theta)$ of a polymer chain at the θ point coincides with that of the hull of the percolating cluster, $d_f(\theta) - d_H$. We also perform extensive simulations of the conventional θ point model—the interacting self-avoiding walk (ISAW)—and the smart kinetic walk (SKW). We demonstrate that the SKW predicts a higher order critical point, termed the θ' point, *which has the same critical behavior as the ISAW.* We conclude that the SKW is a well-defined walk that gives the conformation of a polymer near the θ point in two dimensions. In particular, we report accurate calculations of all three tricritical point exponents that are needed to fully describe the θ point.