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Signatures of the Berezinskii-Kosterlitz-Thouless transition in the location of the zeros of the canonical partition function for the 2D XY-model,

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■In this work we show how one can use the zeros of the canonical partition function, the Fisher zeros, to unambiguously characterize a transition as being in the Berezinskii-Kosterlitz-Thouless (BKT) class of universality.

A "fruit fly" model of the BKT transition is the classical two-dimensional XY-model on a square lattice, defined by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y). \qquad (1)$$

The sum runs over the nearest neighbors, J stands for the exchange coupling constant and S_i^α stands for the component $\alpha = (x, y, z)$ of the i^{th} spin.

We obtained the Fisher's zeros map via recent Monte Carlo simulations techniques (Replica Exchange Wang-Landau) capable of sampling the entire configuration space efficiently in a single simulation and powerful matrix diagonalization procedures.

We found that in a BKT transition the internal border of the zeros map behave in such a way that for $T \leq T_{BKT}$ it coalesces into the real positive axis in the thermodynamic limit, indicating the existence of a line of critical points in this region, as should be expected, and in contrast to what happens for a continuous or discontinuous phase transition, where a single leading zero touches the positive real axis. This behavior is therefore the signature of the BKT transition. The inflection point of the zeros map was successfully used to obtain the BKT temperature, $T_{BKT} = 0.704(3)$, in excellent accordance with the literature.

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