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Partition function zeros for the polymer adsorption transition[1]
MARK TAYLOR, SAMIP BASNET, Dept. of Physics, Hiram College, JUTTA LUETTMER-STRATHMANN, Dept. of Physics, University of Akron — Modern computer simulation techniques, such as the Wang-Landau (WL) algorithm, allow for direct computation of the density of states, and thus the partition function, of a many-body system. The partition function encodes all thermodynamic information including details of phase behavior. Here we describe the application of the WL approach to the adsorption transition for both lattice [1] and continuum chains tethered to an attractive surface. We compute the canonical partition function for chains up to length N=1536 and analyze the zeros of these function in the complex inverse-temperature plane. These zeros define a nearly closed circular region, centered on the origin, intersected near the positive real axis by two flaring tails. With increasing chain length the intersection point pinches down towards the positive real axis, dividing the real axis into two distinct regions or phases in accord with Yang-Lee theory. We apply finite size scaling theory (including corrections to scaling) for the leading partition function zeros to locate the adsorption transition in the thermodynamic limit and obtain values for the polymer crossover, order parameter, and specific heat exponents.

[1] M.P. Taylor and J. Luettmer-Strathmann, J. Chem. Phys. 141, 204906 (2014).

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