Abstract Submitted
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From complex numbers to critical exponents: Partition function zeros for polymer adsorption[1] SAMIP BASNET, MARK TAYLOR, Dept. of Physics, Hiram College — Grafting polymer chains onto a solid provides a means of modifying surface properties in a controlled and tunable manner. For example, in the presence of an attractive surface a polymer can undergo a transition from a desorbed "mushroom" state to an adsorbed "pancake" state resulting in a large change in surface properties. Here we study this adsorption transition of a flexible hard-sphere chain tethered at one end to a flat attractive surface. We have carried out computer simulations for chains up to length N=256 using the Wang-Landau algorithm to determine the density of states. From the density of states we construct the canonical partition function and, following Yang and Lee, we compute the zeros of the partition functions and study their distribution in the complex inverse-temperature plane. These zeros are symmetric about the real axis, defining a nearly closed circular boundary, centered at origin, terminated by two flaring tails. This structure defines a root-free zone about the positive real axis with the leading roots (i.e., the pair with the smallest imaginary part) dividing the axis into the adsorbed and desorbed phases. A finite-size scaling analysis of the leading roots gives the transition temperature and polymer crossover exponent in the long chain limit.

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