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Partition function zeros and phase transitions of a polymer chain[1]

PYIE PHYO AUNG, Dept. of Physics, Hiram College, Hiram OH, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — The zeros of the canonical partition functions for flexible square-well polymer chains have been computed for chains up to length 256 for a range of square-well diameters. We have previously shown that such chain molecules can undergo a coil-globule and globule-crystal transition as well as a direct coil-crystal transition [1]. Here we show that each of these transitions has a well-defined signature in the complex-plane map of the partition function zeros. The freezing transitions are characterized by nearly circular rings of uniformly spaced roots, indicative of a discontinuous transition. The collapse transition is signaled by the coalescence of roots onto an elliptical horse-shoe segment pinching down towards the positive real axis. For sufficiently small square-well diameter the elliptical collapse ring merges with the circular freezing ring yielding the direct coil-crystal transition. The root density of all rings increases with increasing chain length and the leading roots move towards the positive real axis, implying a divergence of the specific heat in the thermodynamic limit (as originally proposed by Yang and Lee).

[1] M.P. Taylor, W. Paul, and K. Binder, J. Chem. Phys. 131, 114907 (2009).

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