

Abstract Submitted
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Exact Calculation of the Thermodynamics of Biomacromolecules on Cubic Recursive Lattice.¹ RAN HUANG, Shanghai Jiao Tong University —

The thermodynamics of biomacromolecules featured as foldable polymer with inner-linkage of hydrogen bonds, e. g. protein, RNA and DNA, play an impressive role in either physical, biological, and polymer sciences. By treating the foldable chains to be the two-tolerate self-avoiding trails (2T polymer), abstract lattice modeling of these complex polymer systems to approach their thermodynamics and subsequent bio-functional properties have been developed for decades. Among these works, the calculations modeled on Bethe and Husimi lattice have shown the excellence of being exactly solvable. Our project extended this effort into the 3D situation, i.e. the cubic recursive lattice. The preliminary exploration basically confirmed others' previous findings on the planar structure, that we have three phases in the grand-canonical phase diagram, with a 1st order transition between non-polymerized and polymer phases, and a 2nd order transition between two distinguishable polymer phases. However the hydrogen bond energy J , stacking energy ε , and chain rigidity energy H play more vigorous effects on the thermal behaviors, and this is hypothesized to be due to the larger number of possible configurations provided by the complicated 3D model. By the so far progress, the calculation of biomacromolecules may be applied onto more complex recursive lattices, such as the inhomogeneous lattice to describe the cross-dimensional situations, and beside the thermal properties of the 2T polymers, we may infer some interesting insights of the mysterious folding problem itself.

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