

Interactions between trivial-ring polymers studied by Monte Carlo simulation

Jiro Suzuki¹, Atsushi Takano² and Yushu Matsushita²

jiro.suzuki@kek.jp

¹ Computing Research Center, High Energy Accelerator Research
Organization

² Nagoya University

The value of Flory's critical exponents, ν , for linear polymers is $1/2$ at the θ -temperature, where the excluded volume of chains is screened by the attractive force between chain segments and the chain conformations can be described by Gaussian, three-dimensional random walks. In this case the value of A_2 for linear polymers, inter-molecular interaction between linear polymer molecules, is zero; the excluded volume of polymer molecule is also screened by the attractive force between segments.

Ring polymers are interesting molecules for scientists, because they do not have chain ends. The θ -temperature for trivial ring polymers is lower than that for linear polymers [1]; at θ -temperature for linear polymers the ν value for trivial ring polymers is $1/2 < \nu << 0.588$, where the excluded volume of chains was screened completely by the attractive force between chain segments and the topology of rings was fixed as 0_1 . At $\nu=1/2$ for trivial-ring polymers conformations of trivial-rings are described by closed-random walks, random polygons [2]. In this study, the A_2 value for trivial-ring polymers in dilute condition was estimated from a Metropolis Monte-Carlo simulation and the temperature dependence of A_2 and ν values were obtained, where the chain topology of rings was also fixed as 0_1 . At $\nu=1/2$ for trivial-ring polymers the A_2 value for trivial rings is larger than zero; repulsive force between trivial-ring molecules, random polygons with fixed topology, is working [3].

References

- [1] J. Suzuki, A. Takano and Yushu Matsushita, *J. Chem. Phys.* **138**, 024902 (2013).
- [2] J. Suzuki, A. Takano and Yushu Matsushita, *J. Chem. Phys.* **139**, 184904 (2013).
- [3] J. Suzuki, A. Takano and Yushu Matsushita, *J. Chem. Phys.* **142**, 044904 (2015).