

Analytic theory of DNA toroids

— from Van der Waals to Coulomb —

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完全屈曲性を持つ高分子ガウス鎖の連続理論は、場の理論による相転移の記述等よく知られている。一方、DNA等のより一般の半屈曲性高分子鎖については、数値計算で一定の理解は得られたが、予言性を持つ解析理論に至っていなかった。我々はこのモデルを経路積分において引力項付きで定式化し、DNA凝縮に特徴的なトロイド状態を解析的に導き出した [1]。更に実験との一致を見、ウィップ-トロイド相転移を発見した。これを発展させ、異なる引力相互作用によるトロイド半径のスケーリング則、例えばクーロン力の場合トロイド半径 r_c が全長 L に対して $r_c \sim L^{-1/3}$ となることを示す [2]。

As a simple model of DNA condensation, a semiflexible homopolymer in a poor solvent condition has been investigated. Simulations using Monte Carlo, Langevin approaches or Gaussian variational method, calculated phase diagram for the semiflexible chain in a poor solvent. In analytical works, existing phenomenological models balance the bending and surface free energies to estimate toroidal properties, assuming a priori toroidal geometry as the ground state with no analytical proof. Recently, we have shown analytically that the toroid is the ground state for a certain DNA condensation [1]. Compared to the theory of coil-globule transition of flexible chains, there was no simple microscopic theory, which demonstrates the whip-toroid transition of the semiflexible polymer. Reviewing our previous works with the nonlinear sigma model on a line segment, we show such a transition, the quantitative agreement with experiments, and the scaling properties of the toroid radii for different attractive potentials. The analysed potentials vary from van der Waals interaction to the Coulomb one, *i.e.*, including the Yukawa interactions, which would allow us to find actual attractive interactions between DNA segments [2].

In the continuum limit, the Green function of a semiflexible polymer chain with attractive interactions can be given by the path integral with an inextensibility constraint $|\vec{u}|^2 = 1$: $G(\vec{0}, \vec{R}; \vec{u}_i, \vec{u}_f; L, W) = \mathcal{N}^{-1} \int_{\vec{r}(0)=\vec{0}, \vec{u}(0)=\vec{u}_i}^{\vec{r}(L)=\vec{R}, \vec{u}(L)=\vec{u}_f} \mathcal{D}[\vec{r}(s)] e^{-\mathcal{H}[\vec{r}, \vec{u}, W]}$. s is the proper time along the chain of length L . $\vec{r}(s)$ is the three dimensional position vector at s while $\vec{u}(s) \equiv \frac{\partial \vec{r}(s)}{\partial s}$ is the unit bond vector at s . \mathcal{N} is the normalisation constant. The dimensionless Hamiltonian can

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be written by $\mathcal{H}[\vec{r}, \vec{u}, W] = \int_0^L ds [H(s) + V_{AT}(s)]$ with the bending $H(s) = \frac{l}{2} \left| \frac{\partial}{\partial s} \vec{u}(s) \right|^2$ and the attraction $V_{AT}(s) = -W \int_0^s ds' \delta(\vec{r}(s) - \vec{r}(s'))$. l is the persistence length and W is a positive coupling constant of attraction between polymer segments. The thermodynamic β is implicit.

Our Hamiltonian with $|\vec{u}(s)|^2 = 1$ can be interpreted as the low energy theory of the $O(3)$ nonlinear sigma model on a line segment with the attractive potential. By minimizing the Hamiltonian, we obtain two types of classical solutions such as $\vec{u}(s) = \text{const.}$ (rod solution) or $\theta = \frac{\pi}{2}$ and $\varphi_u = as + b$ (toroid solution) with constant a, b . Introducing the conformation parameter $c \equiv \frac{W}{2l} \left(\frac{L}{2\pi} \right)^2$, we obtain the energy level: $\mathcal{H}_c(a, l, L, W) = WL \left[\frac{x^2}{4c} + \frac{1}{2x} [x]([x] + 1) - [x] \right]$ where $x \equiv \frac{aL}{2\pi}$, $[x] \equiv N$ is the winding number of the chain. Note that the chain with zero winding number is termed “whip state,” whereas the chain with non-zero winding number is called “toroid state”. By plotting the energy for different values of c , we find that at the critical value of $c = \frac{1}{2}$, the whip phase to whip-toroid co-existence phase transition would occur. At $c = \frac{27}{16}$, when the energy of the $N = 1$ stable toroid state balances with the $x = 0$ whip state, the whip-dominant to toroid-dominant phase transition may occur. Due to the energy barrier between these (meta-)stable states, the conformational transition is first order. Using classical solutions, we also construct the low-energy effective Green function, in a perturbative way, which describes possible conformations such as tadpole or multi-tori.

Next, we consider the finite size effect and predict toroidal properties, which are successfully compared to experimental results of DNA condensation. We then show how different microscopic interactions between chain segments can affect the physical properties of the toroid such as mean toroidal and cross sectional radii. For different interaction potentials, we derive the modified toroidal energy functions. Analyzing them we obtain analytic expressions for the toroidal mean and cross section radii of the dominant toroid states. We find that, depending on the form of interactions, they show qualitatively different scaling behaviours. For instance, the mean radius of the toroid ground state scales as $r_c \sim L^{\nu(N_c)}$ where $\nu(N_c)$ is the exponent as a function of the dominant toroid winding number N_c . In the asymptotic limit ($N_c \rightarrow \infty$), such exponents of the mean toroidal radii are categorized into three distinct species: $\nu = \frac{1}{5}$ for van der Waals type attractions, $\nu = -\frac{1}{3}$ for Coulomb type attractions, $\nu = -1$ for delta function type attractions. Striking feature is that for the intermediate winding number of $N_c = 100 \sim 400$ (realistic winding number of DNA toroids), we have $\nu \simeq 0$ for the Yukawa interaction with inverse screening length $\kappa = 0.5 \sim 1.0$, and $\nu = 0.1 \sim 0.13$ for van der Waals type interaction. These could explain an experimentally well know observation that $r_c \sim L^\nu$ with $\nu \simeq 0$.

References

- [1] Y. Ishimoto, N. Kikuchi, cond-mat/0507477 (2005), cond-mat/0512092 (2006).
- [2] Y. Ishimoto, N. Kikuchi, to appear (2006).