ICFP M2 – Selected Topics in Statistical Field Theory
TD n$^{\text{o}}$ 3 – Filaments & Polymers

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A – Worm-Like Chain: model building

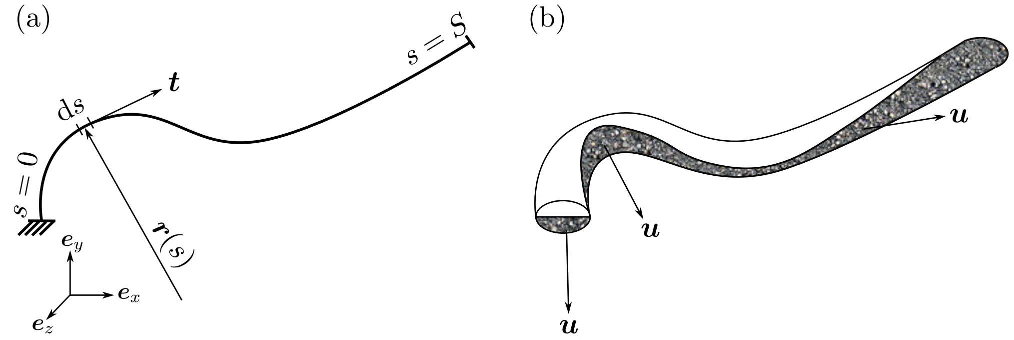

Figure 1: (a) Inextensible filament. (b) Asymmetric inextensible filament.

Consider the inextensible filament represented in Fig. 1(a), the position of which is given by the 3-dimensional vector $\boldsymbol{r}(s)$ where $s \in [0, S]$ is the curvilinear abscissa. The Landau-Ginzburg Hamiltonian reads

$$\mathcal{H}[\boldsymbol{r}] = \int_0^S \mathrm{d}s\ \mathcal{L}_0[\boldsymbol{r}(s)] \cancel{+\mathcal{H}_{\mathrm{int}}[\boldsymbol{r}]}\,,$$

where $\mathcal{L}_0[\boldsymbol{r}(s)]$ is a non-interacting local energy density and $\mathcal{H}_{\mathrm{int}}[\boldsymbol{r}]$ collects the local and non-local interactions that we hereby neglect. Note that, due to the inextensibility of the filament, the field $\boldsymbol{r}(s)$ is constrained by the relation $|\mathrm{d}\boldsymbol{r}/\mathrm{d}s| = 1$.

(1) Using the symmetries of the system, propose an expression for $\mathcal{L}_0[\boldsymbol{r}(s)]$. What is the most-likely configuration?

(2) When the filament is pulled at one end by a force $f\boldsymbol{e}_x$, an external potential $-fL_x$ has to be added to the Landau-Ginzburg Hamiltonian, where $L_x \equiv \boldsymbol{r}(S) \cdot \boldsymbol{e}_x$ is the projected total length. Let us consider the regime of strong enough forces, when the filament is mostly aligned along $\boldsymbol{e}_x$. Show that the constraint on $\boldsymbol{r}(s)$ can be eliminated by working with the two-dimensional field $\boldsymbol{T}(s) \equiv t_y(s)\boldsymbol{e}_y + t_z(s)\boldsymbol{e}_z$ where $\boldsymbol{t} \equiv \mathrm{d}\boldsymbol{r}/\mathrm{d}s$. Write down the corresponding Landau-Ginzburg Hamiltonian and make the connection with an $O(N)$ model. Compute the typical angle $\bar{\theta} \equiv \sqrt{\langle \theta^2 \rangle}$ where $\sin\theta \sim \theta \sim t_y$.

(3) Let us now consider the case of an asymmetric filament which can twist around $\boldsymbol{t}$, as represented in Fig. 1(b). Propose an expression for $\mathcal{L}_0$.

B – Flexible polymers: ideal chain

Let us now consider an ideal flexible polymer in d-dimensional space, composed of $N \gg 1$ monomers of size a, and described by the non-interacting Ginzburg-Landau Hamiltonian

$$\mathcal{H}[\boldsymbol{r}] = \int_0^N \mathrm{d}s \, \frac{1}{2a^2} \dot{\boldsymbol{r}}(s)^2 \, .$$

Note that, contrary to the previous worm-like chain, the field $\boldsymbol{r}(s)$ is not constrained. Let us study this simple Gaussian theory by means of a renormalization group approach.

(1) Discuss why this theory is the one of a random walk. What is the most-likely configuration? Estimate rapidly the scaling exponent ν defined as $\mathcal{R}_{\mathrm{g}} \sim N^{\nu}$ where $\mathcal{R}_{\mathrm{g}}$ is the radius of gyration of the polymer.

(2) Coarse graining. Introducing the Fourier modes *via* $\boldsymbol{r}(s) = \sum_k \boldsymbol{r}(k) \mathrm{e}^{\mathrm{i}ks}$, write down the partition function $\mathcal{Z}$ by separating the fluctuations into two components as, $\boldsymbol{r}(k) = \bar{\boldsymbol{r}}(k)$ for $0 < k < \Lambda/b$ and $\boldsymbol{r}(k) = \tilde{\boldsymbol{r}}(k)$ for $\Lambda/b < k < \Lambda$. Write down the coarse-grained Hamiltonian $\overline{\mathcal{H}}[\bar{\boldsymbol{r}}]$.

(3) Rescaling. Restore the cutoff Λ by setting $k = b^{-1}k'$. Express the new (effective) monomer size $\bar{a}$ in terms of the original a.

(4) Amplify the field $\bar{\boldsymbol{r}} = z\boldsymbol{r}'$ with $z = b^D$ where D has still to be determined, and derive the flow equation for the parameter a by setting $b = \mathrm{e}^l$ and considering an infinitesimal δl. Give the condition on D to obtain a fixed point under RG.

C – Flexible polymers: real chain

Let us now consider the Edwards model where long-range hard-core repulsive interactions are added to the ideal chain:

$$\mathcal{H}[\boldsymbol{r}] = \int_0^N \mathrm{d}s \, \frac{1}{2a^2} \dot{\boldsymbol{r}}(s)^2 + \lambda \int_0^N \mathrm{d}s \int_0^N \mathrm{d}s' \, \delta^d(\boldsymbol{r}(s) - \boldsymbol{r}(s')) \, ,$$

with $\lambda > 0$. Let us perform a poor's man renormalization group analysis.

(1) Coarse graining and rescaling. Let us assume that $\overline{\mathcal{H}}[\bar{\boldsymbol{r}}]$ is well approximated by

$$\overline{\mathcal{H}}[\bar{\boldsymbol{r}}] = \int_0^{N/b} \mathrm{d}s \, \frac{1}{2\bar{a}^2} \dot{\bar{\boldsymbol{r}}}(s)^2 + \bar{\lambda} \int_0^{N/b} \mathrm{d}s \int_0^{N/b} \mathrm{d}s' \, \delta^d(\bar{\boldsymbol{r}}(s) - \bar{\boldsymbol{r}}(s')) \, .$$

Do you expect the effective characteristic length scale $\bar{a}$ to be larger or smaller than in the case of the ideal chain? Justify the following relations (guessed by P. G. de Gennes):

$$\bar{a} = a \, b^{1/2} \, (1 + H_b) \, , \tag{1}$$

$$\bar{\lambda} = \lambda \, b^2 \, (1 - K_b) \, , \tag{2}$$

where H_b and K_b are positive dimensionless functions of the dimensionless parameters $u \equiv \lambda / a^d$, b and d. Justify why $H_b \to 0$ when $u \to 0$.

(2) Amplify the field $\bar{\boldsymbol{r}} = z\boldsymbol{r}'$ with $z = b^D$ where D will be determined later, and derive the flow equations by relating the parameters at the n^{th} RG step, *i.e.* a_{n+1} and u_{n+1}, in terms of a_n and u_n.

(3) Identify the fixed points, a^* and u^*, and the related conditions on D. Discuss the stability of the fixed points and the RG flow.

(4) Scaling law for $\mathcal{R}_\text{g}$. Using dimensional analysis (*i.e.* Buckingham's π theorem), relate the radius of gyration $\mathcal{R}_\text{g}$ with the parameters a, u, and the number of monomers N. Repeat the dimensional analysis for $\mathcal{R}_\text{g}^{(n)}$, the radius of gyration after n RG steps, where n is large enough to ensure that the RG has converged to a fixed point [*i.e.* $(a, u) \to (a^*, u^*)$] and small enough to ensure a large number of effective monomers (*i.e.* $N/b^n \gg 1$). Deduce the universal scaling law for $\mathcal{R}_\text{g}$, and compute the scaling exponent ν defined as $\mathcal{R}_\text{g} \sim N^\nu$.

D – Challenge

The real polymer is now pulled with a force $f\boldsymbol{e}_x$. The force elongates the polymer along the x axis, but is assumed to be sufficiently weak such that it does not affect the local structure of the polymer. Hence, the RG equations on the (local) parameters a and u are unchanged. Repeating the RG and scaling analysis performed in Section B, show that the projected total length, $L_x \equiv \boldsymbol{r}(N) \cdot \boldsymbol{e}_x$, is governed by the following scaling law

$$\frac{L_x}{\mathcal{R}_\text{g}} = \Psi_\nu \left(\beta f / \mathcal{R}_\text{g} \right) , \tag{3}$$

where $\Psi_\nu(x)$ is a universal dimensionless function. Considering the regime of very weak forces, guess the behavior of $\Psi_\nu(x \ll 1)$. In the regime of relatively strong forces, one expects $L \propto N$. Deduce the behavior of $\Psi_\nu(x \gg 1)$.