ICFP M2 – SOFT MATTER PHYSICS
Tutorial 4. Renormalization along a macromolecule ($d = 4 - \epsilon$)

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The aim of this tutorial is to apply the renormalization principle to the case of polymer statistics without involving technical details. We consider a single chain of N monomers, each with size a, and we place ourselves in dimension d. We assume $N \gg 1$. The intermonomeric interaction is described by the Flory parameter χ, or equivalently via the excluded volume $v = a^d\,(1-2\chi)$ or the coupling constant $u = v/a^d$. For a single polymer chain in $d = 4-\epsilon$ dimensions ($\epsilon \ll 1$), we aim at characterizing the crossover onset between the ideal behaviour and non-ideal behaviour in good solvent.

I Elementary transformation

We introduce the integer g, such that $g \ll N$, and we perform an elementary "coarse-graining" transformation which consists of grouping consecutive monomers into larger subunits – each of them containing g monomers.

1 How many such subunits are present in the chain ?

2 What is the average size $a_1^{(0)}$ of a subunit in the ideal case where $v = 0$?

3 Discuss the qualitative effect of having $v > 0$ on the actual size a_1 of a subunit. We introduce the quantity $h = \left(a_1 - a_1^{(0)}\right)/a_1^{(0)}$; specify the sign and dependencies of h, and explain why $a_1 = a\sqrt{g}\,[1 + h(u, g)]$.

4 What is the excluded-volume parameter $v_1^{(0)}$ at the coarse-grained level in the ideal case ? For arbitrarily small v, what is the dominant behaviour ?

5 Discuss the qualitative effect of having a finite and positive v on the actual excluded-volume parameter v_1. We introduce the quantity $\ell = \left(v_1^{(0)} - v_1\right)/v_1^{(0)}$; specify the sign and dependencies of ℓ and give the general expression of v_1.

6 Provide the new coupling constant u_1 after coarse-graining and obtain the sign and dependencies of $k = \left(u_1^{(0)} - u_1\right)/u_1^{(0)}$.

II Iteration and fixed point

We now repeat p times the elementary transformation above to arrive at a coarse-grained polymer problem described by the couple (a_p, u_p).

1 Identify a critical dimension of space for this procedure and explain its meaning.

2 How many subunits are present in the chain at coarse-graining level p? How must p be chosen for the coarse-grained polymer problem to remain relevant?

3 What are the recursive relations between two successive coarse-graining levels?

4 We assume the problem to become scale invariant at large p. What are the implications on u_p, a_p/a_{p-1}, and the inter-unit behaviour? What equation fixes the renormalized coupling constant u^*?

III Scaling law for the chain size

1 By dimensional analysis, what is the general form of the end-to-end distance R in the initial problem?

2 Provide an equivalent expression for R after p coarse-graining steps.

3 In the scale-invariant asymptotic regime, prove the existence of a power-law behaviour of the type $R \sim N^\nu$.

4 Exhibit a general expression as well as a lower bound for ν.

5 What needs to be done in practice to calculate ν?

IV Development in $\epsilon = 4 - d$

We place ourselves near and below dimension $d = 4$. For that purpose, we introduce $\epsilon = 4 - d > 0$.

1 As $\epsilon \to 0$, what do we expect for the quantities k and h, the exponent ν, and the renormalized coupling constant u^*?

2 By doing a perturbation expansion in ϵ, and thus in the renormalized coupling constant $u^*(\epsilon)$, while neglecting the nearest-subunit interactions, Gabay and Garel managed to calculate :

$$h(u^*) \simeq \frac{4}{\pi^2 \epsilon} u^* \tag{1}$$

$$k(u^*) \simeq \frac{32}{\pi^2 \epsilon} u^* , \tag{2}$$

at lowest order in ϵ. What is the expansion of $u^*(\epsilon)$ at the lowest (non-vanishing) order in ϵ?

3 Estimate the exponent ν at linear order in ϵ. Extrapolate the result to $d = 3$; conclusion?