

Comment on “A simple model for DNA denaturation” by T. Garel, C. Monthus and H. Orland

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Garel, Monthus and Orland [1] (to be referred to as GMO) in a study of DNA denaturation transition argued that the effect of mutual repulsion of the two strands can be approximated by a long-range interaction. Such a replacement is unjustified and can lead to disastrous consequences.

The dimensionless Hamiltonian is

$$H = \sum_i^2 \int_0^N ds \frac{1}{2} \left(\frac{\partial \mathbf{r}_i(s)}{\partial s} \right)^2 + \int_0^N ds V(\mathbf{r}_{12}(s)) + H_{\text{ev}}, \quad (1)$$

$$H_{\text{ev}} = u_0 \int_0^N ds ds' \delta_\Lambda(\mathbf{r}_1(s) - \mathbf{r}_2(s')) \quad (2)$$

$$\approx \int_0^N ds \frac{\alpha_d}{|\mathbf{r}_{12}(s)|^{d-2}}, \quad (\text{by GMO}), \quad (3)$$

where $\mathbf{r}_i(s)$ is the d -dimensional position coordinate of a monomer point at a contour length s of chain i , each of length N , V is the base pairing interaction at the same contour length (“directed polymer” interaction), H_{ev} is the mutual excluded volume (ev) interaction represented by the $u_0 > 0$ term with $\delta_\Lambda(\mathbf{r})$ as the usual delta-function with an ultraviolet cut-off Λ in the reciprocal space. The thermodynamic properties come from the partition function $Z = \int \mathcal{D}\mathcal{R} e^{-H}$, where the integration is over the configurations of the polymers. Equation (3) is the replacement advocated by GMO, obtained by a partial sum over the polymer configurations given by the first term on the right-hand side of eq. (1). The base-pairing interaction $V(r)$ has just been added onto this effective repulsion in eq. (16) of ref. [1].

It is well-recognized that the self- and mutually avoiding chains can be described by the prevalent renormalization group approach which predicts that in the large-length-scale limit the chains are described [2] by the stable fixed point $u^* \sim \epsilon \equiv 4 - d$, where u is an appropriate running dimensionless variable. From a dimensional analysis point of view, $[u_0] = [\alpha_d] = L^{d-4}$, where L is a length scale but there is a major difference between the two terms in the renormalization group (RG) framework [3–5]. While the u_0 term flows under renormalization, thereby reaching a fixed point (f.p.) for $\epsilon > 0$, *i.e.*, $d < 4$, the singular α_d term *does not* get renormalized because of the analyticity of the RG transformation [3]. This tells us that for

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$\epsilon \rightarrow 0$ the renormalized dimensionless mutual avoidance, u , goes to zero (chains behave like noninteracting random walkers up to log corrections) but, on the contrary, α_4 does not vanish. In technical terms, α_4 remains *marginal* while u is a marginally *irrelevant* variable at $d = 4$. In fact α_4 leads to continuously varying exponents as GMO also rediscovered (see eq. (33) of ref. [1]). For $\epsilon > 0$, u reaches a f.p. but α *does not*. Therefore, eq. (3), *the replacement proposed by GMO, leads to a major contradiction*, if we do not want to discard RG.

Lastly, the effects of long-range interactions for directed polymers, as done in ref. [1], are already available in refs. [3–5].

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