# Relaxation of a one-dimensional bead-string model

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The one-dimensional (1d) bead-spring model, or 1d Rouse model, consists of $N$ monomers (beads) subject to thermal fluctuations and connected by massless springs. Monomers can thus be viewed as impenetrable random walkers (RWs) interacting through a nearest-neighbour harmonic potential. Here we consider a similar model in which the beads are connected by *strings* rather than by springs. Therefore, our model can be viewed as a modified 1d Rouse model where the harmonic potential is replaced by an extremely soft-hard potential: the square well. Note that the beads (RWs) can diffuse freely in 1d, except for the fact that they cannot cross nor separate from one another beyond a certain distance $\Delta$ ($\Delta$ is the string length or, equivalently, the width of the square-well). We are primarily interested in studying how this system relaxes to its equilibrium state.

It should be noted that our model progressively approaches a standard single-file model (with finite $N$) the larger $\Delta$ or the smaller $t$ becomes; in fact, for $\Delta^2/(4Dt) \to \infty$ (where $D$ is the RW diffusion constant), our model is just the single file model .

In order to obtain an approximate expression for the $N$-particle positional pdf, we make the following factorization ansatz:

$$p(x_1, \ldots, x_N, t; \Delta) = A \prod_{i=1}^{N} G(x_i, t) \prod_{i=1}^{N-1} R(x_{i+1} - x_i, \Delta)$$

where $A$ is the normalization constant, $G(x, t|x_0, t = 0)$ denotes the free-particle Green function (gaussian distribution) and $R(x, \Delta)$ is the rectangular (hat) function of width $\Delta$: $R(x, \Delta) = 1$ for $0 < x < \Delta$ and $R(x, \Delta) = 0$ elsewhere. The exclusion effects arising from the square well potential are accounted for by the hat function. For $\Delta \to \infty$, this ansatz becomes identical with the one used by Aslangul [1] to study the single-file model with a finite RW number $N$. Reduction of $p(x_1, \ldots, x_N, t; \Delta)$ by repeated integration yields the pdf for the position $x_i$ of the $i$-th RW. It turns out that it is possible to find approximate expressions for such pdfs and for the corresponding moments as power series of $\delta \equiv \Delta/(4Dt)^{1/2}$. We subsequently compare the dynamics of the beads predicted by our model (and their corresponding collective "polymer" dynamics) with the outcome of MC simulations. Our simulations show that, starting from a fully compressed polymer or a fully stretched polymer, the relaxation of the polymer length $L$ is well described by a Kohlrausch-Williams-Watts (KWW) law for short and intermediate times, at less for not too large values of $N$ (see Fig. 1). However, for very long times, our ansatz predicts that the $L$-relaxation to its equilibrium state follows the inverse power law $1/t$, which is in full contrast with the exponential decay exhibited by the 3d Rouse model. On the other hand, once the system has attained the equilibrium state, the diffusion constant of each bead (and thus of the polymer as a whole) can be shown to scale as $1/N$, as it is also the case in the 3d Rouse model [2]. It is possible to estimate the full equilibrium pdf for the polymer length $L$ by counting the number of microstates compatible with the equilibrium state. We have also found that the bead-string polymer is Hookean in the sense that the force required to change the equilibrium value of $L$ by an amount of $x$ is proportional to $x$. The elastic constant turns out to be proportional to $\Delta$ and, as in the 3d Rouse model, inversely proportional to $N$.

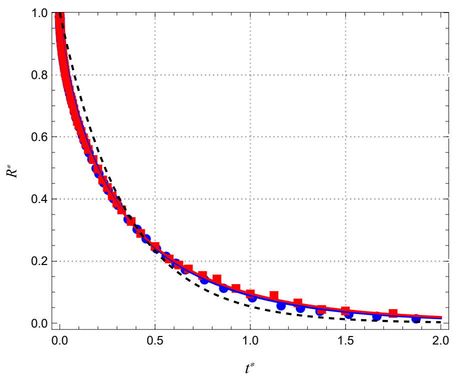


Fig. 1. Relaxation of the scaled relative polymer length $R^* \equiv |L(t) - L_{\text{eq}}|/|L(0) - L_{\text{eq}}|$ as a function of time $t^* = t/\tau$ with $\tau = \Delta^2/(4D)$. We consider both a fully compressed (circles) and a fully stretched (squares) initial condition. Solid lines represent a KWW relaxation law, $\exp(t/t_R)^\beta$, with $\beta \approx 3/4$ and $t_R \approx 1/3$ for both initial conditions. The dashed line is an exponential fit.

[1] Cl. Aslangul,*Classical diffusion of N interacting particles in one dimension: General results and asymptotic laws*, Europhysics Letters, **44** (3) 284–289 (1998).

[2] M. Rubinstein and R. H. Colby, *Polymer Physics* (OUP Oxford, 2003).