Datreat theory: ring2

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theory id-name: ring2
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 Dynamic scattering function for a polymer ring melt as developed in the PRL of S. Goossen
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Parameters(17):
  1: ampli     >      prefactor
  2: diff      > ABS: limiting diffusion (NMR value) in [A**2/ns]
  3: r021      > ABS: reference mean squared displacement at first transition point to medium timed diff.
  4: alpha     > ABS: sub-diffusion  exponent of SHORT time diffusion
  5: r022      > ABS: reference mean squared displacement at second transition point to D0 in [A**2]
  6: beta      > ABS: sub-diffusion  exponent of medium time diffusion
  7: a_cross   > ABS: transition exponent between short and long time diffusion (sharper kink for larger a)
  8: n         > INT: number of segments in one ring
  9: l         > ABS: effective segment length
 10: nue       > ABS: chain statistics exponent (nu=0.5 => random walk, Gaussian)
 11: wl4       > ABS: Rouse rate in [A**4/ns]
 12: pmin      > ABS: transition mode number between simple ring-Rouse and large p modification
 13: pwidth    > ABS: sharpness of transition
 14: f0        > ABS: prefactor f(p) limit for small p values (default 1)
 15: finf      > ABS: prefactor f(p) limit for large p values (default F=0.9??) transitin width is pwidth
 16: tauinf    > ABS: large p tau(p) = tauinf/p**pexinf
 17: pexinf    > ABS: large p tau(p) = tauinf/p**pexinf
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INPUT: Parameters that are extracted from the actual considered data records:
..there may be default assumptions, but better make sure that these parameters are set properly!
  1: q         > q
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OUTPUT: Parameters that are computed and added to the records parameters as information:
  1: Rg        > predicted ring radius of gyration
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cite:  S. Goossen et al., PRL 2014, 113, 168302 !
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Modified polymer ring structure factor with sublinear diffusion with **3 regimes**.

Diffusion factor:

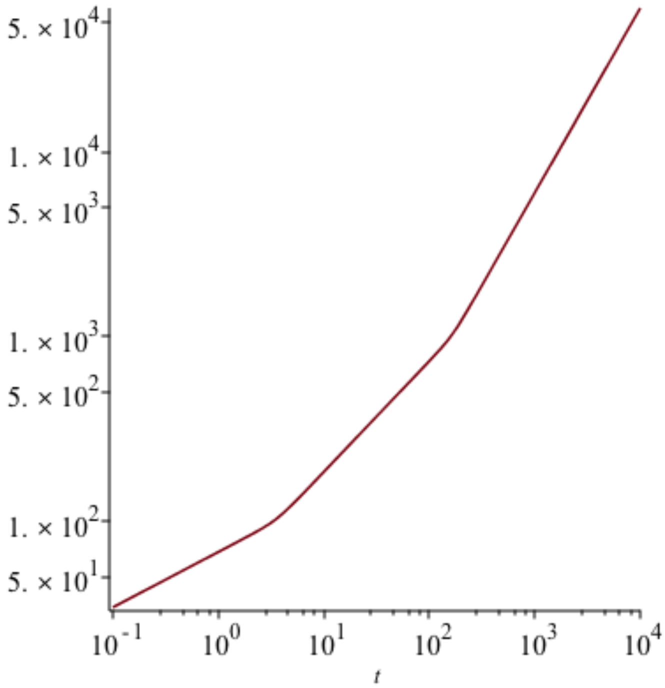
$$\exp\left(-\langle r^2(t)\rangle\, q^2/6\right)$$

with

$$\langle r^2(t)\rangle = \left[\left(e^{\frac{1}{\beta}\left((-\alpha+\beta)\ln\left(\frac{r_1{}^2}{r_2{}^2}\right)+\beta\,\alpha\left(-\ln\left(\frac{r_2{}^2}{6D_0}\right)\right)\right)} r_2{}^2 t^{\alpha}\right)^a + \left(e^{\left(-\ln\left(\frac{r_2{}^2}{6D_0}\right)\right)\beta} r_2{}^2 t^{\beta}\right)^a + \left(6D_0\, t\right)^a\right]^{1/a}$$

describing sublinear-linear center-of-mass diffusion with a normal long time diffusion constant D_0 and a sublinear diffusion with exponent α until the first kink at the msd level r_1^2 and with an exponent β until the second kink at the msd level r_2^2. The sharpness of the transitions is controlled by a, the larger the value the sharper is the transition.
Intended use assumes that $0 < \alpha < \beta < 1$ and $r_1^2 < r_2^2$. This is NOT automatic !

The figure shows $\langle r^2(t)\rangle$ for $r_1^2 = 100\text{Å}^2$; $r_2^2 = 1000\text{Å}^2$; $\alpha = 0.3$ and $\beta = 0.6$ $(a = 20)$.



Ring structure factor (without diffusion):

$$S(q,t) = \frac{1}{N}\sum_{i,j}^{N} \exp\left[\frac{(ql)^2}{6}\left(|i-j|\{N-|i-j|\}/N\right)^{2\nu} - B_{i,j}(t)\right]$$

with

$$B_{i,j}(t) = A\sum_{p,even}\frac{F(p)}{p^2}\cos(p\pi[i-j]/N)\,[1-\exp(-t\Gamma(p))]$$

with the mode p dependent amplitude $F(p)$ and rate $\Gamma(p)$ parameters.
Here

$$A = 2N^{2\nu}(lq)^2/(3\pi^2)$$

and

$$F(p) = F_0[1-T_f(p)] + F_\infty T_f(p)$$

and

$$\Gamma(p) = [1-T_f(p)]p^2/\tau_R + T_f(p)p^\mu/\tau_\infty$$

the transition function is

$$T_f(p) = \{1+\exp([p-p_{min}]/p_{width})\}^{-1}$$

the Rouse time is computed as

$\tau_R = N^2/(W\pi^2)$ with $W = Wl^4/l^4$

Problems (scaling behavior)

The above formulation (and also the following) exhibits only works approximately if we use a (N, l) scaling: $N \to \eta N$ and $l \to l/\eta^{\nu}$!.

In addition I guess the following modification (motivated by the old expression for Zimm in the norbornene dynamics paper, sources for that were Doi-Edwards and papers of Harnau and Winkler (I would have to rework the matter but changes made in analogy to that are shown below) should be made.

$$S(q,t) = \frac{1}{N}\sum_{i,j}^{N} \exp\left[\frac{(ql)^2}{6}\left(|i-j|\{N-|i-j|\}/N\right)^{2\nu} - B_{i,j}(t)\right]$$

with

$$B_{i,j}(t) = A\sum_{p,even}\frac{F(p)}{p^{1+2\nu}}\cos(p\pi[i-j]/N)\,[1-\exp(-t\Gamma(p))]$$

with the mode p dependent amplitude $F(p)$ and rate $\Gamma(p)$ parameters.

Here

$$A = 2N^{2\nu}(lq)^2/(3\pi^2)$$

and

$$F(p) = F_0[1-T_f(p)] + F_\infty T_f(p)$$

and

$$\Gamma(p) = [1-T_f(p)]p^{4\nu}/\tau_R + T_f(p)p^{\mu}/\tau_\infty$$

the transition function is

$$T_f(p) = \{1+\exp([p-p_{min}]/p_{width})\}^{-1}$$

the Rouse time is computed as

$\tau_R = N^2/(W\pi^2)$ with $W = Wl^4/l^4$

Scaling works approximately with $N \to \eta N$ and $l \to l/\eta^{\nu}$!

This formulation (still missing possible modifications for the p^4-terms) is implemented as theory **ring2a.**

Parameter correspondences

Observe units, if not other specified: Angstroems and nano-seconds

$\text{diff} \to D_0$
$\text{r021} \to r_1^2$
$\text{alpha} \to \alpha$
$\text{r022} \to r_2^2$
$\text{beta} \to \beta$
$\text{a\_cross} \to a$
$\text{n} \to N$

l $\rightarrow l$
nue $\rightarrow \nu$
wl4 $\rightarrow Wl^4$
pmin $\rightarrow p_{min}$
pwidth $\rightarrow p_{width}$
f0 $\rightarrow F_0$
finf $\rightarrow F_\infty$
tauinf $\rightarrow \tau_\infty$
pexinf $\rightarrow \mu$