Effect of bending stiffness on a homopolymer inside a spherical cage

Martin Marenz

Institute for Theoretical Physics
University of Leipzig

Outline

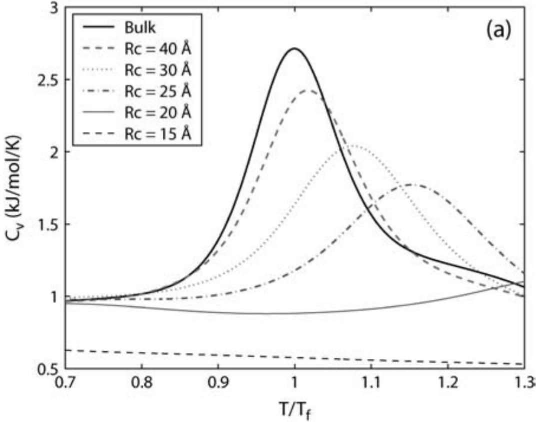


Figure : Effect of a confining potential on the melting of protein SH3.[1]

[1] N. Rathore et al., Biophys. J. **90**, 2006

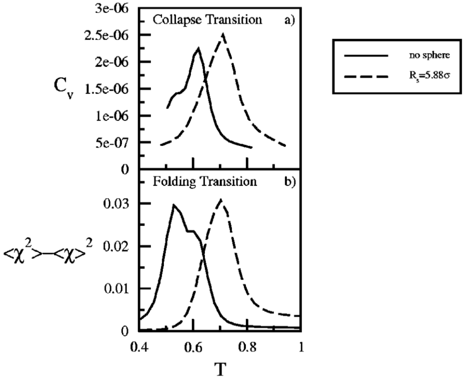
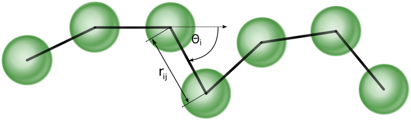


Figure : Effect of a confining potential to a β-barrel protein.[2]

[2] M. Friedel et al., J. Chem. Phys. **118**, 2003

Bead-Stick Homopolymer

bulk case

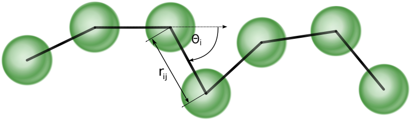


- $H = E_{\text{bend}} + E_{LJ}$
  - $E_{\text{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right)$
  - $E_{\text{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$

κ

With κ one can adjust the stiffness of the polymer.

bulk case

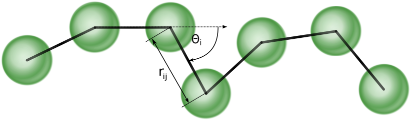


- $H = E_{\text{bend}} + E_{LJ}$
  - $E_{\text{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}}\right)$
  - $E_{\text{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$

κ

With κ one can adjust the stiffness of the polymer.

bulk case

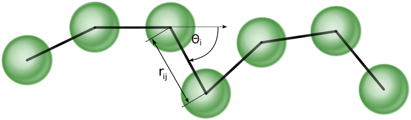


- $H = E_{\mathrm{bend}} + E_{LJ}$
  - $E_{\mathrm{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}}\right)$
  - $E_{\mathrm{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$

κ

With κ one can adjust the stiffness of the polymer.

bulk case

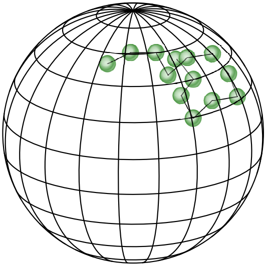


- $H = E_{\text{bend}} + E_{LJ}$
  - $E_{\text{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}}\right)$
  - $E_{\text{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$

κ

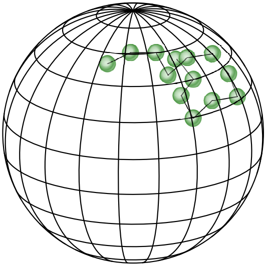
With κ one can adjust the stiffness of the polymer.

constrained case



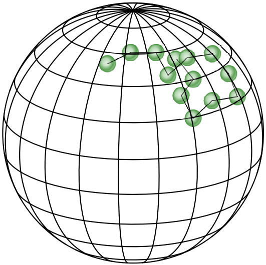
- $H = E_{\text{bend}} + E_{LJ} + V_{\text{Sphere}}$
  - $E_{\text{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$
  - $E_{\text{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} (\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}})$
  - $V_{\text{Sphere}} = \begin{cases} 0 & \text{if all } |r_i| < R_S \\ \infty & \text{if any } |r_i| \geq R_S \end{cases}$

constrained case



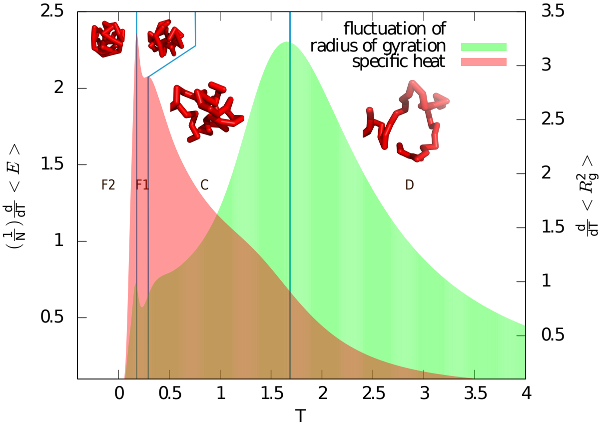
- $H = E_{\mathrm{bend}} + E_{LJ} + V_{\mathrm{Sphere}}$
  - $E_{\mathrm{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$
  - $E_{\mathrm{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} (\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}})$
  - $V_{\mathrm{Sphere}} = \begin{cases} 0 & \text{if all } |r_i| < R_S \\ \infty & \text{if any } |r_i| \geq R_S \end{cases}$

constrained case



- $H = E_{\mathrm{bend}} + E_{LJ} + V_{\mathrm{Sphere}}$
  - $E_{\mathrm{bend}} = \kappa \sum_{i=1}^{N-2} (1 - \cos \Theta_i)$
  - $E_{\mathrm{LJ}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} (\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}})$
  - $V_{\mathrm{Sphere}} = \begin{cases} 0 & \text{if all } |r_i| < R_S \\ \infty & \text{if any } |r_i| \geq R_S \end{cases}$

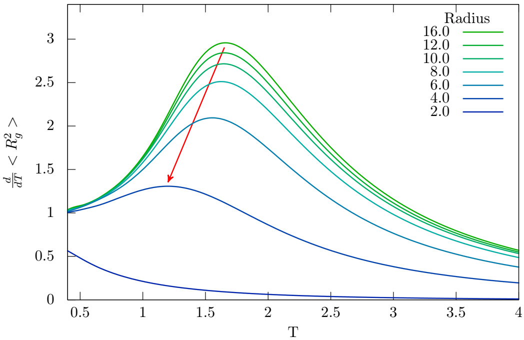
flexible polymer ($\kappa = 0.00$)



Derivative of the energy and radius of gyration of a homopolymer (28 monomers) with $\kappa = 0.00$. Lines indicate pseudo phase transitions between desorbed (D), collapsed (C) and frozen (F1, F2) phases.

Radius	T_c
Free	1.656(3)
20	1.655(2)
16	1.659(2)
12	1.651(2)
10	1.645(2)
8	1.626(2)
6	1.555(2)
4	1.200(2)

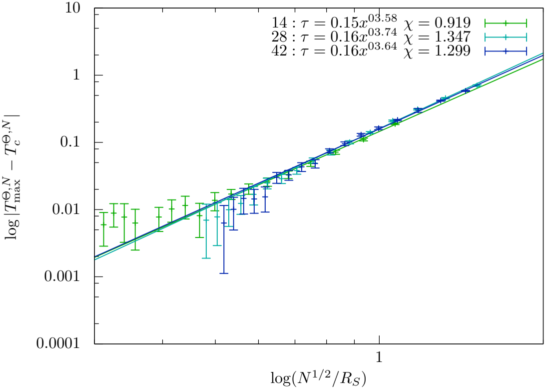
radius dependency of the collapse transition



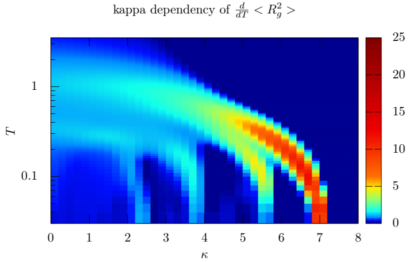
- For $\kappa = 0.00$ collapse transition shifts to lower temperatures.
- Freezing transitions hardly change transition temperature.

For $\kappa = 0.00$ all points fall into one common master curve.

$$|T_{\max}^{\Theta,N} - T_c^{\Theta,N}| \propto \left(\frac{N^{\frac{1}{2}}}{R_S}\right)^{\gamma} \text{ with } \gamma = 3.65(15)$$

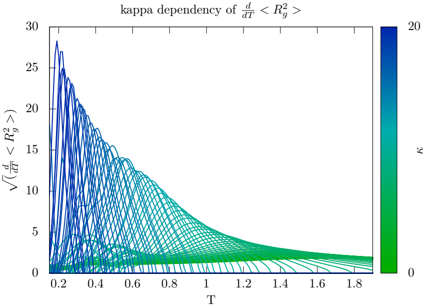


Effect bending stiffness

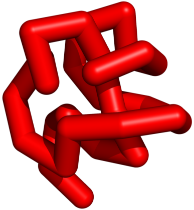


Contour plot of $\frac{d}{dT}\left\langle R_g^2 \right\rangle$ for a free 14mer. Bright colours indicate high thermal activity and thus the location of pseudo phase transitions. Detailed overview of a similar model can be found in the work of D .T. Seaton et al., Phys. Rev. Lett. **110**, 2013.

Plot of $\frac{d}{dT}\left\langle R_g^2 \right\rangle$ for several free 28mer with different κ. The peak in $\frac{d}{dT}\left\langle R_g^2 \right\rangle$ denotes the location of the pseudo phase transition. For higher bending stiffness the peak goes to lower temperatures.



Collapse transition at $\kappa = 0.00$

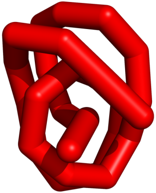


(a) $T = 0.51$

$\leftrightarrow$

(b) $T = 3.00$

Collapse transition at $\kappa = 4.00$

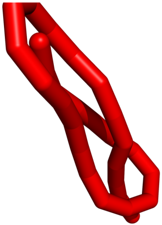


(a) $T = 0.61$

$\leftrightarrow$

(b) $T = 3.00$

Collapse transition at $\kappa = 8.00$

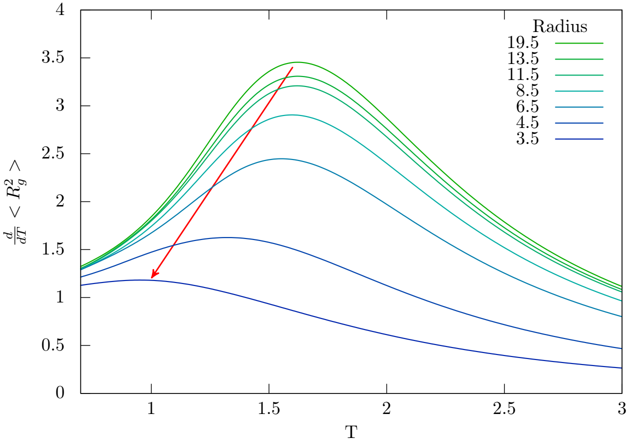


(a) $T = 0.61$

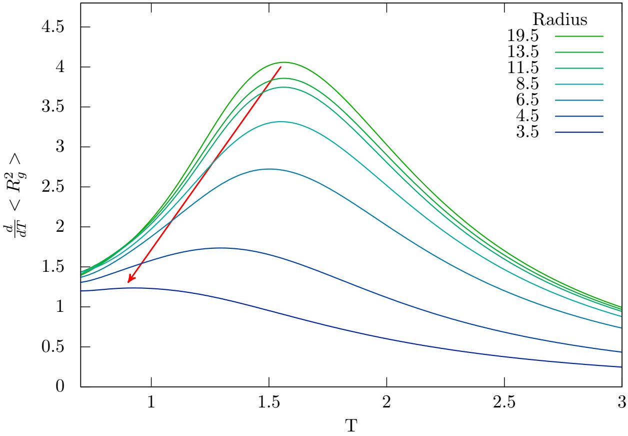
$\leftrightarrow$

(b) $T = 3.00$

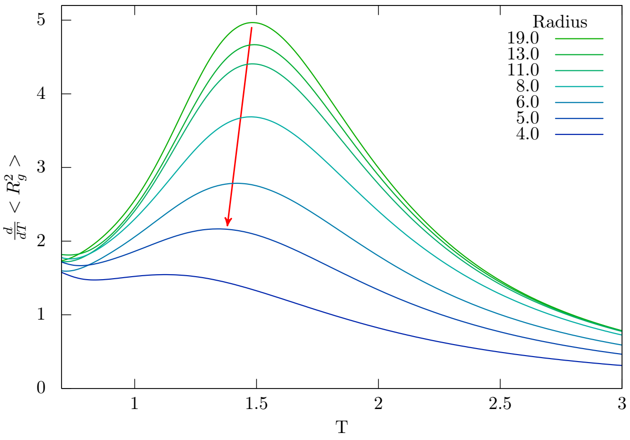
$\frac{d}{dT}\left\langle R_g^2 \right\rangle$ of a 28mer for $\kappa = 1.00$



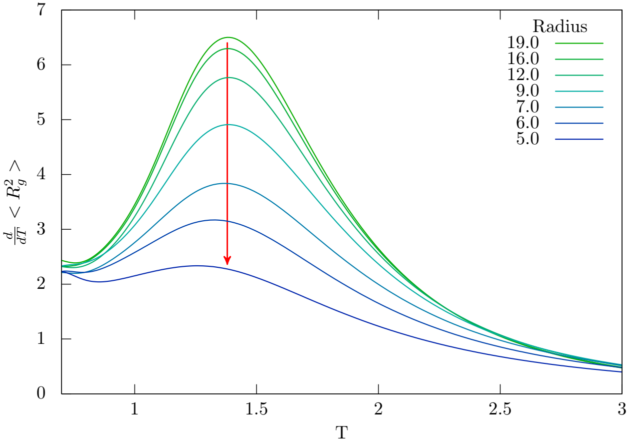
$\frac{d}{dT}\left\langle R_g^2 \right\rangle$ of a 28mer for $\kappa = 2.00$



$\frac{d}{dT}\left\langle R_g^2 \right\rangle$ of a 28mer for $\kappa = 3.00$

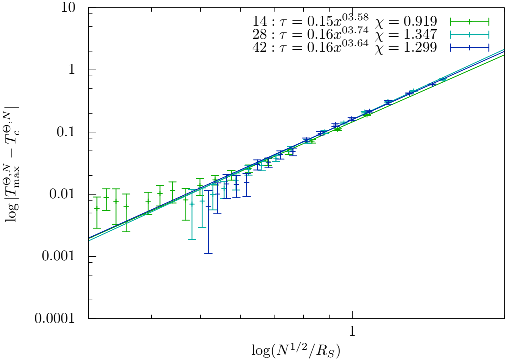


$\frac{d}{dT}\left\langle R_g^2 \right\rangle$ of a 28mer for $\kappa = 4.00$



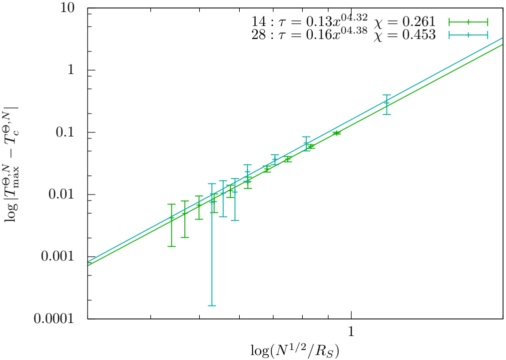
κ	$\gamma(R_g)$
0.00	3.65(15)
1.00	4.34(16)
2.00	4.29(16)
3.00	4.81(18)
4.00	–

$\kappa = 0.00$



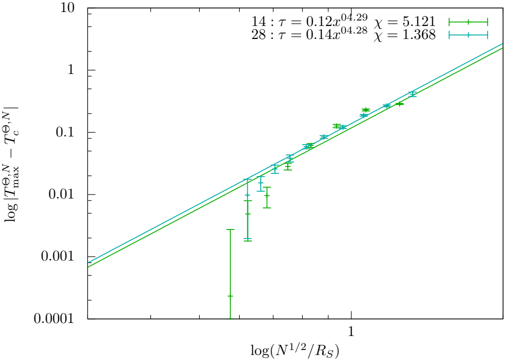
κ	$\gamma(R_g)$
0.00	3.65(15)
1.00	4.34(16)
2.00	4.29(16)
3.00	4.81(18)
4.00	–

$\kappa = 1.00$

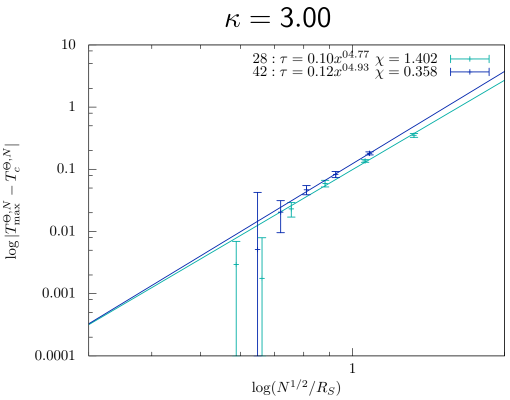


κ	$\gamma(R_g)$
0.00	3.65(15)
1.00	4.34(16)
2.00	4.29(16)
3.00	4.81(18)
4.00	–

$\kappa = 2.00$



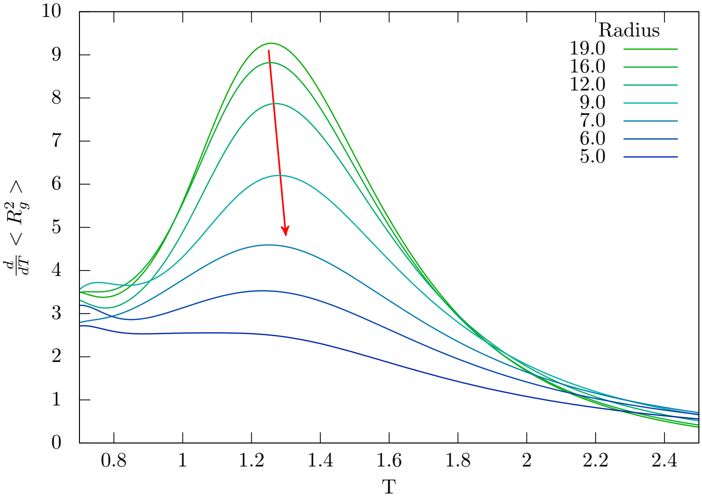
κ	$\gamma(R_g)$
0.00	3.65(15)
1.00	4.34(16)
2.00	4.29(16)
3.00	4.81(18)
4.00	–



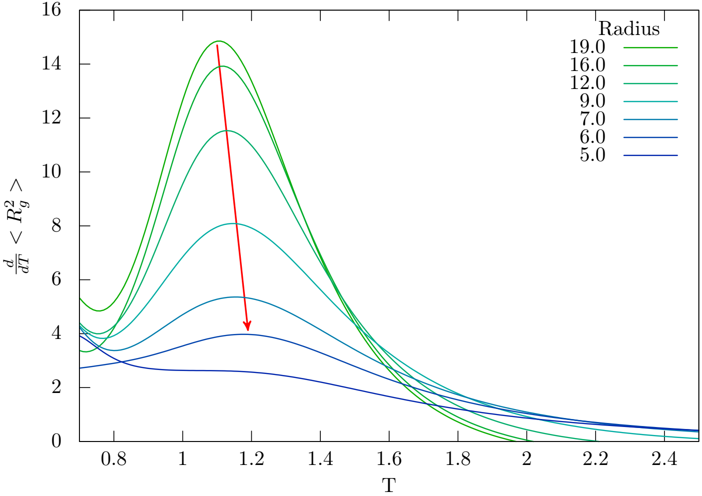
κ	$\gamma(R_g)$
0.00	3.65(15)
1.00	4.34(16)
2.00	4.29(16)
3.00	4.81(18)
4.00	–

?

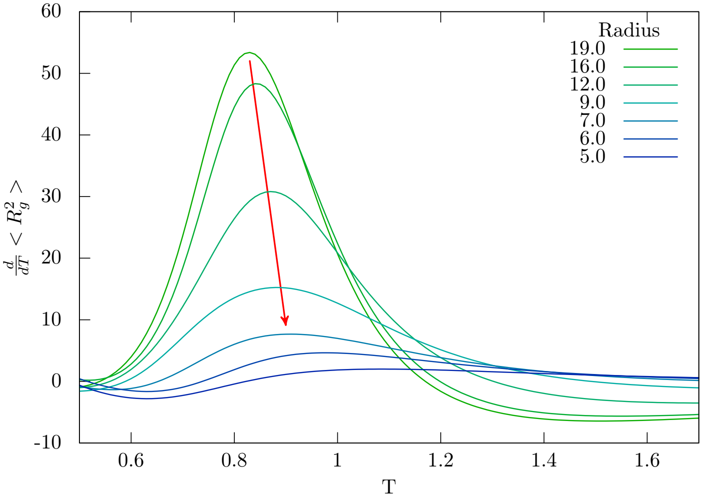
$\frac{d}{dT} < R_g^2 >$ of an 28mer with $\kappa = 5.00$



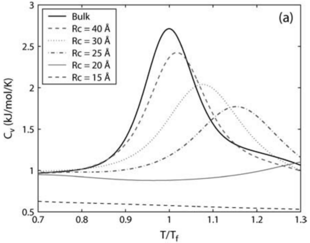
$\frac{d}{dT} < R_g^2 >$ of an 28mer with $\kappa = 6.00$

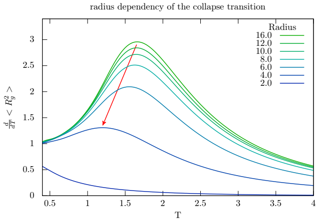


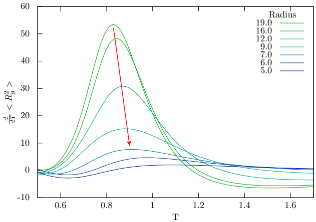
$\frac{d}{dT} < R_g^2 >$ of an 28mer with $\kappa = 8.00$



Summary


Bulk
Rc = 40 Å
Rc = 30 Å
Rc = 25 Å
Rc = 20 Å
Rc = 15 Å
(a)
Cv (kJ/mol/K)
T/Tf


radius dependency of the collapse transition
Radius
16.0
12.0
10.0
8.0
6.0
4.0
2.0
T


Radius
19.0
16.0
12.0
9.0
7.0
6.0
5.0
T