randcopoly

This folder contains Matlab scripts to calculate and plot the structure factor and spinodal decomposition of an A-B semiflexible random copolymer based on a polymer field theoretic formulation [1].

For a given chemical correlation λ, number of monomers N, and monomer length (in Kuhn segments) N_M, this package calculates the melt structure factor (density-density correlations), the spinodal Flory-Huggins parameter χ_S, and critical wavemode of phase segregation q^*. The folder "functions" provides functions `s2invwlc` and `kmaxwlc` that calculate the structure factor of semiflexible (wormlike chain model) random copolymer (`s2invwlc`) and the critical wavemode (location of peak) in the structure factor (`kmaxwlc`). Similar codes can be found for flexible random copolymers based on the Gaussian chain model (`s2invgc` and `kmaxgc`) and for perfectly rigid random copolymers (`s2invrr` and `kmaxrr`).

This package was developed by Shifan Mao, Quinn MacPherson, and Andrew Spakowitz [1]

Installation

Open Matlab and change directory to `randcopoly` . Then add the folder `functions` to path with

```
addpath('functions')
```

Example Usage

Here is an example of using the package to calculate the structure factor (density-density correlations) of rigid, anti-correlated random copolymers.

```
% Example 1: plot density-density correlations vs wavevector at different CHI
N=100;  % total of 100 monomers
NM=0.1; % each monomer has 0.1 Kuhn steps
LAM=-0.75; % anti-correlated random copolymer
FA=0.5;    % equal chemical composition

% find spinodal CHIS
[kval,sval]=kmaxwlc(N,NM,FA,LAM);
CHIS=0.5*sval;
CHI=CHIS*[0 0.2 0.4 0.6 0.8];  % range of CHI values (scaled by spinodal)

RM=sqrt(r2wlc(NM));  % end-to-end distance of a monomers
K0=1e-2;  % minimum wavevector
KF=1e2;    % maximum wavevector
NK=201;  % number of wavevectors
K=transpose(logspace(log10(K0),log10(KF),NK))/RM;

% evaluate s2inv
[SINV]=s2invwlc(N,NM,FA,LAM,K);
figure;hold
for I=1:length(CHI)
    COL=(I-1)/(length(CHI)-1);
    loglog(RM*K,1./(-2*CHI(I)+SINV),'-','LineWidth',2,'Color',[COL 0 1-COL])
end
xlabel('R_Mq');ylabel('S(q)');box on;
set(gca,'xscale','log');set(gca,'yscale','log');axis([K0 KF 1e-2 1e1])
```
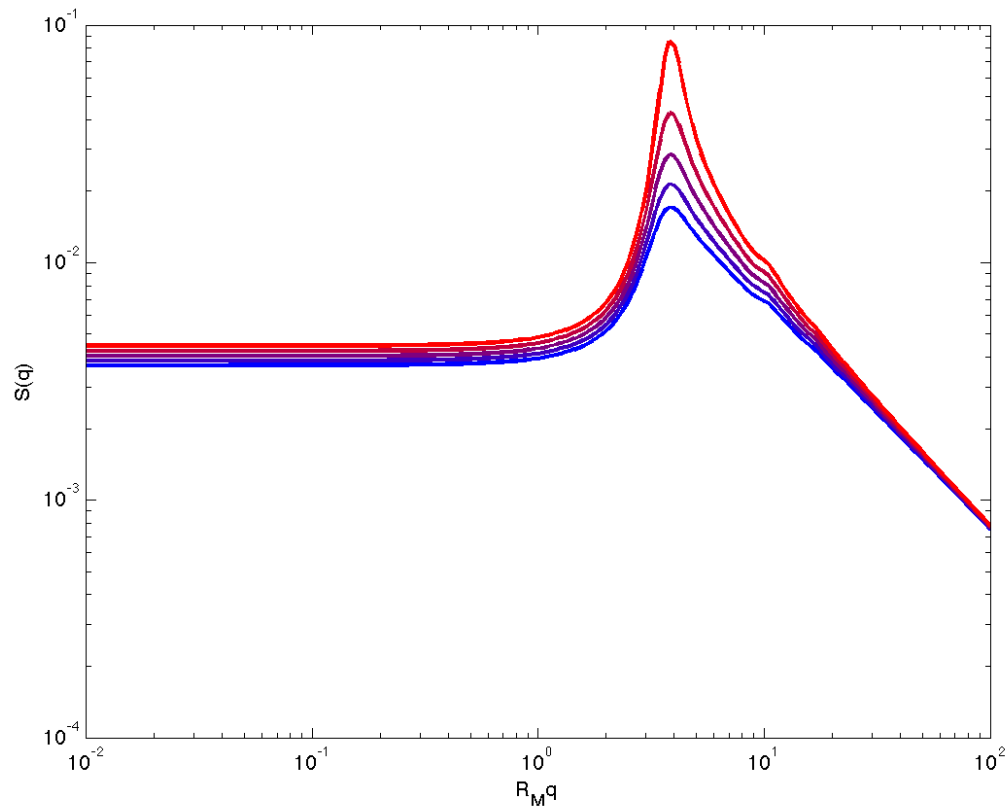
As another example, the spinodal (order-disorder transition) of flexible random copolymers can be calculated as follows

```
% Example 2: find spinodal vs. fraction of A monomers
N=100;  % total of 100 monomers
NM=10; % each monomer has 10 Kuhn steps
LAM=0; % ideal random copolymer

FAV = linspace(0.1,0.9,101);
CHIS = zeros(length(FAV),1);
for ii = 1:length(FAV)
    FA = FAV(ii);
    [kval,sval,d2gam2]=kmaxwlc(N,NM,FA,LAM);
    CHIS(ii)=0.5*sval;  % spinodal
end
figure;plot(FAV,CHIS*NM,'k-','linewidth',2)
xlabel('f_A');ylabel('\chi_S v N_M')
```
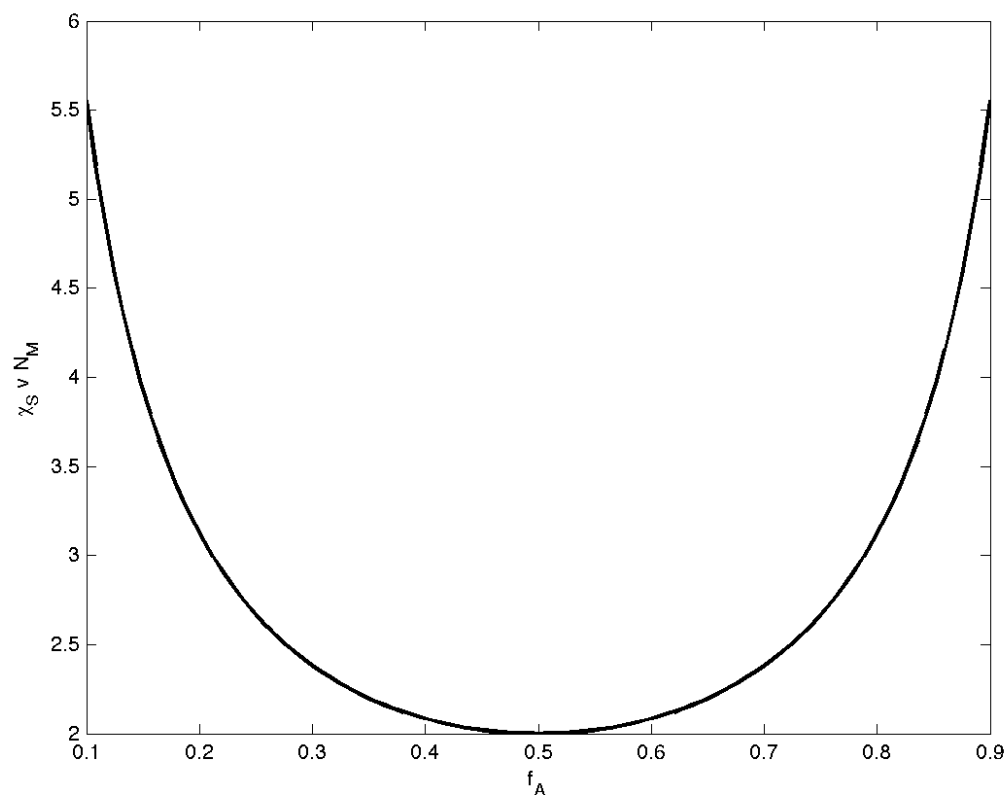
[1] S. Mao, Q. J. MacPherson, S. He, E. Coletta, and A. J. Spakowitz. "Impact of conformational and chemical correlations on microphase segregation in random copolymers," *Macromolecules* in submitted (2015).