

README.md - Grip

randcopoly

This is a package that uses polymer field theory to find phase behavior of random copolymers. The polymers are modeled as wormlike chains. Given chemical correlation λ , number of monomers N , and monomer rigidity NM , it calculates

- structure factor (density-density correlation)
- phase transition Flory-Huggins parameter
- critical wavenumber of phase segregation

The package provides two of functions `s2invwlc()` and `kmaxwlc()`. `s2invwlc()` calculates the structure factor of random copolymers in the homogeneous phase. `kmaxwlc()` finds the critical wavenumber (location of peak) in the structure factor. Similar codes can be found for Gaussian chain (`s2invgc()` and `kmaxgc()`) and perfectly rigid rod (`s2invrr()` and `kmaxrr()`).

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

Installation

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

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

Example Usage

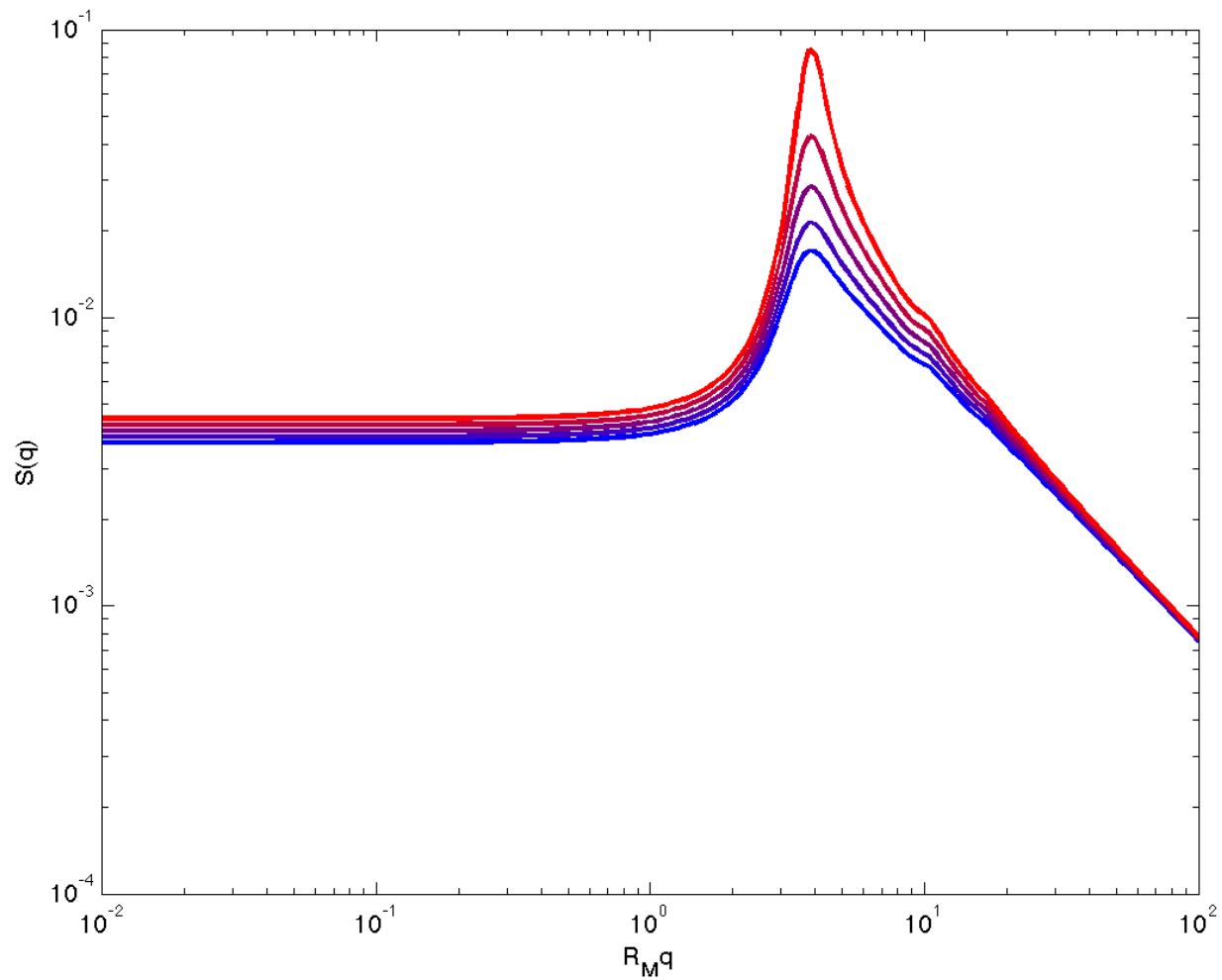
Here is an example of using the code to calculate the structure factor (density-density correlations) of rigid, anti-correlated random copolymers.

```
% 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];

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;

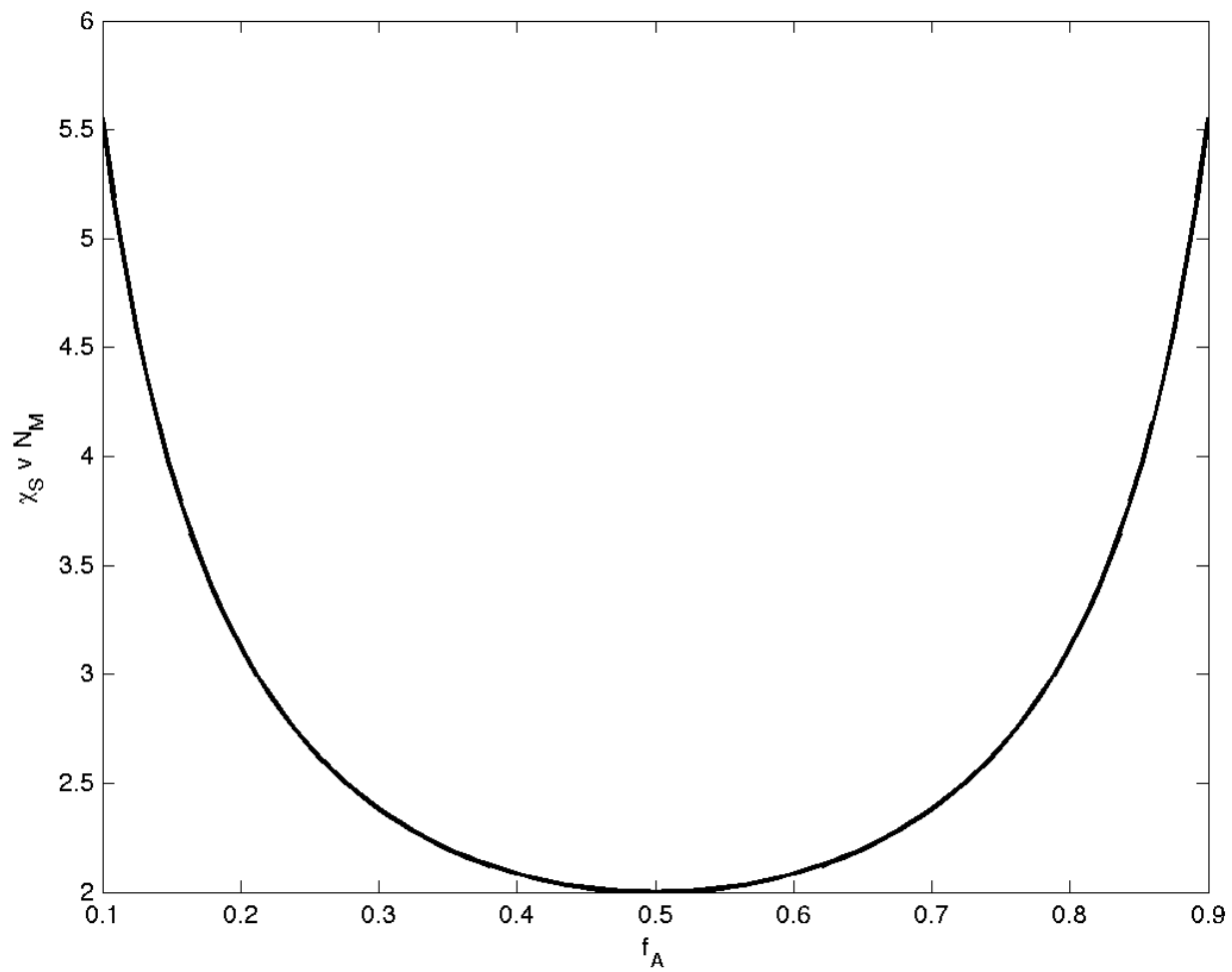
% evaluate s2inv
[SINV]=s2invwlc(N,NM,FA,LAM,K);
figure;hold
for I=1:length(CHI)
    COL=(I-1)/(length(CHI)-1);
    loglog(RM*K,1./(-2*CHI(I)+SINV),'-','LineWidth',2,'Color',[COL 0 1-COL])
end
xlabel('R_Mq');ylabel('S(q)')
set(gca,'xscale','log');set(gca,'yscale','log');
axis([K0 KF 1e-2 1e1])
```



As another example, the spinodal (order-disorder transition) of flexible random copolymers

```
% 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] Mao, S and MacPherson, Q and He, S and Coletta, E and Spakowitz, A "Impact of conformational and chemical correlations on microphase segregation in random copolymers". *Macromolecules in review* (2016)