Finite size scaling II

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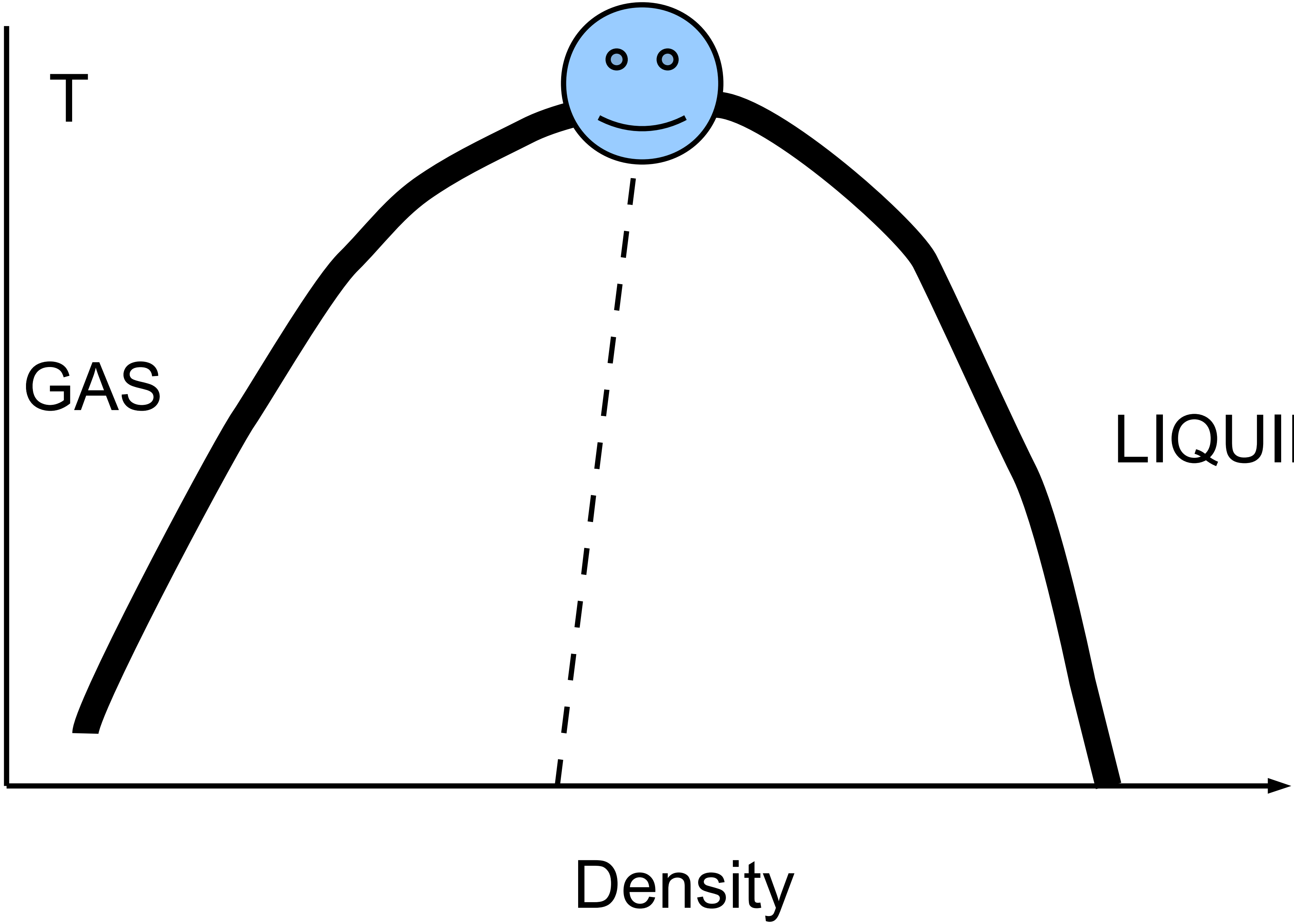
The block analysis (coarse-graining) technique

- Simple to use.
- Ordinary NVT MD or MC suffices.
- Get phase boundaries i.e. coexistence densities, compressibilities of coexistent phases.
- Also get surface tensions, Binder cumulants, scaling functions, scaling fields and scaling exponents.
- Can be generalized to obtain elastic constants etc. (generalized susceptibilities).


T
GAS
LIQUID
Density

The Ising model and lattice gas

The energy of the Ising model is defined to be:

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j ; S_i = \pm 1$$

For each pair, if

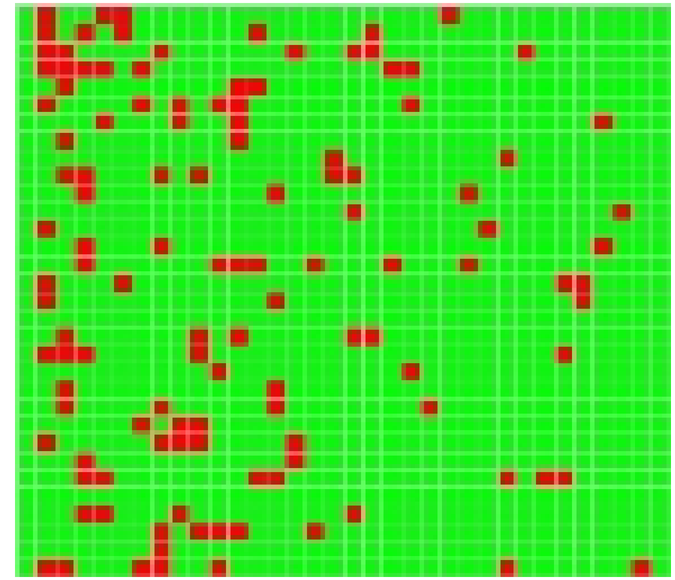
J_{ij} > 0 the interaction is called ferromagnetic

J_{ij} < 0 the interaction is called antiferromagnetic

J_{ij} = 0 the spins are noninteracting

A ferromagnetic interaction tends to align spins, and an antiferromagnetic tends to anti align them.

Ising “lattice” gas

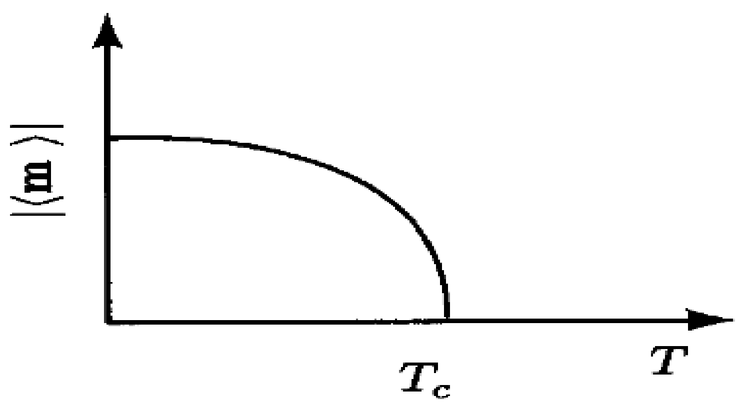


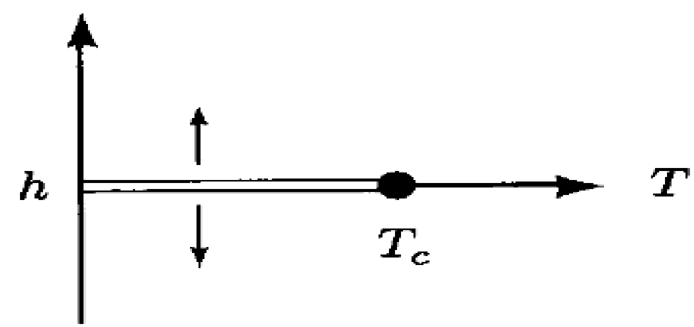
$H = -١/٢ \sum_{\langle ij \rangle} ε J B_i B_j - \sum_i \mu B_i$

$B_i = ١,٠$

$S_i = ٢ B_i - ١$

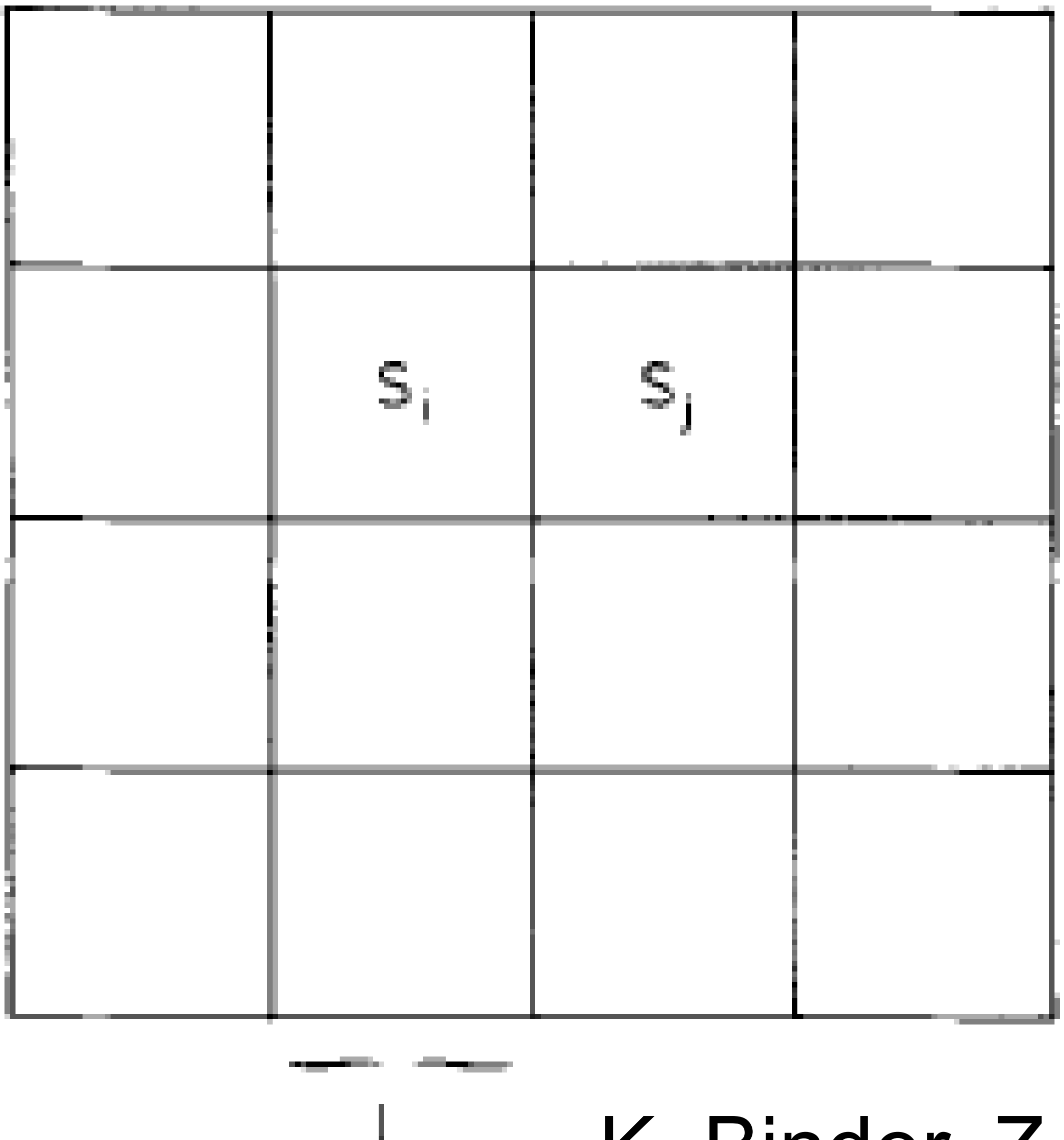
$m = \sum_i S_i$





$m \equiv \rho \,; h \equiv \mu$

Block analysis for the Ising model



Constant magnetization = NVT

$$s_i = \sum_{I \in i} S_I$$

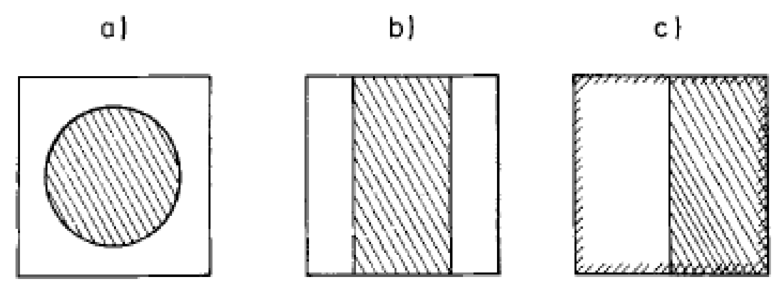


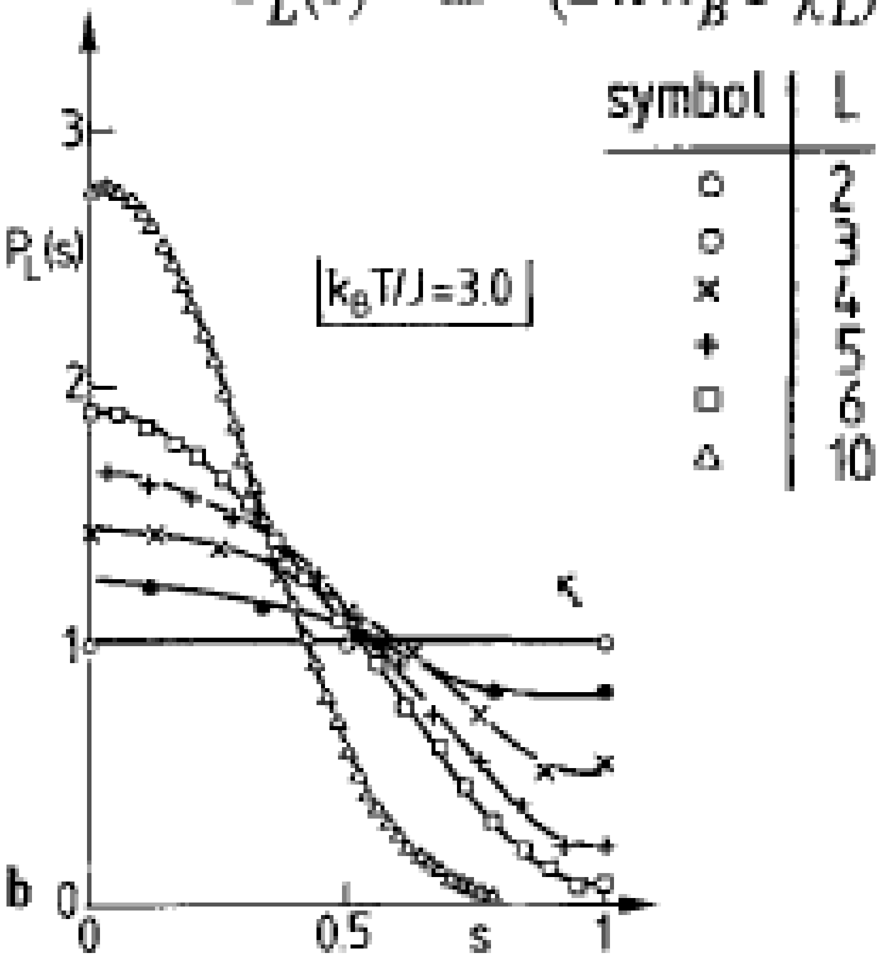
Fig. 2. Typical configurations of twodimensional blocks for $L \gg \xi$, $s \approx 0$, in the cases where the block is a subsystem of a large system **(a)** or where it is an isolated finite system with periodic **(b)** or free **(c)** boundary conditions. Shaded areas indicate domains of negative magnetization, white areas have positive magnetization

K. Binder, Z. Phys. B 43, 119 (1981)

Block analysis for the Ising model

$T > T_c$

$$P_L(s) = L^{d/2}(2\pi k_B T \chi_L)^{-1/2} \exp[-s^2 L^d/(2k_B T \chi_L)],$$

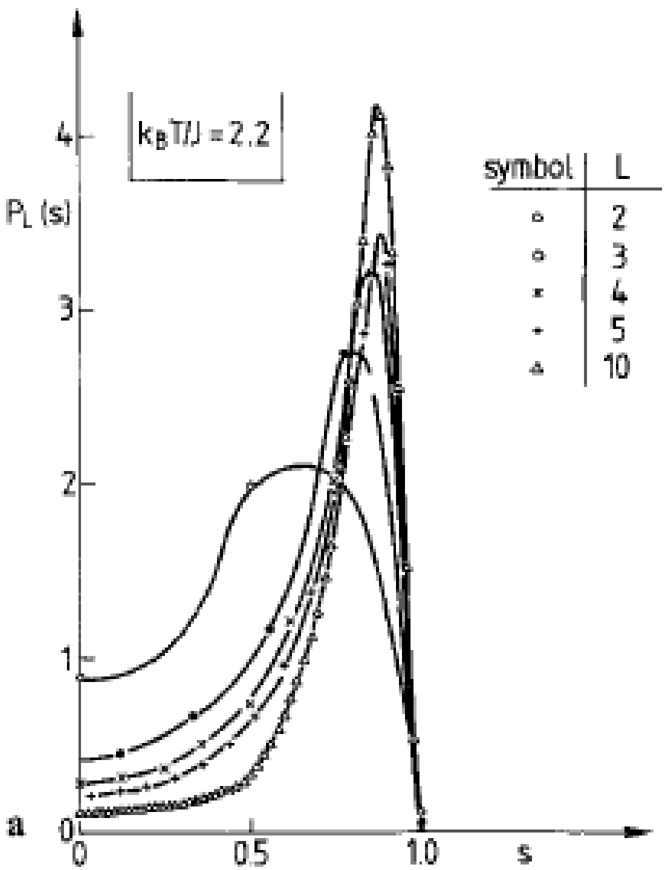


$$\chi_L = \frac{\partial s_L}{\partial h}$$

$$\chi_L^{-1} = \frac{\beta}{N}[\langle s^2 \rangle - \langle s \rangle^2]$$

Block analysis for the Ising model

$T \leq T_c$



$$P_L(s) \cong \frac{1}{2} L^{d/2} (2\pi k_B T \chi_L)^{-1/2}$$
$$\{\exp[-(s - \langle |s| \rangle_L)^2 L^d/(2 k_B T \chi_L)]$$
$$+ \exp[-(s + \langle |s| \rangle_L)^2 L^d/(2 k_B T \chi_L)]\}.$$

But this works only for T << T_c

In general P(0) is underestimated

$P(0) \sim \exp(-L^d)$ instead of $\sim \exp(-L^{d-1})$

Block analysis for the Ising model

Near the critical point: Finite size scaling !!

$$P_L(s) = L^y \hat{P}\, \tilde{P}(asL^y, \xi/L) \qquad y = \frac{\beta}{\nu}$$

$$P_L(s) = L^y \hat{P}\, \tilde{P}(z, z')$$

Use (1) normalization (2) scaling relations (3) FSS of the Binder cumulant to finally get ..

$$\tilde{P}(z, z') = \frac{C_0 A_1}{2\sqrt{\pi}} z'^{-\gamma/2\nu} \{\exp[-A_1^2 z'^{-d}(z z'^{\beta/\nu} - A_2)^2] + \exp[-A_1^2 z'^{-d}(z z'^{\beta/\nu} + A_2)^2]\}, \quad (40)$$

Block analysis for the Ising model

$$A_1 = \sqrt{\frac{\hat{\chi}^+}{\hat{\chi}^-}\left(\frac{\hat{\xi}^+}{\hat{\xi}^-}\right)^{-\gamma/\nu}}, \qquad A_2 = \hat{M}(\hat{\xi}^-)^{\beta/\nu}\, a.$$

Also one can get the surface tension by taking the limit, $\lim_{z\to 0} P(z, z')$

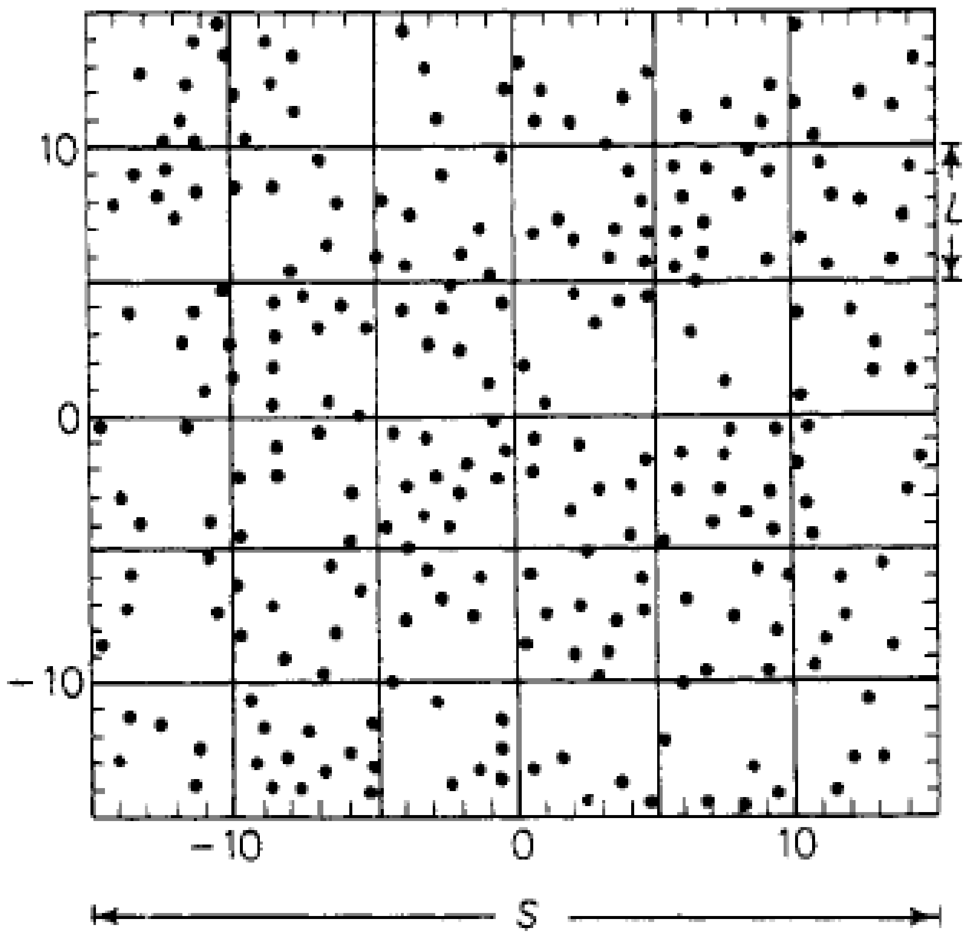
$$\tilde{P}(0, z') = \frac{C_0 A_1}{2\sqrt{\pi}} z'^{-\gamma/2\nu} \exp[-A_3 (z')^{1-d}], \; z' \to 0,$$

$$A_3 = \hat{F}_s S_d [2 V_d / (\hat{\xi}^-)^d]^{-(d-1)/d}. \quad \sim L^{d-1}$$

From a single simulation you get:

(1) coexistence densities (magnetizations).
(2) Magnetic susceptibilities from constant M simulations at $h = 0$!!
(3) ratio of critical amplitudes (universal values).
(4) surface tensions.

Block analysis for liq-gas transitions



Block analysis for liq-gas transitions

$$\frac{\chi_T^{(L)}}{\chi_T^0} = \frac{\langle N^2 \rangle_L - \langle N \rangle_L^2}{\langle N \rangle_L}, \qquad \chi_T^0 = 1/\rho k_B T$$

$$\chi_T^{(L)} = \left(1 - \frac{L^2}{S^2}\right) \chi_T + \chi_T^{(b)} L^{-1} + O(L^{-2}).$$

Constant volume !!

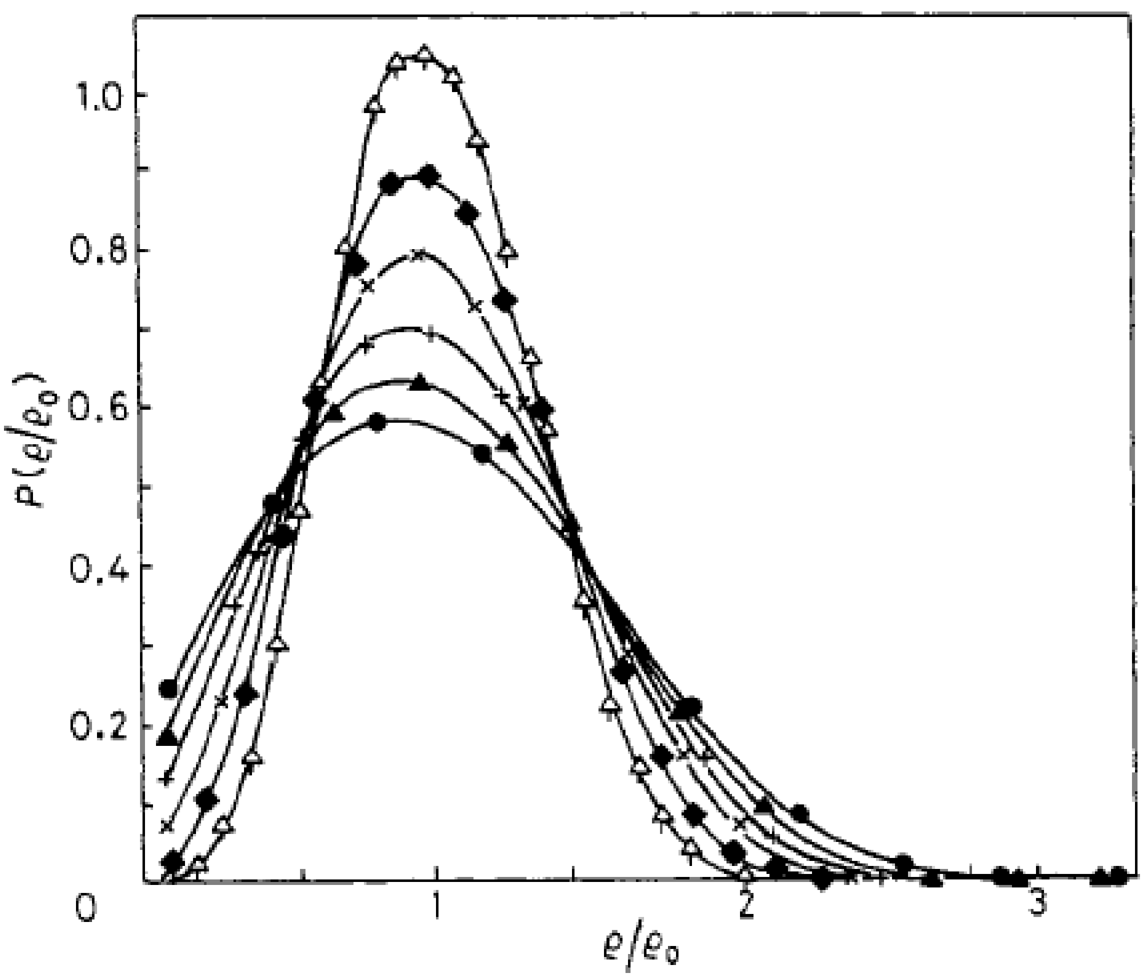
$$\chi_T^{(L)} = \chi_T + \chi_T^{(b)} L^{-1} + O(L^{-2})$$

Constant pressure

Roman, White and Velasco Europhys. Lett. 42, 371, (1998)

Block analysis for liq-gas transitions

Rovere, Heerman, Binder, Europhys. Lett. **6**, 585 (1988)



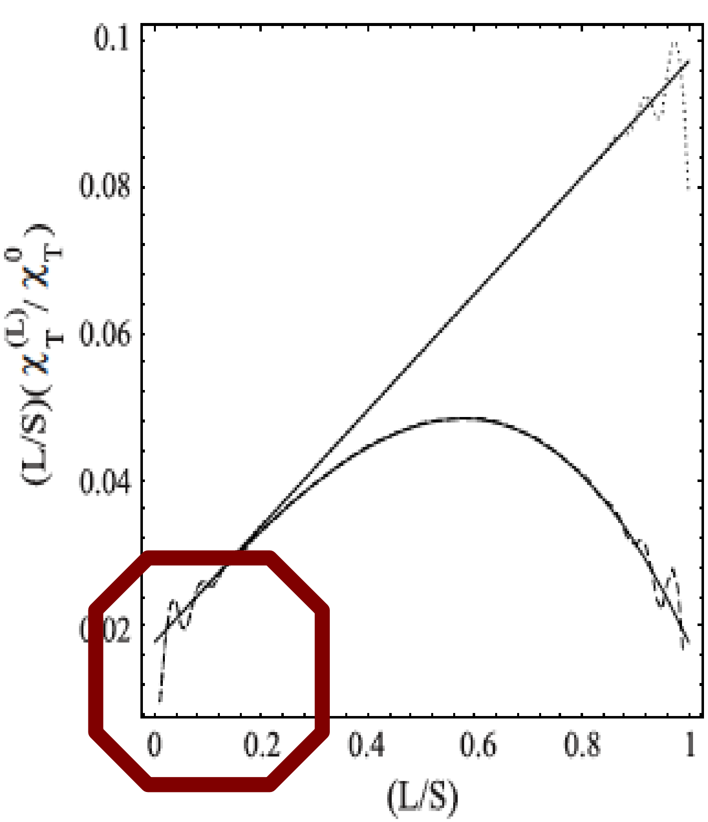


Fig. 1

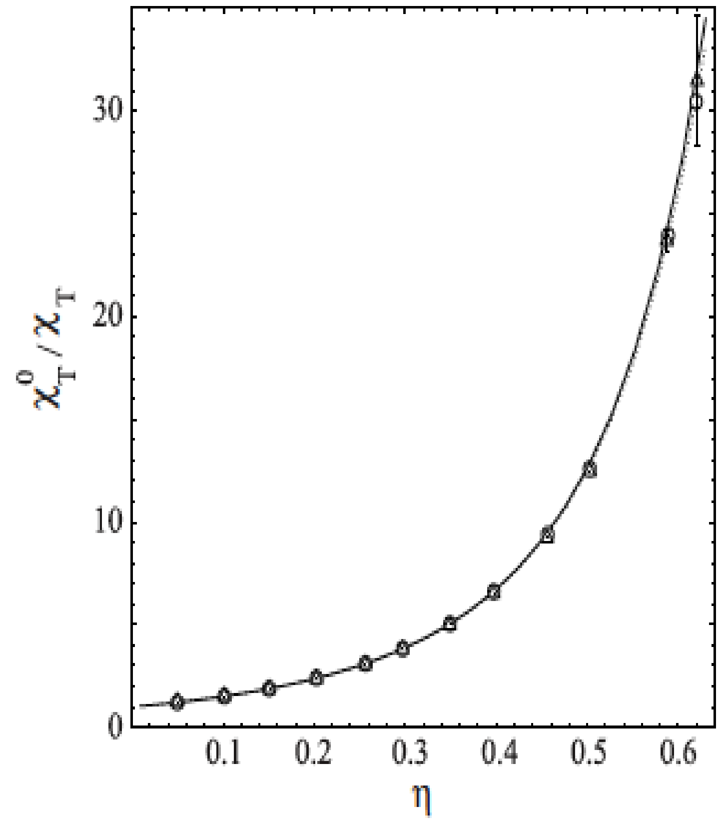


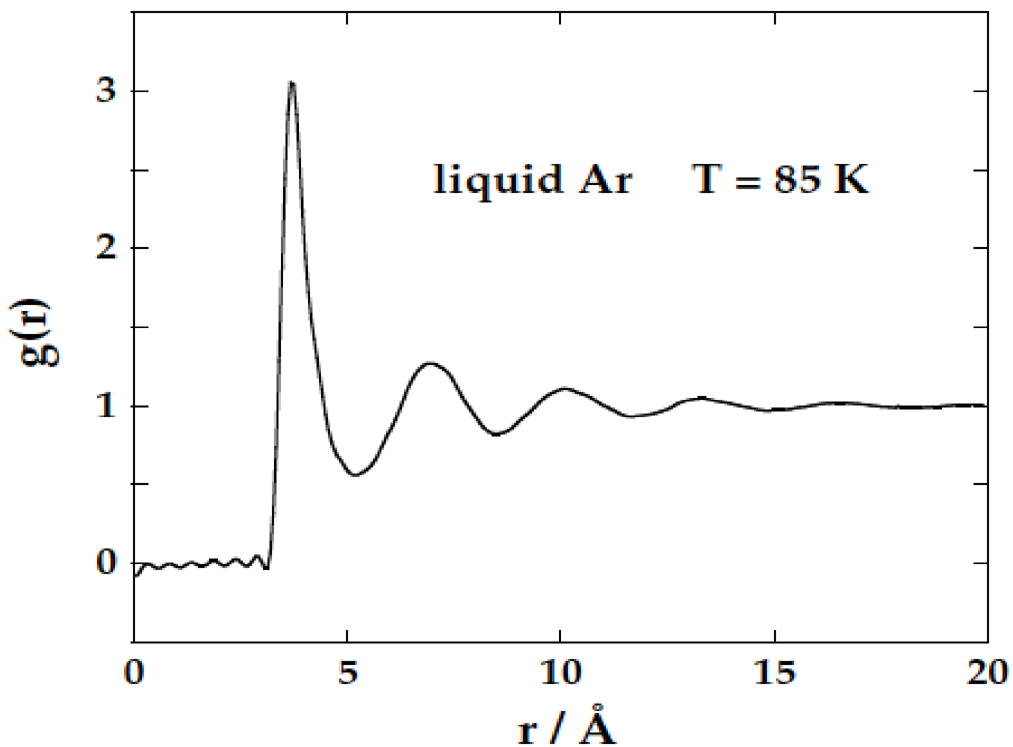
Fig. 2

Fig. 1. – Plot of $(L/S)\chi_T^{(L)}$ *vs.* L/S at a packing fraction $\eta = 0.5$. Dashed line: CEMC data from a system of $N = 256$ hard disks (7.8×10^6 MCS). Dotted line: GCEMC data from a system of $\langle N \rangle = 256$ hard disks (7.8×10^6 MCS). The thin lines correspond to the results of the fit to (4) and (3), respectively (see text).

Fig. 2. – Inverse isothermal compressibility of a hard-disk fluid. Triangles: extrapolated results from a CEMC simulation; $N = 256$, MCS $= 7.8 \times 10^6$. Circles: extrapolated results from GCEMC data; $\langle N \rangle = 256$, MCS $= 7.8 \times 10^6$. The lines correspond to the results obtained from the compressibility factor of Henderson (eq. (5)) with $a = 0.128$, $b = 0.043$ (solid line) and $a = 0.125$, $b = 0$ (dotted line).

$$1 + \rho \int [g(r) - 1] \, d\mathbf{r} = \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle} = \rho k_B T \chi_T$$

$$\rho k_B T \chi_T = 1 + \rho \hat{h}(0) \qquad S(\mathbf{k}) = 1 + \rho_0 \hat{h}(\mathbf{k})$$



Scaling Fields and Universality of the Liquid-Gas Critical Point

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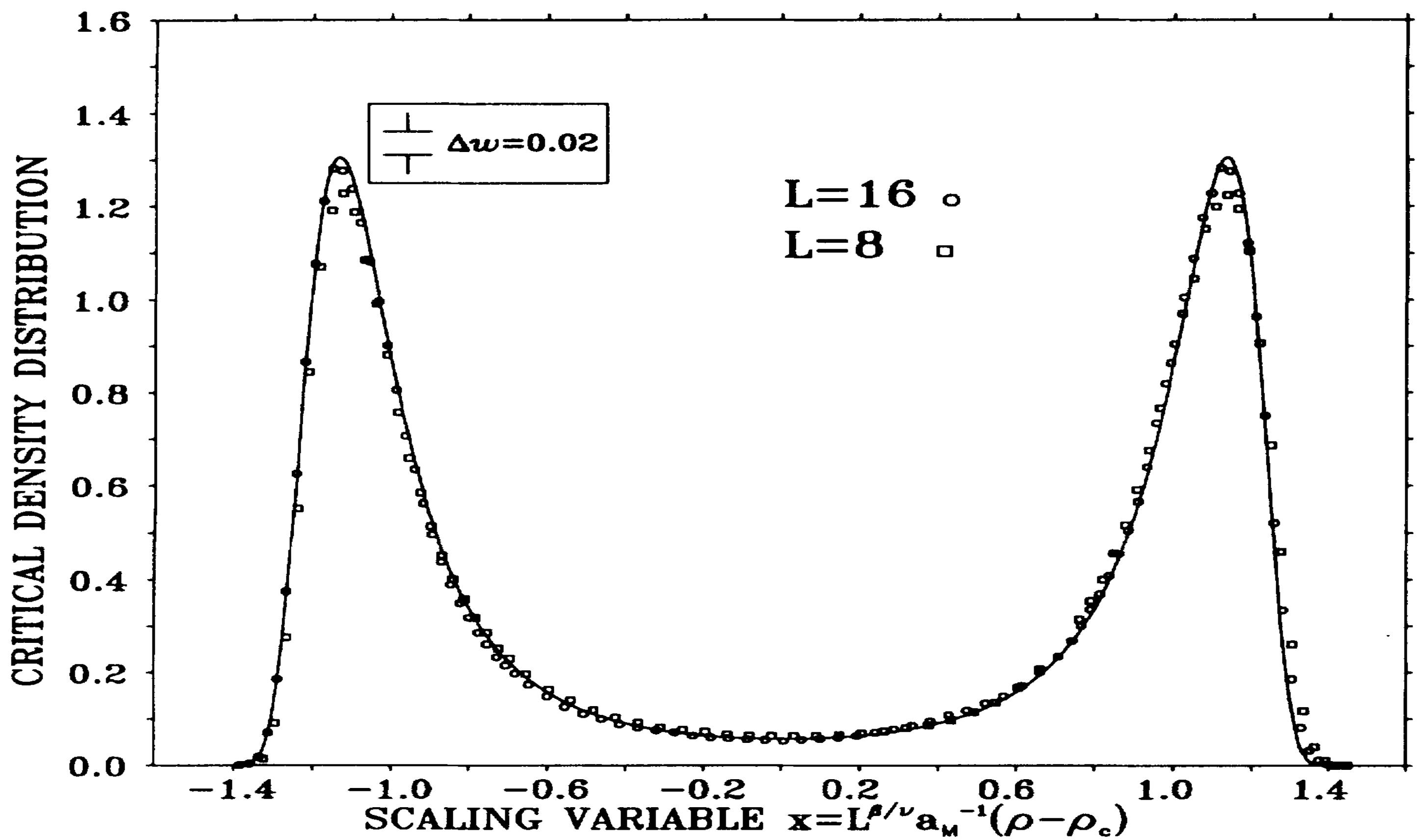
(Received 16 September 1991)



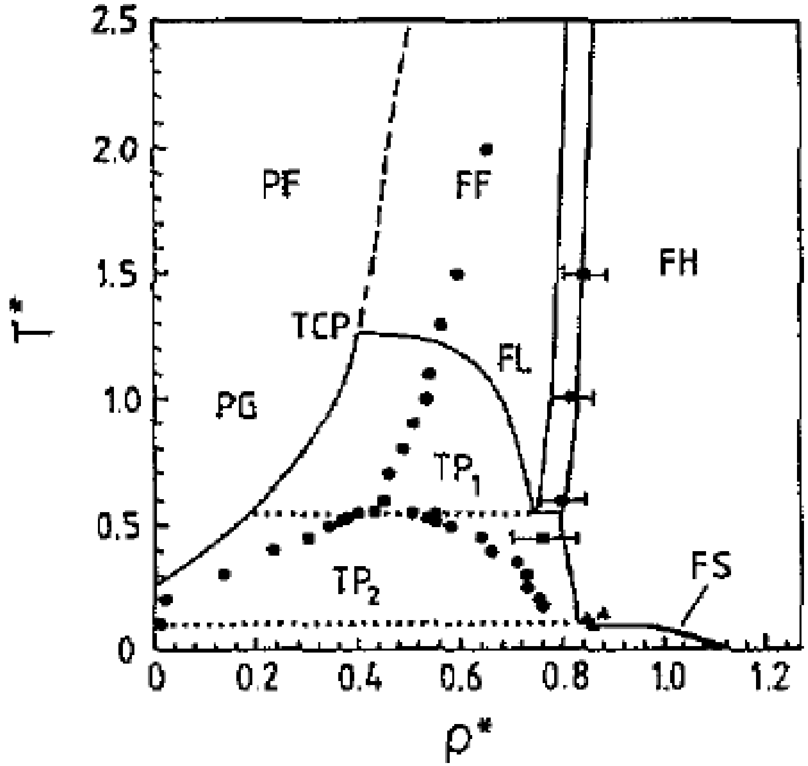


Figure 1. Phase diagram including paramagnetic fluid (PF), ferromagnetic fluid (FF), paramagnetic gas (PG), ferromagnetic liquid (FL), ferromagnetic hexagonal solid (FH), and ferromagnetic square solid (FS) phases. Special points are the tricritical point (TCP) and two triple points (TP_1, TP_2). Curves: MF/DFT predictions. (Full curve: first-order transitions; broken curve: second-order transitions; dotted lines: triple lines). Circles and triangles (FS coexistence densities): block-analysis PIMC data. Squares (FH coexistence densities): local structure analysis PIMC data.

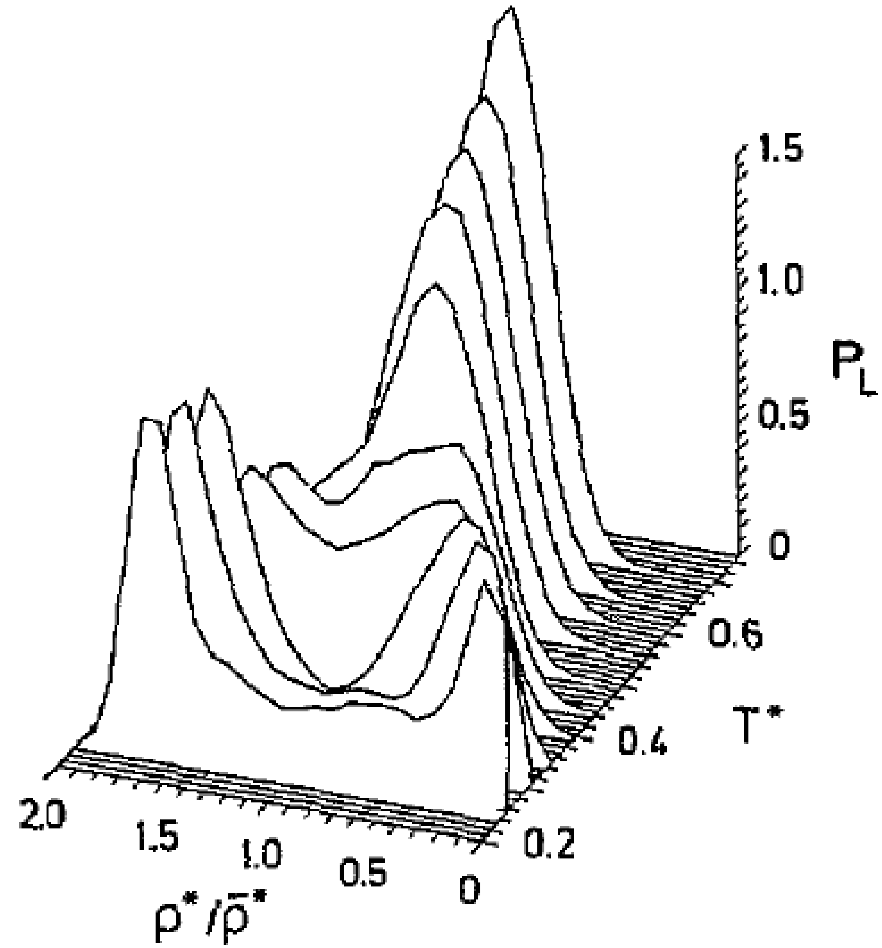


Figure 2. Normalized block density distributions $P_L(T^*, \rho^*/\bar{\rho}^*)$ for $\bar{\rho}^* = 0.45$ and $M_b = 4$ ($L = [N/\bar{\rho}^*]^{1/2}/M_b$); connecting lines are guides to the eye.

```
CC
CC THE BLOCK ANALYSIS
CC
      DO 31 I = 1,10
         NB =  5 +   (I-1)
         DL = 1.0/DFLOAT(NB)
         DO 32 J = 1,NB
            DO 33 K = 1,NB
               PKNT = 0
               DO 34 L = 1,N
                  XT = X(L) + 0.5
                  YT = Y(L) + 0.5
                  IF(XT.LT.J*DL.AND.XT.GE.(J-1)*DL)THEN
                  IF(YT.LT.K*DL.AND.YT.GE.(K-1)*DL)THEN
                  PKNT = PKNT + 1
                  ENDIF
                  ENDIF
34               CONTINUE
               BINDEN = PKNT+1
               IF(BINDEN.GT.MAXBND)BINDEN=MAXBND
               IF(BINSPN.GT.MAXBNS)BINSPN=MAXBNS
               HISDN(I,BINDEN) = HISDN(I,BINDEN) + 1
33            CONTINUE
32         CONTINUE
31    CONTINUE
      RETURN
      END
```

Block analysis for solids

- Solids are very incompressible
- Number fluctuations are (almost) nonexistent
- Block densities suffer from discretization and/or commensurability-incommensurability effects
- Liq-solid density difference is small + it is first order
- No critical scaling properties can be used.
- Block analysis for liq-solid boundary = bad idea

Some examples of gas/liquid/solid phase coexistence

PHYSICAL REVIEW E VOLUME 49, NUMBER 2 FEBRUARY 1994

Phase diagram of a model anticlustering binary mixture in two dimensions: A semi-grand-canonical Monte Carlo study

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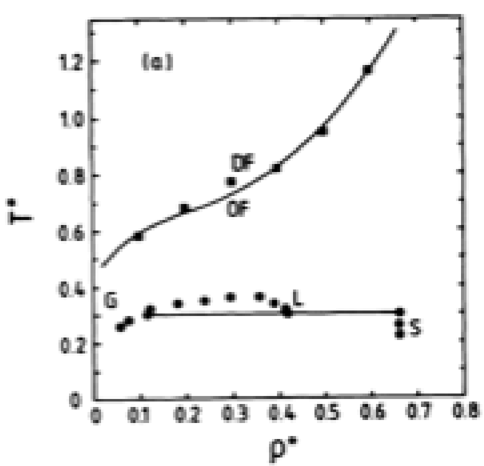
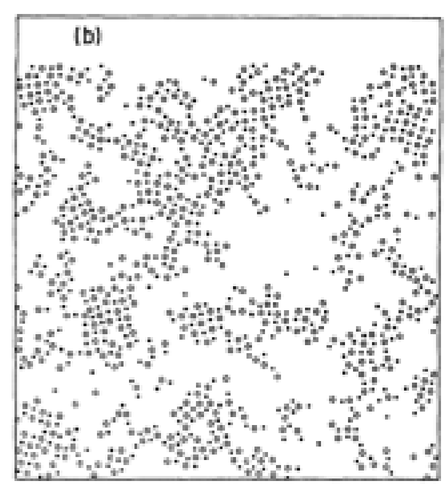
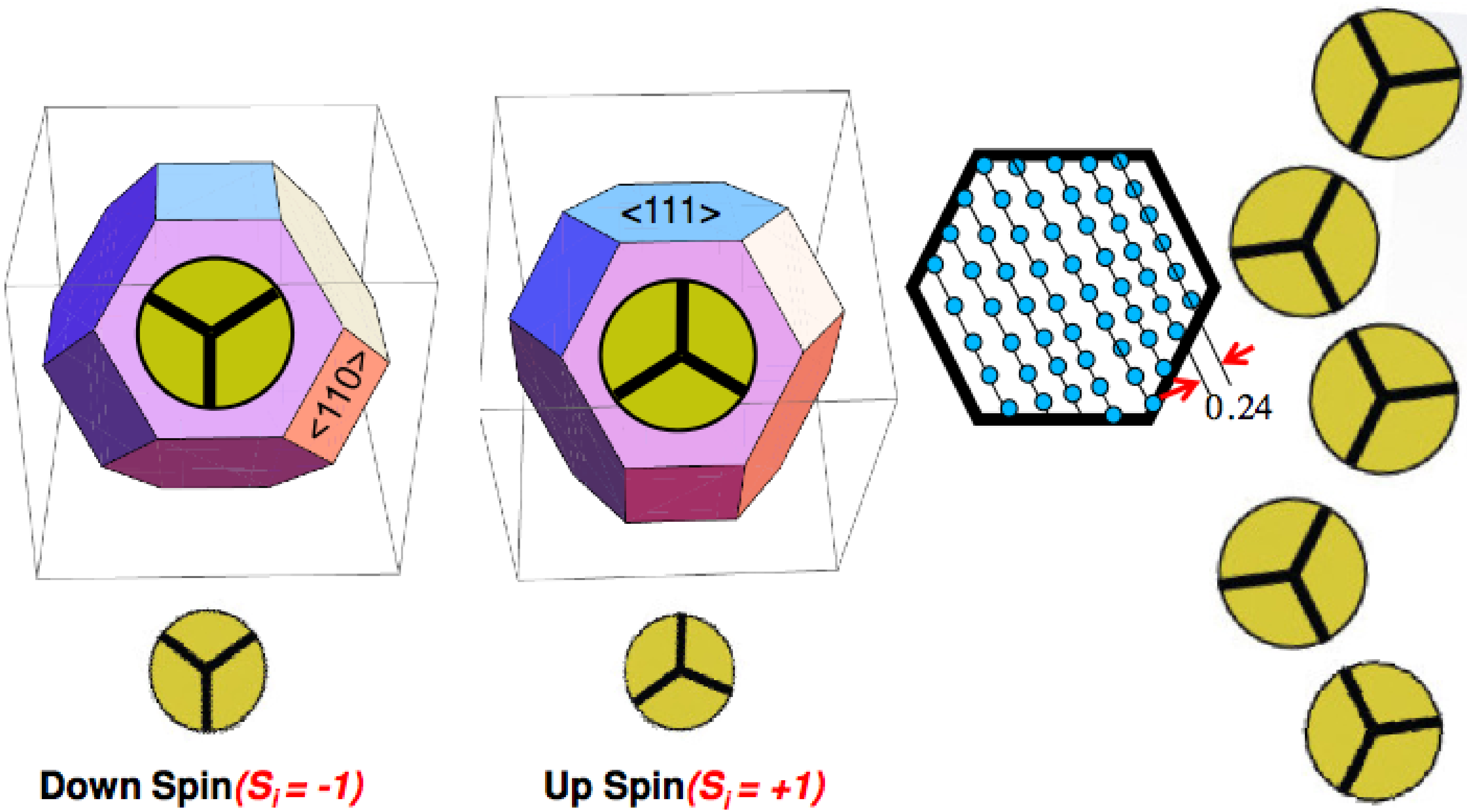
(Received 30 September 1993)

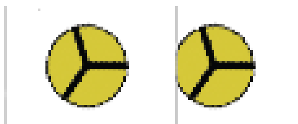




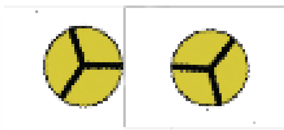
Construction of the Model System



Construction of the Potential



Same Spin Repel *(SiSj = +1)*



Opposite Spin Attract (*SiSj = -1*)

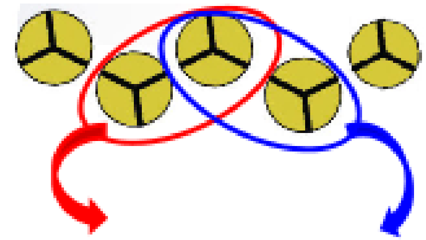


Fig.1 (θ = 240) *Fig.2* (θ = 120)

- The angle θ is always measured from the up spin to the downspin

$$u(r) = u_{attr}(r) + u_{rep}(r)$$

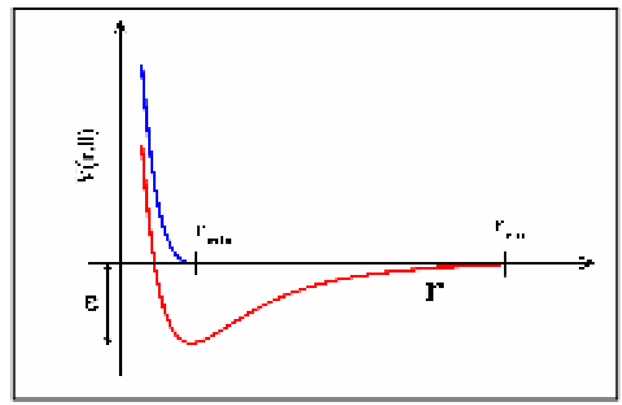
$$u_{attr}(r) = -\varepsilon\left(\frac{s_i s_j - 1}{2}\right)\left(\frac{-Cos(3\theta_{ij}) - 1}{2}\right) - E_{cut} \; ; r \le r_{min}$$

$$u_{attr}(r) = u_{LJ}(r)\left(\frac{s_i s_j - 1}{2}\right)\left(\frac{-Cos(3\theta_{ij}) - 1}{2}\right) - E_{cut} \; ; r > r_{min}$$

$$u_{rep}(r) = u_{LJ}(r) + \varepsilon \; ; r \le r_{min}$$

$$u_{rep}(r) = 0 \; ; r > r_{min}$$

$$u_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$



Here,

$r = |\vec{r_{ij}}|$ is the interparticle separation

s_i is the spin of the i^{th} particle

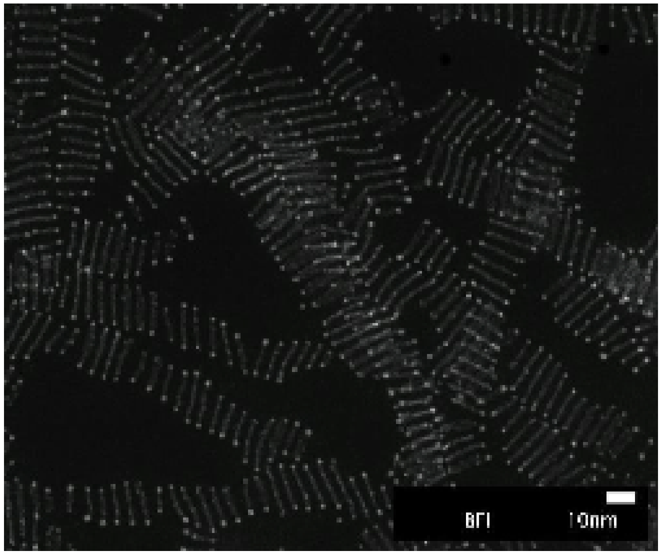
θ_{ij} is the angle between i^{th} and j^{th} particle

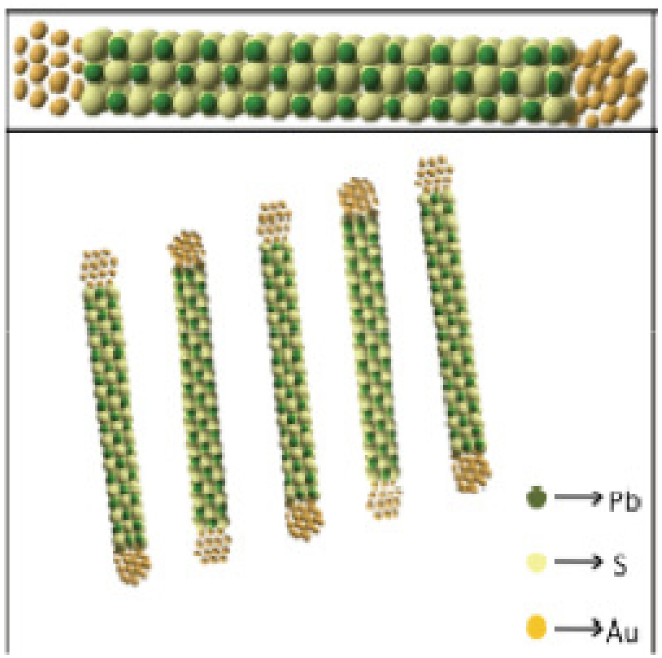
The pair potential was calculated using a minimum image convention with a spherical cut-off at $r_{cut}^2 = 2.5\sigma^2$ and $E_{cut} = u_{LJ}(r_{cut})$; $r_{min}^2 = 2^{1/3}\sigma^2$ is the position of the minima of the L-J pair potential.

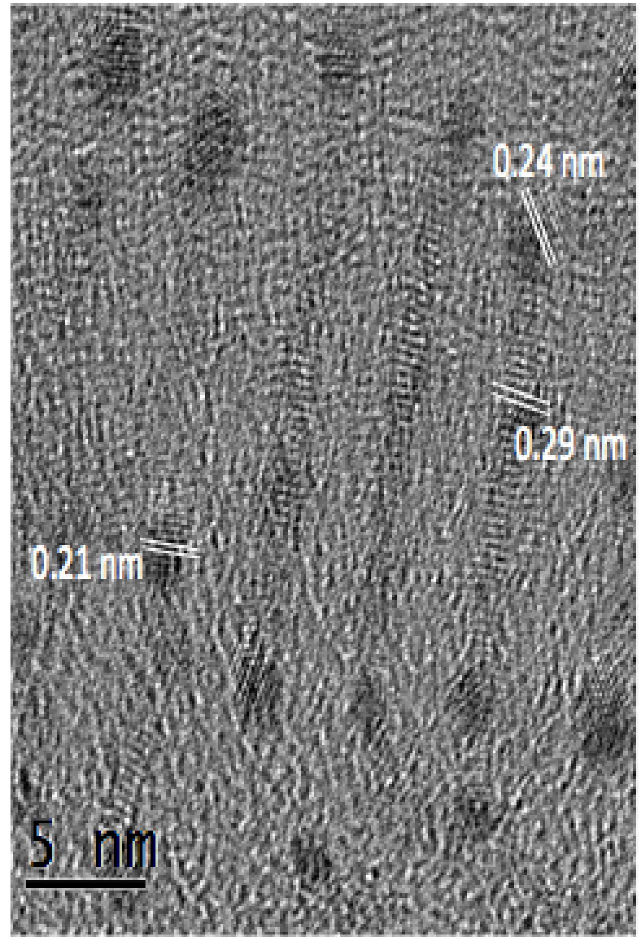
Block analysis (coarse – graining) for solids

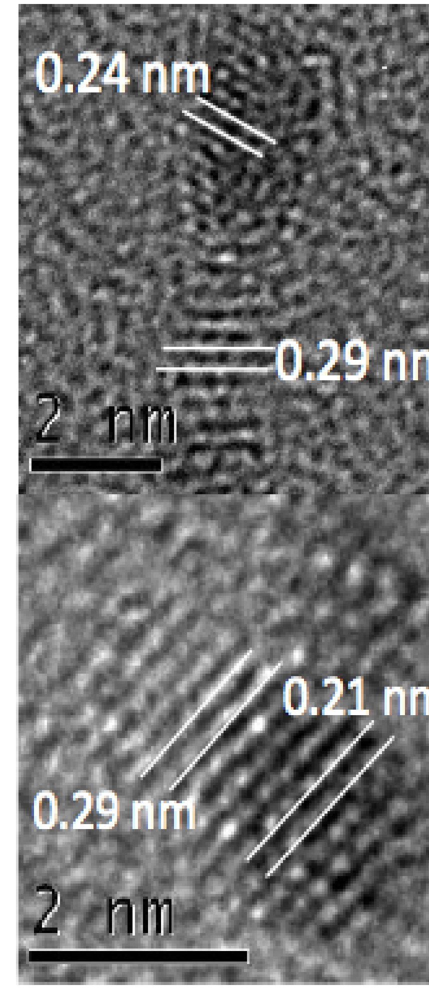
- Fluctuations of block strains
- No external stress both NVT and NPT will do
- Can be applied to experiments
- “Model independent” (almost)
- Can be used to get non-local elasticity etc.

Introduction and Motivation

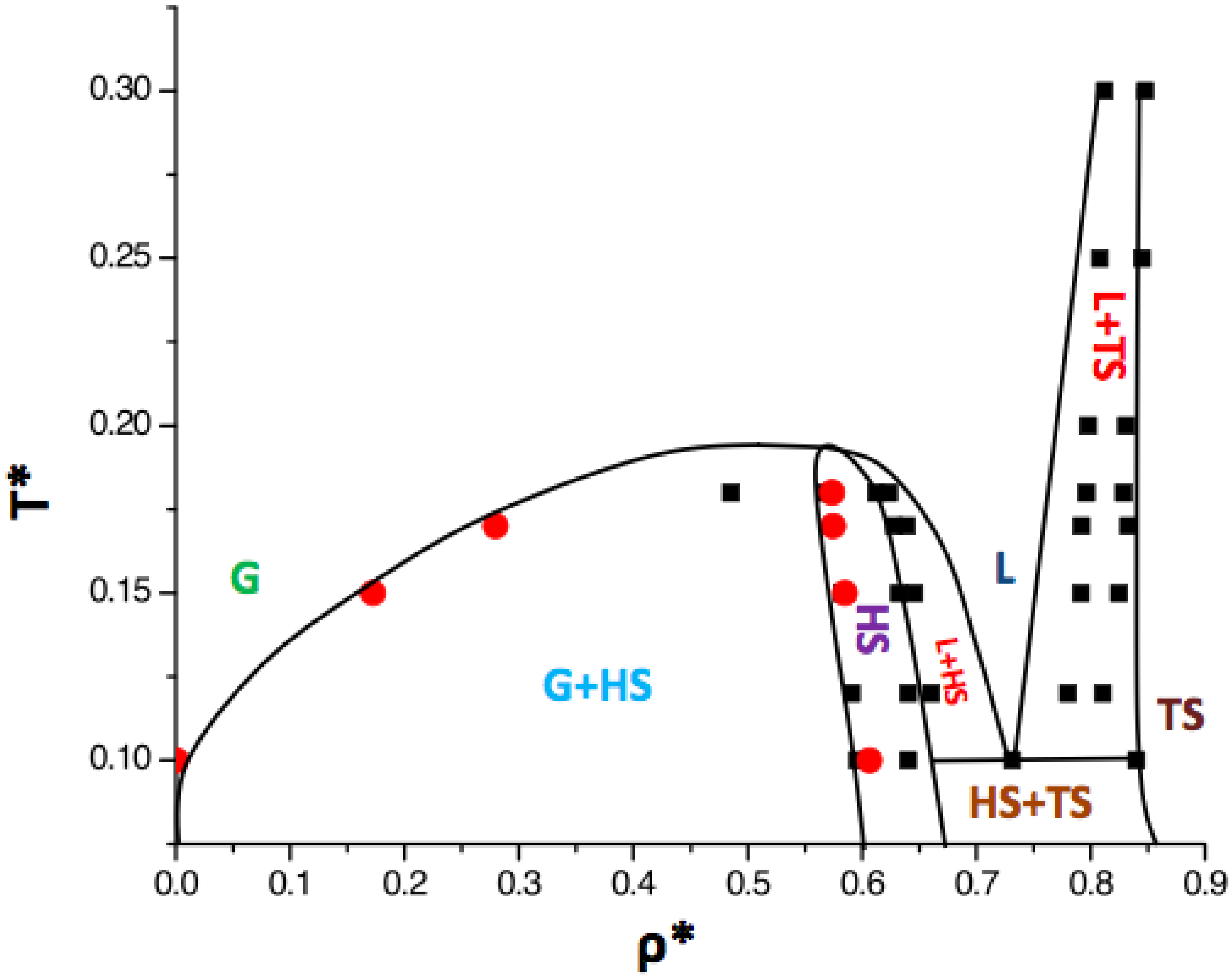








- **Points to be noted :**
  - The chains are formed with alternate Au <111> and <110> planes
  - The bottom end of the chains are just the mirror image of the top end



T*
0.30
0.25
0.20
0.15
0.10
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
ρ*
G
G+HS
HS
L+HS
L
L+TS
TS
HS+TS

PHYSICAL REVIEW E 78, 026106 (2008)

Nonlocal elastic compliance for soft solids: Theory, simulations, and experiments

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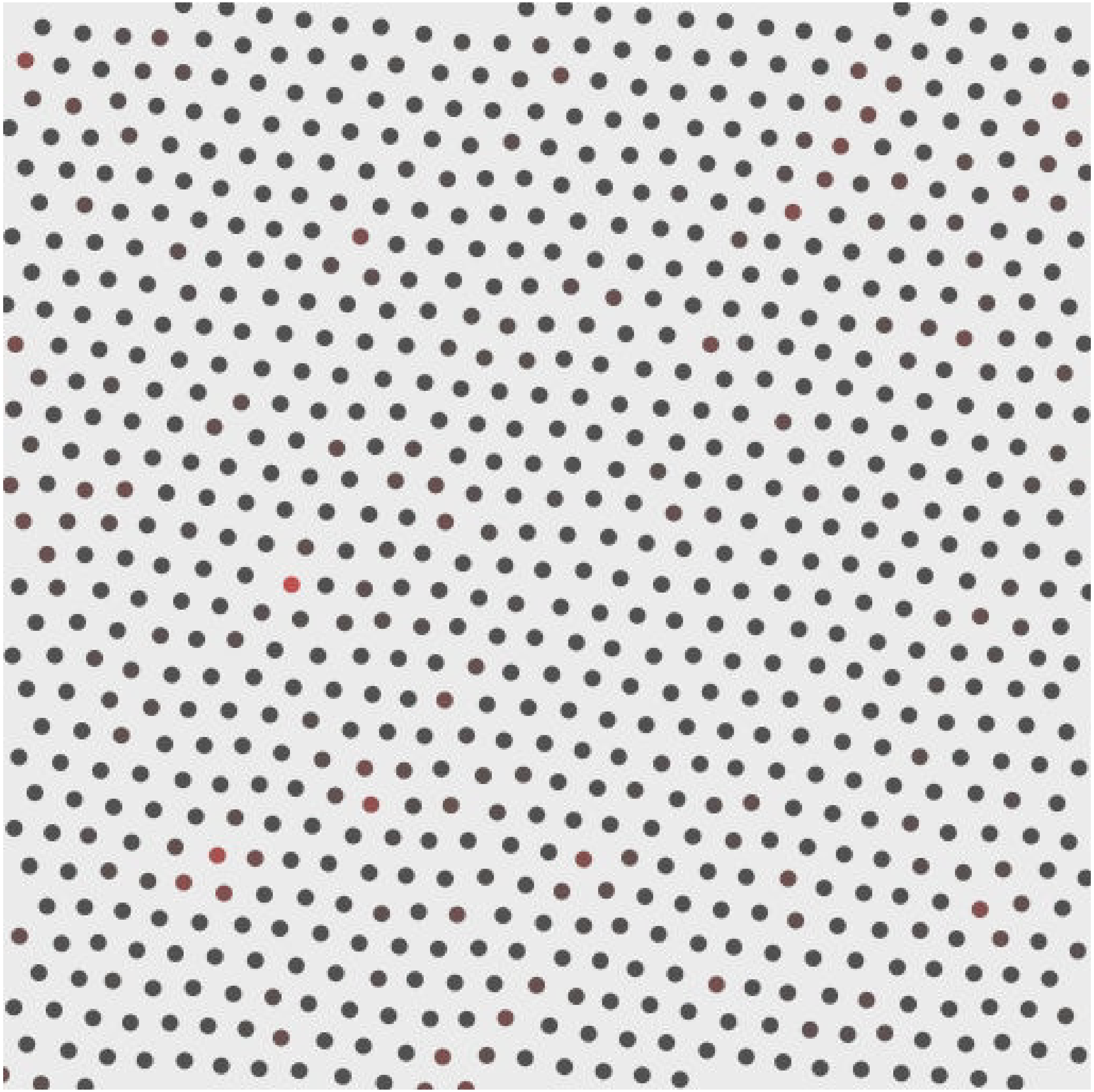
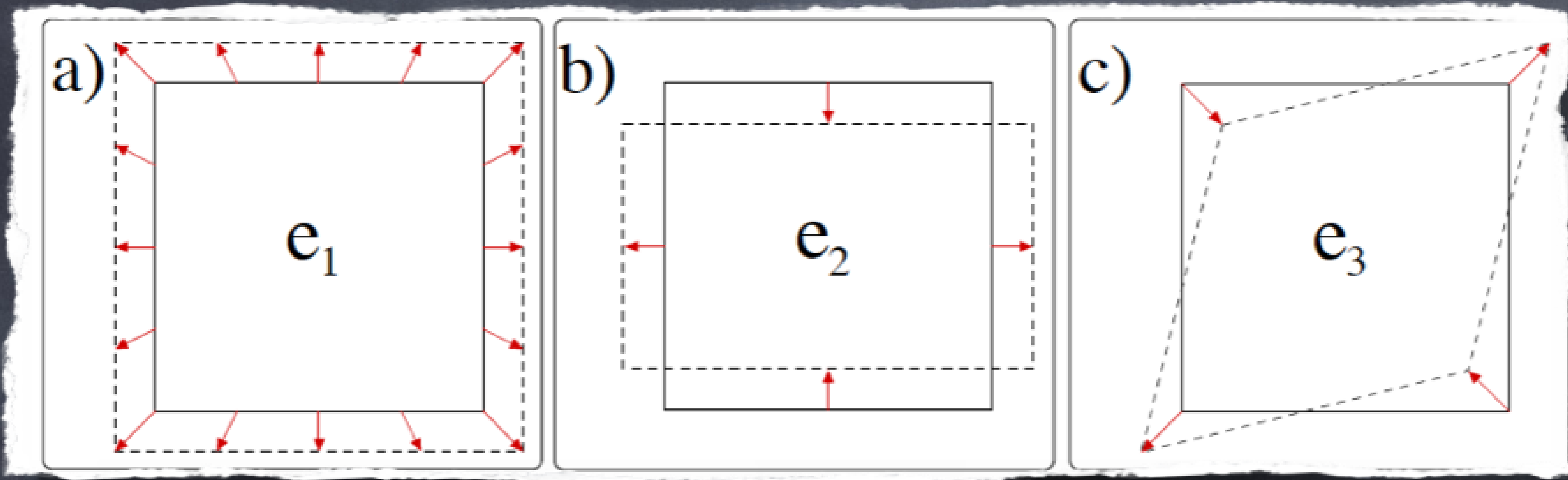
The nonlocal elastic response function is crucial for understanding many properties of soft solids. This may be obtained by measuring strain-strain autocorrelation functions. We use computer simulations as well as video microscopy data of superparamagnetic colloids to obtain these correlations for two-dimensional triangular solids. Elastic constants and elastic correlation lengths are extracted by analyzing the correlation functions. We show that to explain our observations displacement fluctuations in a soft solid need to contain affine (strain) as well as nonaffine components.

DOI: 10.1103/PhysRevE.78.026106 PACS number(s): 62.20.D−, 05.10.Ln, 82.70.Dd



Local elastic (or affine) excitations of the 2d solid



$$e_1 = \partial u_x / \partial x + \partial u_y / \partial y \quad \text{(volume)},$$
$$e_2 = \partial u_x / \partial x - \partial u_y / \partial y \quad \text{(deviatoric)},$$
$$e_3 = (\partial u_x / \partial y + \partial u_y / \partial x)/2 \quad \text{(shear)}.$$

$\varepsilon_{xx} + \varepsilon_{yy}$

$\varepsilon_{xx} - \varepsilon_{yy}$

$\varepsilon_{xy} = \varepsilon_{yx}$

+ local rotations $\Theta = \partial u_x / \partial y - \partial u_y / \partial x$

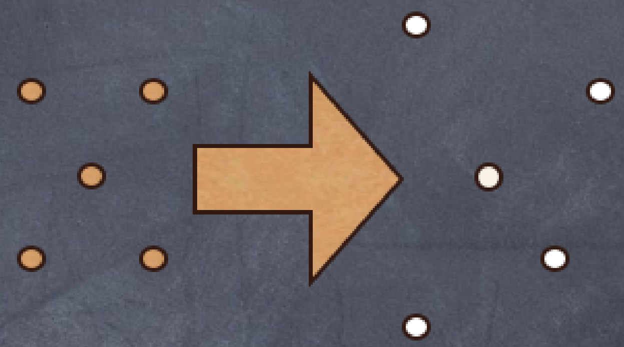
Coarse graining

N.P.T. ensemble M. C. simulations of a 2d triangular "harmonic net".

coarse grain over an "interaction volume"

affine transformation:

$r_m(t) - r_0(t) = (1 + \varepsilon(t))(R_m - R_0)$



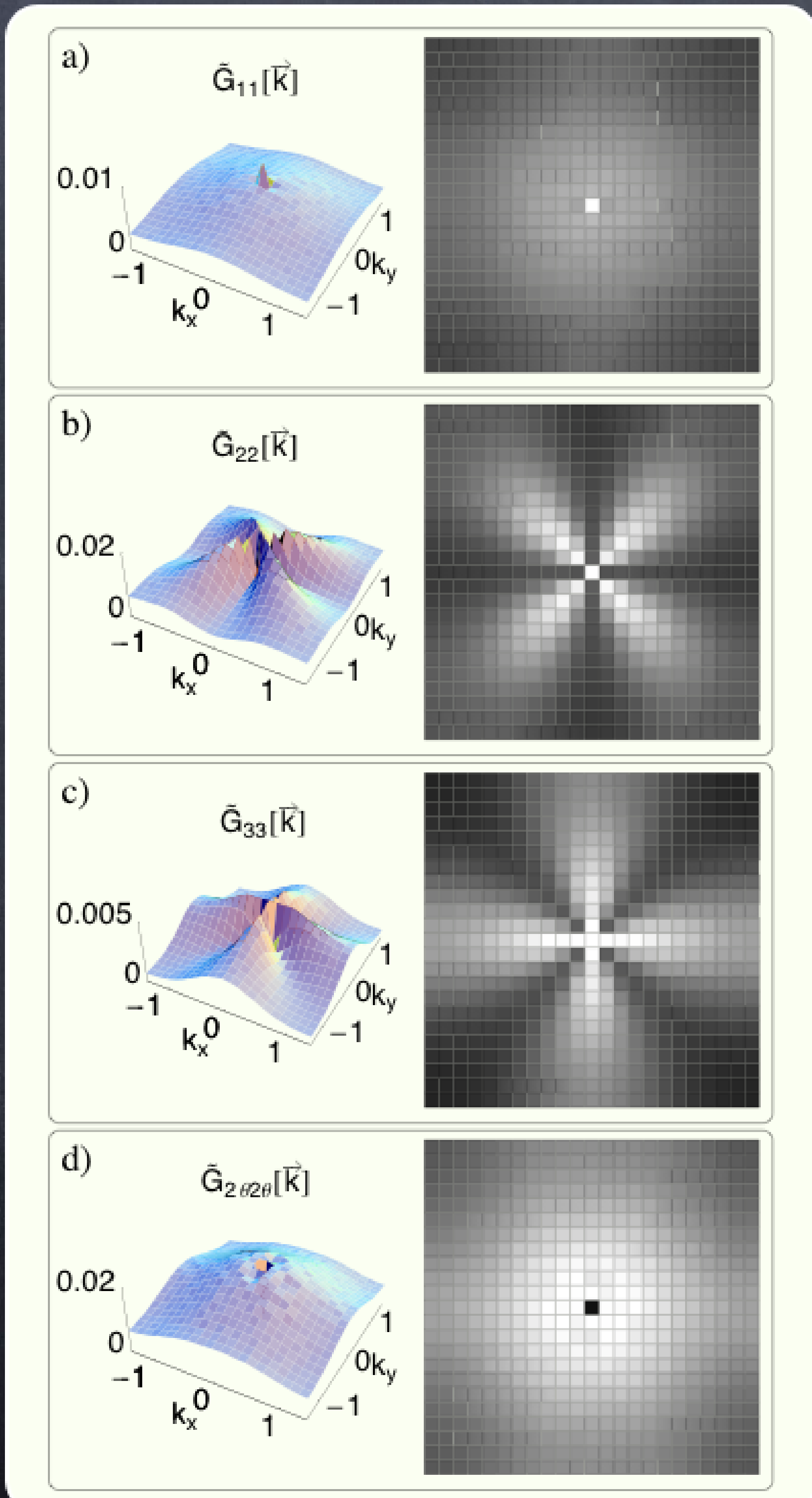
M. L. Falk and J. S. Langer, Phys. Rev. E 57, 7192 (1998)

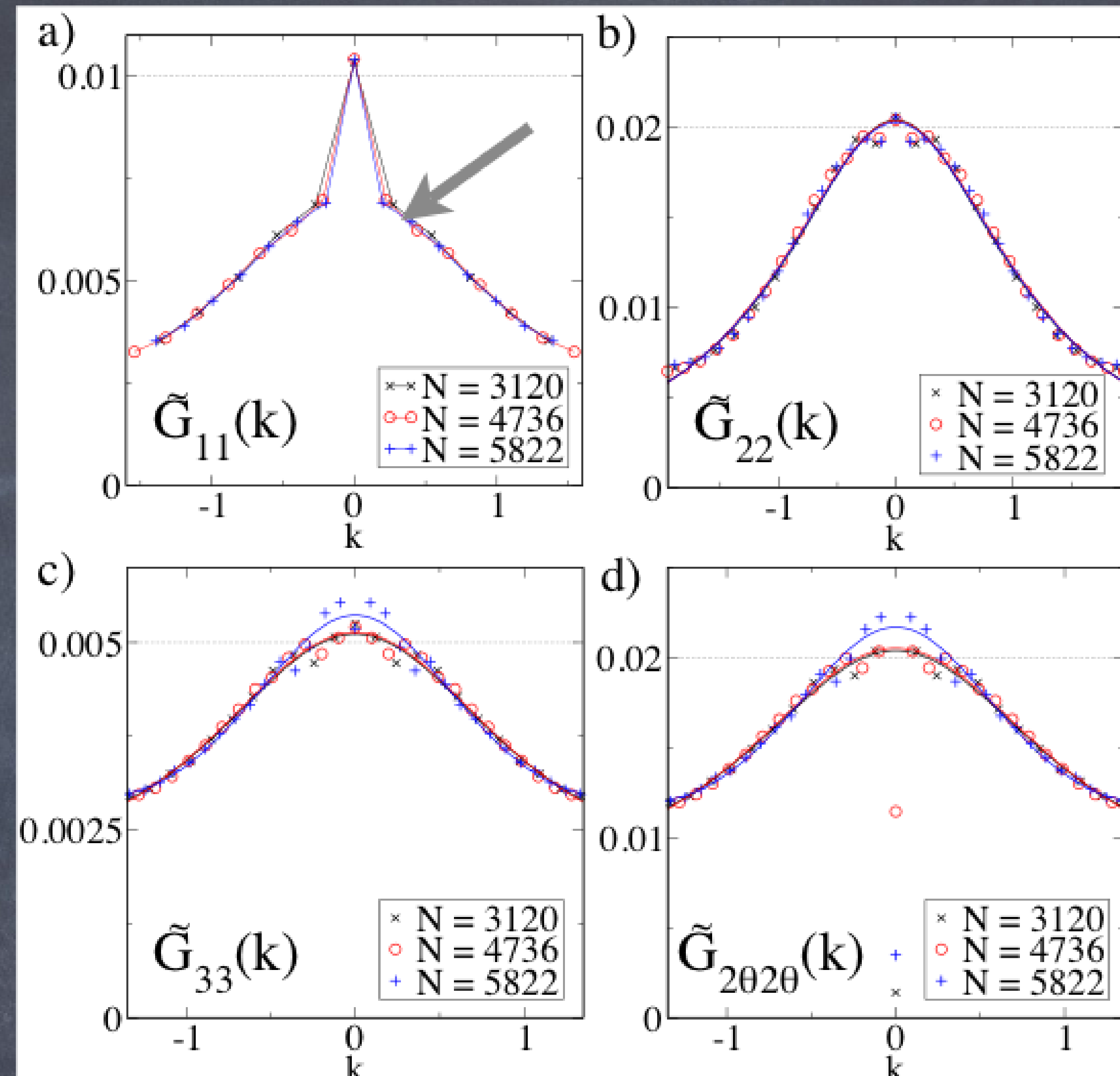
$$\chi = \Sigma_{m=1,N}\, \Sigma_{i=1,2}\, \{r_m^i - r_0^i - \Sigma_{j=1,2}\, (\delta_{ij}+\varepsilon_{ij})\, [R_m^j - R_0^j]\}^2$$

- One needs to minimize the "error" χ with respect to choices of the local strain tensor ε.
- The residual value of χ measures "non-affineness" of the transformation.

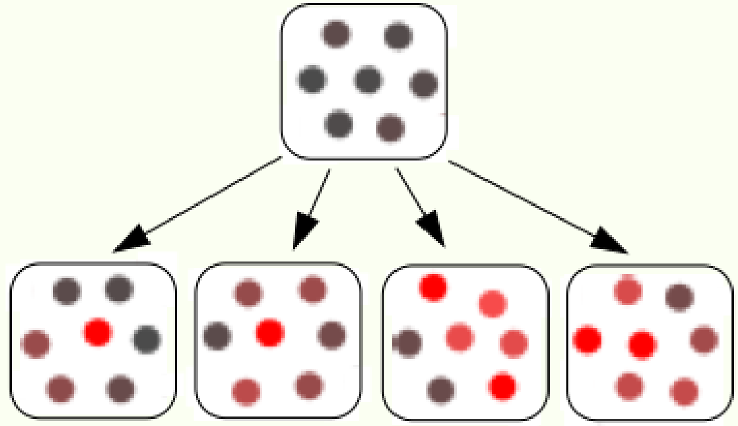
Strain-strain correlation functions

i) highly anisotropic
ii) strongly coupled
iii) singular at k=0
iv) limit k→0 gives
elastic constants





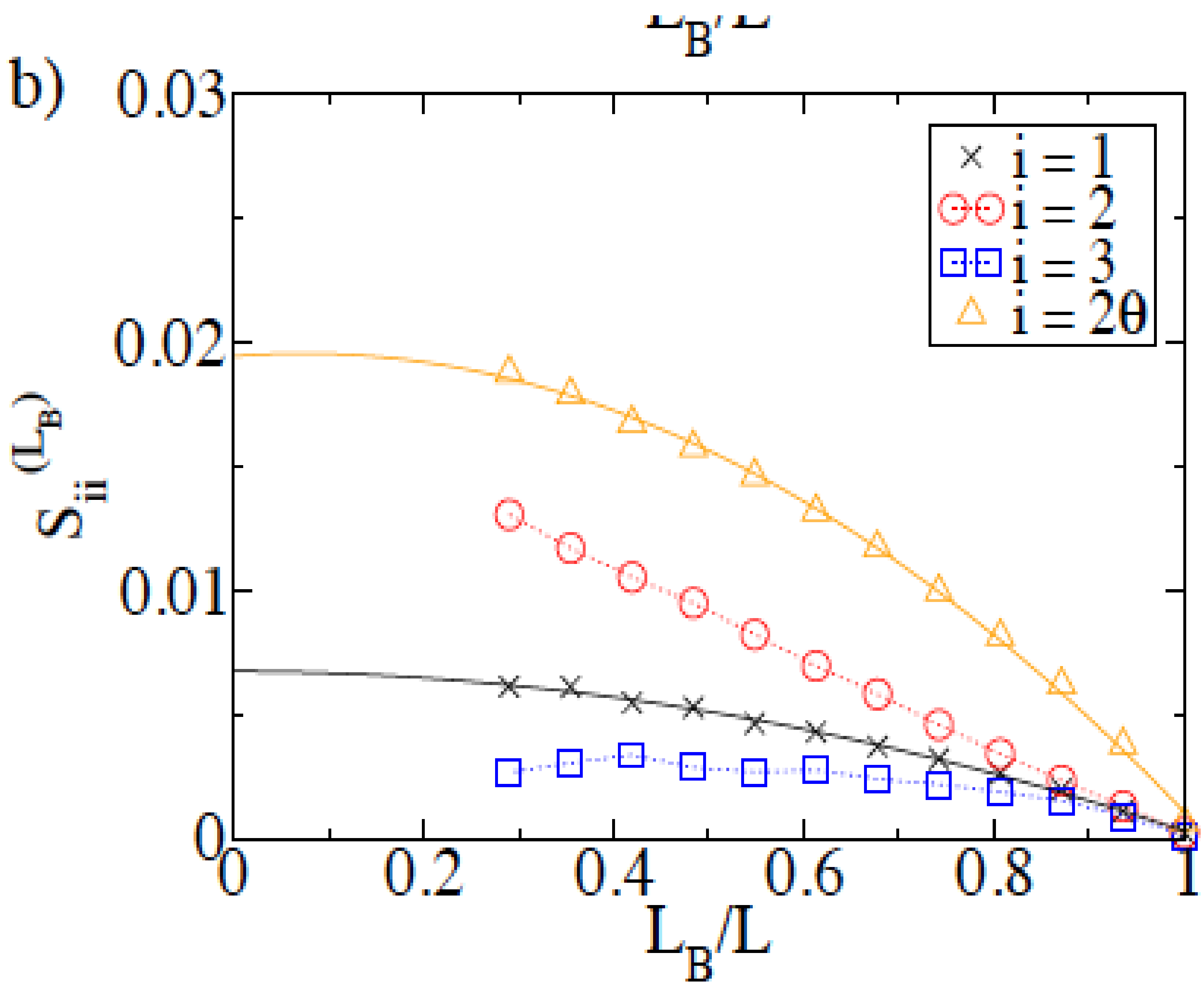
- All elastic constants recovered from $k \to 0$ limits.
- for $k \neq 0$ deformations, the solid is 20-25 times softer for volume fluctuations.



coarse-graining leads to non-affineness.

Total, $\Delta\rho/\rho = e_1 = e_1^A + e_1^P$ (i.e. $\nabla \cdot u$ + non-affine "defects")
such that: $\langle e_1^P \rangle = 0$ (total defects = 0)
and $\langle e_1^P(r) e_1^A(r') \rangle = 0$. (affine and non-affine parts are uncorrelated)

Then any $\langle e_1^P(0) e_1^P(r) \rangle \sim \exp(-r/\lambda) - \lambda$, which satisfies the constraints, explains the results. $\lambda \sim 5$ lattice spacings



L_B/L
b)
0.03
0.02
0.01
0
$S_{ii}^{(L_B)}$
0
0.2
0.4
0.6
0.8
1
L_B/L
i = 1
i = 2
i = 3
i = 2θ

	a_1	a_2	a_3
calculated from f	$100\ /\beta a^2$	$50\ /\beta a^2$	$200\ /\beta a^2$
from fluctuations of h	$98.9\ /\beta a^2$	$49.4\ /\beta a^2$	$196.7\ /\beta a^2$
from $\tilde{G}(\vec{k}=\vec{0})$	$96.8\ /\beta a^2$	$48.6\ /\beta a^2$	$190.8\ /\beta a^2$
from fits of $\tilde{G}(\vec{k}\neq\vec{0})$	-	$49.1\ /\beta a^2$	$195.7\ /\beta a^2$

Thanks for everything !!