Statistical Mechanics of Elongated Hard Particles in One Dimension

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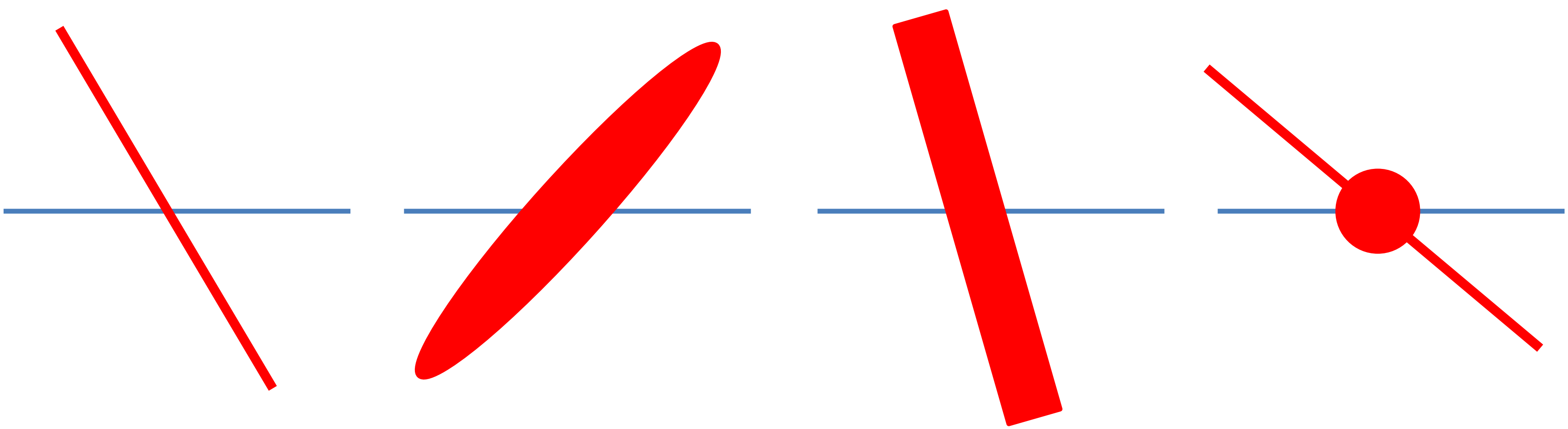

Needle   Ellipse   Rectangle   Metronome

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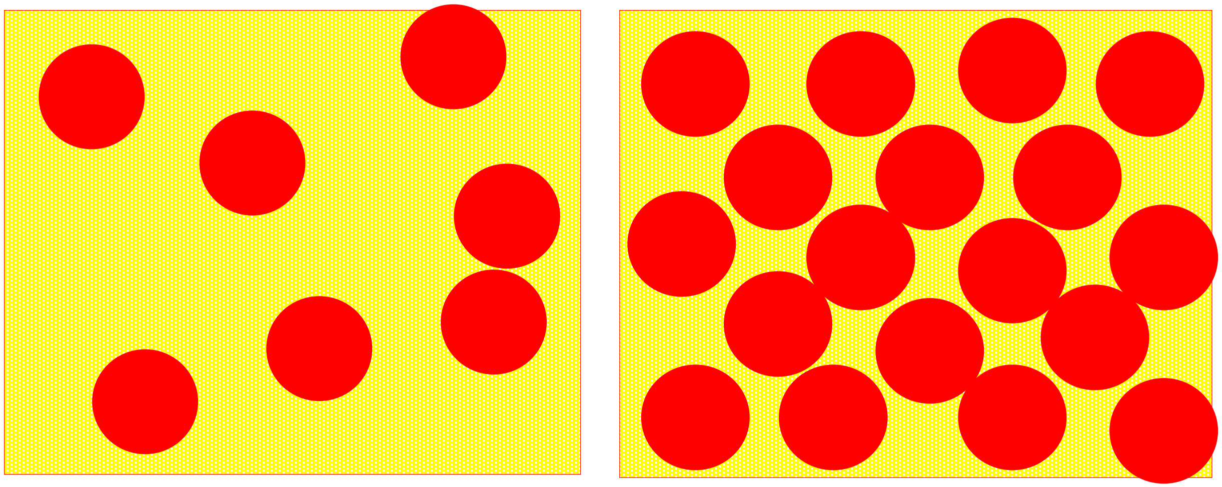
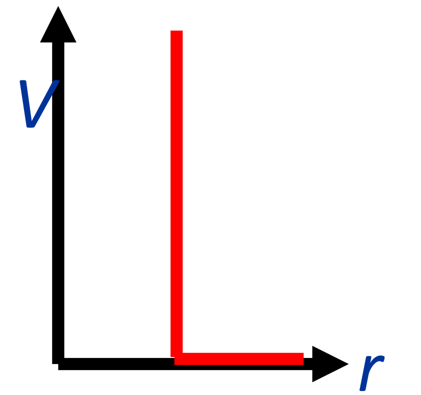
Statistical Mechanics Day III, Weizmann Inst., June 16, 2010

Outline

- Why hard potentials are interesting?
- Why do we use one dimensional systems?
- Directional correlations of elongated particles
- Universality in the jamming limit
- Conclusions

Entropy-Dominated Systems



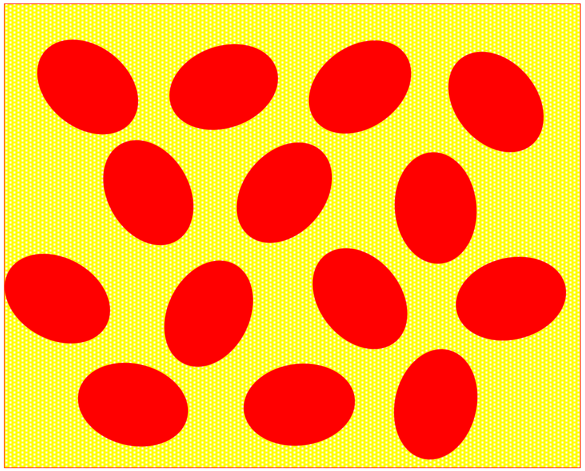


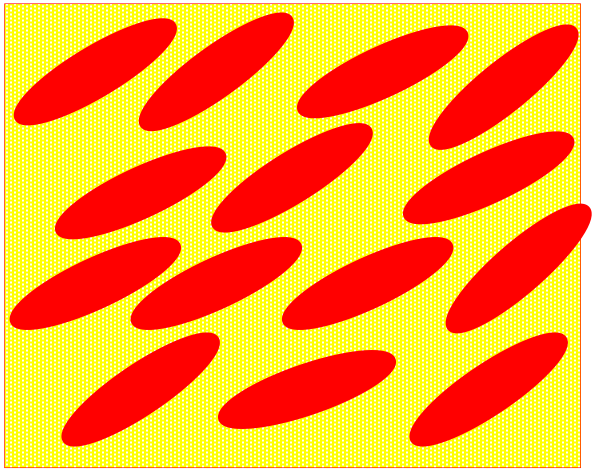
Hard sphere repulsion

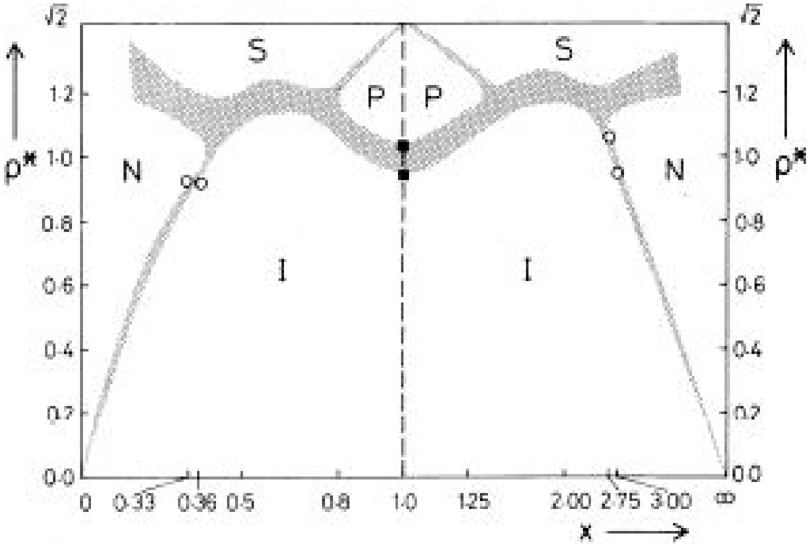
P. W. Bridgman, Phys. Rev. 3, 153 (1914).
J. G. Kirkwood, J. Chem. Phys. 7, 919 (1939).
J. G. Kirkwood, E. K. Maun and B. J. Alder, J. Chem. Phys. 18, 1040 (1950).
W. W. Wood and J. D. Jacobsen, J. Chem. Phys. 27, 1207 (1957).
B. J. Alder and T. E. Wainwright, J. Chem. Phys. 27, 1208 (1957).

Metropolis et al. JCP 21 (53)
Alder,Wainwright JCP 27 (57)
Pusey,Magen Nature 320 (86)
Mitus et al. PRE 55 (97)
Jaster EPL 42 (98)

Spheroids – phase diagram



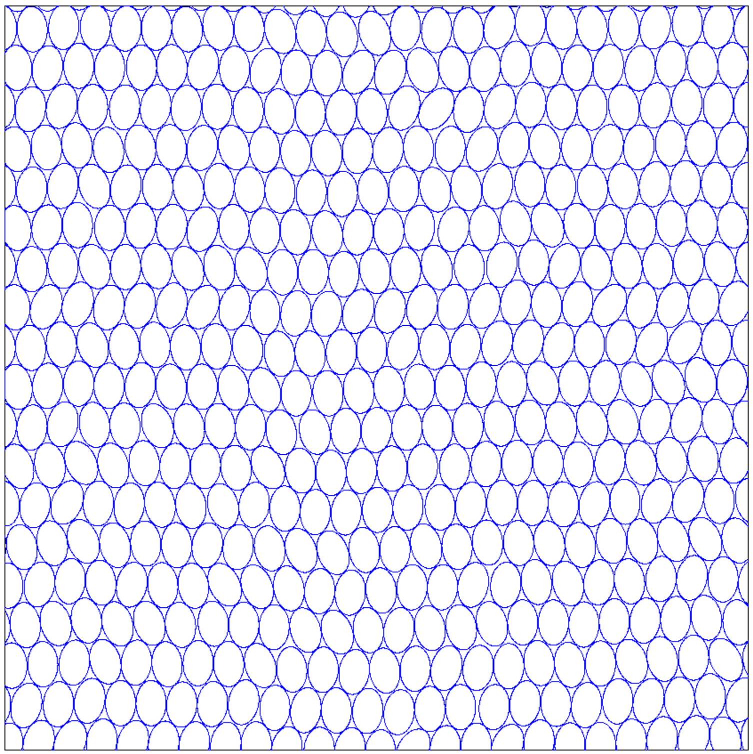


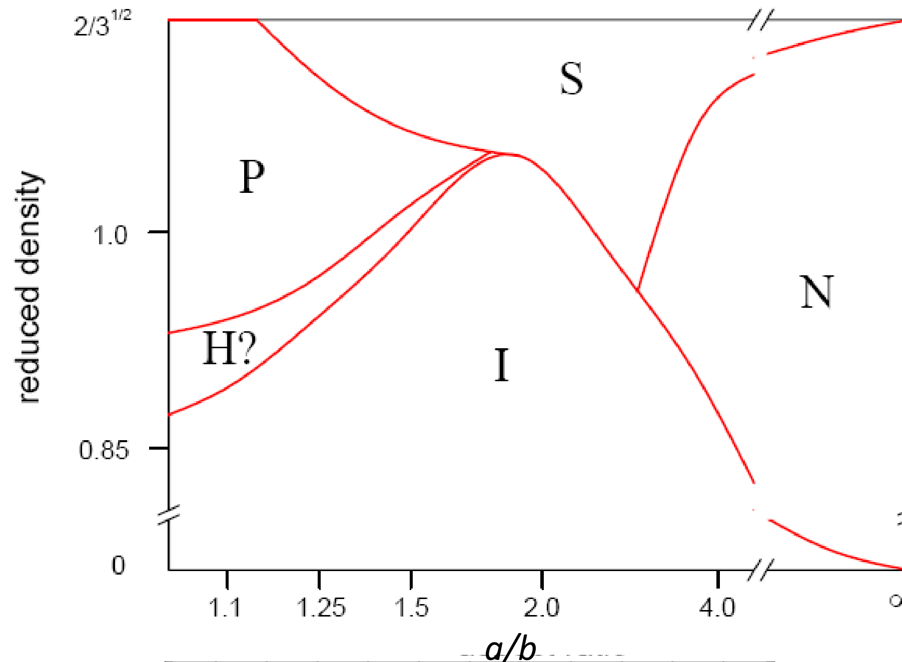


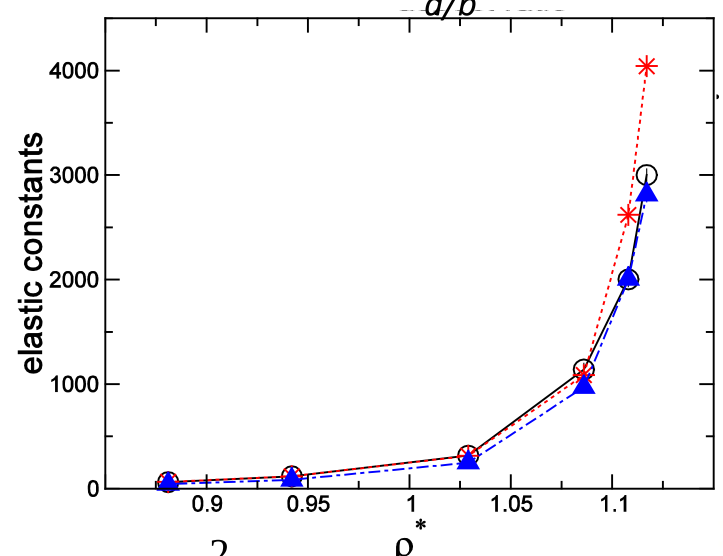
D.Frenkel, B.M.Mulder, J.P.McTague, PRL52,287 (1984)

Hard ellipses - 2D phase diagram

"Oriented" solid



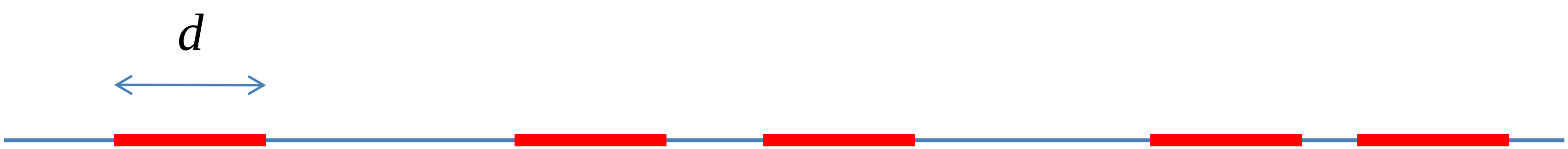




M. Murat, Y. Kantor, PRE74,031124 (2007)

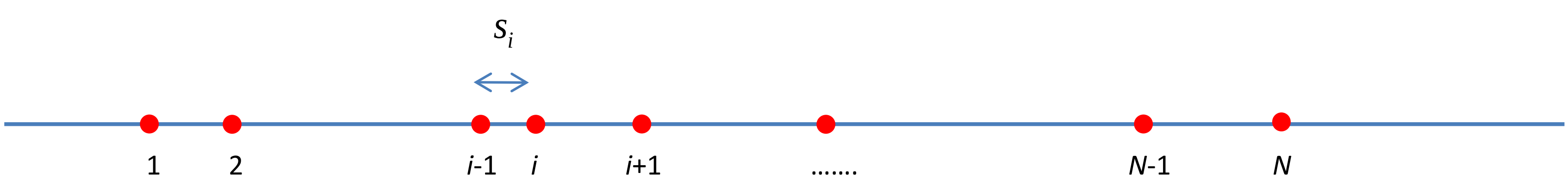
$$\rho^* \equiv \rho \cdot 4ab, \quad \max \rho^* = \frac{2}{\sqrt{3}} \approx 1.155...$$

Why 1D systems are "simple"



$$p(L - Nd) = Nk_B T$$

Tonks gas R. Tonks, Phys. Rev. **50**, 955 (1936)



$$Z_G = \int \prod_{j=1}^{N} dx_j \, \mathrm{e}^{-\beta \sum_{i=1}^{N} V(x_i - x_{i-1}) - \beta p x_N}$$

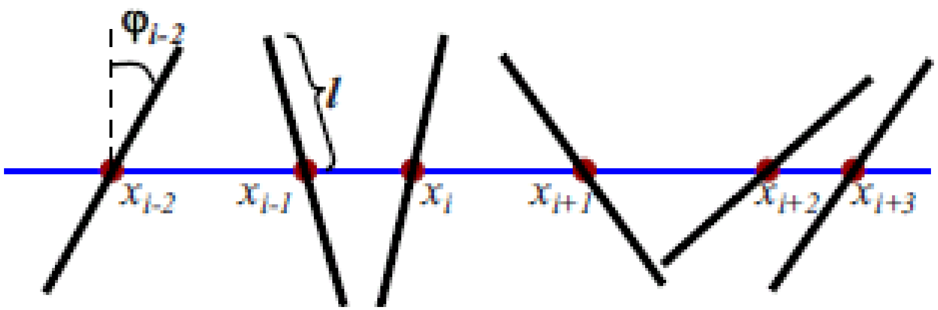
H. Takanishi,Proc.Math.-Phys Soc. Jpn. **24**, 60 (1942)

$$= \int \prod_{j=1}^{N} ds_{j,j-1} \, \mathrm{e}^{-\beta \sum_{i=1}^{N} (V(s_{i,i-1}) - p s_{i,i-1})}$$

$$\beta = \frac{1}{k_B T}$$

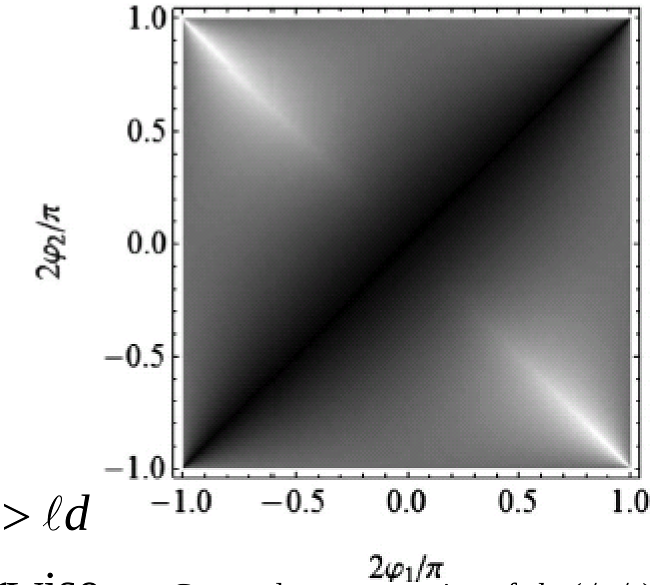
$$= \left(\int ds \, \mathrm{e}^{-\beta V(s) - \beta p s} \right)^N$$

1D gas of needles



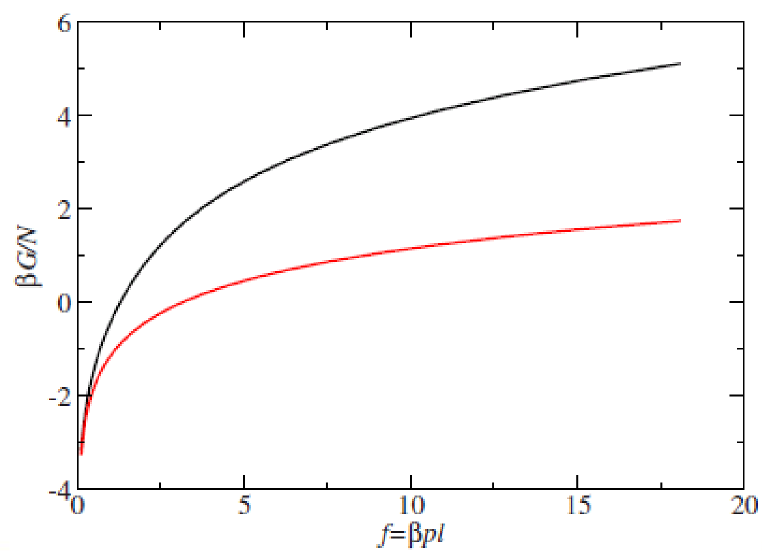
$$Z_G = \int \prod_{j=1}^{N} ds_{j,j-1} \prod_{j=1}^{N} d\phi_j \, e^{-\beta \sum_{i=2}^{N} (V(s_{i,i-1},\phi_{i-1},\phi_i) - p s_{i,i-1})}$$

$$= (\beta p)^{-N} \int \prod_{j=1}^{N} \left[d\phi_j \, e^{-\beta p \ell d_{i-1,i}(\phi_{i-1},\phi_i)} \right], \text{because } e^{-\beta V} = \begin{cases} 1, \text{ for } s > \ell d \\ 0, \text{ otherwise} \end{cases}$$



Greyscale representation of $d_{1,2}(\phi_1,\phi_2)$.
White $d = 2$, black $d = 0$ (for $\ell = 1$)

$$d_{i-1,i}(\phi_{i-1},\phi_i) = \frac{\sin|\phi_i - \phi_{i-1}|}{\max[\cos(\phi_{i-1}),\cos(\phi_i)]}$$

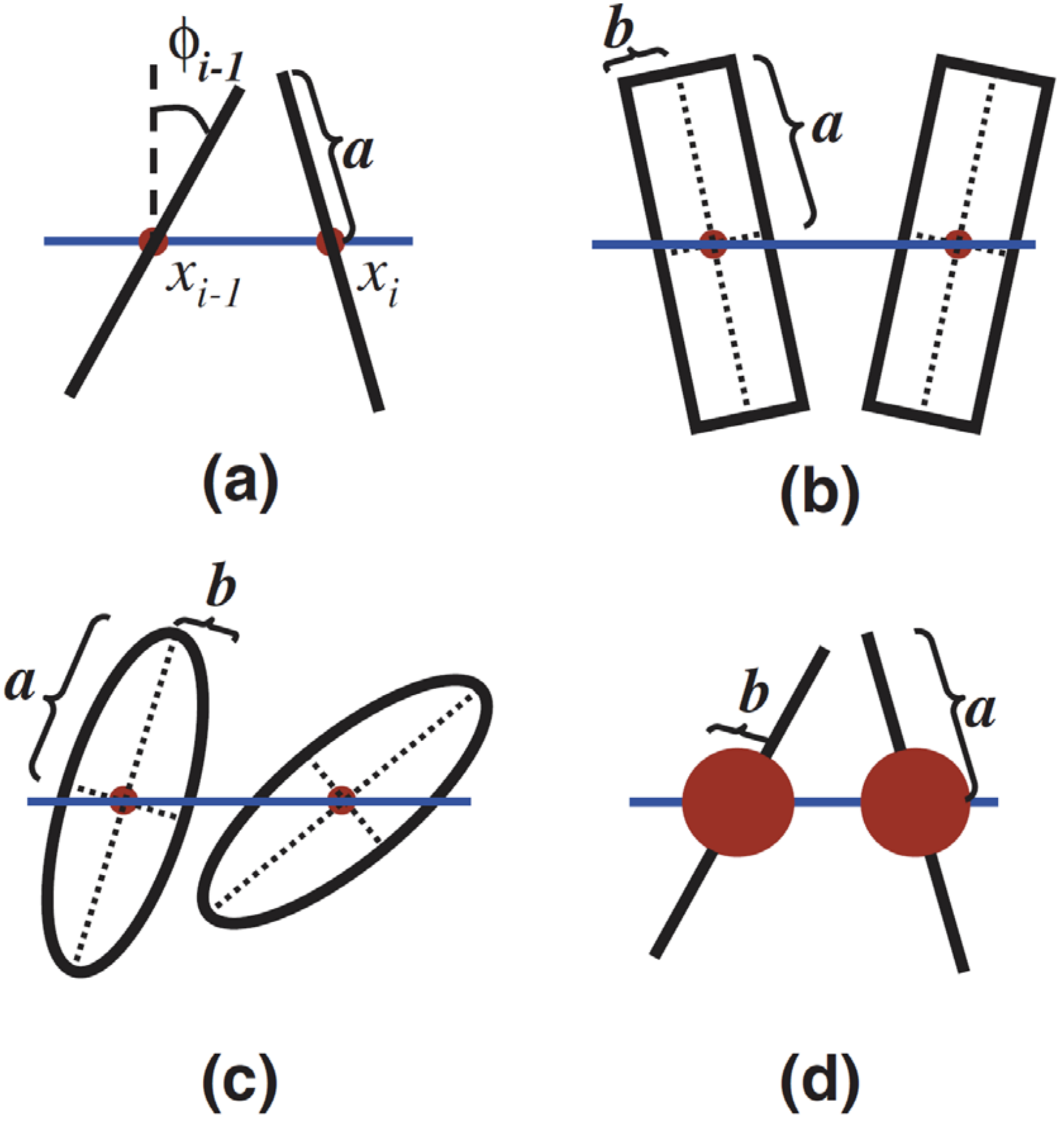


$$\beta = \frac{1}{k_B T}$$

Upper curve Gibbs free energy per particle, lower curve – noninteracting particles

Y. Kantor, M. Kardar, Phys. Rev. E**79**, 401109 (2009)

Various elongated particles



$\alpha = b/a$

aspect ratio

Y. Kantor and M. Kardar, Europhys. Lett. **87**, 60002 (2009).

Variance of direction as a function of pressure for rectangles

$\alpha = b/a$ aspect ratio

$$\sigma^2 \simeq \begin{cases} \frac{1}{2f\sqrt{1+4\alpha f}}, & \text{for rectangles,} \\ \frac{\sqrt{\alpha}}{\sqrt{f(1+4\alpha f)}}, & \text{for ellipses,} \end{cases}$$

σ^2 = variance of direction angle ϕ

$f = \beta p a$ dimensionless pressure

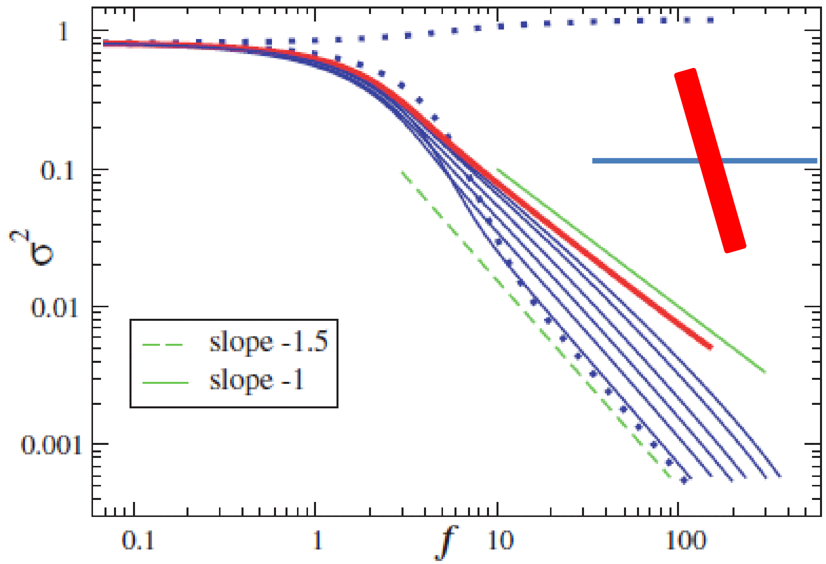


Fig. 2: (Color online) Variance of the angle as a function of the dimensionless pressure $f = \beta pa$ for rectangles. The rightmost (red) solid line is for needles ($\alpha = 0$), while the remaining solid lines correspond to aspect ratios $\alpha = 0.01, 0.02, 0.05, 0.1, 0.2, 0.5$ (right-to-left). The lower dotted line demonstrates the fast decay for $\alpha = 0.7$, while the almost horizontal dotted line corresponds to a square particle $\alpha = 1$. Short straight segments of slopes -1 and -1.5 are included for visual comparison.

Y. Kantor and M. Kardar, Europhys. Lett. **87**, 60002 (2009).

Variance of direction as a function of pressure for ellipses

$$\alpha = {}^{b}\!/\!_{a} \quad \text{aspect ratio}$$

$$\sigma^2 \simeq \begin{cases} \dfrac{1}{2f\sqrt{1+4\alpha f}}, & \text{for rectangles,} \\ \dfrac{\sqrt{\alpha}}{\sqrt{f(1+4\alpha f)}}, & \text{for ellipses,} \end{cases}$$

$\sigma^2 =$ variance of direction angle ϕ

$f = \beta p a$ dimensionless pressure

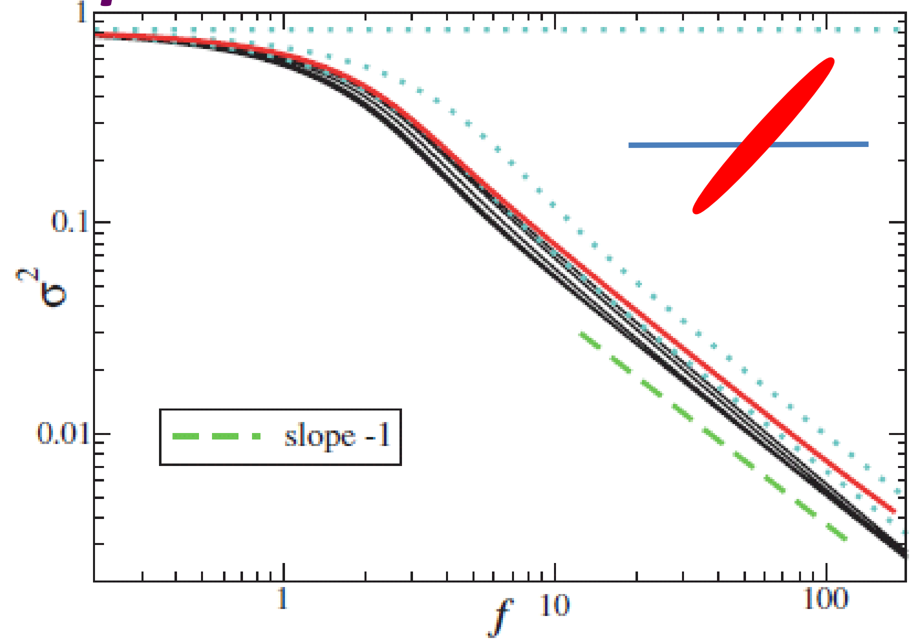
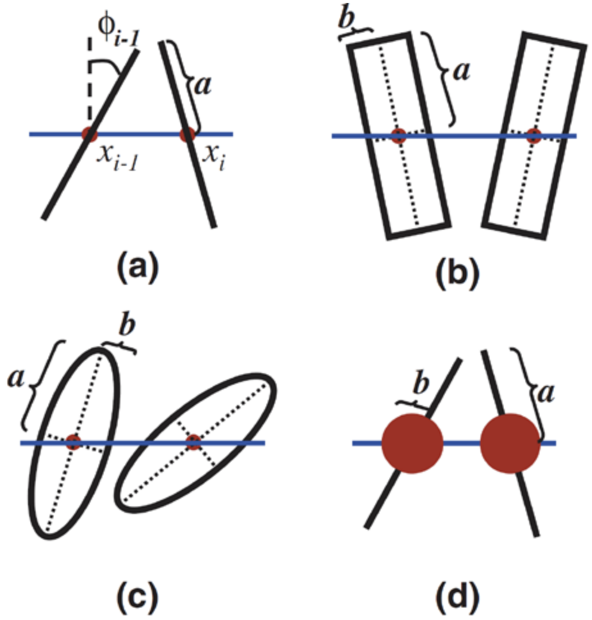


Fig. 3: (Color online) Variance of the angle as a function of the dimensionless pressure f for ellipses. The rightmost (red) solid line is for needles ($\alpha = 0$), while the remaining solid lines correspond to aspect ratios $\alpha = 0.01, 0.02, 0.05, 0.1, 0.2$ (right-to-left). Dotted lines (left-to-right) demonstrate the function for $\alpha = 0.5, 0.7$, while the horizontal dotted line correspond to a circular particle $\alpha = 1$. The short straight segment of slope -1 is included for visual comparison.

Y. Kantor and M. Kardar,
Europhys. Lett. **87**, 60002 (2009).

Various elongated particles



$$\text{(a)}\ d(\phi,\phi') = a\frac{\sin|\phi-\phi'|}{\max[\cos\phi,\cos\phi']}$$

$$\text{(b)}\ d(\phi,\phi') = 2b + \frac{b}{2}(\phi^2+\phi'^2) + a|\phi-\phi'| + \ldots$$

$$\text{(c)}\ d(\phi,\phi') = 2b + \frac{b}{2}\left(1-\frac{b^2}{a^2}\right)(\phi^2+\phi'^2) + \frac{a^2}{4b}\left(1-\frac{b^2}{a^2}\right)^2(\phi-\phi')^2 + \ldots$$

$$\text{(d)}\ d(\phi,\phi') = 2b + 0 + 0 + \ldots$$

Correlation length as a function of pressure

$$\alpha = {}^{b}\!/_{a} \quad \text{aspect ratio}$$

$$c(n) \equiv \langle \cos\phi_i \cos\phi_{i+n} \rangle - \langle \cos\phi_i \rangle^2 \sim e^{-n/\xi}$$

$$\xi^2 \simeq \begin{cases} \dfrac{f^2}{1+4\alpha f}, & \text{for rectangles,} \\ \dfrac{f}{4\alpha(1+4\alpha f)}, & \text{for ellipses.} \end{cases}$$

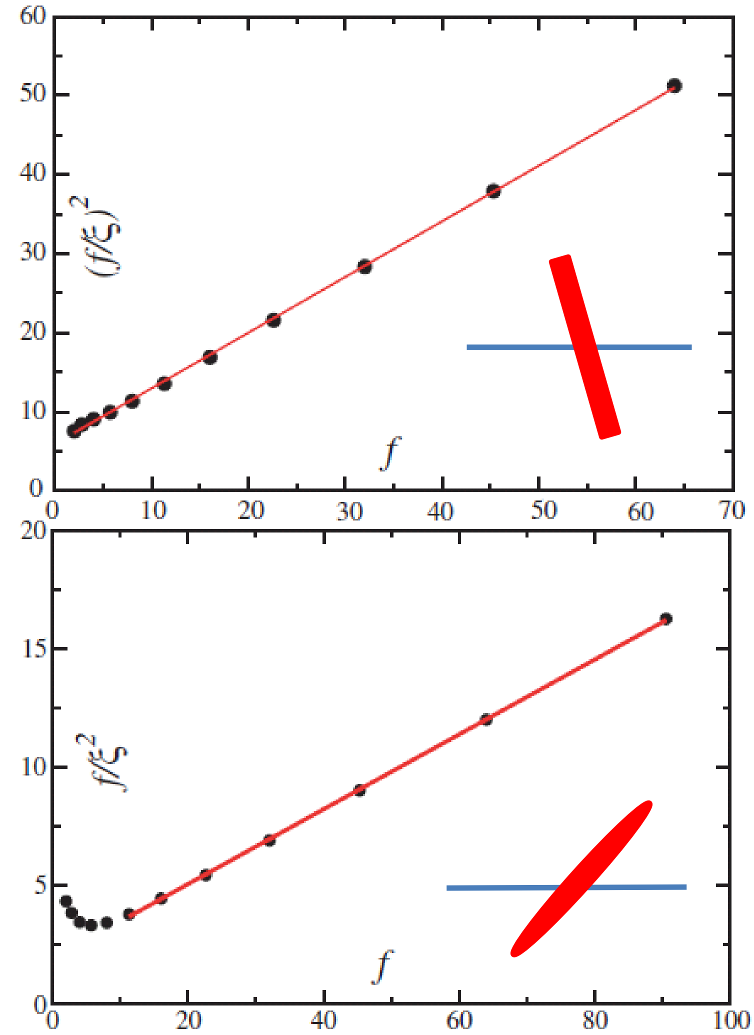


Fig. 4: (Color online) Numerical verification of eqs. (12) for the asymptotic relation between the correlation length ξ and the dimensionless pressure f. The top panel is for rectangles with aspect ratio $\alpha = 0.05$, and the bottom panel is for ellipses with aspect ratio $\alpha = 0.1$.

Y. Kantor and M. Kardar, Europhys. Lett. **87**, 60002 (2009).

Conclusions

- *1D systems provide a non-trivial check of higher-dimensional expressions (such as elasticity)*
- *Directional correlation correlations of elongated objects are sensitive to the curvature*
- *Properties of entropy-dominated systems are not always evident from simple symmetry considerations*
- *Possible extensions: shapes of interparticle contacts can be varied*