Anisotropic complex plasma crystals

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Anisotropic complex plasma crystals?

Anisotropy:

Anisotropy is the property of being directionally dependent, i.e. systems with axis along which isotropy symmetry is broken

Why study anisotropic systems?

- scientific interest (phase diagrams, collective phenomena,. . .)

Anisotropic complex plasma crystals?

Anisotropy:

Anisotropy is the property of being directionally dependent, i.e. systems with axis along which isotropy symmetry is broken

Why study anisotropic systems?

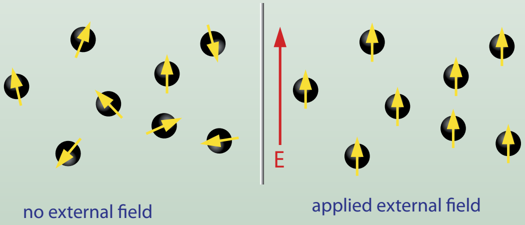
- scientific interest (phase diagrams, collective phenomena, . . .)
- buzzword: *smart materials*: materials with properties that can be changed in a controlled fashion
  - well known: liquid crystals (i.e. LCD)
  - here: electro- and magnetorheological systems (ER / MR)

Electro- and magnetorheological Systems

A short retrospection:
permanent dipoles embedded in media (also called: Stockmayer-fluids)
Interaction:

$$u_{dipol}(i,j) = \frac{(\vec{\mu}_i \cdot \vec{r})(\vec{\mu}_j \cdot \vec{r}) - (\vec{\mu}_i \cdot \vec{\mu}_j) r^2}{r^5}$$

Dipolar fluids:

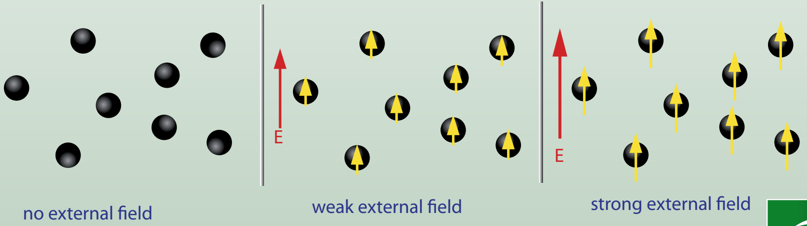


Electro- and magnetorheological Systems

Electro- or magnetorheological fluids: particles with *induced* moments (may be both magneto or electrostatic) in media:
Interaction:

$$u_{rheo}(i,j) = -m^2 \frac{(\vec{e}_z \cdot \vec{e}_r)^2 - 1}{r^3} = -d \frac{1}{r^3} P_2(cos\theta)$$

ER/MR fluids:



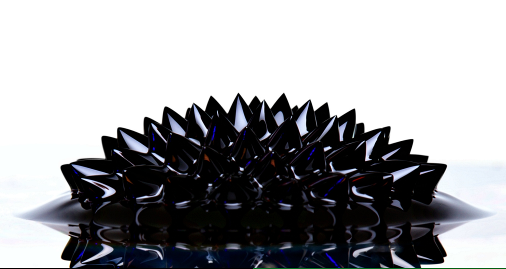
Applications | Mechanics

Tunable mechanical properties

ER/MR fluids can be switched to fluid or solid state:

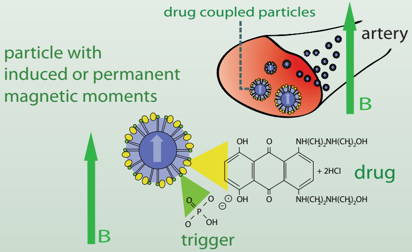
- Adaptive shock absorbers[a]
- Electrostatic switchable valves and hydraulic flow control
- Lock-less breaks (hydraulic bridge circuits)[b]

[a] R Stanway et al. , Smart Materials 5 (1996) 464
[b] S.B. Choi et al., Smart Materials 14 (2005) 1483



Applications | Medical Science

Magnetofection



drug is delivered by an activated trigger molecule

- a tool for biological chemistry and medicine [a]
- Intention: place drugs only in affected tissues
- Use nano-sized particles as a vehicle(+tigger) (colloidial MR-fluid)
- affected tissue is exposed to external magnetic fields

[a] C. Plank et al.,Biological Chemistry 384 (2003) 737

Applications | Photonic crystals

PhoC

Blue-Morpho-Butterfly (a natural PhoC, no colored pigments)

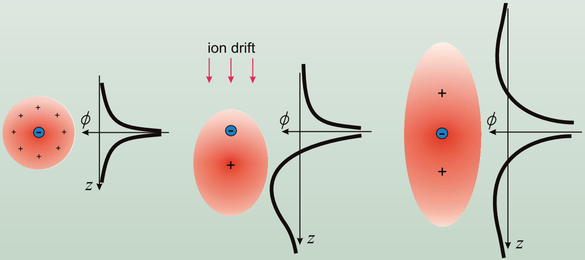
- Photonic crystals control the way electromagnetic waves (modes) propagate
  - *in no way* restricted to visible light
  - open issue: design and manufacturing (i.e. lithographic methods), usually anisotropic structures
- ER / MR systems provide tunable crystals [a]

[a] R. Tao, D. Xiao, Appl. Phys. Letters 80 (2002) 4702

Electrorheological plasmas

- Basic principle: Application of RF-discharges: (PK-3)[1]
- Applied RF-amplitude: *tunable* dipolar-dipolar interaction:

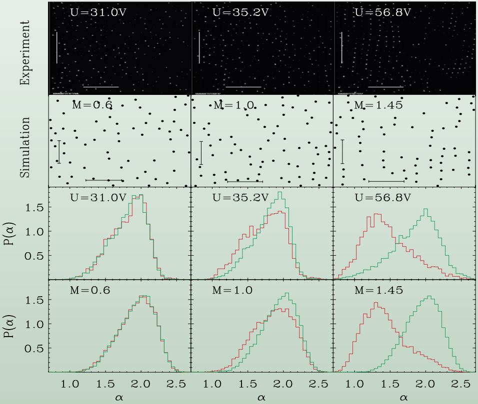
$$W(r,\theta) = Q^2 \left(\frac{\exp(-r/\lambda)}{r} - d\,\frac{M_T^2 \lambda^2}{r^3} P_2(\cos\theta) \right)$$



[1] R. Kompaneets, PhD-Thesis (2007)

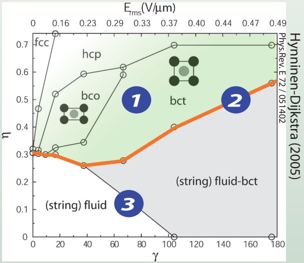
Electrorheological plasmas

- Discovery of electrorheological plasmas in PK-3[2]
- Advantage: interaction is determined by plasma parameters
- Experimental results: string fluids, observations on the kinetic level



[2]A.V. Ivlev et al., PRL 100 (2008) 095003

Theory of ER/MR - Systems



Simulations

Monte Carlo simulations and molecular dynamics:

- MC simulation using almost 300 particles
- sophisticated problem: dipol-dipol interaction causes lattice sums to be *conditionally* convergent
- thus every sweep requires an Ewald summation (DFT)

Also: Molecular dynamics (Goyal et. al.: step potentials[a])

[a] PRE 77 (2008) 031401

Variational approach

Alternative: Bogoliubov-Inequality

- Bogoliubov inequality provides an upper limit for the Helmholtz free energy F
- assuming the free energy F_0 of a reference system H_0 is known:

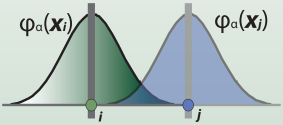
$$F = -\beta^{-1} \int d\Gamma \exp(-\beta H) \qquad \beta = \frac{1}{k_B T}$$

$$F \leq F_0 + \langle H - H_0 \rangle_0$$

- a reference system for classical solids: Einstein-Model

$$H_0 = \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + \frac{k}{2} \left(\mathbf{r}_i - \mathbf{r}_i^0 \right)^2 \right],$$

Variational approach



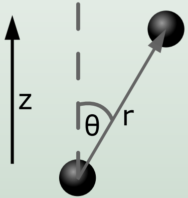
Variational free energy:

$$\tilde{F} = F_0 + \frac{1}{2}\epsilon \sum_{i\neq j}^{N} W(\mathbf{x}_{ij}^0) - \frac{3}{2} N k_\mathrm{B}$$

$$W(\mathbf{x}_{ij}^0) = \int d\mathbf{x}_i d\mathbf{x}_j \, \varphi_\alpha(\mathbf{x}_i) \, \phi(\mathbf{x}_{ij}) \, \varphi_\alpha(\mathbf{x}_j)$$

$$\varphi_\alpha(\mathbf{x}_i) = \left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\alpha(\mathbf{x}_i - \mathbf{x}_i^0)^2}$$

Variational approach | Model



Approximated interaction

- binary particle-particle interaction separation:

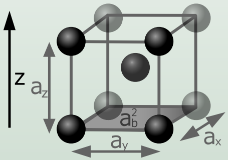
$$V(\mathbf{r}) = \epsilon\left[\phi_I(r) + \xi\phi_A(r,\theta)\right]$$

- sophisticated: dipol-dipol interaction $\propto r^{-3}$ (conditionally convergent lattice sums, divergences $r \rightarrow 0$) requires an approximation (chosen here GCM):

$$\phi_I(r) = \frac{\sigma}{r} e^{-\kappa(r/\sigma - 1)} \quad (1)$$

$$\phi_A(r,\theta) = \exp\left(-\left(\frac{r}{\sigma R}\right)^2\right) P_2(\cos\theta) \quad (2)$$

Variational approach | Variation

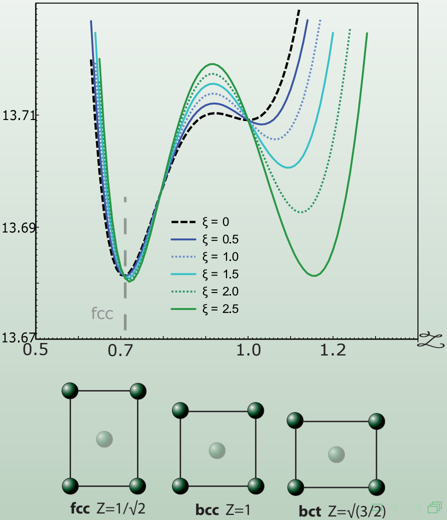


Approximated interaction

- W_I and W_A can be evaluated analytically
- hence: for a given lattice structure F viz. f can be evaluated using lattice sums (by variation)
- variational parameters: $\mathcal{Y} = \sqrt{\frac{a_y}{a_x}} \geq 1$, $\mathcal{Z} = \sqrt{a_x a_y}/a_z$
- chosen here: two classes of lattices bco (including fcc, bct, bcc), and hcp

Variational approach | Variation

A *toy* variation: ($\mathcal{Z}$ only)

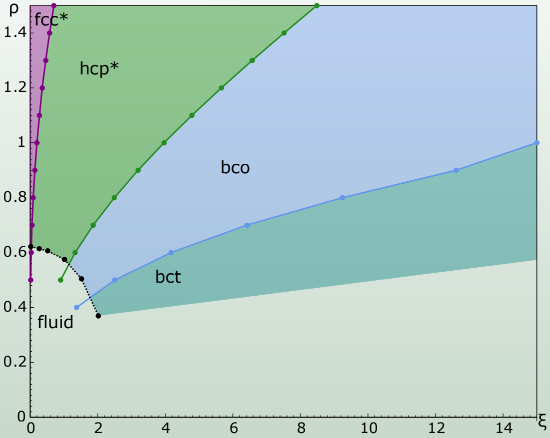


Variational approach | Phase diagrams

Phase diagrams

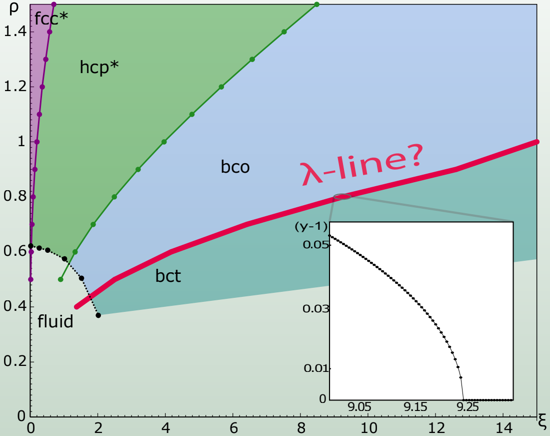
- Variation in the full parameter space $(\alpha, \mathcal{Y}, \mathcal{Z})$: phases and regimes
- Numerical minimization: downhill-simplex algorithm & quadratic optimization
- depending on the *hardness* κ of the isotropic core ϕ_I at least three different regimes of phase diagrams exist: here named as soft, medium and hard
- Additional parameters
  - ρ: particle number density
  - ξ: anisotropic strength (viz. strength of the external field
  - ϵ: strength of interaction

Medium regime



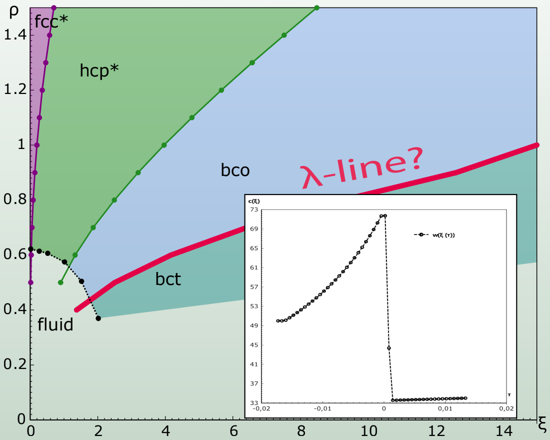
- ($\kappa = 7$) sequence of phases: fcc $\rightarrow$ hcp $\rightarrow$ bct $\rightarrow$ bco
- three fluid-solid-solid triple points

Medium regime | λ-line candidate



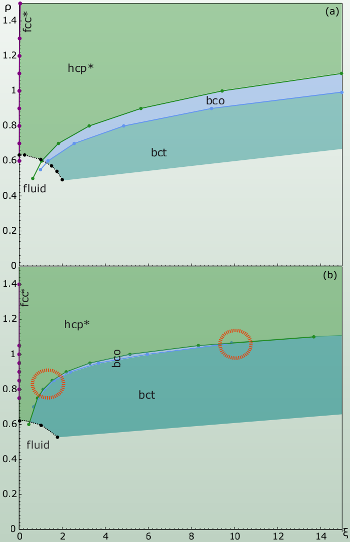
- a candidate for a second order (continuous) transition?
- continous phase transition $\longrightarrow$ critical phenomena

Medium regime | λ-line candidate



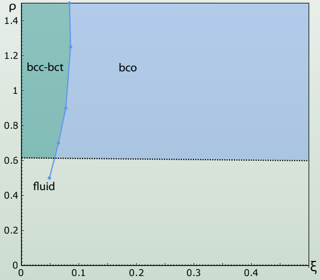
- specific "heat": $c(\tau) = -\xi \frac{\partial^2 \tilde{f}}{\partial \xi^2}$
- results: compatible with mean field critical exponents

Hard regime



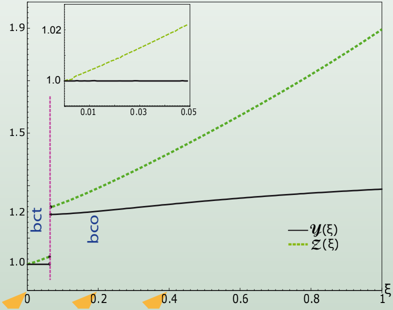
- Phase diagrams for $\kappa = 15$ viz. $\kappa = 35$
- fcc(*) is almost wiped out ($\xi \leq 4 \times 10^{-3}$)
- dominating phase: hcp
- new topology for high values of κ “bco-lens”
- likely bco is eliminated for even higher values of κ (i.e. hard spheres)

Soft regime diagram



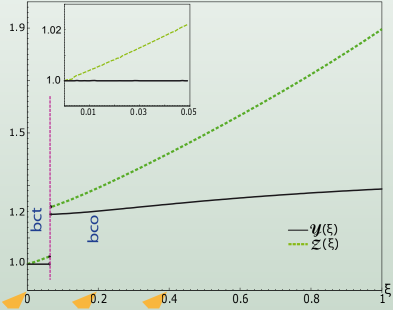
- phase diagram for $\kappa = 1$
- only two phases bcc-bct and bco
- at $\xi = 0$: bcc
- here: first-order transition
- speculative: tricrticial point in $1 < \kappa < 4$?
- no other structures observed (i.e. hcp)

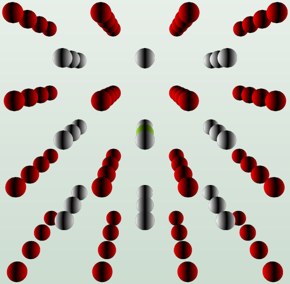
Soft regime diagram | Applications?



- defomations in terms of $\mathcal{Y}$, $\mathcal{Z}$ shown for $\kappa = 1$
- precisely tunable bct and bco structures
- colloidial systems: *tunable* photonic crystals?
- all these structures are accessible for quite small values of the *anisotropic* parameter ξ

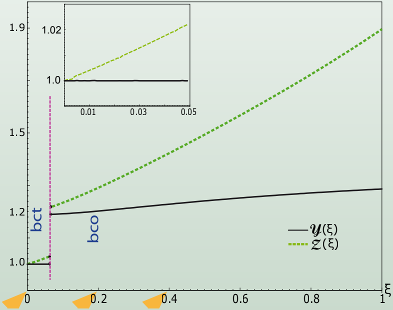
Soft regime diagram | Applications?

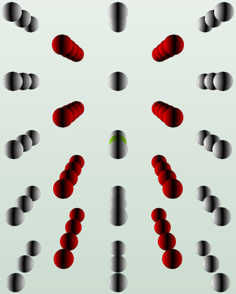




$$\xi = 0$$

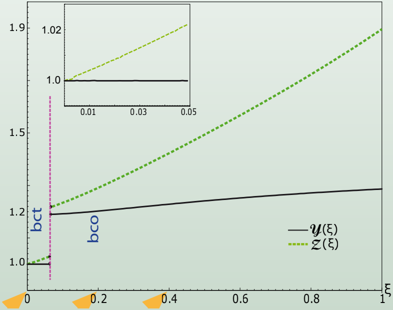
Soft regime diagram | Applications?

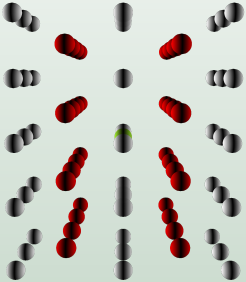




$\xi = 0.2$

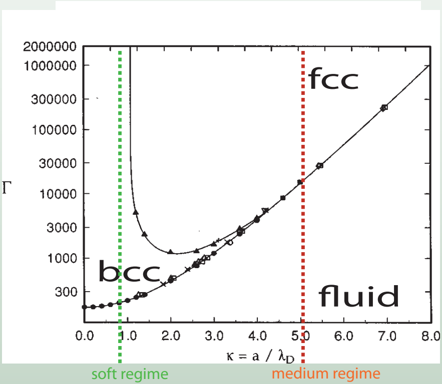
Soft regime diagram | Applications?





$\xi = 0.4$

Discussion | ER-Plasmas

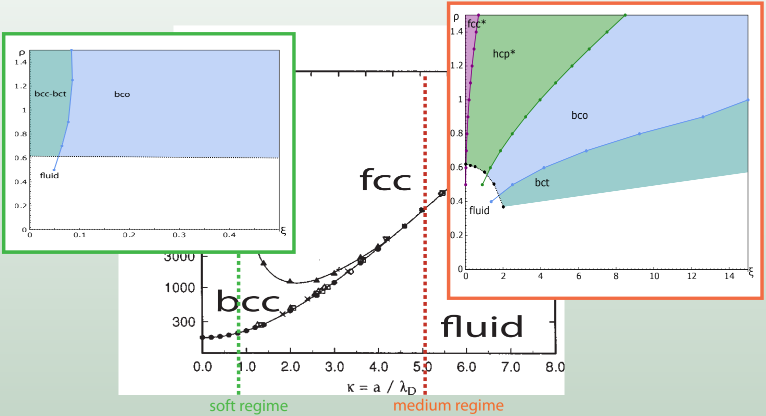


- these results can be mapped on the well-known phase diagram for plasma crystals (Yukawa) [a] [b]
- acceptable results for solid-solid line (≈ 6%), less accurate fluid-solid (≈ 15%)

[a] V. E. Fortov et al., Phys. Rep. 421(2005)1

[b] S. Hamaguchi et al., PRE 56(1997) 4671

Discussion | ER-Plasmas



Results

Conclusions

- ER / MR (electro- and magnetorheological) systems: enablers for smart materials
- complex plasmas as ER systems:
  - soft and medium regime accessible
  - critical phenomena research (λ-line candidate)
  - and a "toolbox" of solid-solid phase transitions
- open issue: fluid phases?

Thank you for your kind attention.