Simple estimations of thermodynamic properties of Yukawa systems

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Knowledge for Tomorrow

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Motivation

- Equation of state for complex (dusty) plasmas
    - Thermodynamics
    - Hydrodynamic description of the particle component
    - Waves and instabilities

- Specifics of complex plasmas
    - Open systems
    - Particle charge depends on particle density (charge cannibalism)
    - Plasma composition can vary

- Strategy
    - Develop simple analytical approximations for the “basic” case
    - Study relative importance of various specific phenomena

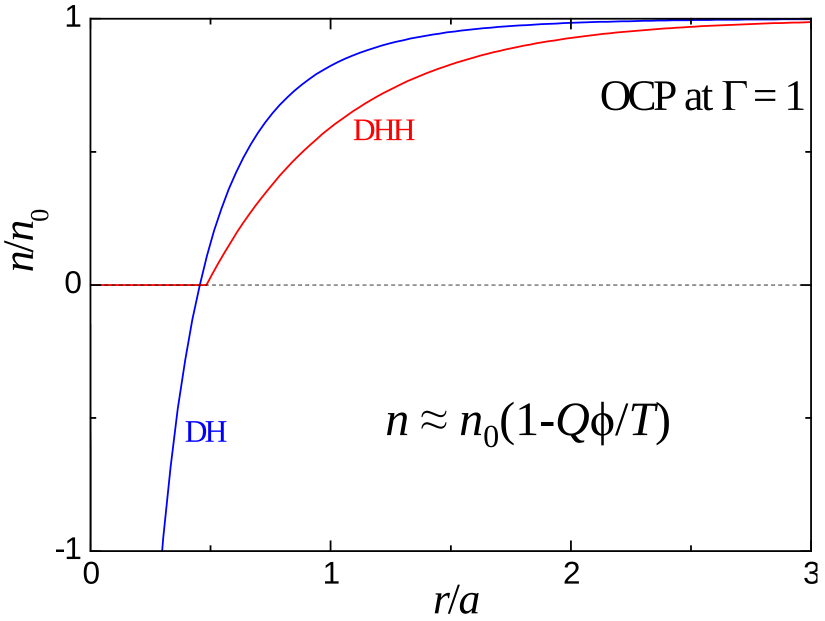
Model

- Two–component system consisting of
    - Point-like particles of charge Q and density n_0
    - Neutralizing background (uniform – OCP; linear response - Yukawa)

- Main parameters
    - Wigner-Seitz radius $a = (3/4\pi n_0)^{1/3}$ and the screening length λ
    - Coupling parameter, $\Gamma = Q^2/aT$
    - Screening parameter, $\kappa = a/\lambda$

- Main quantities of interest (in reduced units)
    - Internal energy, $u = U/NT$
    - Helmholtz free energy, $f = F/NT$
    - Pressure, $p = PV/NT$

Debye-Hückel + Hole (DHH) Approximation



- Conventional Debye-Hückel approach results in unphysical negative density
- Main idea behind DHH is to introduce a cut off (hole radius) *h*, below which the particle density is zero
- The hole radius, *h,* has to be found self-consistently via electrostatic consideration

DHH has been explicitly introduced for the OCP by Nordholm (1984)
Similar relations have been known earlier, e.g. Gryaznov&Iosilevskiy (1973)

DHH for Yukawa systems: Procedure

- Solve Poisson equation

$$\Delta\phi = -4\pi(Qn - en_{\rm m})$$

- Two solutions, inside and outside the hole

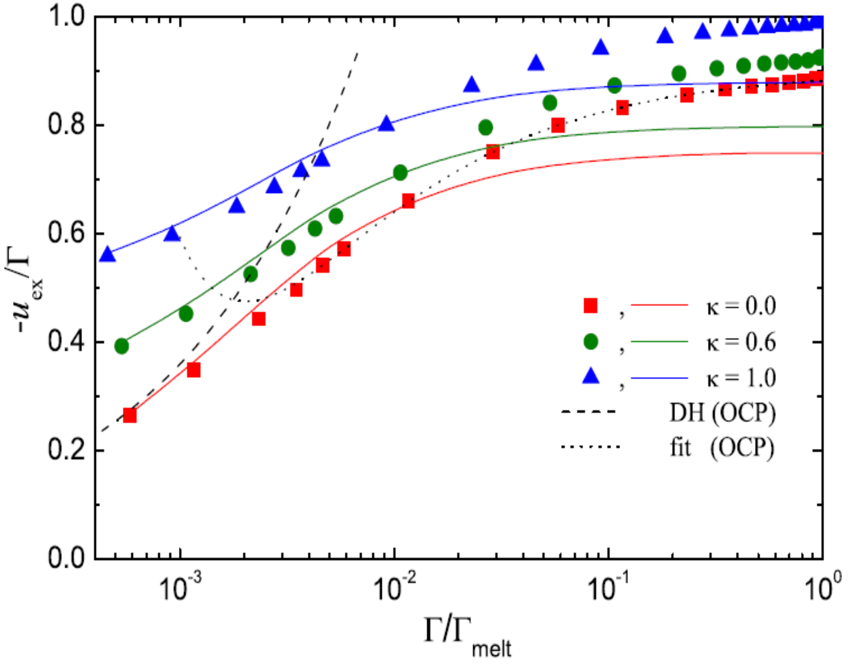
$$n = \begin{cases} 0, & r \leqslant h \\ n_0(1 - Q\phi/T), & r > h \end{cases}$$

- Match the two solutions at the hole boundary to determine *h* and one unknown parameter in the expression for ϕ inside the hole

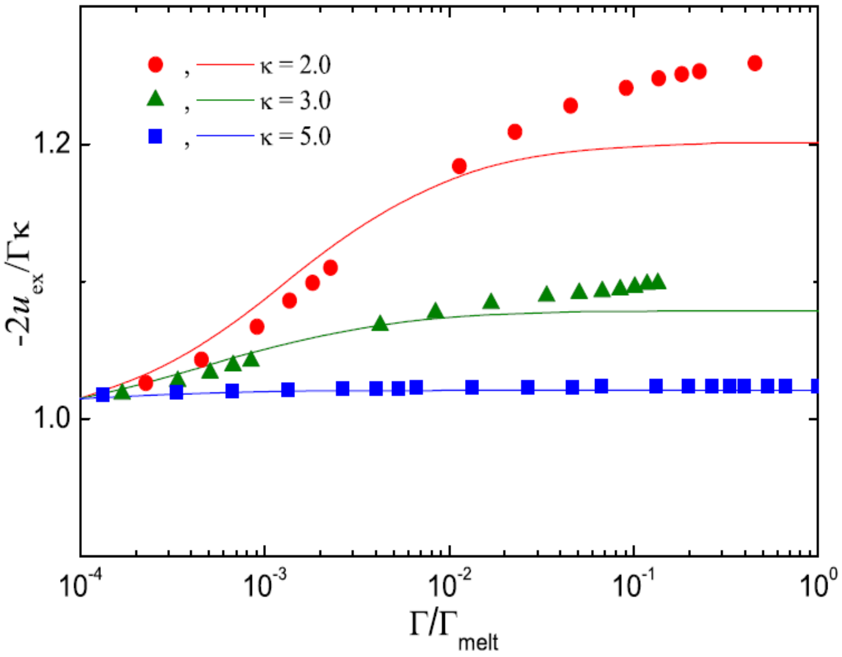
- Determine excess energy via the conventional expression

$$u_{\rm ex} = \frac{1}{2}\frac{Q}{T}\left[\phi(r) - \frac{Q}{r}\right]_{r\to 0}$$

Results: Excess Energy



Week screening



Strong screening

Numerical results from Hamaguchi et al. (1996, 1997)

Results: Helmholtz Free Energy at Weak Coupling

Excess free energy:

$$f_{\rm ex} = \int_0^{\Gamma} d\Gamma' u_{\rm ex}(\kappa,\Gamma')/\,\Gamma'$$

Debye-Hückel (DH) approximation:

$$u_{\rm ex}(\kappa,\Gamma) = -\tfrac{1}{2}\Gamma\kappa\sqrt{1+3\Gamma/\kappa^2}$$

$$f_{\rm ex}(\kappa,\Gamma) = -\frac{\kappa^3}{9}\left[\left(1+\frac{3\Gamma}{\kappa^2}\right)^{3/2}-1\right]$$

$f_{\rm ex}(\kappa,1)$

κ	MD	DH	DHH
0.0	−0.4368	−0.577	−0.460
0.2	−0.4495	−0.588	−0.471
0.4	−0.4809	−0.617	−0.502
0.6	−0.5284	−0.660	−0.548
0.8	−0.5866	−0.715	−0.606
1.0	−0.6541	−0.778	−0.673
1.2	−0.7304	−0.848	−0.747
1.4	−0.8103	−0.922	−0.826
2.0	−1.0710	−1.169	−1.084
2.6	−1.3504	−1.435	−1.360
3.0	−1.5424	−1.619	−1.549
3.6	−1.8326	−1.900	−1.838
4.0	−2.0274	−2.091	−2.033
4.6	−2.3223	−2.380	−2.326
5.0	−2.5200	−2.574	−2.523

MD results from Hamaguchi et al. (1997)

Application: Dust Acoustic Waves (DAW) at strong coupling

- Simplest hydrodynamic approach (particles)

$$\frac{\partial N_d}{\partial t} + \nabla(N_d \mathbf{V}_d) = 0,$$

$$\frac{\partial \mathbf{V}_d}{\partial t} + (\mathbf{V_d} \cdot \nabla)\mathbf{V_d} = \frac{Q\boldsymbol{E}}{M_d} - \frac{\nabla(P_d)}{M_d N_d}$$

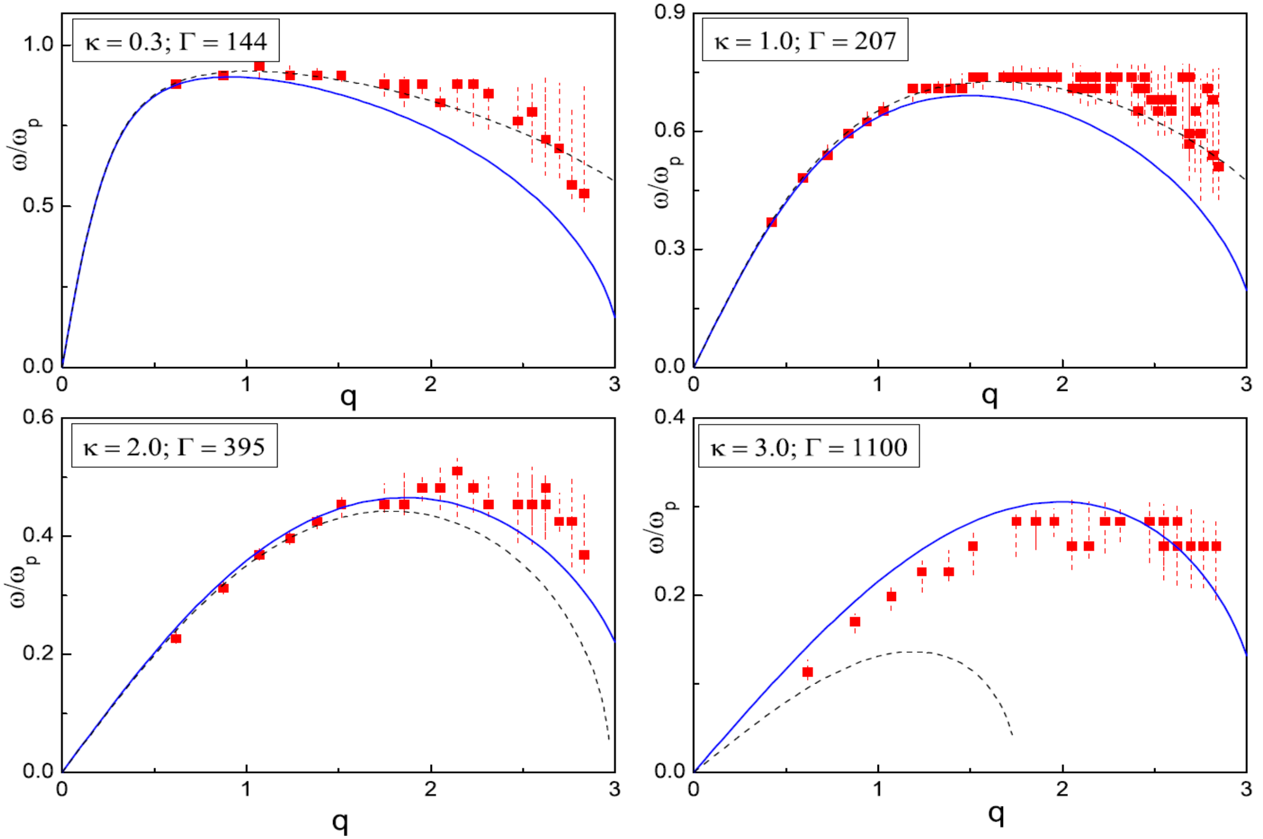
- Boltzmann response of the neutralizing medium + Poisson equation

- Resulting dispersion relation

$$\boxed{\frac{\omega^2}{\omega_{\mathrm{p}}^2} = \frac{q^2}{q^2+\kappa^2} + \frac{q^2}{3\Gamma}\gamma\mu_{\mathrm{p}}}$$

where $q = ka$, $\gamma \approx 1$, and $\mu_{\mathrm{p}} = 1 + p_{\mathrm{ex}} + \frac{\Gamma}{3}\frac{\partial p_{\mathrm{ex}}}{\partial \Gamma} - \frac{\kappa}{3}\frac{\partial p_{\mathrm{ex}}}{\partial \kappa}$

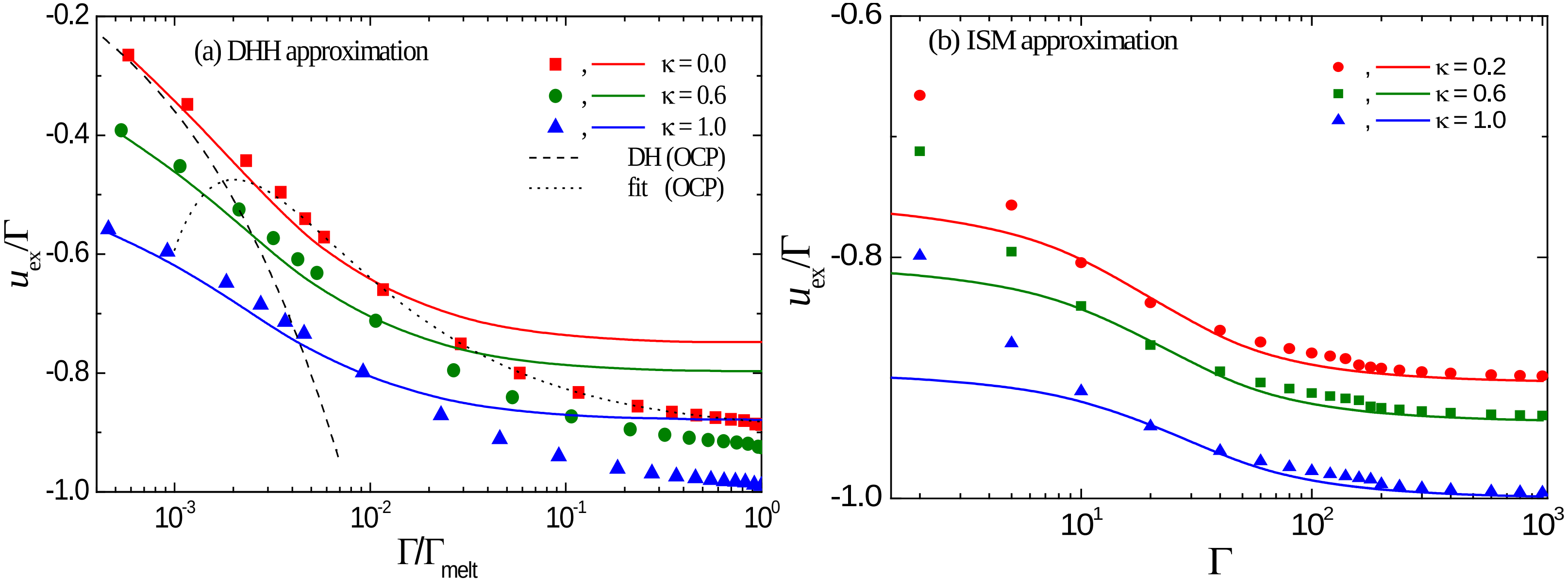
Dust Acoustic Waves at Strong Coupling



Numerical results: Ohta & Hamaguchi (2000);
Solid curves: Hydrodynamics with DHH, Dashed curves: sum rule analysis OCP

Recent Developments: Ion Sphere Model (ISM)

- Fixed hole radius = Wigner-Seitz radius
- Pure electrostatics to estimate the static excess energy, u_{ex}
- Simple approximation to estimate the thermal contribution to u_{ex}
- ISM is simple and more accurate than DHH at strong coupling



Numerical results from Hamaguchi et al. (1996, 1997)

Conclusion

- The ultimate goal of these studies is to produce reliable equation(s) of state for complex (dusty) plasmas
- The first element of the project is to develop simple analytic approximations for the “basic” case
- Two such approximations have been proposed
- DHH approximation is an extension of the DH approach and is suitable in the weak/moderate coupling regime
  - see S. Khrapak et al. Phys. Rev. E **89**, 023102 (2014)
- ISM approximation is more appropriate in the moderate/strong coupling regime
  - paper in preparation

Thank you for your attention!

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