Properties of collective modes in complex (dusty) plasmas and related systems

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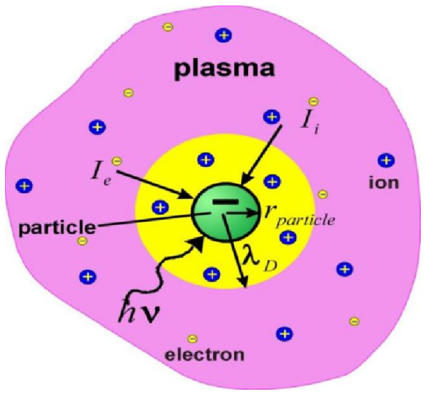
Motivation:

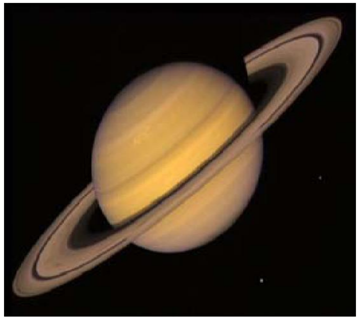
- Theory of collective motion in liquids is active area of research since the second half of XX century (starting from neutron scattering measurements)
- In particular, the theory for monoatomic liquids (liquid metals and rare gases) has been worked out
- To which extent the developed theories are applicable to complex (dusty) plasmas, representing classical systems of strongly interacting particles?
- Alternatively, using complex (dusty) plasmas is it possible to check the accuracy and applicability limits of these early theories?

Complex Plasma: Interdisciplinary Research Field

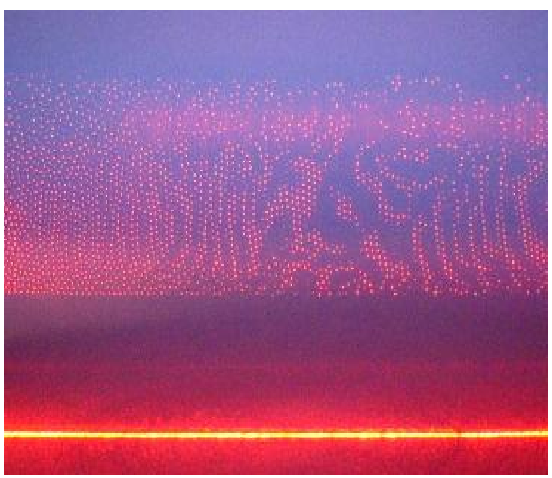


- Solid particles in the plasma background
- Particles are charged (mainly by collecting electrons and ions)
- Classical system of strongly interacting particles
- Interdisciplinary research area

Astrophysical topics:



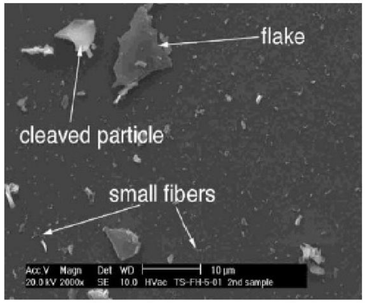
Laboratory:

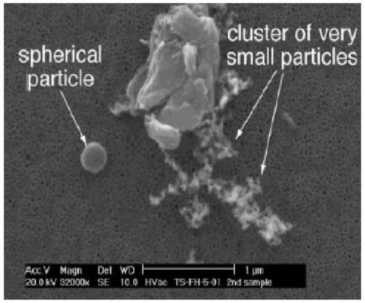


From Kretschmer, Selwyn, Sharpe, et al.

Industry:

Fusion:





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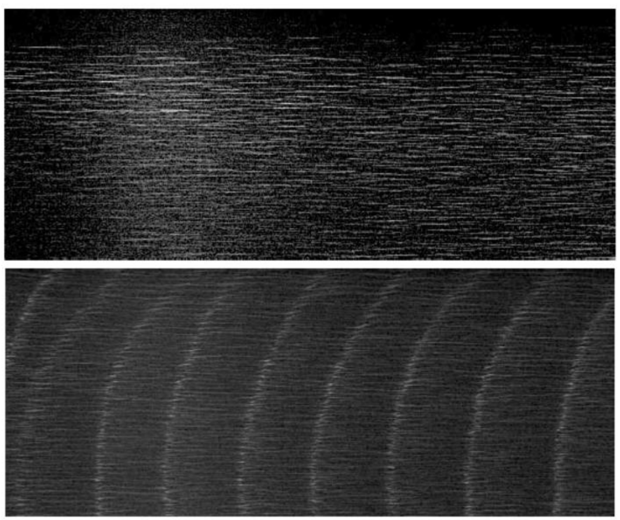
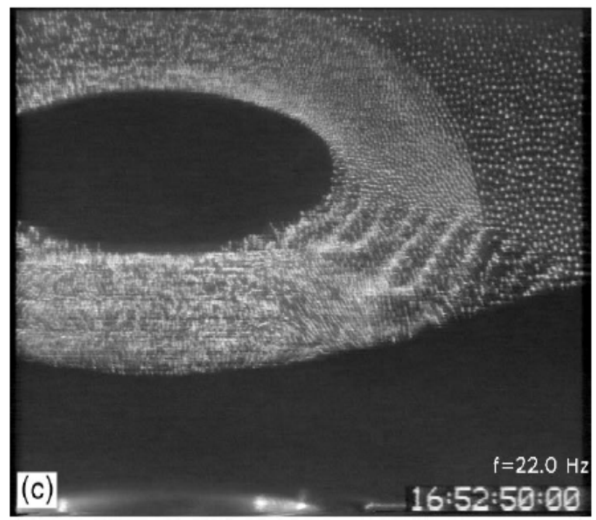
Waves in complex plasmas (few examples)

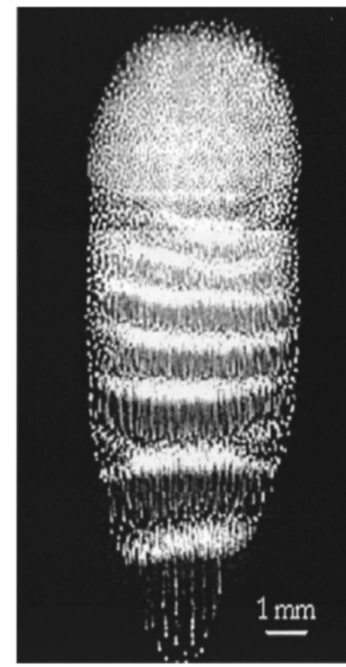
- Low damping due to particle-neutral gas collisions
- Simple determination of dispersion relation
- Individual particle motion can often be resolved



Ratynskaia et al. (2004)



Yaroshenko et al. (2004)



Fortov et al. (2000)

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Theory of dust acoustic waves (DAW)

- Continuity and momentum equations for the particle component

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

$$\frac{\partial \mathbf{v}_d}{\partial t} + (\mathbf{v}_d \cdot \nabla)\mathbf{v}_d = -\frac{eZ}{m_d}\nabla\phi - \frac{\nabla(n_d T_d)}{m_d n_d} - \sum_{\beta} \nu_{d\beta}(\mathbf{v}_d - \mathbf{v}_\beta) \ .$$

- Boltzmann distribution for ions and electrons

$$n_{e(i)} \simeq n_0 \exp(\pm e\phi / T_{i(e)}).$$

- Poisson equation

$$\nabla^2 \phi = -4\pi e (n_i - n_e + Z n_d)$$

- Standard linearization procedure (all perturbations are proportional ~exp(i**kr**-iωt))

$$\frac{\omega^2}{k^2} = \gamma_d v_{T_d}^2 + \frac{\omega_{\rm pd}^2 \lambda_{\rm D}^2}{1 + \lambda_{\rm D}^2 k^2}$$

Rao, Shukla, Yu (1990)

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Dust acoustic velocity

- In the long-wavelength limit DAW exhibits acoustic dispersion with the DA velocity

$$C_{\mathrm{DA}} = \omega_{\mathrm{pd}} \lambda_{\mathrm{D}} \equiv \sqrt{|Z| \frac{T_i}{T_d}} \sqrt{\frac{P\tau}{1 + (1 + P)\tau}} v_{T_d}$$

- Here $P = |Z| n_d / n_e$ is the Havnes parameter, $\tau = \frac{T_e}{T_i}$ is the electron–to–ion temperature ratio (normally ~ 100), Z is the particle charge number (normally ~ 1000)

- DA velocity can be remarkably higher than the thermal velocity (plasma related effect)

Strong coupling effects

- Electric charge of particles is very high
- The energy of interparticle interaction can be remarkably higher than the particle kinetic energy (temperature)
- Strong coupling effects can be dominant
- Description of waves at strong coupling
    - Generalyzed Hydrodynamics (GH)
    - **Quasi-localized charge approximation (QLCA)**

Fluid approach with proper thermodynamics

- The standard expression for the sound velocity of single-component fluids reads

$$c_s = v_T\sqrt{\gamma\mu}$$

where $\gamma = C_P/C_V$ is the adiabatic index, $\mu = (1/T)(\partial P/\partial n)_T$ is the isothermal compressibility modulus, and v_T is the particle thermal velocity

- Proper equation of state is required.

- The simple practical equations of state for 3D Yukawa fluids and crystals have been recently worked out in papers by Khrapak and Thomas (2015); Khrapak, Kryuchkov, Yurchenko and Thomas (2015)

- DA sound velocity can be considerably modified due to strong coupling

Dependence on coupling and screening

- Weak-coupling (conventional DA velocity) scale

$$c_0 = \omega_p \lambda_D.$$

- Weak dependence of c_s/c_0 on Γ deep in the fluid regime
- c_s/c_0 is sensitive to the screening parameter
- c_s/c_0 drops by almost one order on the way from near-OCP to κ = 5.

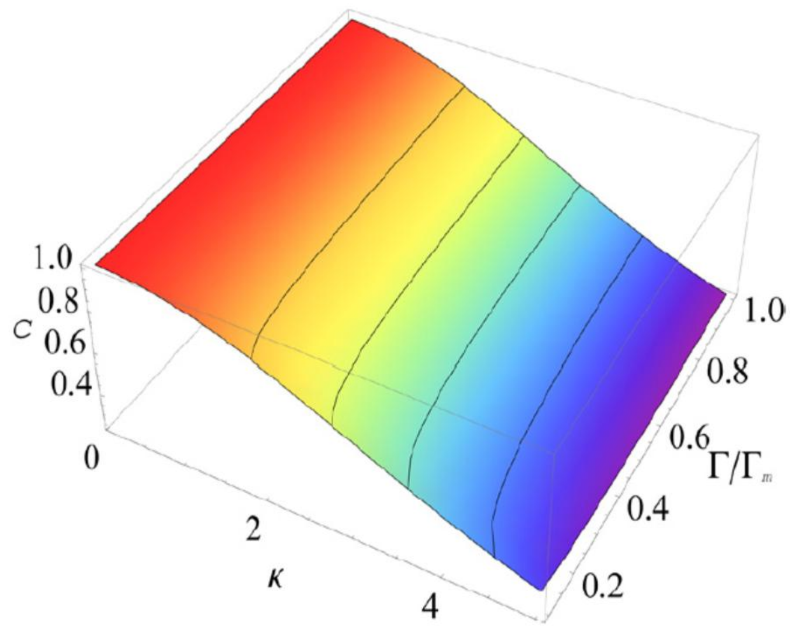

Figure 5. Three-dimensional plot of the reduced sound velocity $c \equiv c_s/c_0$ as function of Yukawa system state variables κ and Γ/Γ_m.

Khrapak and Thomas (2015)

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Quasi-localized charge approximation (QLCA)

- Generic expressions for the longitudinal and transverse dispersion relations:

$$\omega_L^2 = \frac{n}{m}\int \frac{\partial^2 V(r)}{\partial z^2} g(r)\left[1-\cos(kz)\right]d\mathbf{r},$$

$$\omega_T^2 = \frac{n}{m}\int \frac{\partial^2 V(r)}{\partial y^2} g(r)\left[1-\cos(kz)\right]d\mathbf{r}.$$

are equivalent to the model of collective motion in liquids by Zwanzig (1967), quasi-crystalline approximation (QCA) by Hubbard&Beeby (1969), Takeno&Goda (1971). Similar expressions occur from the analysis of frequency moments of $S(k,\omega)$.

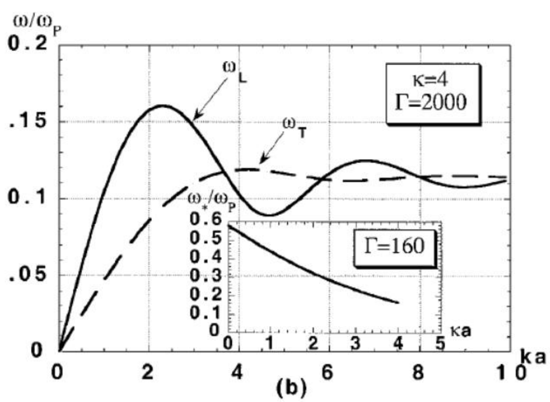
- In the context of plasma physics is known as QLCA after Kalman and Golden applied the approximation to one-component-plasma and related systems

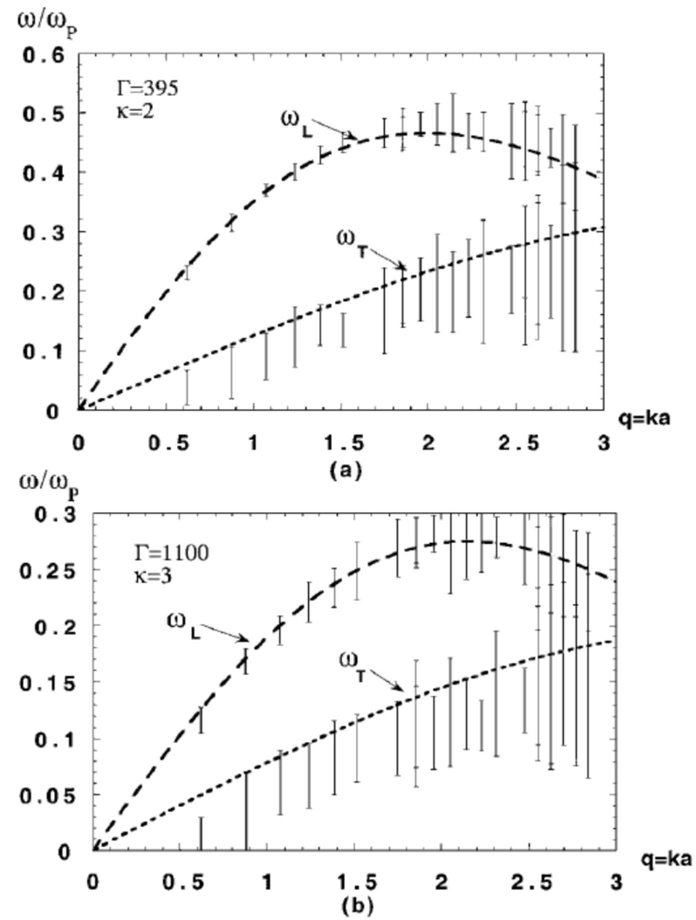
History of application to complex (dusty) plasmas

- **Yukawa interaction potential**

- First applied by Rosenberg and Kalman (1997) in the regime of long-wavelengths and weak screening

- Kalman et al. (2000) computed *g*(*r*) using the HNC scheme get results in good agreement with MD modeling by Ohta and Hamaguchi (2000)





Kalman et al. (2000)

Relations between the fluid (thermodynamic) and QLCA approaches

- The sound velocities evaluated using the fluid thermodynamic approach and QLCA are very close, QLCA yields systematically slightly higher values

- The difference is because QLCA is a theory for high-frequency perturbations

TABLE I. Reduced sound velocity $c_s/\omega_p a$ of Yukawa fluids as calculated from the QLC approximation and present fluid model for several phase state points. QLCA data are from Ref. [29]. For details see the text.

κ	Γ/Γ_m	QLCA	Fluid
1.0	0.12	0.96	0.95
1.0	0.70	0.96	0.94
2.0	0.12	0.42	0.41
2.0	0.70	0.41	0.39
3.0	0.12	0.23	0.21
3.0	0.70	0.21	0.19

QLCA results by Kalman et al. (2000) and Donko et al. (2008)

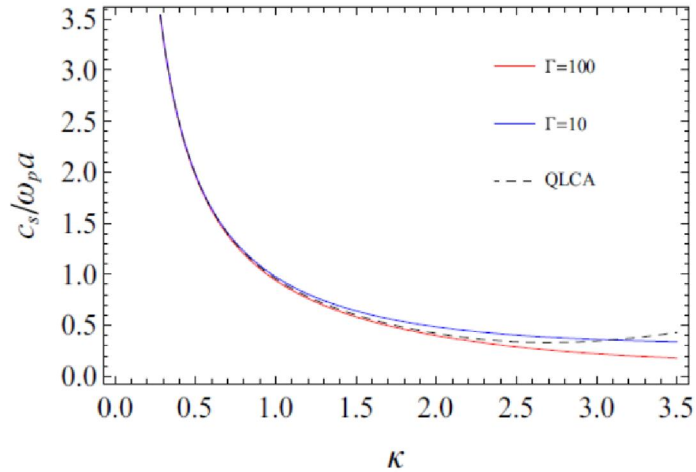
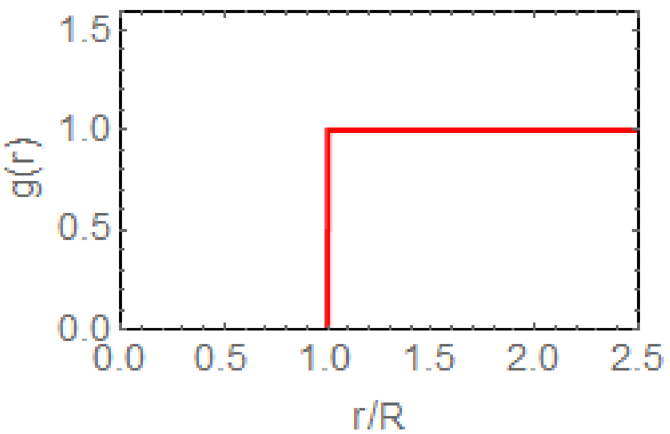


FIG. 2. (Color online) Reduced sound velocity of Yukawa fluids, $c_s/\omega_p a$, as a function of the screening parameter κ. The solid curves correspond to the results of the simple fluid approach of this paper for $\Gamma = 10$ (blue curve) and $\Gamma = 100$ (red curve). The dashed curve is plotted using QLCA result of Ref. [28], given by Eqs. (21) and (22).

Khrapak and Thomas (2015)

How accurately RDF should be known?

- The simplest model which takes into account excluded volume effects
- The integration can be performed analytically
- The parameter *R* is evaluated requiring consistency for energy or pressure



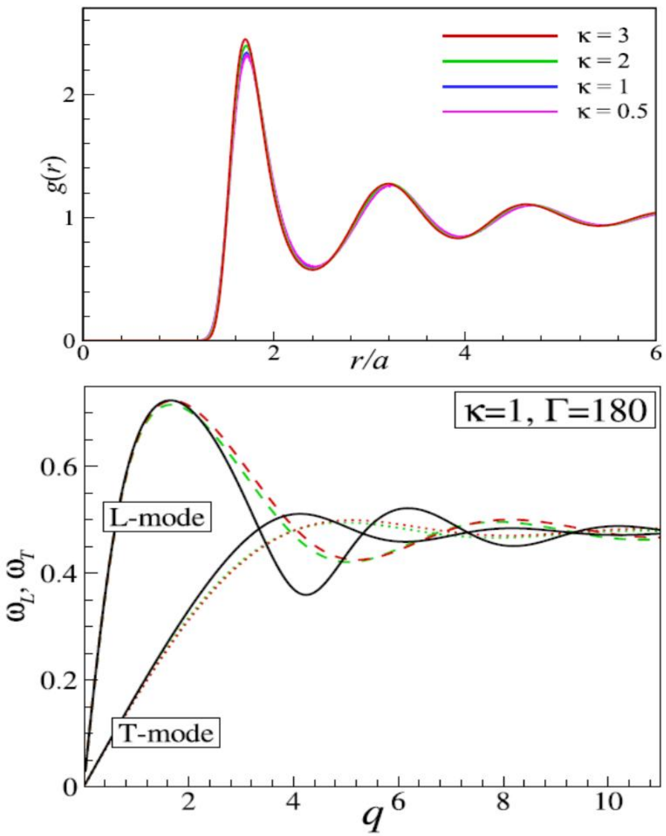
$$\omega_L^2 = \omega_p^2 e^{-R\kappa}\left[(1+R\kappa)\left(\frac{1}{3}-\frac{2\cos Rq}{R^2q^2}+\frac{2\sin Rq}{R^3q^3}\right) - \frac{\kappa^2}{\kappa^2+q^2}\left(\cos Rq + \frac{\kappa}{q}\sin Rq\right)\right].$$

$$\omega_T^2 = \omega_p^2 e^{-R\kappa}(1+R\kappa)\left(\frac{1}{3}+\frac{\cos Rq}{R^2q^2}-\frac{\sin Rq}{R^3q^3}\right).$$

Khrapak et al. (2016)

QLCA with model and accurate RDFs

- Accurate RDF can be calculated in MD simulations and substituted into QLCA expressions
- The overall agreement between calculations with simple and accurate RDF is not very good
- From experimental point of view, large wavelengths are most interesting ($q \leq 1$)



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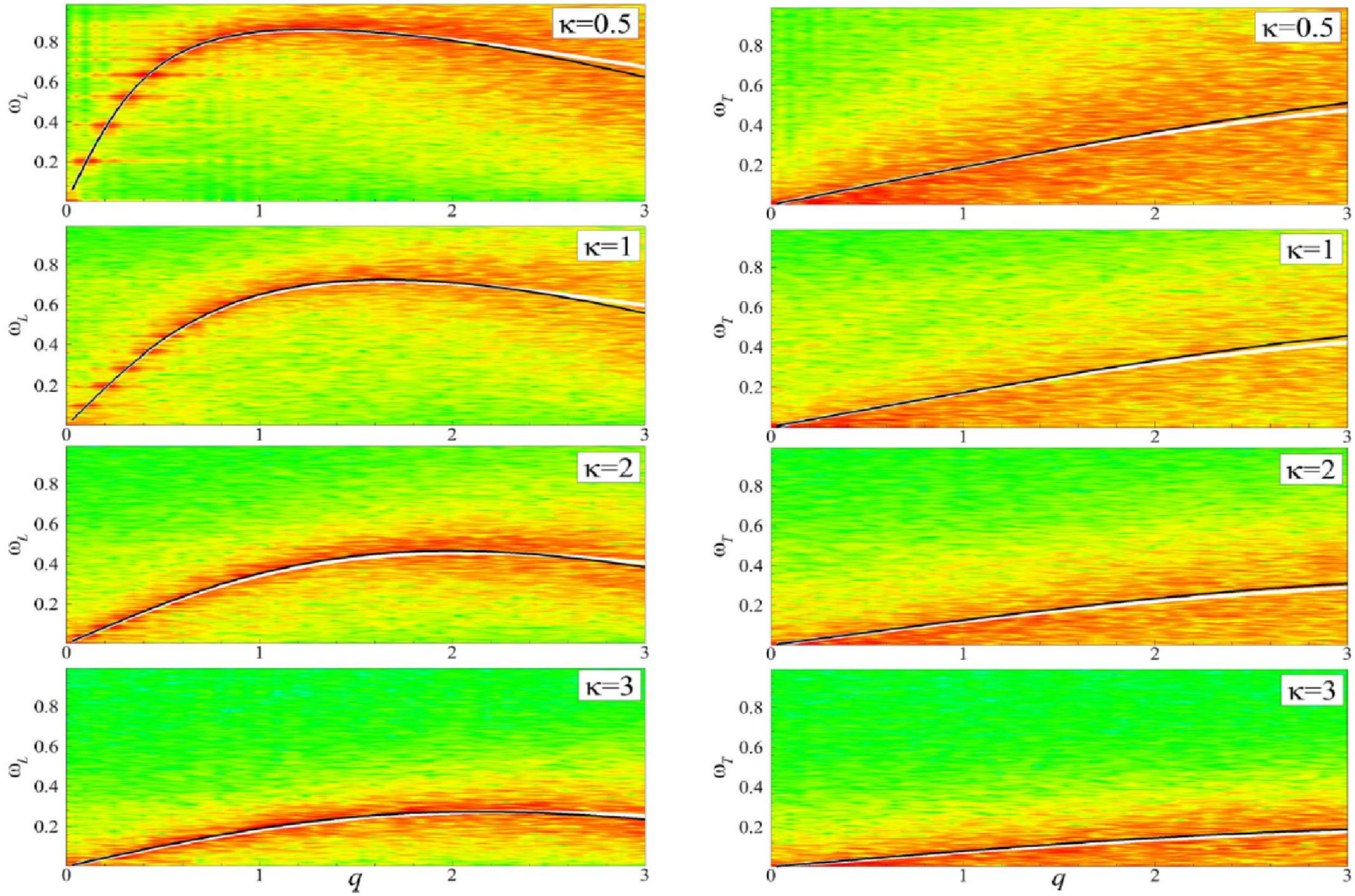
Long-wavelength regime

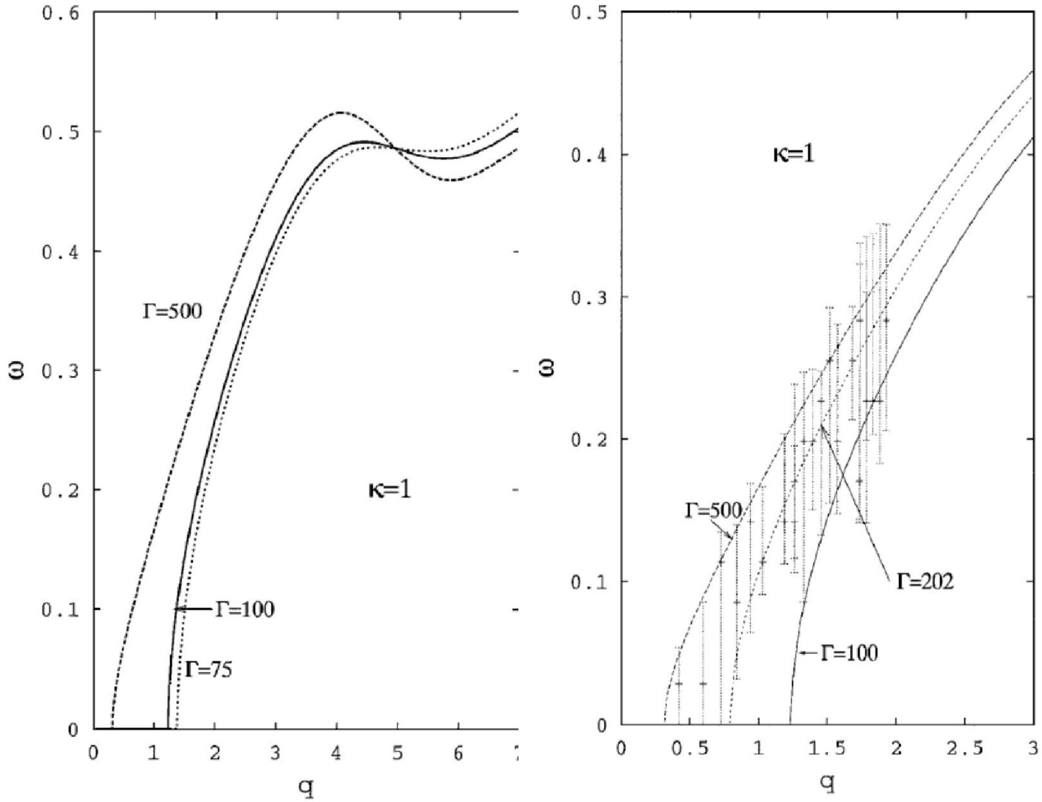


- **In the long-wavelength regime the full (dark) and simplified (white) QLCA produce almost identical results**

Khrapak et al. (2016)

Remark about the transverse modes in fluids

- At sufficiently strong coupling fluids can support transverse (shear) modes
- However, they exist only at sufficiently short wavelengths (above critical wave vector)
- The transverse sound velocity is not very well defined, but is nevertheless a useful quantity



Murillo (2000)

Relations between the sound velocities

- If the velocities are expressed in units of thermal velocity, the following general relations exist:

$$c_L^2 - 3c_T^2 = 2p_{\rm ex}$$

$$c_L^2 - \frac{4}{3}c_T^2 = c_{\rm Th}^2$$

TABLE II. The longitudinal (c_L) and transverse (c_T) sound velocities (in units of thermal velocity) of strongly coupled Yukawa fluids in 3D evaluated using the QLCA approach with the input of RDFs from direct MD simulations.[27] The excess pressure, $p_{\rm ex}$, and the thermodynamic sound velocity, $c_{\rm Th}$, are obtained using the expressions from Refs. 22 and 29, respectively.

κ	Γ	c_L	c_T	$c_L^2 - 3c_T^2$	$2p_{\rm ex}$	$\sqrt{c_L^2 - \frac{4}{3}c_T^2}$	$c_{\rm Th}$
0.5	145	41.29	3.98	1657.34	1657.56	41.03	41.06
1.0	180	22.29	4.07	447.15	446.30	21.79	21.81
2.0	370	13.83	4.26	136.83	135.28	12.93	12.93
3.0	990	11.55	4.41	75.06	73.79	10.37	10.37

Khrapak (2016)

Sound velocity near the fluid solid phase transition

- It is well known that the ratio of the sound to thermal velocity of many liquid metals and metalloids has about the same value at the melting temperatures

$$c_s/v_T|_{T=T_m} = \chi \sim 10.$$

- Rosenfeld (1999) pointed out that this "quasi-universal" property is also shared by the hard sphere (HS) model. Using thermodynamic definition

$$c_s/v_T = \left[p(\eta) + \eta dp(\eta)/d\eta + \tfrac{2}{3}p(\eta)^2\right]^{1/2}$$

- This yields $\chi \simeq 12.6$ at $\eta_F = 0.494$ using Carnahan-Starling EoS

- **What about soft spheres?**

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Sound velocity near the fluid solid phase transition

- Consider inverse-power-law (IPL) potential

$$V(r) = \epsilon(a/r)^{\alpha}.$$

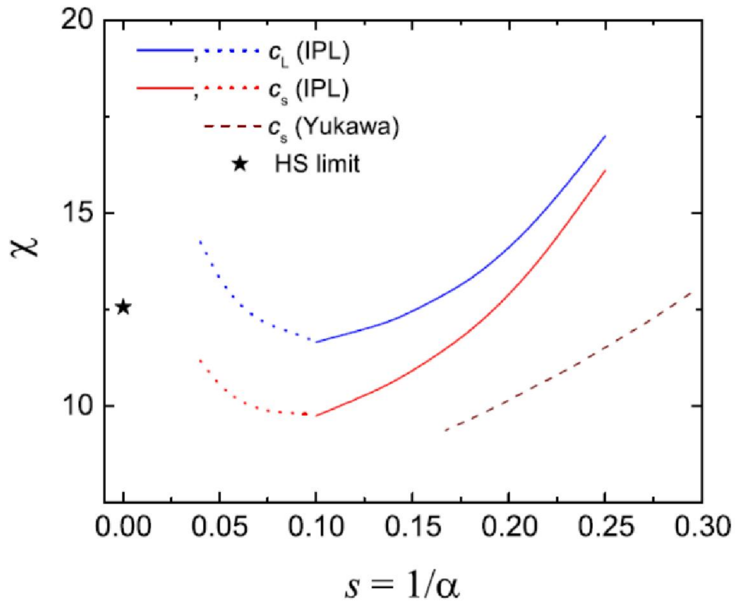
- The longitudinal elastic sound velocity

$$c_L = v_T\sqrt{p_{ex}(3\alpha + 1)/5}.$$

- The thermodynamic (instantaneous) sound velocity $c_s^2 = c_L^2 - \frac{4}{3}c_T^2$ is then

$$c_s = v_T\sqrt{p_{ex}(\alpha + 3)/3}.$$

- Over a wide range of softness χ is practically constant, close to the value predicted by the HS model



Observe: QLCA predicts divergence of the sound velocity in the limits of soft (correct) and steep (incorrect) interaction

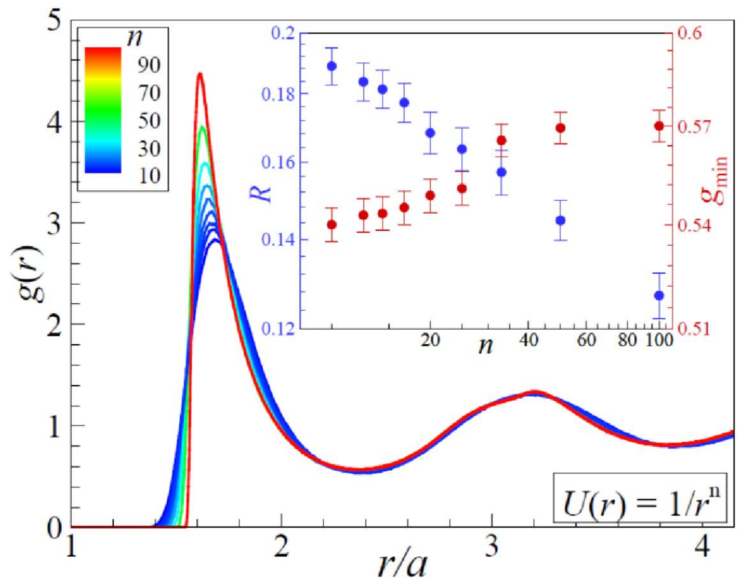
Khrapak (2016)

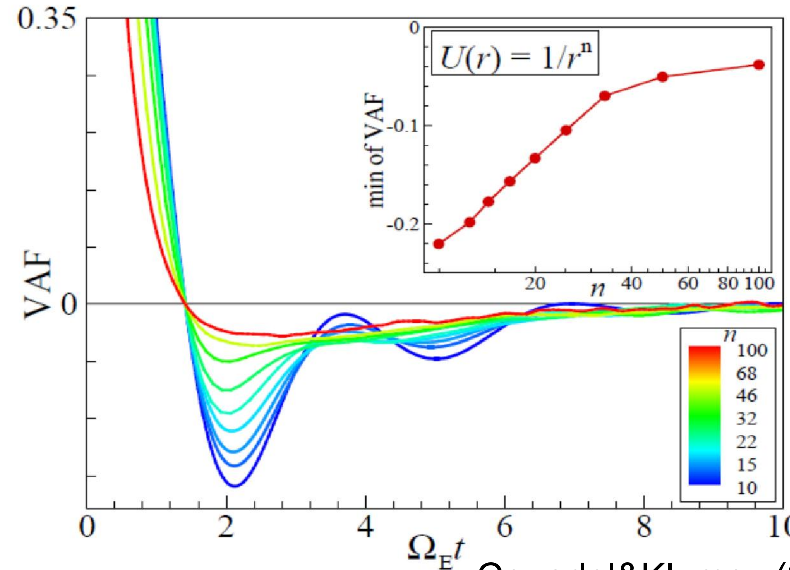
Systematic study of the IPL system near freezing

- Agrawal&Kofke (1995) data on coexistence fluid densities of the IPL model
- MD simulations for a number of IPL exponents ($10 \leq n \leq 100$)
- Analysis: Structure, dynamics, longitudinal mode dispersion

Structure (RDF) and dynamics (VAF)

- With increasing the exponent *n* structure and dynamics tend to HS-like
- Raveche-Mountain-Streett criterion of freezing is not very accurate when potential softness varies in a wide range
- More accurate criterion can be based on the height of the minimum of *g*(*r*)





Couedel&Klumov (2016)

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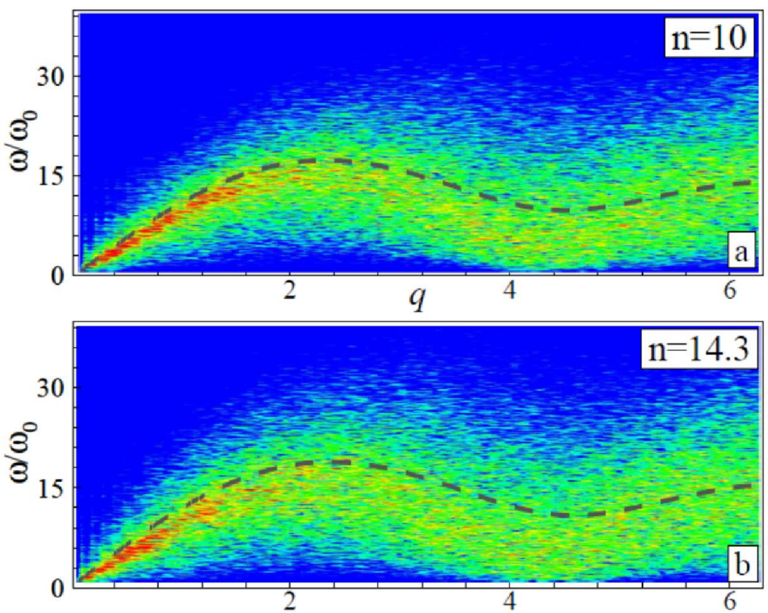
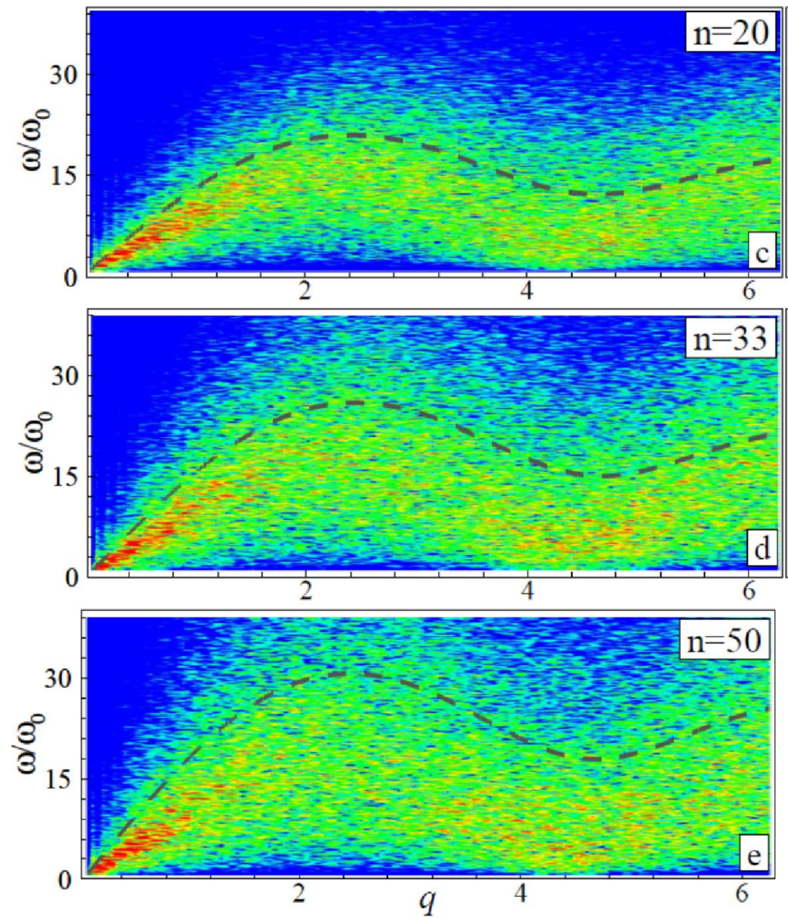
Dispersion of the longitudinal mode

- QCA/QLCA is reasonably accurate for *n* < 20
- Not applicable for steeper interactions





Couedel&Klumov (2016)

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Actual interactions in complex plasmas

- Electron and ion collection ➔ Power-law long-range asymptotes
- Non-linear ion-particle interaction ➔ Variability of the effective screening length
- Plasma production and loss ➔ Double-Yukawa interaction potential
- Ion flows ➔ Wake-mediated interaction
- **Can QLCA be used to discriminate between different interactions in complex plasmas?**

Representative examples of interaction

- Double-Yukawa potentials

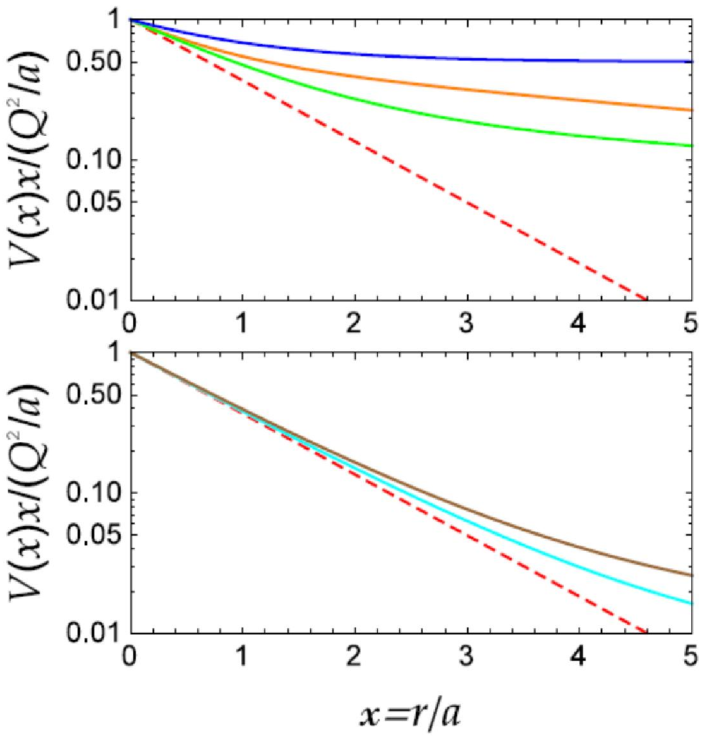
$$V(r) = \frac{Q^2}{r}\left[\epsilon_1 \exp(-r/\lambda_1) + \epsilon_2 \exp(-r/\lambda_2)\right]$$

- Yukawa + inverse square r

$$V(r) = \frac{Q^2}{r}\left[(1-\epsilon)e^{-r/\lambda_D} + (\epsilon\lambda_D/r)\left(1-e^{-r/\lambda_D}\right)\right]$$

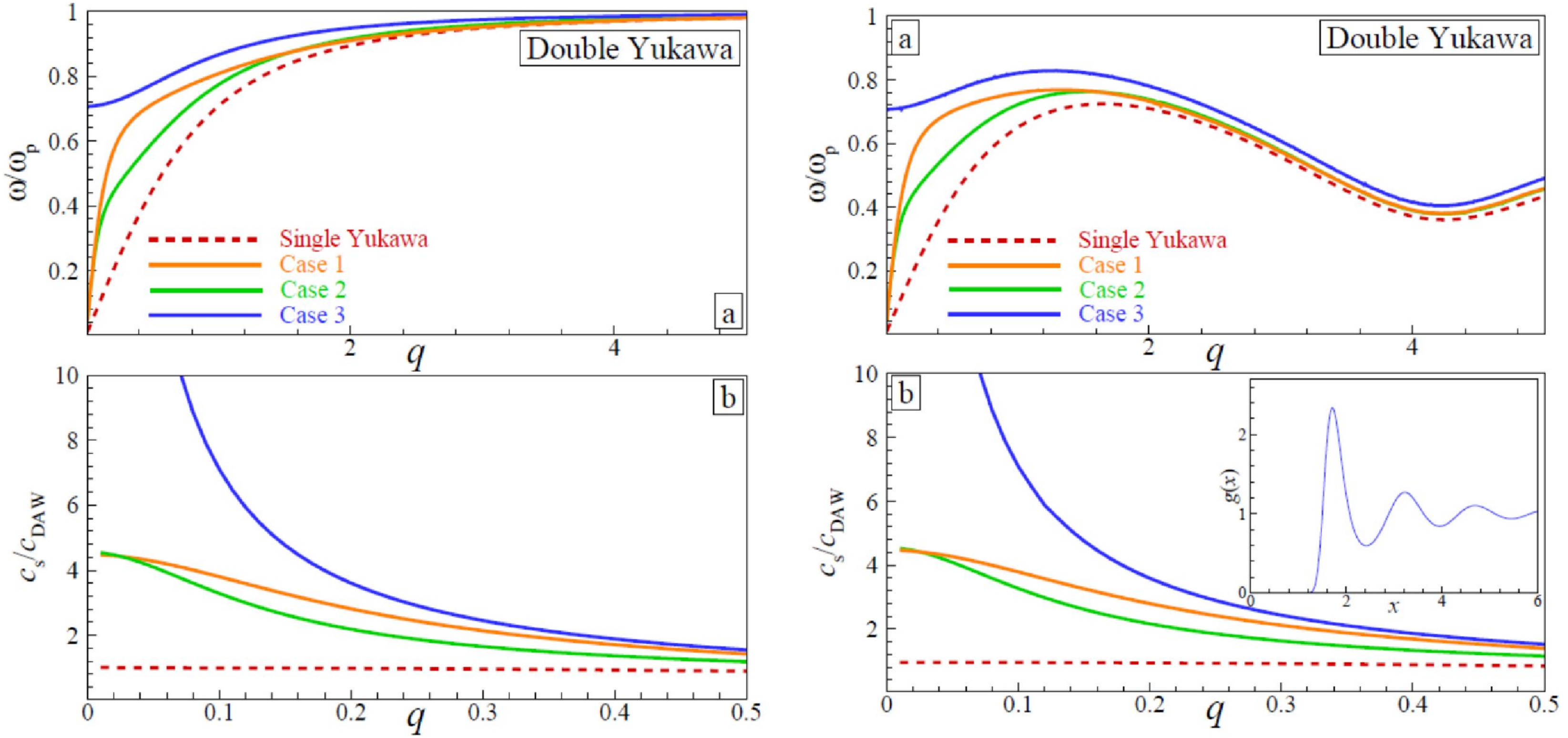
TABLE I. Summary of the model interaction potentials considered in this study (Cases 1 - 5).

Case	Functional form	Parameters
1	Eq. (2)	$\epsilon_1 = \epsilon_2 = 0.5$, $\lambda_1 = 0.7\lambda_D$, $\lambda_2 = 6.3\lambda_D$
2	Eq. (2)	$\epsilon_1 = 0.8$, $\epsilon_2 = 0.2$, $\lambda_1 = \lambda_D$, $\lambda_2 = 10\lambda_D$
3	Eq. (2)	$\epsilon_1 = \epsilon_2 = 0.5$, $\lambda_1 = \lambda_D$, $\lambda_2 = \infty$
4	Eq. (3)	$\epsilon = 0.05$
5	Eq. (3)	$\epsilon = 0.1$



Fingerprints of interactions: Double Yukawa class

Long-range asymptote of the interaction potential affects the dispersion at long wavelengths, which can be measured experimentally



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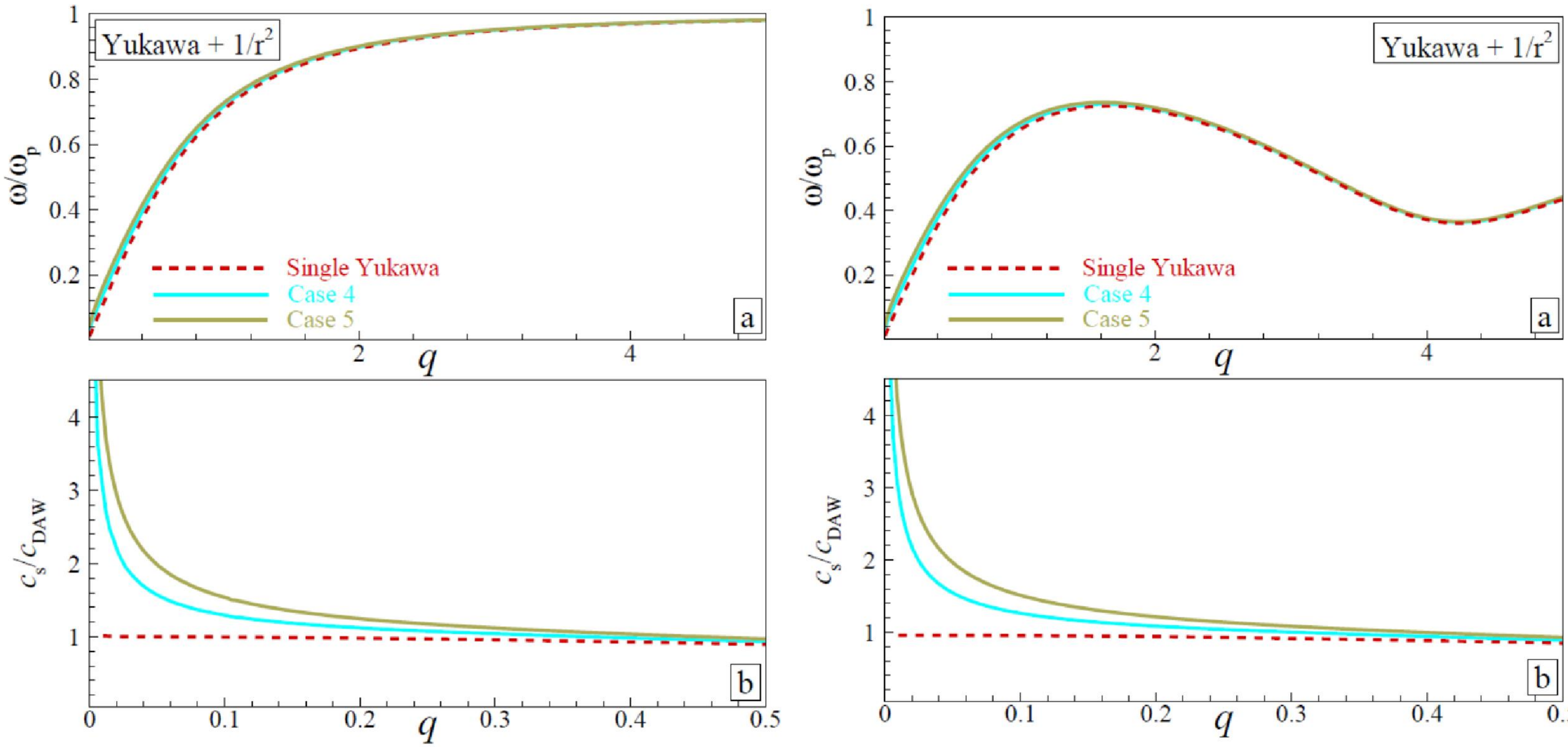
Fingerprints of interactions: Yukawa + $1/r^2$

Long-range asymptote of the interaction potential affects the dispersion at long wavelengths, which can be measured experimentally



Khrapak&Klumov (2016)

Conclusion

- We have discussed different aspects of describing theoretically collective modes in simple fluids/soft matter fluids/complex (dusty) plasmas
- QLCA/QCA approach
    - Relation between sound velocities
    - Limits of applicability
    - Possibility to discriminate between different interactions

Thank you for your attention!

Acknowledgments

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