Theory of strongly correlated plasmas:

Phase transitions, transport, quantum and magnetic field effects

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Outline: Strongly correlated plasmas

I. Structural properties and phase transitions
one-component plasma, dusty plasmas, coupling parameters

II. First principle results for transport properties
diffusion and heat conductivity

III. Correlations and strong magnetic fields
Collective modes, transport

IV. Quantum and spin effects
ab initio simulations. Quantum hydrodynamics

V. Conclusions

One-component plasma

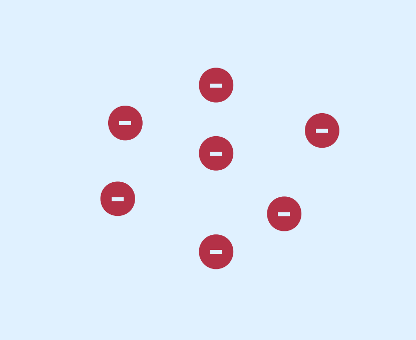
OCP → most basic system to theoretically study strong coupling effects

Classical coupling parameter

$$\Gamma = \frac{Q^2}{4\pi\epsilon_0 a}\frac{1}{k_B T} > 1$$

a ~ Wigner-Seitz radius

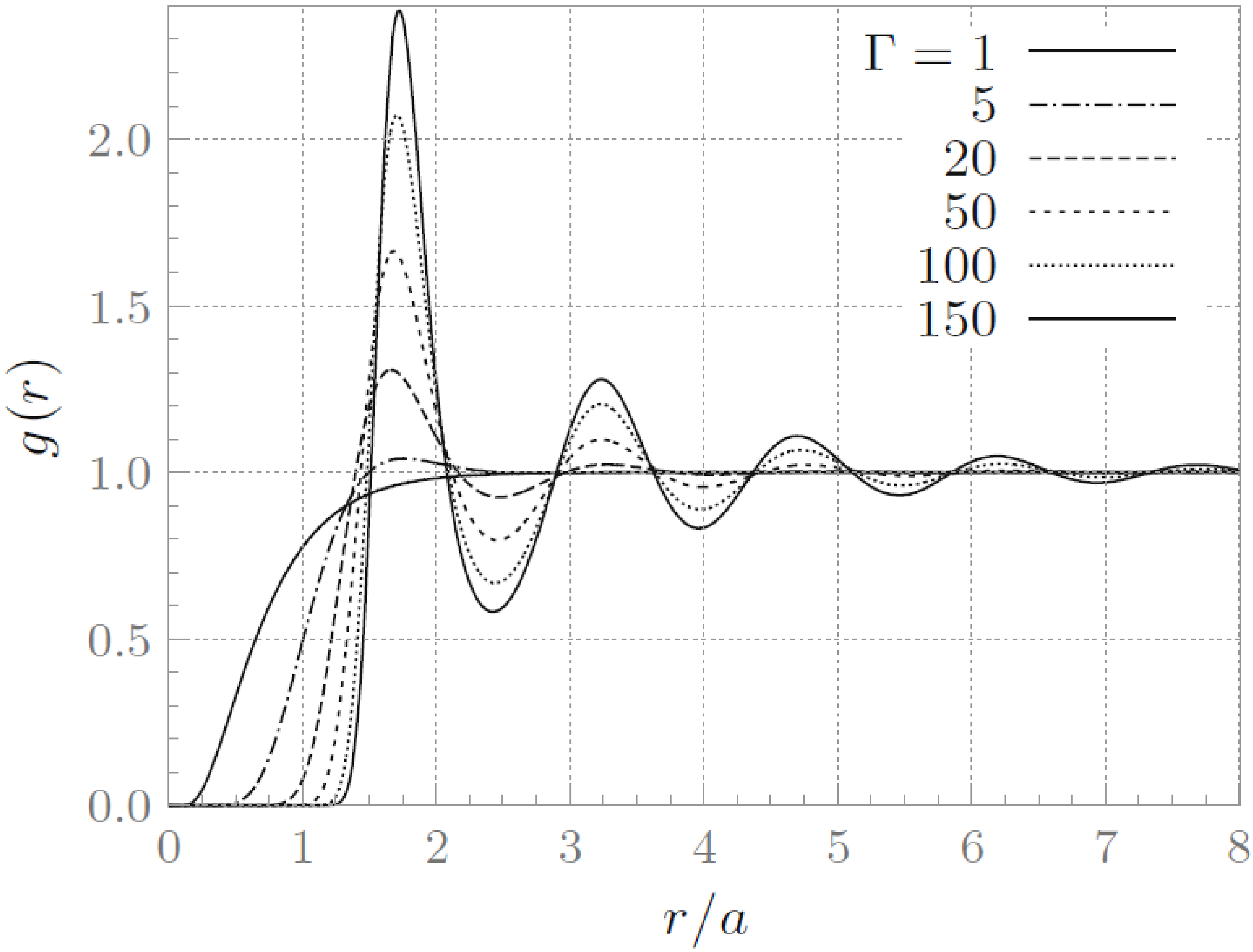
$\Gamma << 1$	weakly coupled
$\Gamma > 1$	strongly coupled *liquid-like,*
$\Gamma >> 1$	*Coulomb (Wigner) crystal*



Note: Γ is only a qualitative measure for pure Coulomb systems

Pair distribution function (2-particle probability)

microscopic measure of strong coupling effects



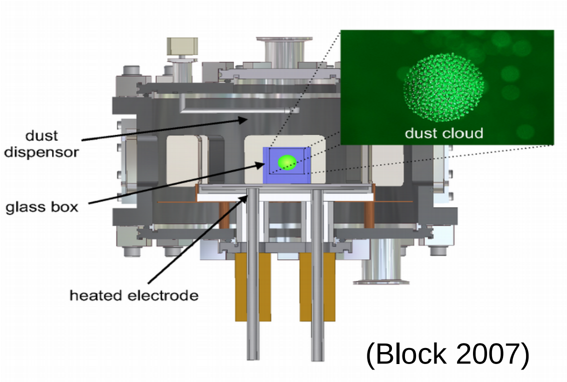
$\int_0^\infty dr\, r^2 g(r) = 1$, for ideal plasma: g(r) = 1

from: M. Bonitz, *Quantum Kinetic Theory*, 2^{nd} ed. (Springer 2016)

Examples of strongly coupled plasmas

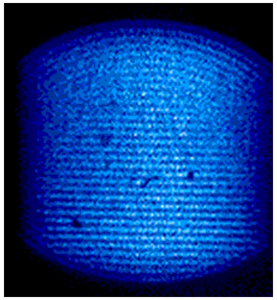
$$\Gamma = \frac{Q^2}{4\pi\epsilon_0 a}\frac{1}{k_\mathrm{B}T} > 1$$

Note: this applies only to classical plasmas



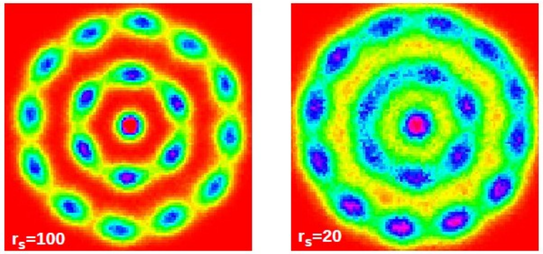
(Block 2007)

dusty plasmas



(Jensen 2004)

ultracold neutral plasmas



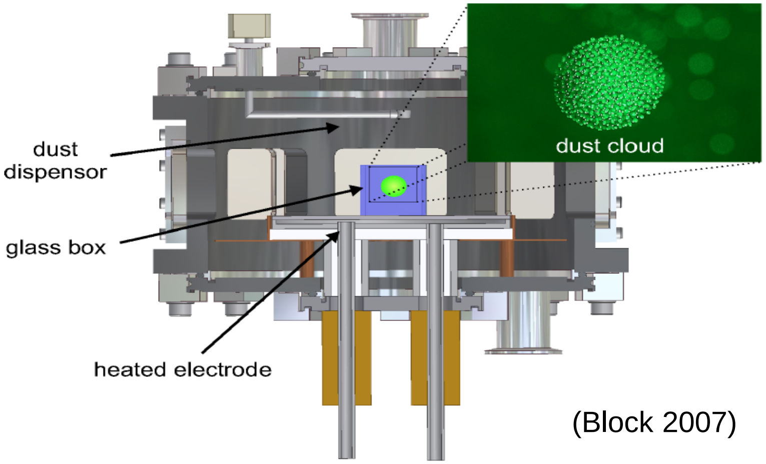
electrons in quantum dot

A. Filinov, M. Bonitz, and Yu.E. Lozovik, PRL 2001

M. Bonitz, C. Henning, and D. Block, Reports Progress Physics **73**, 066501 (2010)

M. Bonitz et al. (eds.), “Introduction to Complex Plasmas”, Springer 2010

Example: complex (dusty) plasmas



(Block 2007)

Advantages:
- strongest correlations
- single-particle diagnostics

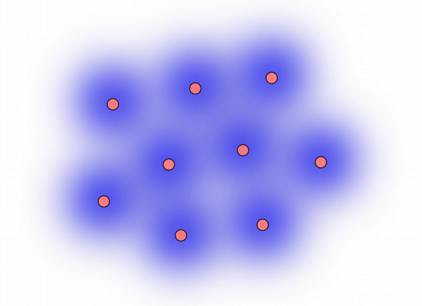
Dusty plasmas are complicated:

- multiple species: electrons, ions, neutrals, dust
- streaming components, electric field
- charge fluctuations

reasonable model [1]

“Yukawa OCP”

2 independent parameters



$$V(r)=\frac{Q^2}{r}e^{-\kappa r}$$

$$\kappa = a/\lambda_D$$

$$\Gamma = Q^2/(ak_BT)$$

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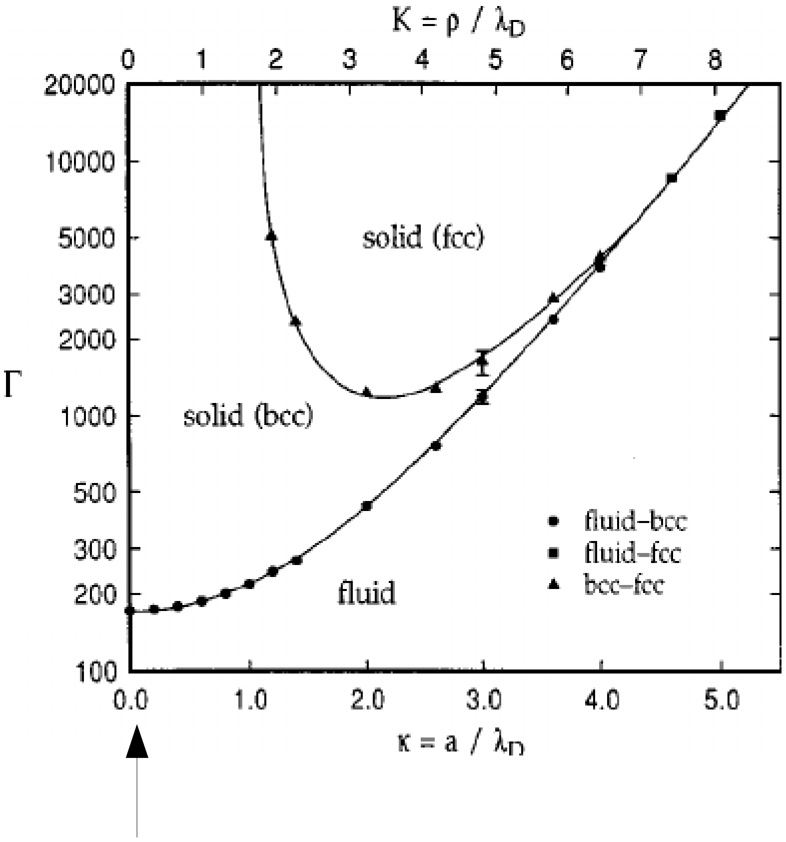
[1] M. Bonitz, *et al.*, PRL (2006)

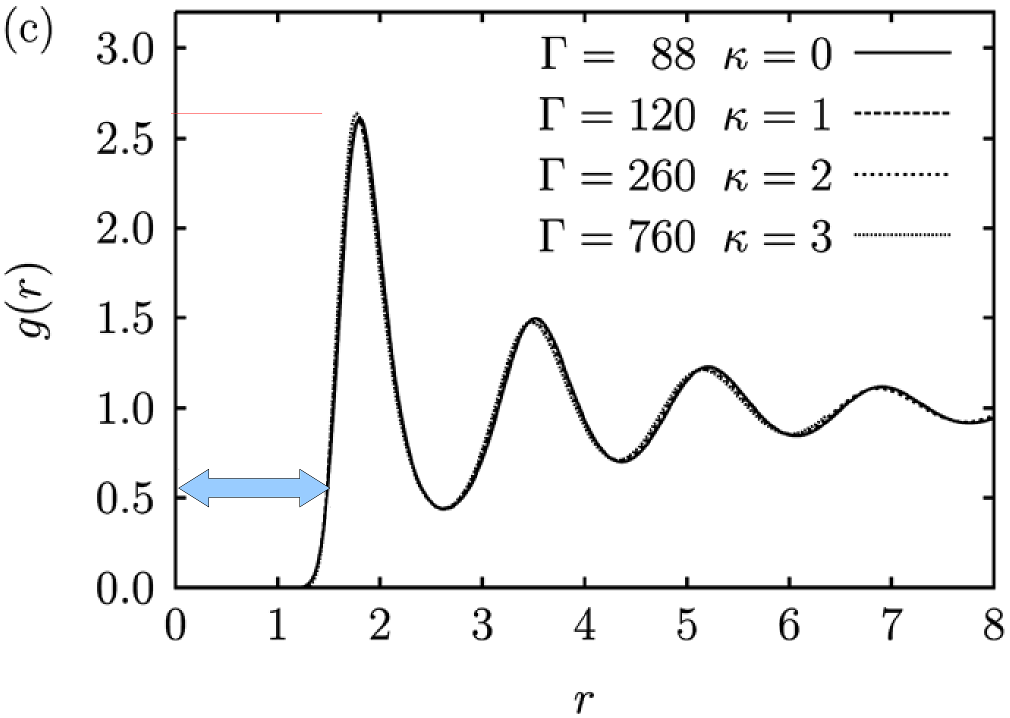
M. Bonitz et al. (eds.), “Introduction to Complex Plasmas”, Springer 2010

Macroscopic Yukawa OCP: phase diagram [1]



$$\Gamma = \frac{Q^2}{a\,k_B T}$$

Pair distribution function



accurate Yukawa coupling parameter
from peak height and with of void
of g(r) [2, 3]

Particle coordinates directly accessible in experiments

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[1] Hamaguchi, *et al.*, PRE (1997)

[2] Ott, Stanley, Bonitz, Phys. Plasmas (2011), [3] Ott, Bonitz, Stanton, Murillo, Phys. Plasmas (2014)

Mesoscopic Yukawa OCP in spherical trap [1]

- particles arranged on shells
- phase diagram N-dependent
- multi-stage melting:
  - radial (RM)
  - inter-shell (ISM)
  - intra-shell disordering (ID)

- Several quantities needed:

- Pair distribution (PDF), g(r1,r2)
- three-particle distribution (TPD)
- center two-particle distrib (C2P)
- reduced entropy
- reduced specific heat

- rigorous derivation from reduced s-particle distribution functions

- particle coordinates directly accessible in dusty plasma experiments
- controlled melting via laser heating [2]

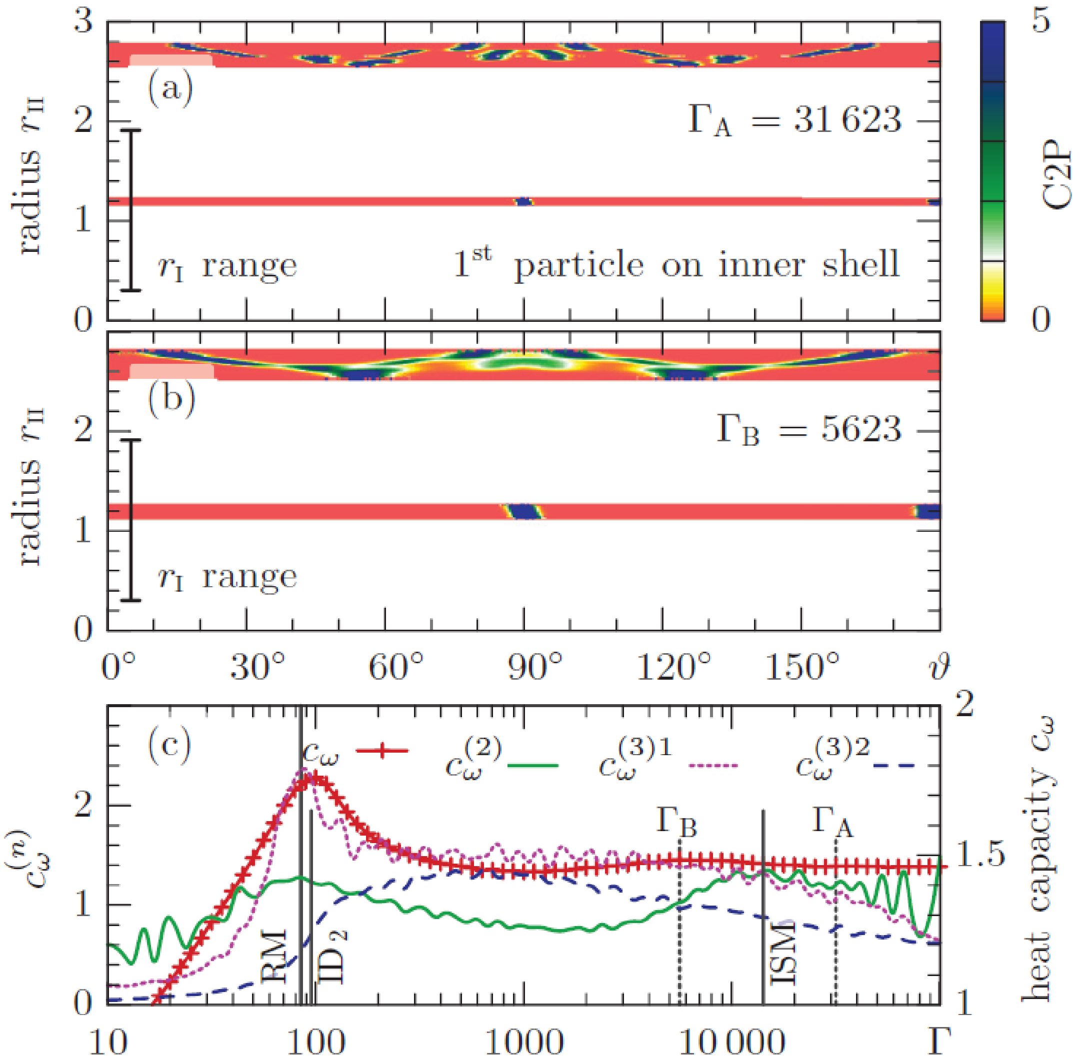

FIG. 6. (Color online) Intershell angular melting (ISM) in the spherical 3D Coulomb cluster with $N = 38$ particles. (a, b) C2P (the first particle radius is averaged over the inner shell) below (above) the melting temperature. The length scale is r_0. (c) Specific heat and reduced specific heat vs Γ. While radial melting (RM) is seen in c_ω and $c_\omega^{(2)}$, ISM is clearly visible only in $c_\omega^{(2)}$, based on the C2P.

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[1] Thomsen and Bonitz PRE (2015)

[2] Thomsen et al., J. Phys. D (2014)

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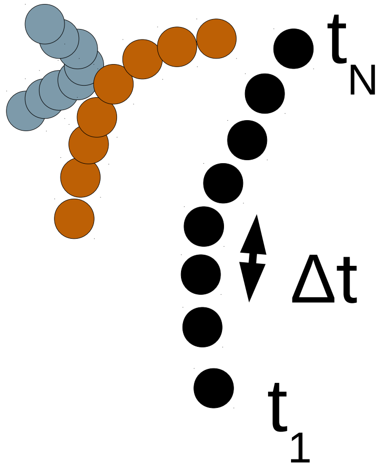
Exact transport properties via molecular dynamics

- solve equations of motion of N particles by time-discretization
- Newton's equations*:

$$\boxed{m\ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i + q\,\dot{\boldsymbol{r}}_i \times \boldsymbol{B}}$$

$$\boldsymbol{F}_i = -\frac{q^2}{4\pi\varepsilon_0}\sum_{j=1}^{N}{}' \left(\nabla \frac{e^{-r/\lambda_D}}{r}\right)\Bigg|_{\boldsymbol{r}=\boldsymbol{r}_i-\boldsymbol{r}_j}$$

$$\boldsymbol{B} = B \cdot \boldsymbol{e}_z$$



- Ewald summation for long-ranged forces
- exact incorporation of arbitrary magnetic fields
  in a quasi-symplectic scheme

T. Ott and M. Bonitz, PRL (2011)

*Langevin dynamics: add friction and fluctuating force

Exact diffusion coefficient D (3D)

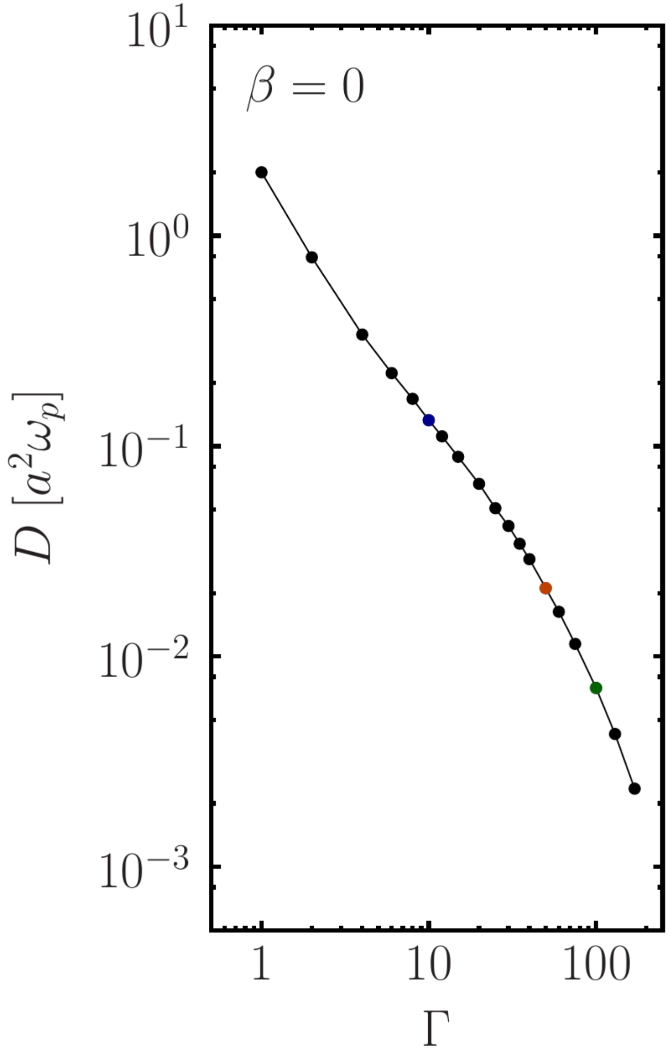
Snapshot of trajectories

$\Gamma=2 \quad \omega_p t=5$

$\Gamma=100 \quad \omega_p t=50$

T. Ott and M. Bonitz, PRL (2011)

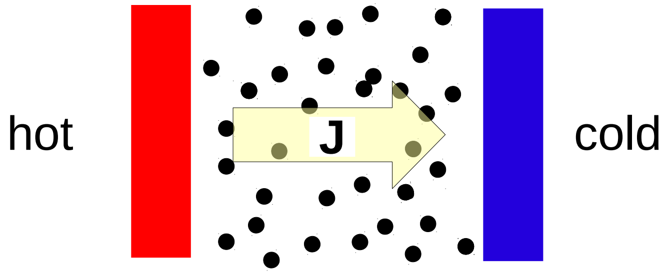
- D follows from velocity auto-correlation function (Green-Kubo relations)



Correlations dramatically reduce D

Exact heat conductivity λ

- λ follows from energy current auto-correlation function (Green-Kubo relations)



$$\boxed{\mathbf{J} = -\lambda \nabla T}$$

$$\lambda = \lim_{\tau\to\infty} \frac{1}{VkT^2} \int_0^\tau \langle J_\alpha(t) J_\alpha(0) \rangle dt$$

$$J_\alpha = \sum_{i=1}^{N} v_{i\alpha} \left[\frac{1}{2} m |\mathbf{v}_i|^2 + \frac{1}{2} \sum_{j\neq i}^{N} \Phi(r_{ij}) \right] - \frac{1}{2} \sum_{i=1}^{N} \sum_{j\neq i}^{N} (\mathbf{r}_i \cdot \mathbf{v}_i) \frac{\partial \Phi(r_{ij})}{\partial r_{ij}}$$

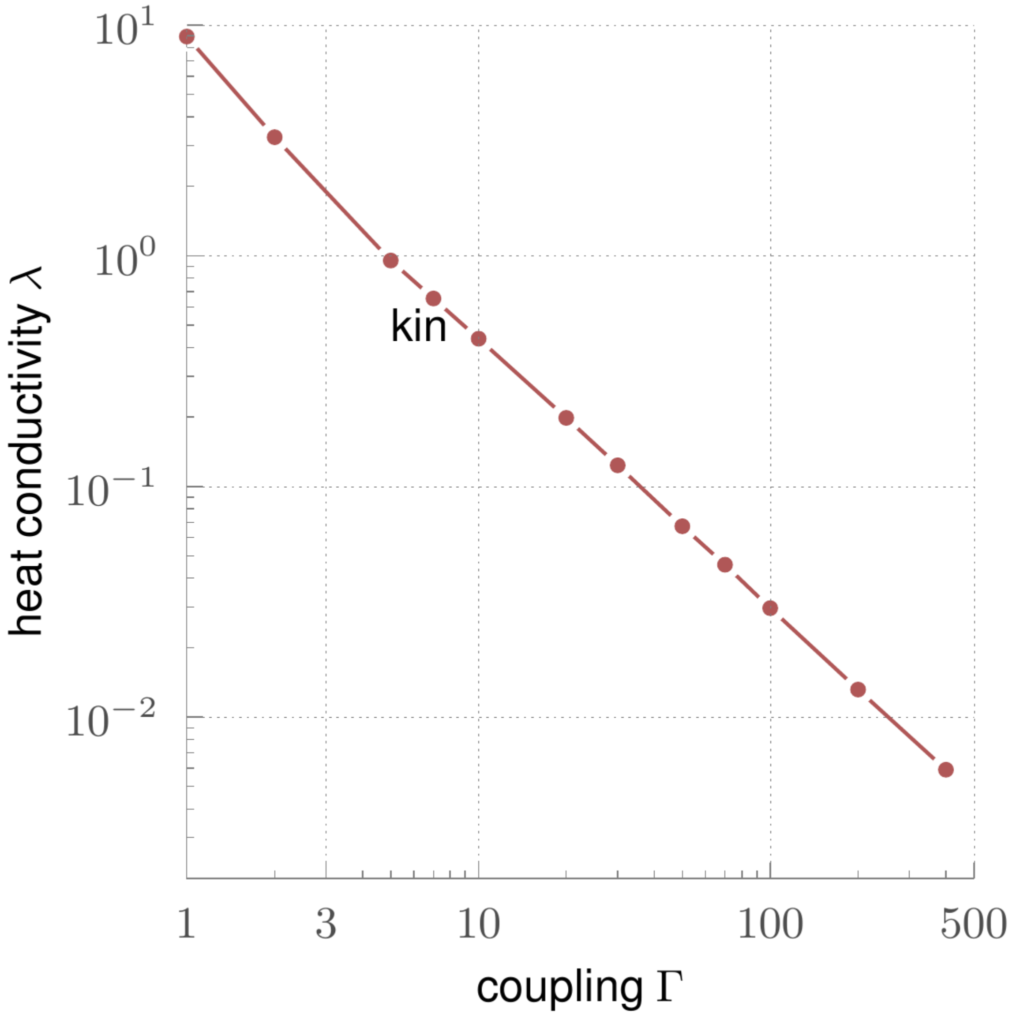
kinetic potential collisional

1-particle terms momentum exchange

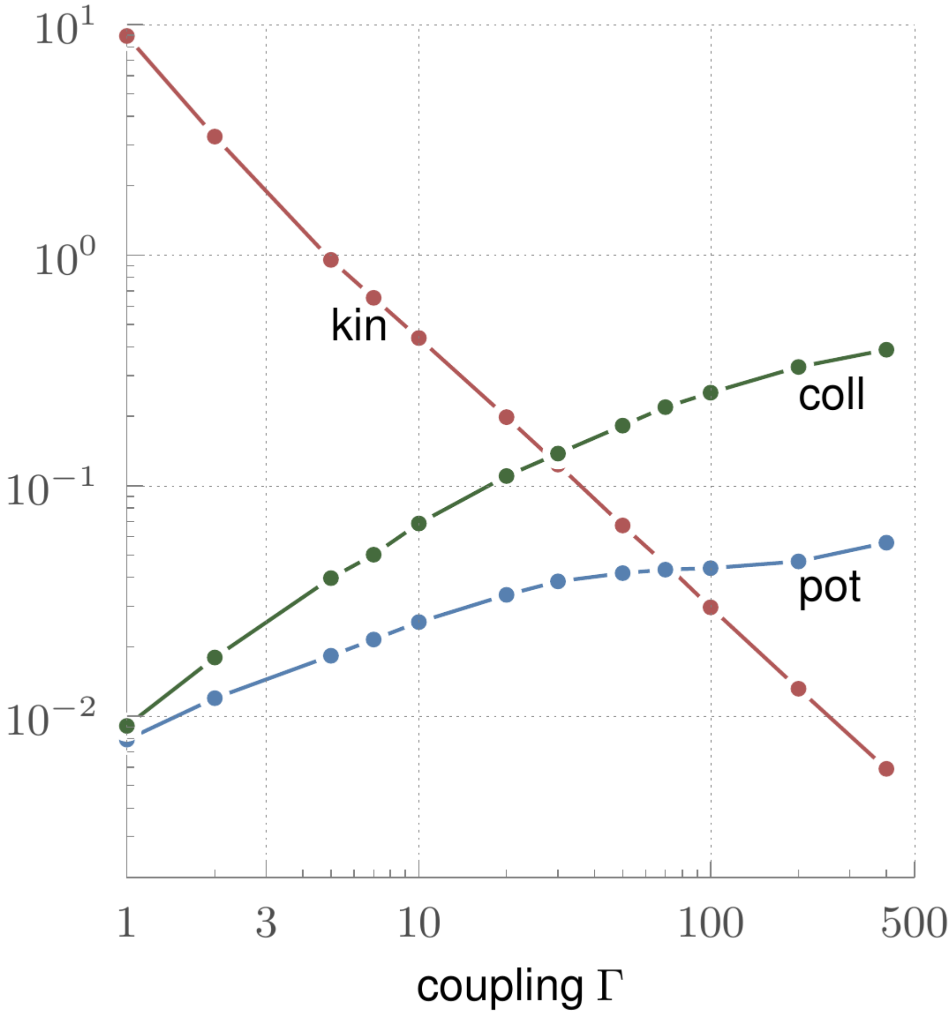
Ott, Bonitz, Donko, Phys. Rev. E (2015)

Exact heat conductivity λ: effect of correlations

reduction of mobility (D)



excitation of collective modes

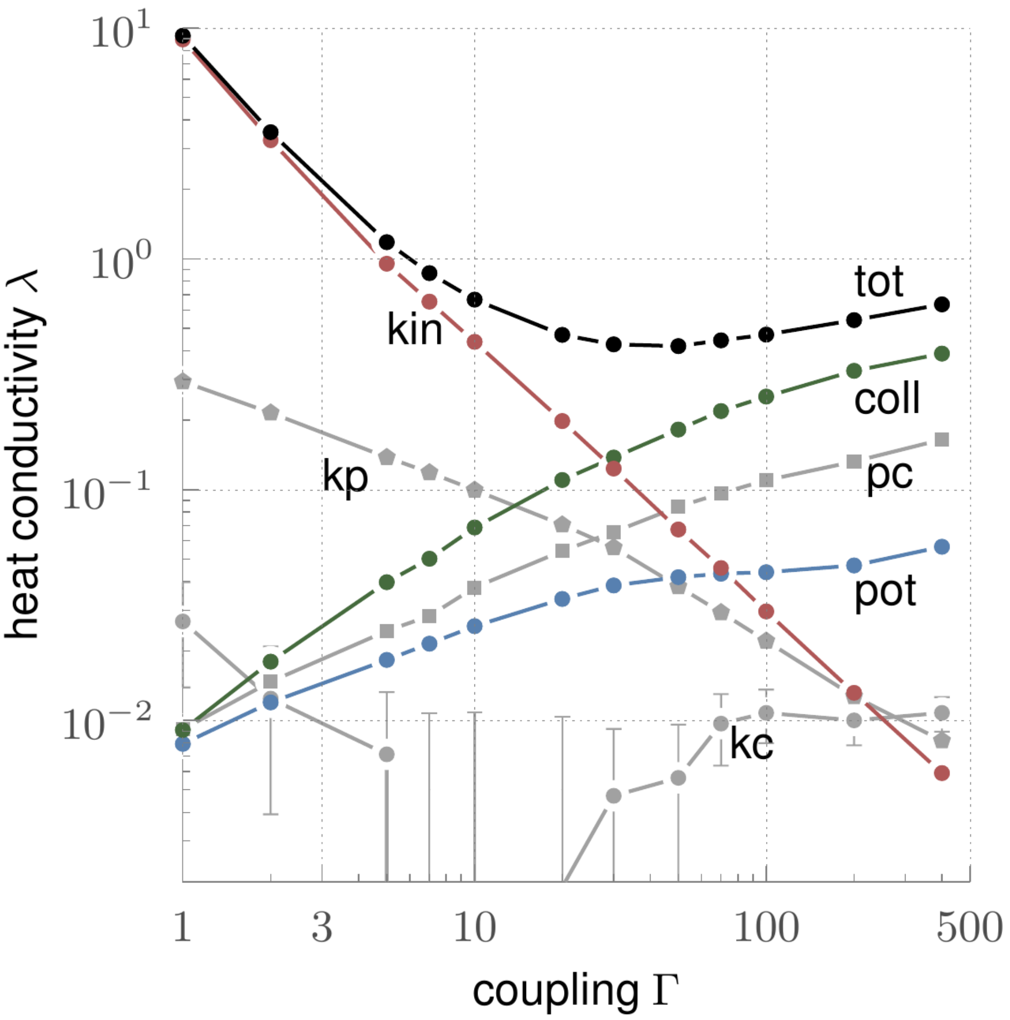


Ott, Bonitz, Donko, Phys. Rev. E (2015)

Exact heat conductivity λ: nontrivial coupling dependence

Single-particle conductivity dominates

Many-particle conductivity dominates



Ott, Bonitz, Donko, Phys. Rev. E (2015)

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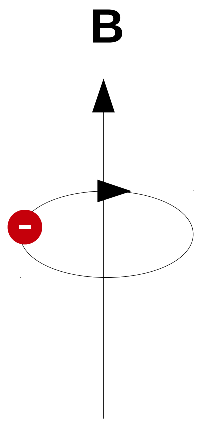
Magnetization and correlations (2D OCP)

One-component plasma in an external magnetic field
Three relevant parameters: Γ, κ, β

$$\boxed{\beta = \frac{\omega_\mathrm{c}}{\omega_\mathrm{p}}} \sim \frac{\lambda_D}{r_c}$$

$$\omega_\mathrm{c} = \frac{QB}{m}$$

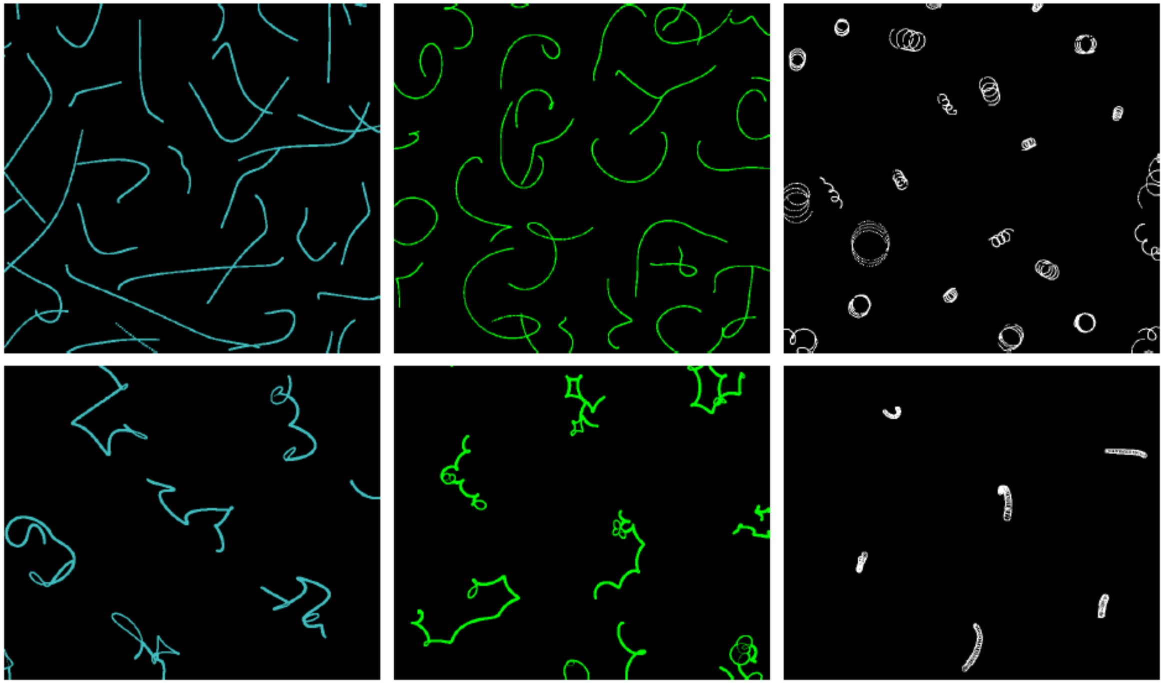


β=0
unmagnetized

β=1

→

β=4
strongly magnetized



moderate coupling (Γ = 2)

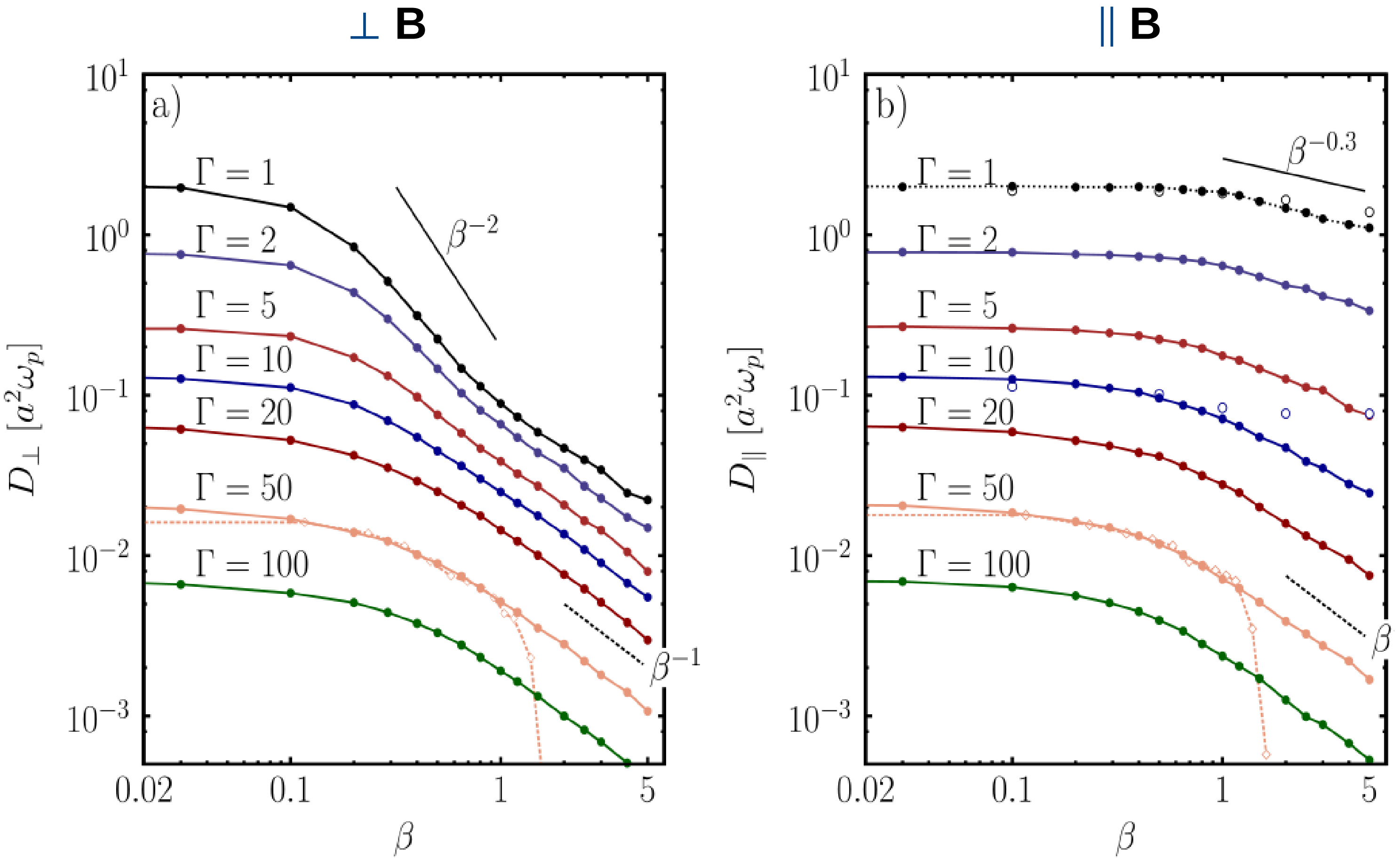
strong coupling (Γ = 100)

2D OCP, MD simulation: T. Ott; M. Bonitz *et al.*, PSST (2013)

Diffusion in magnetized strongly coupled OCP (3D)

Weak coupling (Braginskii 1965): quadratic reduction of D ⊥ B
no effect on D || B

Strong magnetization [1]: - B inhibits diffusion, even along **B**
- at strong B: Bohm diffusion ~ 1/B



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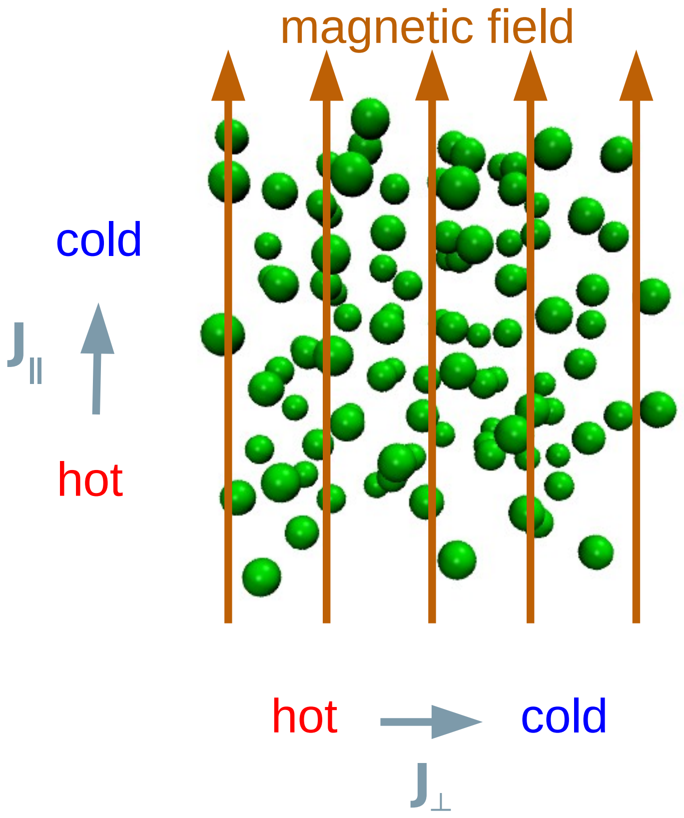
[1] T. Ott and M. Bonitz, PRL (2011)

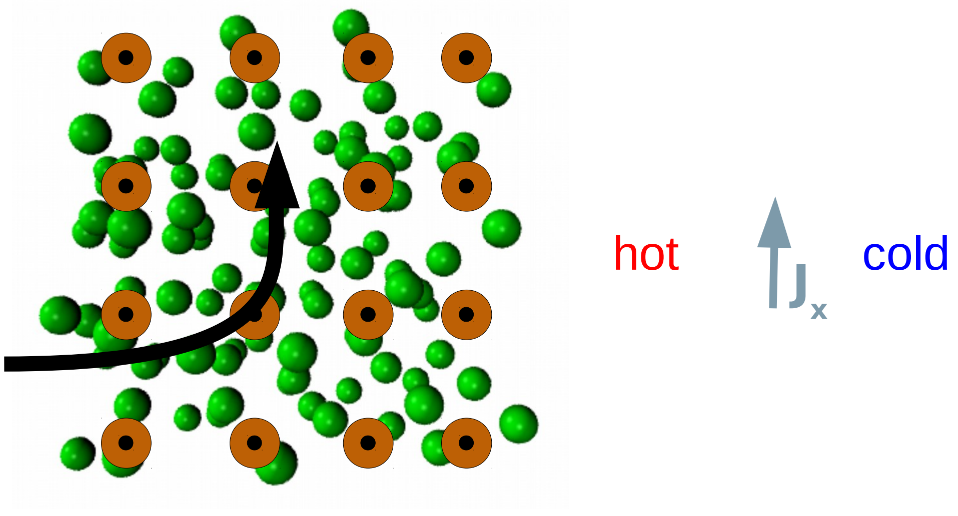
extension to 2D and binary systems:
T. Ott, H. Löwen, and M. Bonitz, PRE (2014)

Heat conductivity in magnetized strongly coupled OCP [1]

side view:



top view:



heat flux analogon of Hall effect:
Righi-Leduc effect

$$\boxed{\mathbf{J} = -\lambda \nabla T} \longrightarrow \boxed{J_a = -\lambda_{ab}(\nabla T)_b}$$

$$\underline{\underline{\lambda}} = \begin{pmatrix} \lambda_{\perp} & \lambda_{\times} & 0 \\ -\lambda_{\times} & \lambda_{\perp} & 0 \\ 0 & 0 & \lambda_{\parallel} \end{pmatrix}$$ tensor

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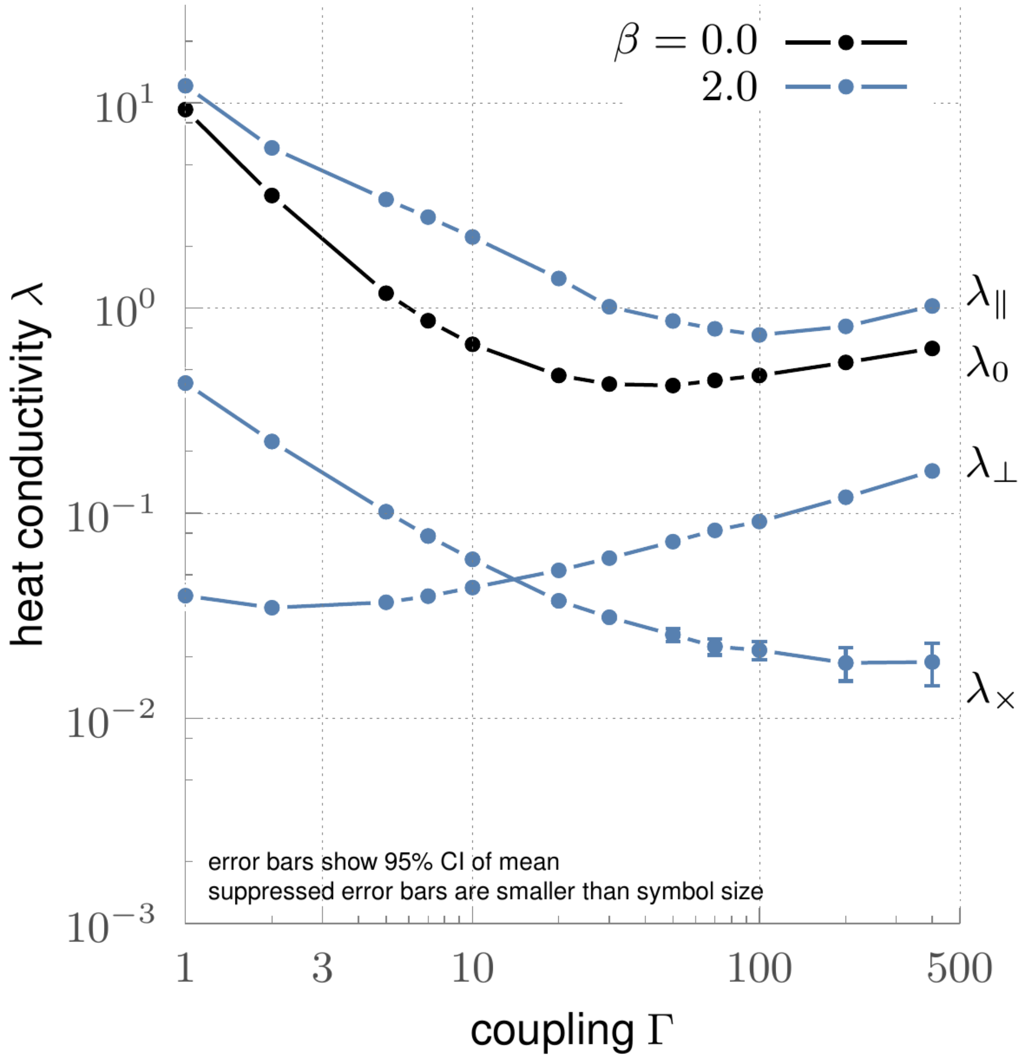
[1] Ott, Bonitz, Donko, Phys. Rev. E (2015)

Heat conductivity in magnetized strongly coupled OCP [1]



error bars show 95% CI of mean
suppressed error bars are smaller than symbol size

parallel: increase

perpendicular: decrease

Righi-Leduc: new

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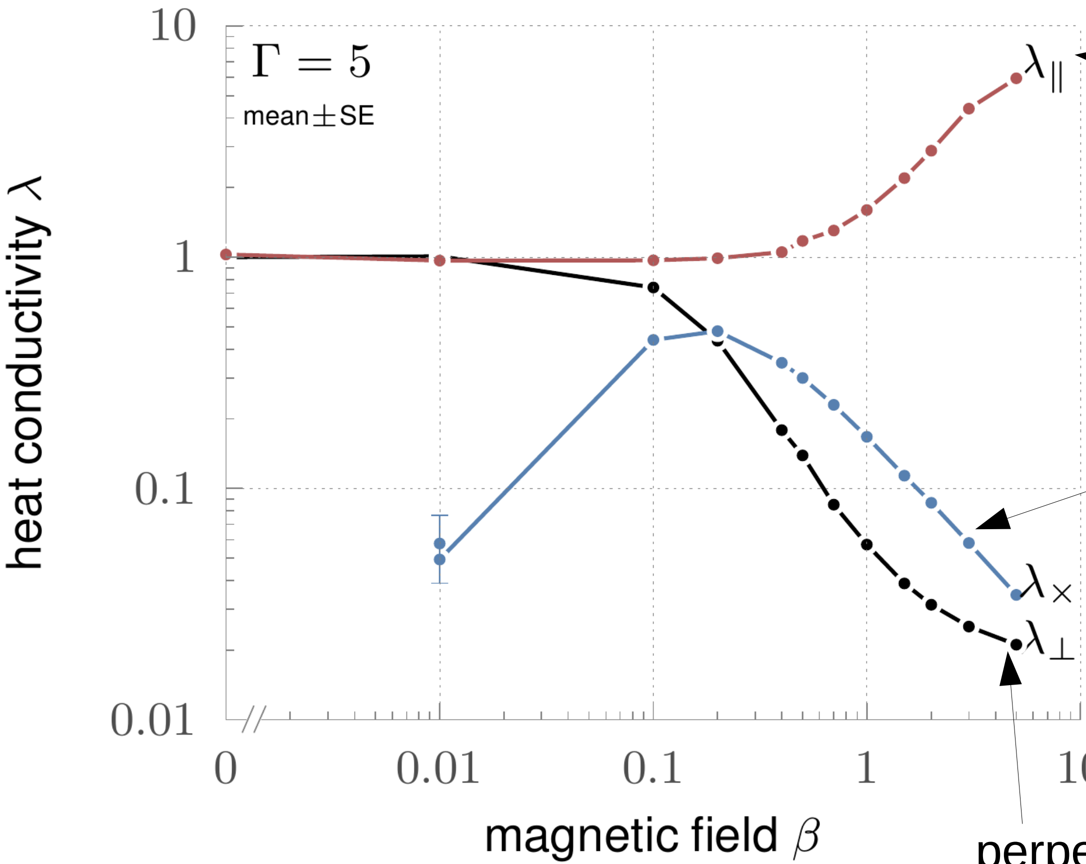
[1] Ott, Bonitz, Donko, Phys. Rev. E (2015)

Heat conductivity in magnetized strongly coupled OCP [1]



parallel: increase

Righi-Leduc: peaked

perpendicular: decrease

→ **At strong coupling, B field can drastically increase transport coefficients**

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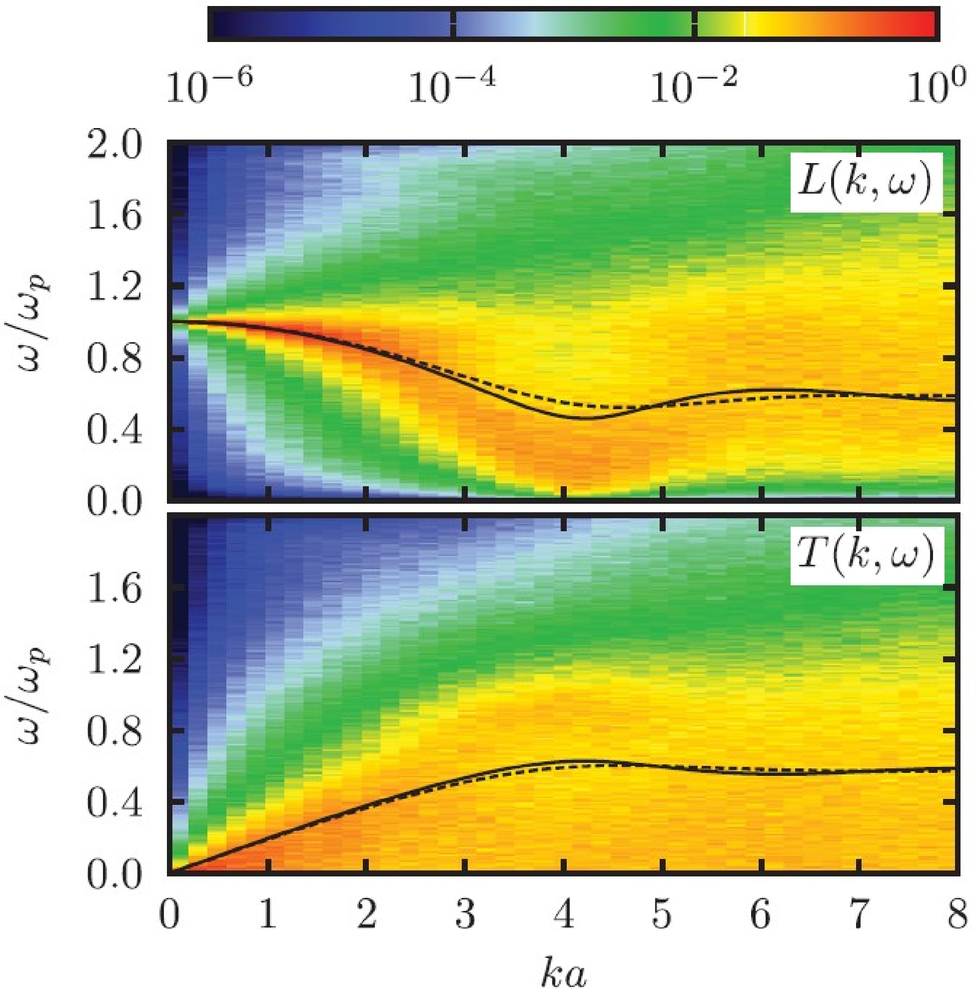
[1] Ott, Bonitz, Donko, Phys. Rev. E (2015)

Spontaneous generation of temperature anisotropy
Ott, Bonitz, Hartmann, Donko, Phys. Rev. E (2017)

Waves in the strongly coupled OCP (B=0)



QLCA [1] vs. MD simulation at Γ = 150 [2]

Strong deviation from ideal plasmon spectrum

plasmon: $\omega_{\mathrm{P}}(k) = \sqrt{\omega_{\mathrm{p}}^2 + D_L(k)}$

One longitudinal mode: **q** || **k,** q: displacement

shear modes: $\omega_{\mathrm{OS}}(k) = \sqrt{D_T(k)}$

two degenerate transverse modes: **q** $\perp$ **k**

$D_L(k)$ and $D_T(k)$ from QLCA
input: pair distribution function g(r)

MD: compute longitudinal (L) and transverse (T) density response [2]

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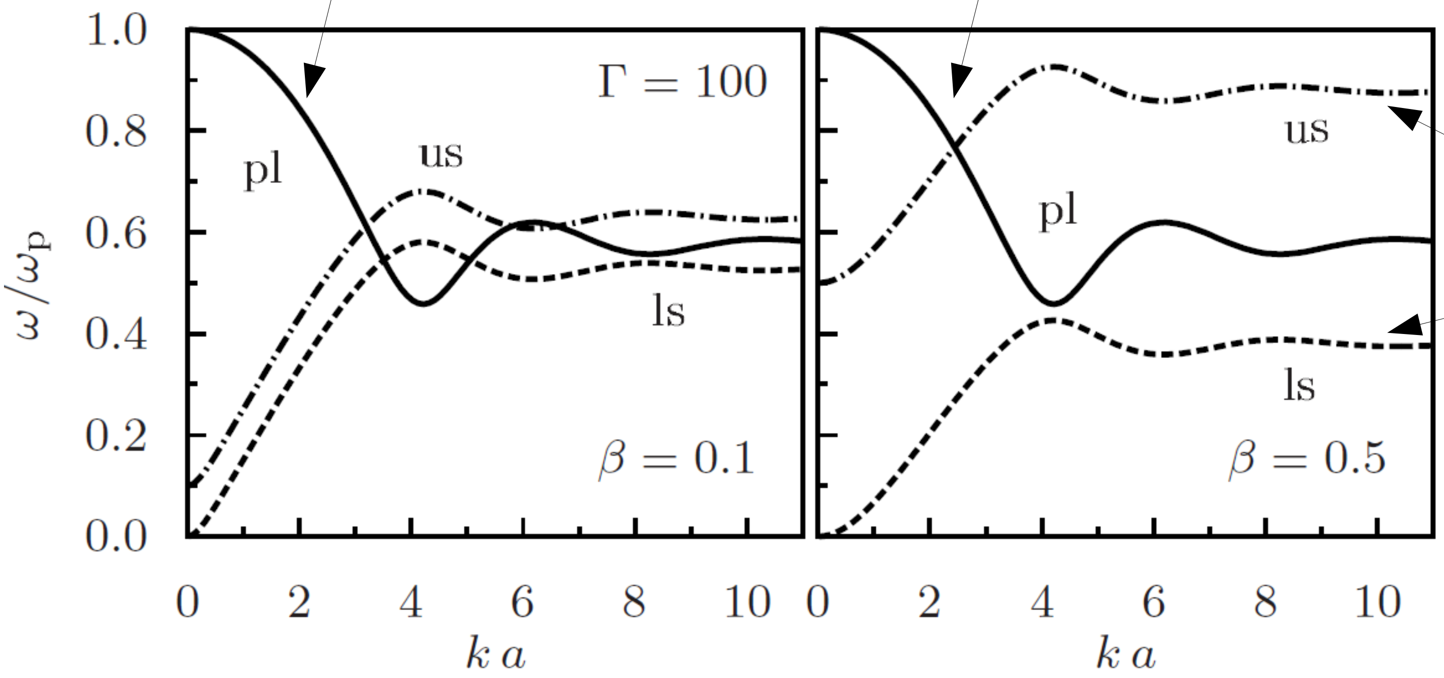
[1] K. I. Golden, G. J. Kalman, and P. Wyns, Phys. Rev. A **46**, 3454 (1992)
[2] T. Ott, H. Kählert, A. Reynolds, and M. Bonitz, Phys. Rev. Lett. (2012)

Magnetized correlated OCP: parallel wave

$\boldsymbol{k} \parallel \boldsymbol{B}$

plasmon (pl) unaffected by magnetic field (**q** || **B**)



degeneracy of shear modes lifted

upper/lower shear (us, ls) circular polarization

q ⊥ **B**

Dispersion relation

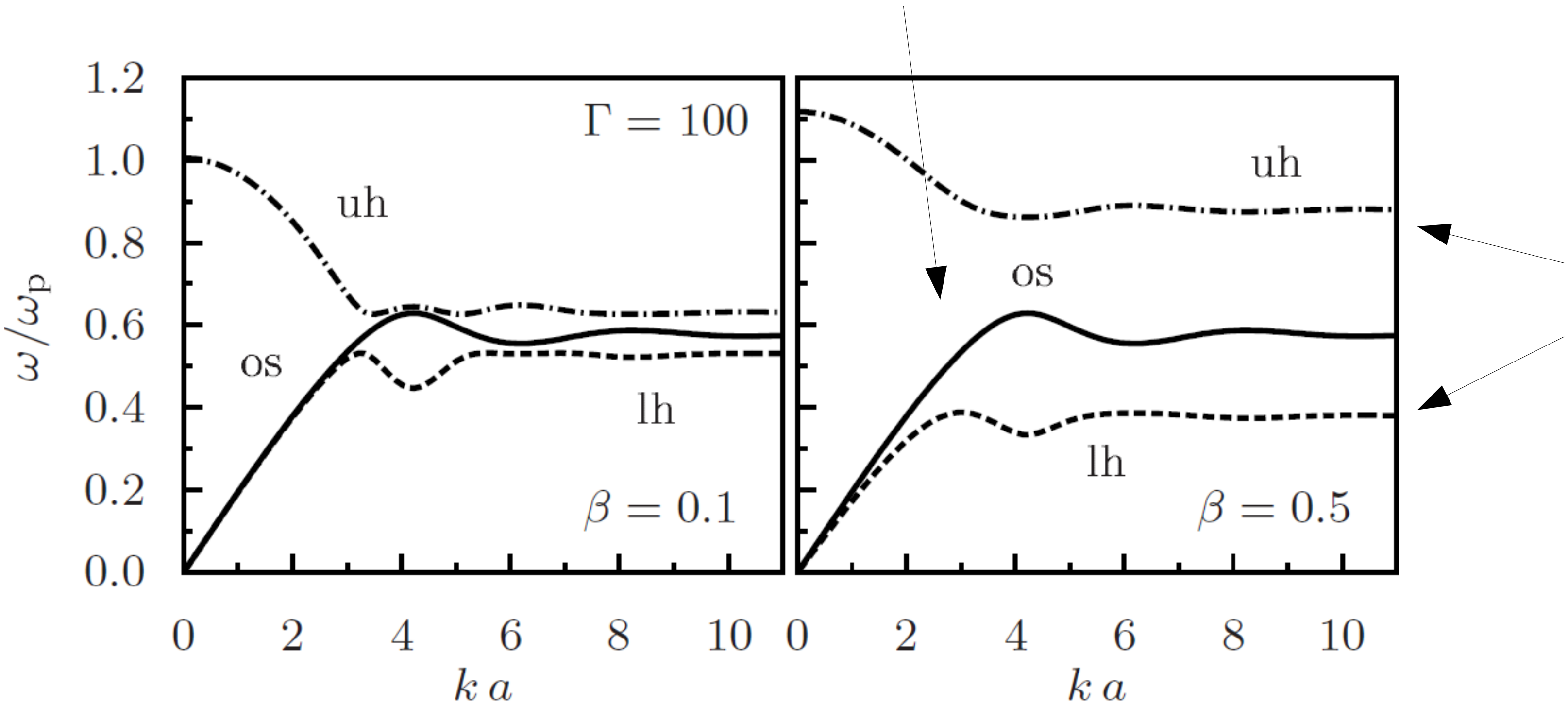
$$\omega_\mathrm{pl}(k) = \sqrt{\omega_\mathrm{p}^2 + D_L(k)}$$

$$\omega_\mathrm{us,ls}(k) = \frac{1}{2}\left[\sqrt{\omega_\mathrm{c}^2 + 4D_T(k)} \pm \omega_\mathrm{c}\right]$$

Magnetized correlated OCP: perpendicular wave

$$\boldsymbol{k} \perp \boldsymbol{B}$$

Ordinary shear mode (os) with **q** || **B** unaffected by magnetic field



Plasmon & 2nd shear

upper/lower hybrid modes (uh, lh)

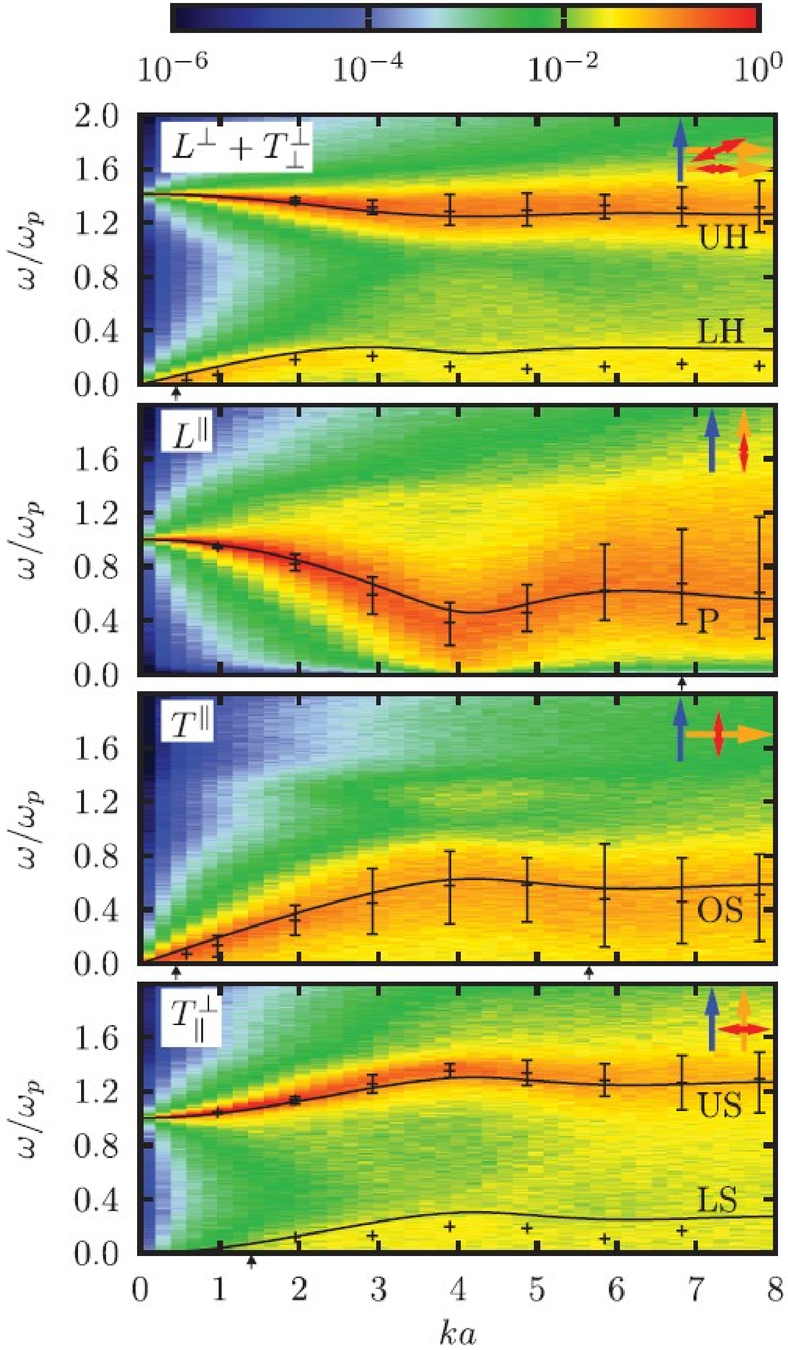
q ⊥ **B**
elliptical motion
In plane ⊥ B

Dispersion relation

$$\omega_{\mathrm{os}}(k) = \sqrt{D_T(k)}$$

$$\omega_{\mathrm{uh,lh}}(k) = \frac{1}{\sqrt{2}} \left[\omega_{\mathrm{c}}^2 + \omega_{\mathrm{p}}^2 + D_T(k) + D_L(k) \pm \tau(k)\right]^{1/2}$$

Exact wave dispersions from MD simulation [1]



Γ = 100 β = 1

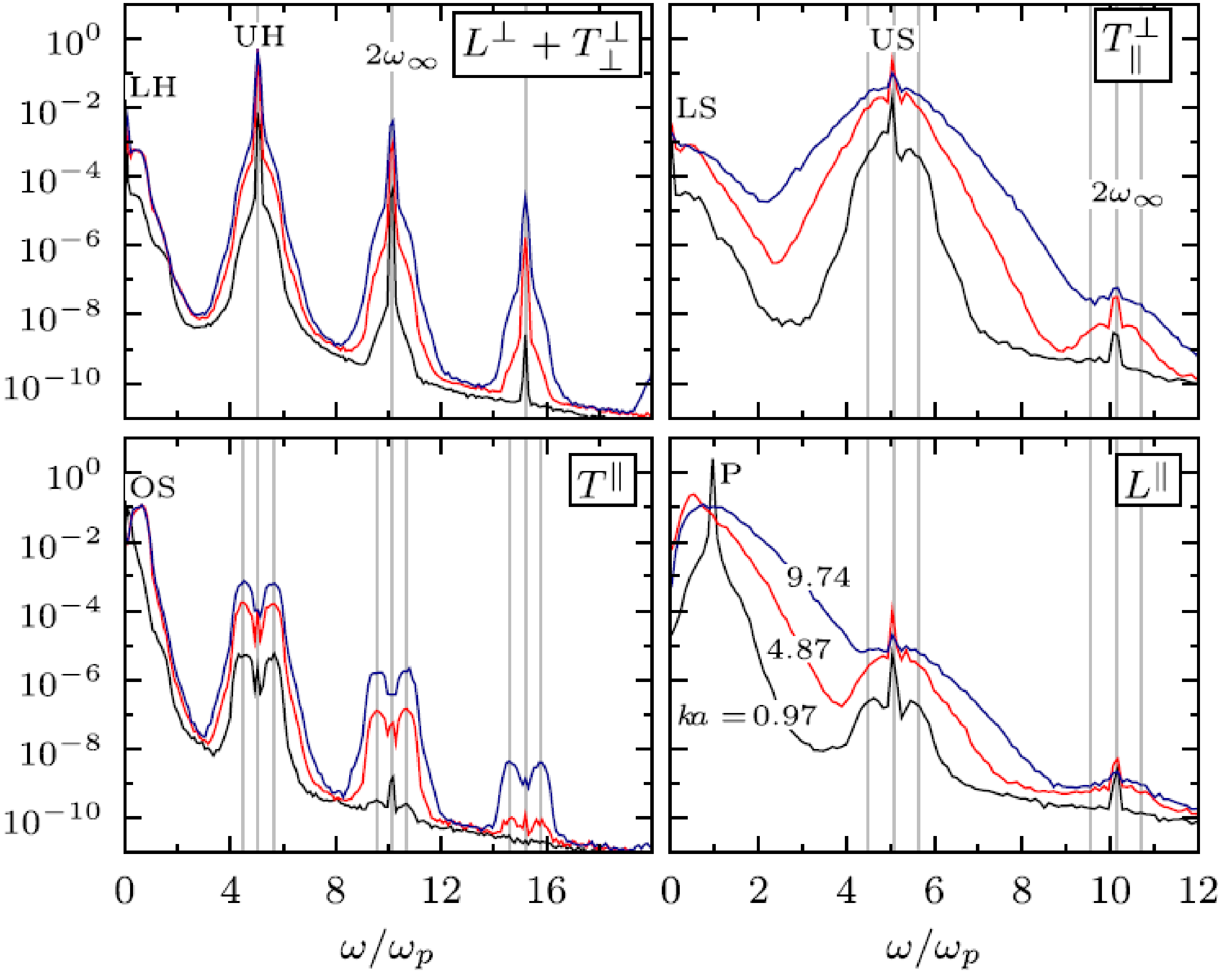
magnetic field
wave vector
displacement

- QLCA frequencies in good agreement with MD
- damping of low-frequency shear modes not contained in QLCA formalism

[1] T. Ott, H. Kählert, A. Reynolds, and M. Bonitz, PRL (2012)

Extension to oblique angles: H. Kählert, T. Ott, A. Reynolds, G. J. Kalman, and M. Bonitz, Phys. Plasmas (2013)

Nonlinear effects: harmonics and mode coupling: MD [1]



- left: **B _|_ k**
- right: **B || k**
- strong B field: β = 5

- higher harmonics of upper hybrid* (UH) and upper shear (US) mode
- appear also in other spectra, interact with ordinary shear mode (OS) and plasmon (P)

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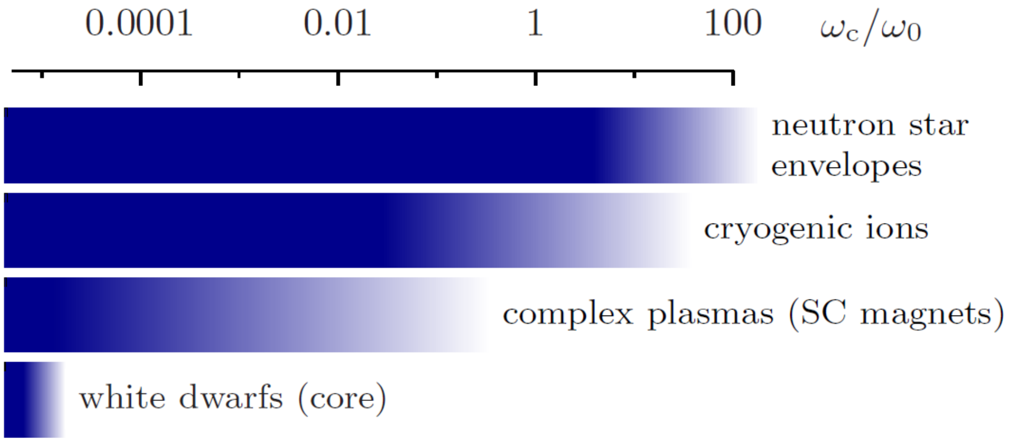
[1] T. Ott, H. Kählert, A. Reynolds, and M. Bonitz, PRL (2012)

Similar spectra in magnetized 2D Yukawa plasmas, M. Bonitz, Z. Donko , T. Ott, H. Kählert, and P. Hartmann, PRL (2010)

Magnetized strongly coupled plasmas: Experiment

$$\beta = \frac{\omega_c}{\omega_p} \propto \frac{B}{\sqrt{m\,n}}$$



Dusty plasmas: magnetization of heavy particles difficult

- small particles carry less charge, not strongly coupled
- Superconducting magnets (B~4T): filamentation of discharge

Alternative ideas needed [1]

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[1] H. Kählert *et al.*, PRL (2012)

“Quasi-magnetization” of the dust particles

Consider a dusty plasma in a rotating gas flow (Langevin dynamics)

- harmonic confinement

$$V(\rho, z) = \frac{m}{2}\left(\omega_\perp^2 \rho^2 + \omega_z^2 z^2\right)$$

- uniformly rotating gas (rotation frequency Ω)

$$\boldsymbol{u}(\boldsymbol{r}) = (\Omega \hat{e}_z) \times \boldsymbol{r}$$

$$\boxed{m\ddot{\boldsymbol{r}}_i = -\nabla_i V(\rho_i, z_i) + \sum_{j\neq i}^{N} \boldsymbol{F}_{ij}^{\text{int}} - \nu m \left[\dot{\boldsymbol{r}}_i - \boldsymbol{u}(\boldsymbol{r}_i)\right] + \boldsymbol{f}_i .}$$

dust-dust
interaction

dust-neutral
friction coefficient

random force

“Quasi-magnetization” of the dust particles

Equation of motion in the rotating frame $(r \to \bar{r})$

$$m\ddot{\bar{\boldsymbol{r}}}_i = -\bar{\nabla}_i \bar{V}(\bar{\rho}_i, \bar{z}_i) + \sum_{j\neq i}^{N} \bar{\boldsymbol{F}}_{ij}^{\mathrm{int}} + \bar{\boldsymbol{F}}_{\mathrm{Cor}}(\dot{\bar{\boldsymbol{r}}}_i) - \nu m \dot{\bar{\boldsymbol{r}}}_i + \bar{\boldsymbol{f}}_i$$

Centrifugal force

$$\bar{V}(\bar{\rho}, \bar{z}) = \frac{m}{2}\left(\bar{\omega}_\perp^2 \bar{\rho}^2 + \omega_z^2 \bar{z}^2\right)$$

$$\bar{\omega}_\perp = \sqrt{\omega_\perp^2 - \Omega^2}$$

Coriolis force

$$\bar{\boldsymbol{F}}_{\mathrm{Cor}}(\dot{\bar{\boldsymbol{r}}}) = m\dot{\bar{\boldsymbol{r}}} \times (2\,\Omega\,\hat{\boldsymbol{e}}_z).$$

equivalent to Lorentz force (Larmor theorem)

$$\boldsymbol{B}_{\mathrm{eff}} = (2m\Omega/Q)\hat{\boldsymbol{e}}_z$$

$$\omega_{\mathrm{c}} = 2\Omega$$

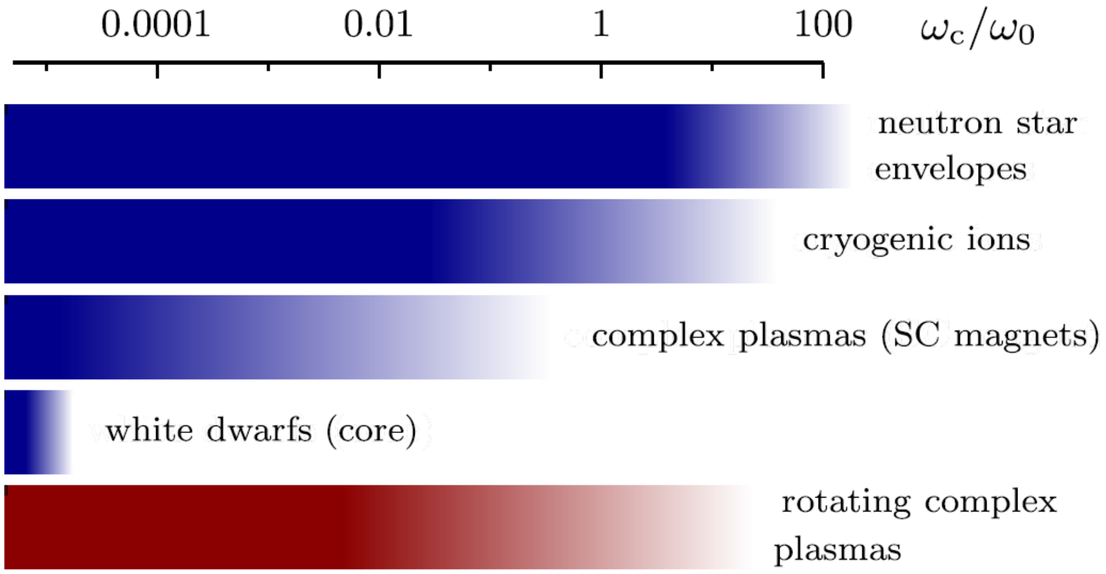
“Quasi-magnetization” of the dust particles [1]

replace Lorentz force with Coriolis force

basically no effect on electrons and ions

$\Omega \sim 10$ Hz, $Q \sim 10^4$ e, $m \sim 10^{-12}$ kg

$\longrightarrow \quad B_{\mathrm{eff}} \sim 10^4$ T



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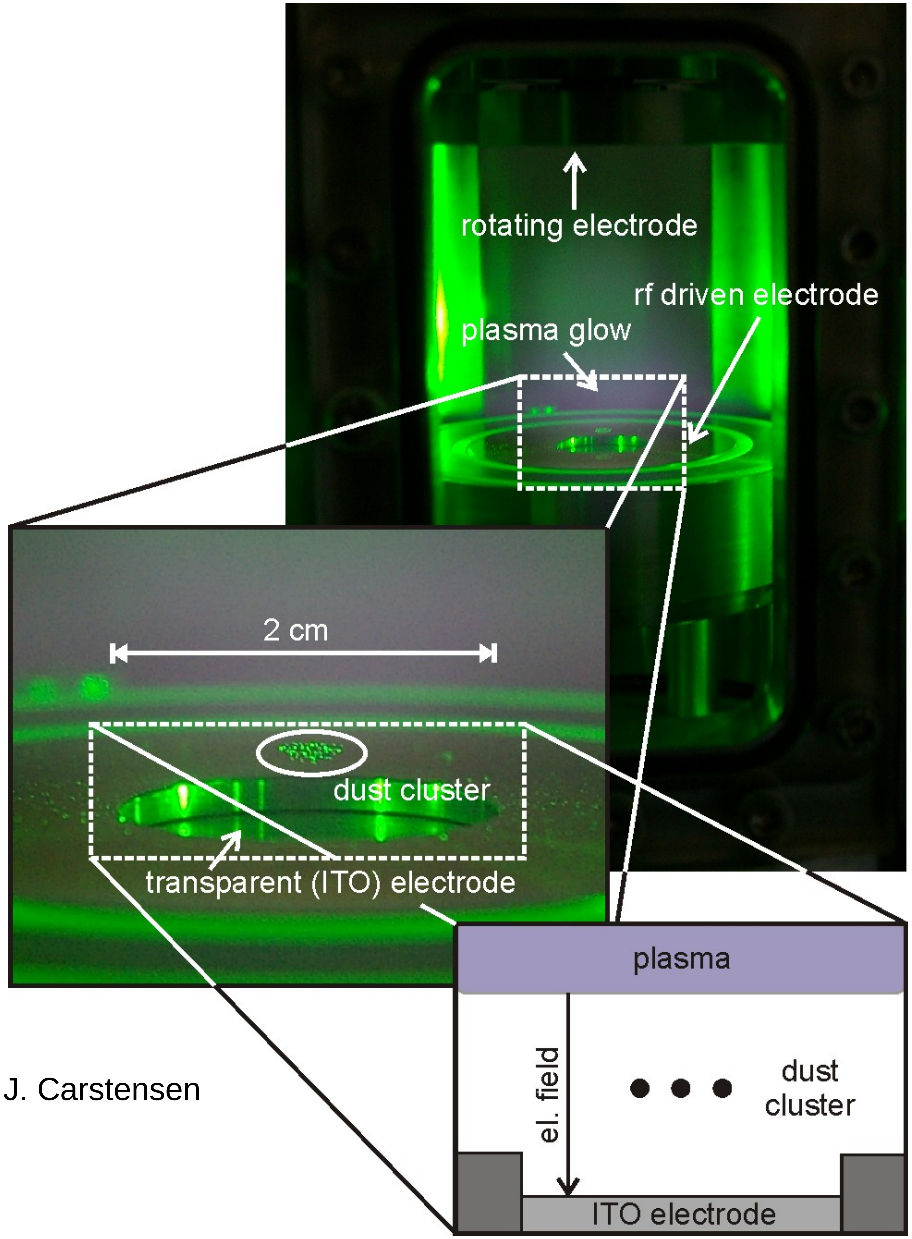
[1] H. Kählert *et al.*, PRL (2012); Bonitz, Kählert, Ott, Löwen, PSST (2013)

*) - similar concepts used in the context of cold quantum gases, e.g., P. Rosenbusch *et al.*, PRL **88**, 250403 (2002)
- vortex frequency in Penning traps, D. H. E. Dubin and T. M. O’Neil, Rev. Mod. Phys. **71**, 87 (1999)

Experimental realization of dust "quasi-magnetization"



J. Carstensen

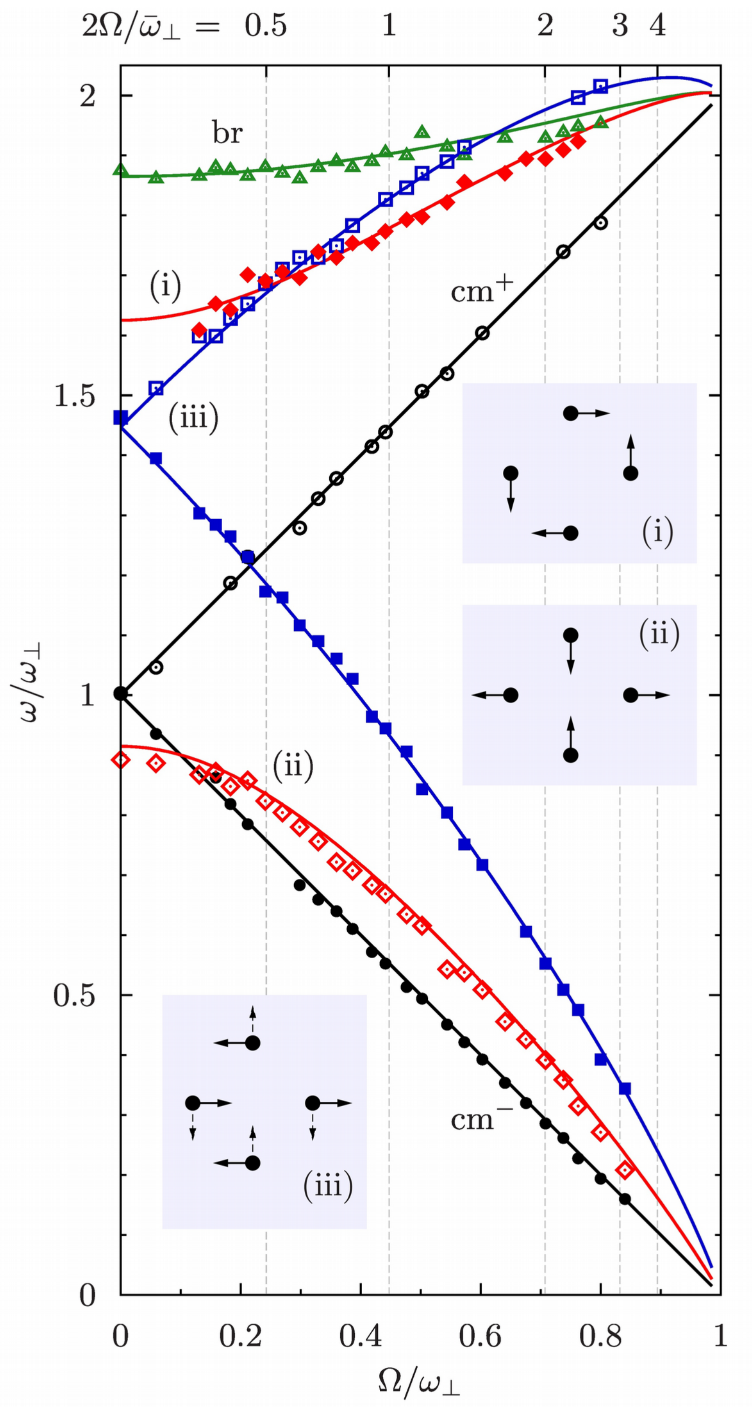
- Rotating electrode, introduced in

J. Carstensen, F. Greiner, L.-J. Hou, H. Maurer, and A. Piel, Phys. Plasmas **16**, 013702 (2009)

- vertically sheared rotation of neutral gas column
- uniform in-plane rotation

H. Kählert, J. Carstensen, M. Bonitz, H. Löwen, F. Geiner and A. Piel, PRL (2012)

Experimental proof: normal modes of a rotating cluster (N=4)



- Symbols: eigenmodes measured in rotating system [1]

- Lines: theory for magnetized plasma (non-rotating)

M. Kong, W. P. Ferreira, B. Partoens,
and F. M. Peeters,
IEEE Trans. Plasma Sci. **32**, 569 (2004)

[1] H. Kählert, J. Carstensen, M. Bonitz, H. Löwen, F. Greiner, and A. Piel, PRL (2012)

Second proof: *magnetoplasmons of macroscopic 2D Yukawa OCP:*
Hartmann, Donko, Ott, Kählert, Bonitz, PRL (2013)

Outline: Strongly correlated plasmas

I. Structural properties and phase transitions
one-component plasma, dusty plasmas, coupling parameters

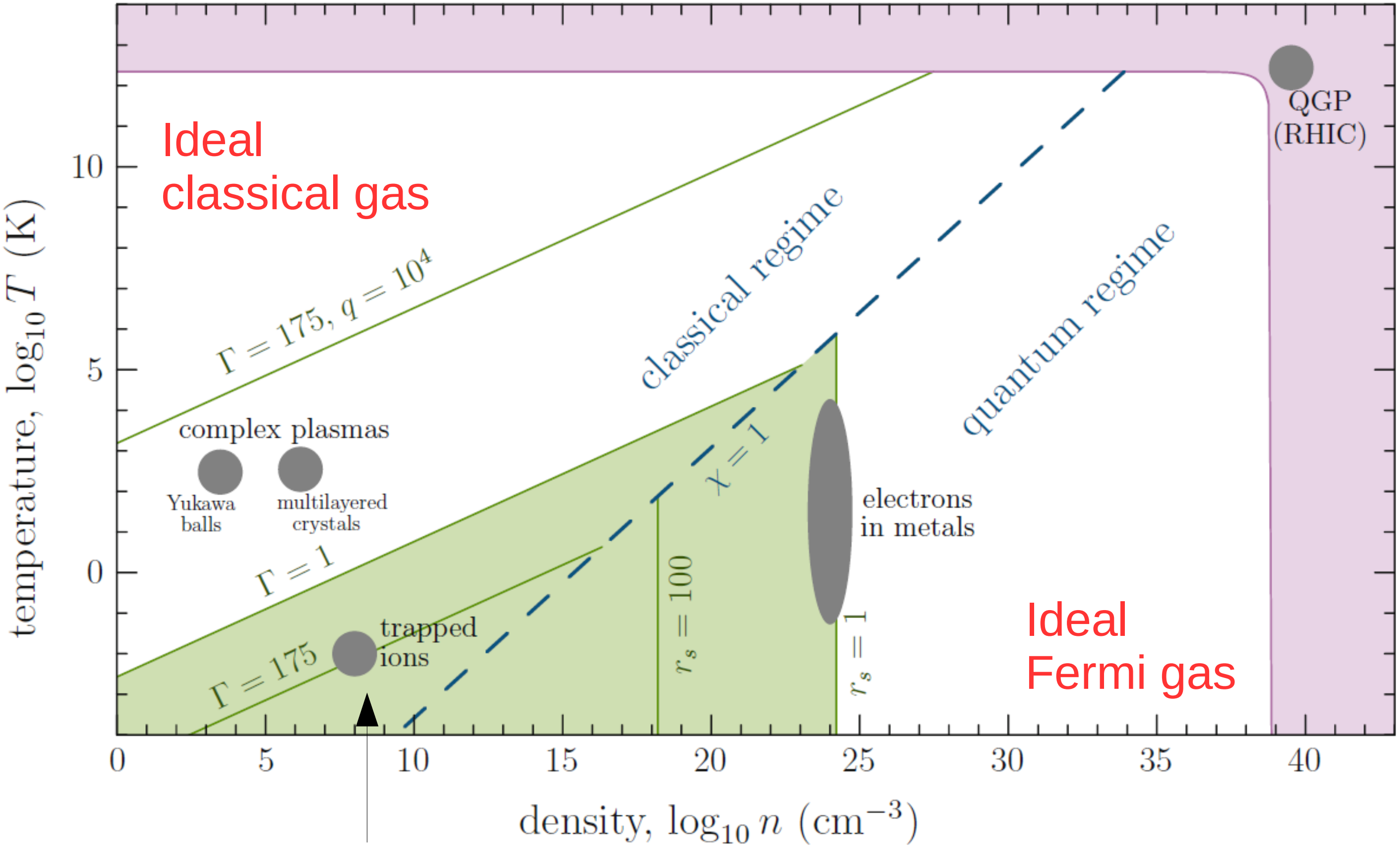
II. First principle results for transport properties
diffusion and heat conductivity

III. Correlations and strong magnetic fields
Collective modes, transport

IV. Quantum and spin effects
ab initio simulations. Quantum hydrodynamics

V. Conclusions

One-component plasma: quantum effects



Strong correlations

Quantum effects:

- finite electron extension
- exchange effects
- Fermi statistics
- quantum correlations

quantum coupling parameter:

$$\Gamma_{qa} \equiv \left(\frac{\hbar\omega_{pa}}{E_{Fa}}\right)^2 \sim$$

$$r_s \equiv \frac{d_a}{a_B} \sim n_a^{-1/3}$$

quantum degeneracy parameter

$$\chi_a = n_a \Lambda_a^3 \sim \left(\frac{\Lambda_a}{d}\right)^3 \sim \left(\frac{E_{Fa}}{k_B T}\right)^{3/2} \equiv \Theta_a^{-3/2}; \qquad \Lambda_a^2 = \frac{h^2}{2\pi m_a k_B T}$$

DeBroglie wavelength, Fermi energy

M. Bonitz, *Quantum Kinetic Theory*, 2nd ed. (Springer 2016)

Ab initio approaches to quantum plasmas

Quantum chemistry (many-body Schrödinger eq.)

Density functional theory

Quantum kinetic theory [1]

Nonequilibrium Green functions [1]

Quantum Monte Carlo [2]

…………………………….

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[1] M. Bonitz, *Quantum Kinetic Theory*, 2nd ed. (Springer 2016)

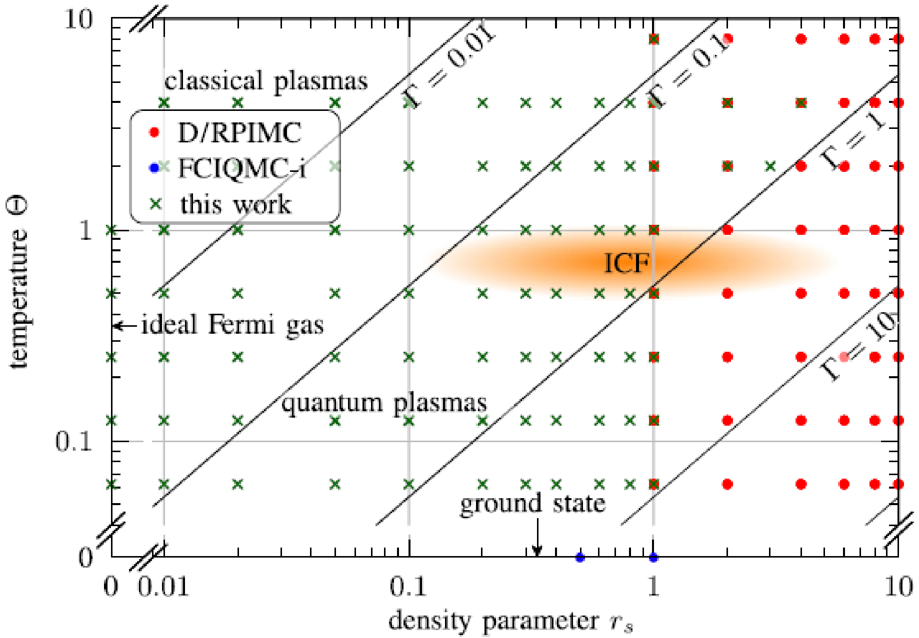
[2] M. Bonitz, J. Lopez, K. Becker, and H. Thomsen, *Complex Plasmas*, (Springer 2014)

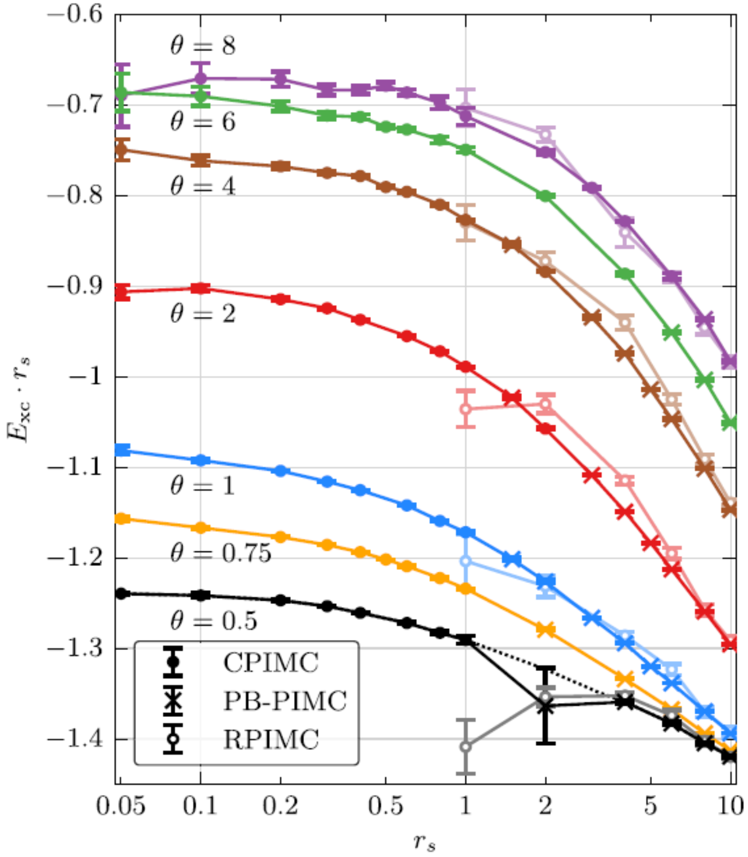
Ab initio results for the quantum electron gas at finite T

- developed two novel Quantum Monte Carlo methods: CPIMC [1] and PB-PIMC [2]
- their combination allows to avoid the notorious fermion sign problem

- obtained the first complete *ab initio* thermodynamic results for the electron gas [3-5]

- key input for warm dense matter and DFT





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[1] T. Schoof *et al.,* Contrib. Plasma Phys. (2011), [2] T. Dornheim et al., New J. Phys. (2014)

[3] T. Schoof *et al.,* PRL (2015); [4] T. Dornheim *et al.,* PRL (2016); [5] S. Groth *et al.*, PRL (2017)

Simplified apprach: quantum hydrodynamics (QHD)

Madelung (1926), Bohm (1952): mapping of Schrödinger equation of **1 electron** on fluid equations

Gross, Pitaevskii (1961): mean field (fluid) form of **many-boson** dynamics in condensate

Manfredi, Haas (2001): QHD equations for many ideal fermions (derivation problematic [1])

$$\frac{\partial}{\partial t} n\left(\mathbf{r},t\right) + \nabla\left[\mathbf{j}\left(\mathbf{r},t\right)\right] = 0,$$

$$m\frac{\partial}{\partial t}\mathbf{j}\left(\mathbf{r},t\right) - n\left(\mathbf{r},t\right) e\mathbf{E}(\mathbf{r},t) = -\nabla\cdot\mathbf{P}(\mathbf{r},t)$$

classical fluid equations
with kinetic pressure

$$-\nabla P_F[n(\mathbf{r},t)] - n\left(\mathbf{r},t\right)\nabla V_B[n(\mathbf{r},t)]$$

obtain QHD, by substituting
Fermi pressure, Bohm potential

$$\frac{\hbar^2}{8m}\left(\left|\frac{\nabla n}{n}\right|^2 - 2\frac{\nabla^2 n}{n}\right)$$

1-electron expression
applies only in special case [2]

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[1] Khan, Bonitz, in: *Complex Plasmas*, (Springer 2014)

[2] Moldabekov *et al.,* Phys. Plasmas (2015)

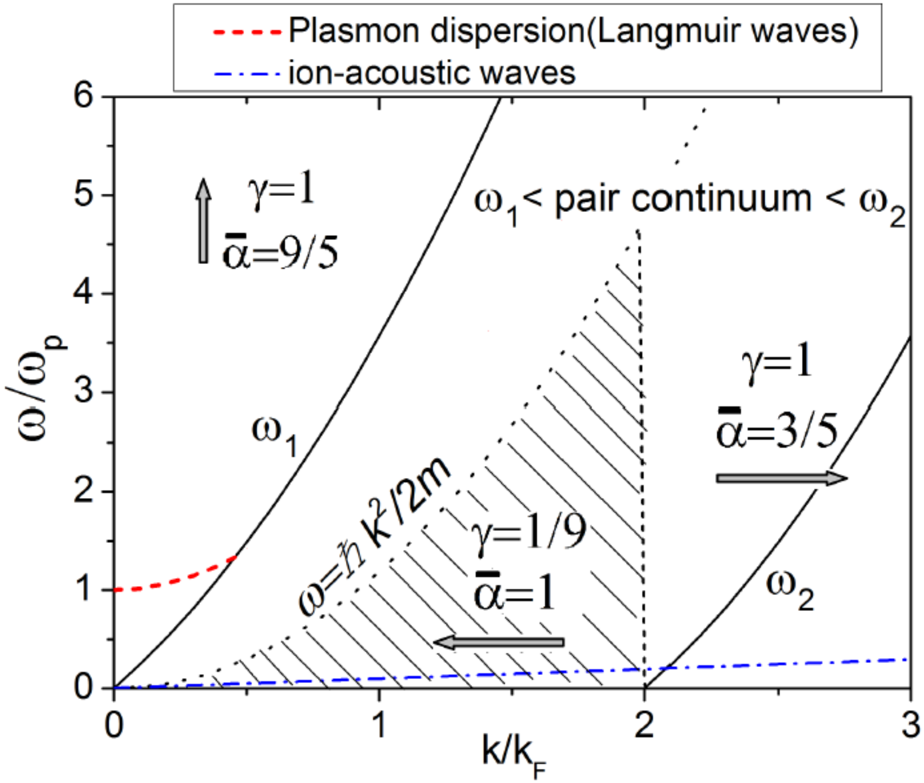
Improved quantum hydrodynamics for plasmas

extend QHD to finite temperature and exchange and correlation corrections [2]

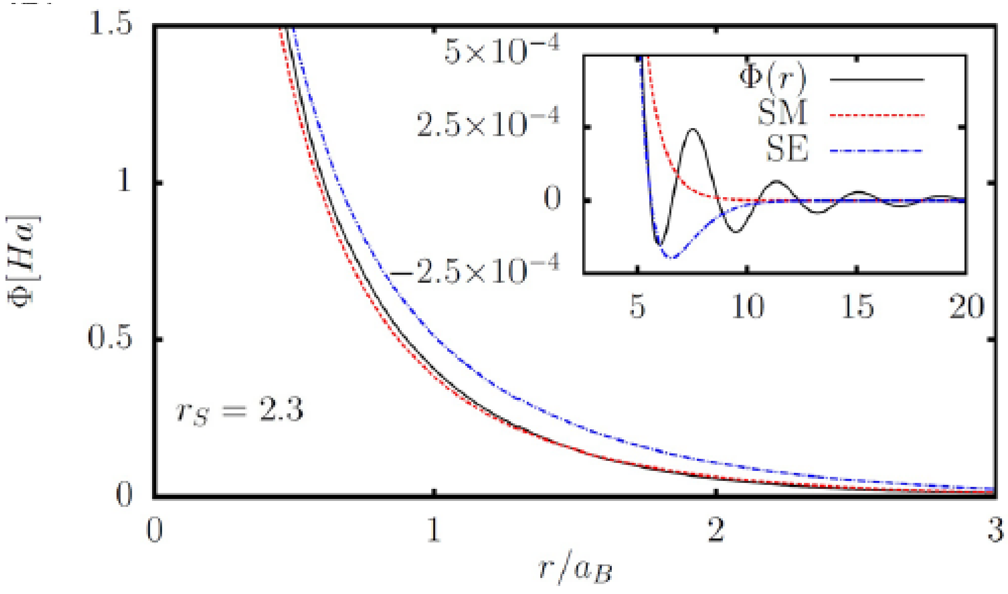
Starting point: free energy functional $F[n]=F_0[n]+\int dr\, a_2[n]|\nabla n(r)|^2+F_{xc}[n]$

Fermi pressure ~ $\bar{\alpha} E_F=\dfrac{\delta F_0[n]}{\delta n}$

$$V_B(\omega,k)=\gamma(\omega,k)\frac{\hbar^2}{8m}\left(\left|\frac{\nabla n}{n}\right|^2-2\frac{\nabla^2 n}{n}\right)$$



Screened ion potential (RPA, Friedel oscillations)
SE: attraction [3] is artefact of wrong Bohm potential
SM: correct prefactor 1/9 [1]



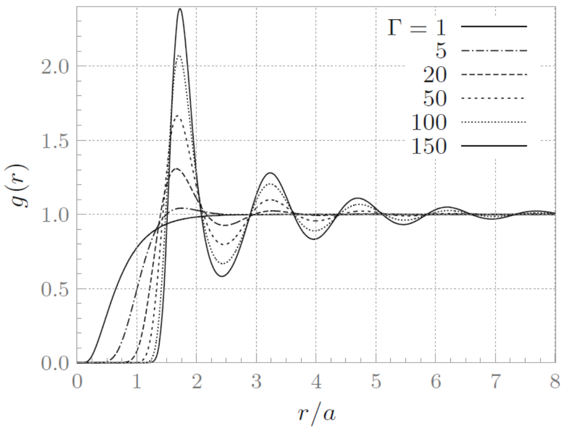
[1] Michta, Graziani, Bonitz, Contrib. Plasma Phys. (2015)

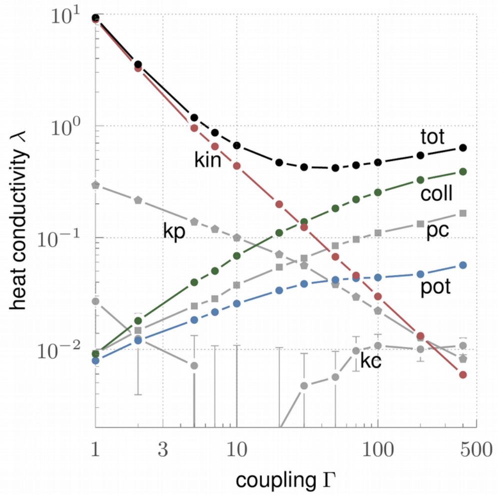
[2] Moldabekov *et al.*, Phys. Plasmas (2017), arxiv:1709.02196

[3] Shukla, Eliasson, PRL (2012)

[4] Bonitz, Pehlke, Schoof, PRE (2013)

Summary





Structure
phase transitions

Transport
***ab initio* results**

Strongly coupled plasmas

Magnetization effects

Quantum and spin effects