Theory of strongly correlated plasmas:

Phase transitions, transport, quantum and magnetic field effects

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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

\[ \Gamma = \frac{Q^2}{4\pi\varepsilon_0 a} \frac{1}{k_B T} \geq 1 \]

\( a \sim \text{Wigner-Seitz radius} \)

\( \Gamma \ll 1 \) weakly coupled

\( \Gamma > 1 \) strongly coupled

\( \text{liquid-like,} \)

\( \Gamma >> 1 \) Coulomb (Wigner) crystal

Note: \( \Gamma \) is only a qualitative measure for pure Coulomb systems
Pair distribution function (2-particle probability)

microscopic measure of strong coupling effects

\[ \int_0^\infty dr \, r^2 g(r) = 1, \quad \text{for ideal plasma: } g(r) = 1 \]

from: M. Bonitz, *Quantum Kinetic Theory*, 2nd ed. (Springer 2016)
Examples of strongly coupled plasmas

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

Note: this applies only to classical plasmas

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

M. Bonitz et al. (eds.), “Introduction to Complex Plasmas”, Springer 2010
Dusty plasmas are complicated:

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

reasonable model [1]

“Yukawa OCP”

2 independent parameters

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

\[ \kappa = a / \lambda_D \]

\[ \Gamma = Q^2 / (a k_B T) \]


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

\[ g(r) \]

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

Particle coordinates directly accessible in experiments


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), \( g(r_1,r_2) \)
  - 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]

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Exact transport properties via molecular dynamics

- solve equations of motion of $N$ particles by time-discretization

- Newton's equations*:

$$m \ddot{r}_i = F_i + q \dot{r}_i \times B$$

$$F_i = -\frac{q^2}{4\pi\varepsilon_0} \sum_{j=1}^{N'} \left( \nabla \frac{e^{-r/\lambda_D}}{r} \right) \bigg|_{r=r_i-r_j}$$

$$B = B \cdot e_z$$

- 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)

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

$\Gamma = 2 \omega_p t = 5$

$\Gamma = 100 \omega_p t = 50$

Correlations dramatically reduce $D$

T. Ott and M. Bonitz, PRL (2011)
Exact heat conductivity $\lambda$

$\lambda$ follows from energy current auto-correlation function (Green-Kubo relations)

$$J = -\lambda \nabla T$$

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

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

1-particle terms

Exact heat conductivity $\lambda$: effect of correlations

- **reduction of mobility ($D$)**
- **excitation of collective modes**

Exact heat conductivity $\lambda$: nontrivial coupling dependence

Single-particle conductivity dominates

Many-particle conductivity dominates

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One-component plasma in an external magnetic field
Three relevant parameters: $\Gamma$, $\kappa$, $\beta$

\[
\beta = \frac{\omega_c}{\omega_p} \sim \frac{\lambda_D}{r_c}
\]

$\omega_c = \frac{QB}{m}$

$\beta = 0$
unmagnetized

$\beta = 1$
strongly magnetized

$\beta = 4$

moderate coupling ($\Gamma = 2$)

strong coupling ($\Gamma = 100$)

2D OCP, MD simulation: T. Ott; M. Bonitz et al., PSST (2013)
Weak coupling (Braginskii 1965): quadratic reduction of $D \perp B$
no effect on $D \parallel B$

Strong magnetization [1]:
- $B$ inhibits diffusion, even along $B$
- at strong $B$: Bohm diffusion $\sim 1/B$

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extension to 2D and binary systems:
T. Ott, H. Löwen, and M. Bonitz, PRE (2014)
Heat conductivity in magnetized strongly coupled OCP [1]

heat flux analogon of Hall effect: Righi-Leduc effect

\[ \mathbf{J} = -\lambda \nabla T \]
\[ J_a = -\lambda_{ab}(\nabla T)_b \]

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

Heat conductivity in magnetized strongly coupled OCP [1]

\[ \beta = 0.0 \quad 2.0 \]

parallel: increase
perpendicular: decrease
Righti-Leduc: new

Heat conductivity in magnetized strongly coupled OCP [1]

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


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 $\Gamma = 150$ [2]

Strong deviation from ideal plasmon spectrum

**plasmon:**
$$\omega_p(k) = \sqrt{\omega_p^2 + D_L(k)}$$

One longitudinal mode: $q \parallel k$, $q$: displacement

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

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]


Magnetized correlated OCP: parallel wave propagation

plasmon (pl) unaffected by magnetic field \((\mathbf{q} \parallel \mathbf{B})\)

Degeneracy of shear modes lifted
upper/lower shear (us, ls) circular polarization
\(\mathbf{q} \perp \mathbf{B}\)

Dispersion relation

\[
\omega_{pl}(k) = \sqrt{\omega_p^2 + D_L(k)}
\]

\[
\omega_{us,ls}(k) = \frac{1}{2} \left[ \sqrt{\omega_c^2 + 4D_T(k)} \pm \omega_c \right]
\]
Magnetized correlated OCP: perpendicular wave propagation

Ordinary shear mode (os) with \( q \parallel B \) unaffected by magnetic field

\( k \perp B \)

Plasmon & 2nd shear upper/lower hybrid modes (uh, lh)

\( q \perp B \)
elliptical motion In plane \( \perp B \)

Dispersion relation

\[
\omega_{\text{os}}(k) = \sqrt{D_T(k)}
\]

\[
\omega_{\text{uh, lh}}(k) = \frac{1}{\sqrt{2}} \left[ \omega_c^2 + \omega_p^2 + D_T(k) + D_L(k) \pm \tau(k) \right]^{1/2}
\]
Exact wave dispersions from MD simulation [1]

Gam = 100  beta = 1

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


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

- 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)

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

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

- harmonic confinement

- uniformly rotating gas (rotation frequency $\Omega$)

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

\[
\mathbf{u}(\mathbf{r}) = (\Omega \hat{e}_z) \times \mathbf{r}
\]

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

- dust-dust interaction
- dust-neutral friction coefficient
- random force
"Quasi-magnetization" of the dust particles

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

\[
m \ddot{\bar{r}}_i = -\nabla_i \bar{V}(\bar{\rho}_i, \bar{z}_i) + \sum_{j \neq i}^{N} \bar{F}_{ij}^{\text{int}} + \bar{F}_{\text{Cor}}(\dot{\bar{r}}_i) - \nu m \dot{\bar{r}}_i + \bar{f}_i
\]

Centrifugal force

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

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

Coriolis force

\[
\bar{F}_{\text{Cor}}(\dot{\bar{r}}) = m \dot{\bar{r}} \times (2 \Omega \hat{e}_z).
\]

equivalent to Lorentz force (Larmor theorem)

\[
B_{\text{eff}} = (2m\Omega/Q)\hat{e}_z
\]

\[
\omega_c = 2\Omega
\]
“Quasi-magnetization” of the dust particles [1]

replace Lorentz force with Coriolis force
basically no effect on electrons and ions

\[ \Omega \sim 10 \text{ Hz}, \; Q \sim 10^4 \text{ e}, \; m \sim 10^{-12} \text{ kg} \]

\[ B_{\text{eff}} \sim 10^4 \text{ T} \]

**Diagram:**
- Neutron star envelopes
- Cryogenic ions
- Complex plasmas (SC magnets)
- White dwarfs (core)
- Rotating complex plasmas

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*) - similar concepts used in the context of cold quantum gases, e.g., P. Rosenbusch et al., PRL 88, 250403 (2002)
Rotating electrode, introduced in


vertically sheared rotation of neutral gas column

uniform in-plane rotation

Experimental realization of dust “quasi-magnetization”
Experimental proof: normal modes of a rotating cluster (N=4)

- Symbols: eigenmodes measured in rotating system [1]

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


Second proof: magnetoplasmons of macroscopic 2D Yukawa OCP:
Hartmann, Donko, Ott, Kählert, Bonitz, PRL (2013)
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One-component plasma: quantum effects

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

Quantum coupling parameter:
\[ \Gamma_{qa} \equiv \left( \frac{\hbar \omega_{pa}}{E_{Fa}} \right)^2 \sim \]
\[ r_s \equiv \frac{d_a}{d_B} \sim n_a^{-1/3} \]

Strong correlations

quantum degeneracy parameter

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

DeBroglie wavelength, Fermi energy

M. Bonitz, Quantum Kinetic Theory, 2nd ed. (Springer 2016)
Quantum chemistry (many-body Schrödinger eq.)
Density functional theory
Quantum kinetic theory [1]
Nonequilibrium Green functions [1]
Quantum Monte Carlo [2]

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

Simplified approach: 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])

\[
\frac{\partial}{\partial t} n (r, t) + \nabla [j (r, t)] = 0,
\]
\[
m \frac{\partial}{\partial t} j (r, t) - n (r, t) eE(r, t) = -\nabla \cdot P(r, t)
\]
\[
- \nabla P_F[n(r, t)] - n (r, t) \nabla V_B[n(r, t)]
\]
\[
\frac{\hbar^2}{8m} \left( \left| \frac{\nabla n}{n} \right|^2 - 2 \frac{\nabla^2 n}{n} \right)
\]

classical fluid equations with kinetic pressure

obtain QHD, by substituting Fermi pressure, Bohm potential

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


Improved quantum hydrodynamics for plasmas

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

Starting point: free energy functional

\[ F[n] = F_0[n] + \int dr \alpha_2[n] |\nabla n(r)|^2 + F_{xc}[n] \]

Fermi pressure \[ \bar{\alpha} E_F = \frac{\delta F_0[n]}{\delta n} \]

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

Screened ion potential (RPA, Friedel oscillations)

SE: attraction [3] is artefact of wrong Bohm potential

SM: correct prefactor 1/9 [1]

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Summary

http://www.itap.uni-kiel.de/theo-physik/bonitz

Structure
phase transitions

Transport
ab initio results

Magnetization
effects

Strongly coupled
plasmas

Quantum and
spin effects

\[
\Gamma = \begin{align*}
1 & \quad 5 \\
20 & \quad 20 \\
50 & \quad 50 \\
100 & \quad 100 \\
150 & \quad 150
\end{align*}
\]

\[
g(r) \quad 10^1 \\
10^0 \\
10^{-1} \\
10^{-2}
\]

\[
\text{heat conductivity } \Lambda \\
k_\text{kin} \\
k_\text{tot} \\
k_\text{kp} \\
k_\text{pc} \\
k_\text{pot} \\
k_\text{kc}
\]

\[
\frac{\omega_c}{\omega_0} \\
0.0001 \\
0.01 \\
1 \\
100
\]

- neutron star envelopes
- cryogenic ions
- complex plasmas (SC magnets)
- white dwarfs (core)
- rotating complex plasmas

\[
E_\text{eff} \quad r_s \\
\theta = 8 \\
\theta = 6 \\
\theta = 4 \\
\theta = 2 \\
\theta = 1 \\
\theta = 0.75 \\
\theta = 0.5
\]

CPMC
PB-PIMC
RPMC