Physics of dense plasmas – correlations, magnetic fields and quantum effects

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Christian-Albrechts-Universität zu Kiel



A. Piel, D. Block, F. Faupel (Kiel),

- A. Melzer, H. Fehske (Greifswald), T. Ott, H. Löwen (Düsseldorf)
- Yu. Lozovik, V. Filinov, V. Fortov (Moscow), S. Smolyansky (Saratov),
- J.W. Dufty (Florida), H. Kählert, G. Kalman (Boston),
- P. Hartmann, Z. Donko (Budapest),
- K. Balzer, M. Drescher (Hamburg), T. Brabec (Ottawa)





Bundesministerium für Bildung und Forschung





A

Plasmas in the Universe and in the Lab



Plasma: hot gas of charged particles

Ideal gas Simple physics

?

From Contemporary physics education project 2010 (NSF, DOE sponsored) http://www.cpepphysics.org/fusion.html

Plasmas in the Universe and in the Lab



Lots of exciting plasmas missing!

Dense space plasmas:

- Cores of giant planets
- dwarf stars
- neutron stars

From Contemporary physics education project 2010 (NSF, DOE sponsored) http://www.cpepphysics.org/fusion.html

Dense plasma in White dwarf star



Structure of the interior of a white dwarf star, showing how the elements are distributed. EBIT-RETRAP recreates the thermodynamic conditions shown in the yellow section, where the ion plasmas crystallize. D. Schneider, LLNL classical fluid and crystal in "quantum sea" of electrons

Size ~ our Earth Mass ~ our Sun \rightarrow density: $\rho \cong 10^6 \rho_{erde}$

 $B = 10^3 \dots 10^7 T$

Dense plasma in Neutron stars



crystal and quantum fluid of Fe-nuclei

in "quantum sea" of electrons

Radius ~ 10km Mass ~ our Sun

 $\rho \cong 10^{15} \, g \, cm^{-3}$

 $B = 10^6 \dots 10^{11} T$

Source: Coleman, UMD

Plasmas in the Universe and in the Lab



Lots of exciting plasmas missing!

Dense space plasmas:

- Cores of giant planets
- dwarf stars
- neutron stars

Dense laboratory plasmas:

- laser plasmas
- ion beam produced plasmas
- ICF

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Plasmas in the Universe and in the Lab



Lots of exciting plasmas missing!

Strong correlations Cooperative behavior

Coulomb liquid and crystal states

- mass asymmetry
- quantum effects
- nonequilibrium
- magnetic fields
- → Theory challenging!

From Contemporary physics education project 2010 (NSF, DOE sponsored) http://www.cpepphysics.org/fusion.html

Outline

1. Correlation effects in plasmas: liquids and crystals

- dusty plasmas: the perfect test system

2. Attraction of identical particles

- from balls to strings

3. Dense plasmas in a strong magnetic field

- diffusion, normal modes
- "Magnetizing" a complex plasma without a magnet

4. Dense two-component quantum plasmas

- status of the theory
- towards multi-scale simulations

5. Conclusions and outlook

Prediction of spontaneous spatial ordering (crystallization)



E. Wigner, Physical Review 46, 1002 (1934):

computed exchange and correlation energy of the electron gas in metals

"If the electrons had no kinetic energy, they would settle in configurations which correspond to the absolute minima of the potential energy. These are close-packed lattice configurations, with energies very near to that of the body-centered lattice...."

But: no electron crystal in metals observed yet

Ongoing search with other types of charged particles



Gradual crystallization upon cooling

Particles settle in potential minima when kinetic energy below threshold

MD simulation (Torben Ott): steady cooling

video _____

Coulomb coupling parameter

$$\Gamma \equiv \frac{Q^2}{\bar{r} k_B T}$$

kT↓

U: total potential energy

Х

Freezing for Gamma > 175

Strongly coupled Coulomb systems



How to achieve Coulomb crystallization (1)



lons in traps, mk temperature

How to achieve Coulomb crystallization (2)



(predicted)

Filinov, Bonitz, Lozovik, PRL 2001

How to achieve Coulomb crystallization (3)



lons in traps, mk temperature

electrons in quantum dots (predicted)

Filinov, Bonitz, Lozovik, PRL 2001

1986: Theoretical prediction Phys. Fluids **29**, 1764 (1986)

Coulomb solid of small particles in plasmas



H. Ikezi

GA Technologies Inc., P. O. Box 85608, San Diego, California 92138

(Received 11 December 1985; accepted 11 March 1986)

Small particles in plasmas can form a coulomb lattice. The conditions for solidification in a laboratory plasma are discussed.

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Small particles in plasmas can form a coulomb lattice. The conditions for solidification in a laboratory plasma are discussed.

1994: Experimental observation

Y. Hayashi et al., Jap J. Appl. Phys. 33, L 804 (1994)

H. Thomas et al., Phys. Rev. Lett. 73, 652 (1994)

A. Melzer et al., Phys. Lett. A **191**, 301 (1994)

Tremendous activity By many groups...

Coulomb crystal in complex plasma



Filinov, Bonitz, Lozovik, PRL 2001



lons in traps, mk temperature

electrons in quantum dots (predicted)

Filinov, Bonitz, Lozovik, PRL 2001

Complex Plasmas





Challenging large parameter space and the diversity of physical conditions	
Plasma size:	From large and stable plasmas to <i>micro and nano plasmas</i>
Plasma pressure:	From low pressure to atmospheric and higher pressure
Plasma chemistry:	From rather simple rare-gas plasmas to more complex and <i>reactive molecular plasmas</i> (e.g., oxygen, hydrocarbons, fluorocarbons) and their interaction with condensed matter
Time scales:	From electron and ion dynamics to <i>chemical reactions</i> and <i>Collective behaviour</i> of massive dust particles

Trapping of Complex (Dusty) Plasma layer



Slight curvature of electrode provides lateral confinement

Picture: A. Melzer

Stereoscopic imaging: 3 video cameras



Plasma optically transparent Slow time scales, room temperature → single-particle resolution! Unique diagnostics of correlation effects!

AG Melzer, EMAU Greifswald

M. Bonitz, Ch. Henning, and D. Block, Rep. Progr. Phys. 73, 066501 (2010)

3D dust crystals without void

RF discharge, Argon









Foto: S. Käding, U Greifswald

- gravity compensated by thermophoretic force and electric fields
- glass box prevents formation of void region inside the dust cloud
- confinement (almost) isotropic
- dust in plasma bulk (slowly streaming ions)

O. Arp et al., Phys. Plasmas 12, 122102 (2005)

3D Spherical Dust Crystals



- Particles arranged on concentric spherical shells
- Optically transparent crystal

Arp, Block, Piel & Melzer, Phys. Rev. Lett. 93, 165004 (2004)

shell structure theoretically explained by Yukawa potential: Bonitz et al. Phys. Rev. Lett. **96**, 075001 (2006)

Accurate diagnostics:

- Video stereoscopy or
- Digital holography







Cold fluid theoy for Yukawa systems

Sensitive diagnostics. Direct comparison with simulations and experiment Current work: inclusion of correlations [Kählert, Bonitz, Kalman 2013]

Kählert, MB, Phys. Rev. E **82**, 036407 (2010) Kählert, MB, Phys. Rev. E **83**, 056401 (2011)

Crystallization (Shell Formation) Dynamics

1.0 0.8 (a) $\omega_0 t =$ (d 0.8 0.6 $n(r) a^3$ MF ----rla 0.6 0.4 0.4 0.2 0.2 0.0 0.0 2.5 3.0 (b) (e) 2.5 2.0 2.0 $u^{(L)}$ rla 1.5 1.0 0.5 0.5 0.0 0.0 (f) C $n(r)a^3$ r/arla wot

Rapid cooling of weakly coupled initial state

screening

H. Kählert and M. Bonitz, PRL 104, 015001 (2010)

Correlation effects in plasmas: liquids and crystals

 dusty plasmas: the perfect test system

2. Attraction of identical particles - from balls to strings

- 3. Dense plasmas in a strong magnetic field
 - diffusion, normal modes
 - "Magnetizing" a complex plasma without a magnet
- 4. Dense two-component quantum plasmas
 - status of the theory
 - towards multi-scale simulations
- **5. Conclusions and outlook**

String Formation in Vertically Elongated 3D Confined Dusty Plasmas







N. Sato et al. (2001)

M. Kroll, J. Schablinski, D. Block, and A. Piel, Phys. Plas. **17**, 013702 (2010)

Vertical alignment not explainable with repulsive Yukawa potential! Effective particle-particle attraction

Origin of attractive force

1997 Schweigert, Melzer, Piel...



wake-field behind charged grain \rightarrow non-reciprocal grain interaction

 \rightarrow vertical grain alignment

Origin of attractive force

1997 Schweigert, Melzer, Piel...



wake-field behind charged grain
→ non-reciprocal grain interaction
→ vertical grain alignment

Effective potential of single particle



Confirmed by simulations (PIC): Hutchinson, Schneider, Miloch...

But: can treat only 1...3 particles

Fig.: Ivlev et al, PRL 100, 095003 (2008)

Other wake fields:

- Surfing

....

- Laser wake field acceleration

- Electrons in undulator

Linear response: dynamically screened potential

$$\Phi_i(\mathbf{r},t) = \int \frac{d^3k}{2\pi^2} \frac{q}{k^2} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}_i t)}}{\epsilon^{\mathrm{l}}(\mathbf{k},\mathbf{k}\cdot\mathbf{v}_i)}$$

Dust grains are "dressed", mediated by dielectric function

Fourier transform of bare Coulomb potential

Linear response: dynamically screened potential

$$\Phi_i(\mathbf{r},t) = \int \frac{d^3k}{2\pi^2} \frac{q}{k^2} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}_i t)}}{\epsilon^1(\mathbf{k},\mathbf{k}\cdot\mathbf{v}_i)}$$

Dust grains are "dressed", mediated by dielectric function



$$\epsilon^{l}(\mathbf{k},\omega) = 1 + \frac{1}{k^{2}\lambda_{De}^{2}} + \frac{1}{k^{2}\lambda_{Di}^{2}} \begin{bmatrix} 1 + \zeta_{i}Z(\zeta_{i}) \\ 1 + \sqrt{2}kv_{T_{i}} \\ \sqrt{2}kv_{T_{i}} \end{bmatrix} \stackrel{\text{electrons: statical screening }(u_{e} < V_{Te})}{\underset{(collisionless)}{}} \\ \lambda_{D_{\alpha}}^{2} = \frac{v_{T_{\alpha}}^{2}}{\omega_{p}^{2}} = \frac{\varepsilon_{0}k_{B}T_{\alpha}}{n_{\alpha}q_{\alpha}^{2}} \\ \text{bar Coulomb} \\ \text{potential} \rightarrow \text{Yukawa potential}} \quad \text{dynamical screening} \\ \rightarrow \text{ wake effects} \quad \text{lon-neutral scattering} \\ \rightarrow \text{ collisional damping}$$

$$\zeta_i = \frac{\mathbf{k}(\mathbf{v}_d - \mathbf{u}_i) + i\nu_{in}}{\sqrt{2}kv_{T_i}} - \text{ion neutral collison}$$
frequency
thermal velocity $v_{T_{\alpha}} = \sqrt{\frac{k_B T_{\alpha}}{m_{\alpha}}}$

M. Lampe, G. Joyce, et al., Phys. Plasmas **7**, 3851 (2000) P. Ludwig, W. Miloch, H. Kählert, and M. Bonitz, New J. Phys. **14**, 053016 (2012)



No ion flow: Yukawa Potential



Plasma parameters (Argon): n=2x10⁸ cm⁻³, T_e=2.585eV (30000K), T_e/T_i=30, ν_{in} =0.1 ω_{pi} , λ_{De} =0.845mm

Potential for Streaming Ions: M=0.250

Dynamically screened Coulomb potential: 'wake' potential (first peak height: 10.9mV @ z=0.29mm)

Mach number $M\equiv rac{u_i}{c_s}$, Bohm speed $c_s\equiv \sqrt{rac{k_{
m B}T_e}{m_i}}$

P.Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. **14**, 053016 (2012)

Plasma parameters (Argon): $n=2x10^{8}$ cm⁻³, $T_{e}=2.585$ eV (30000K), $T_{e}/T_{i}=30$, $\upsilon_{in}=0.1\omega_{pi}$, $\lambda_{De}=0.845$ mm

Potential for Streaming Ions: M=0.500

Dynamically screened Coulomb potential: 'wake' potential (first peak height: 31.2mV @ z=0.46mm)

Mach number
$$M\equiv \frac{u_i}{c_s}$$
, Bohm speed $c_s\equiv \sqrt{\frac{k_{\rm B}T_e}{m_i}}$

P.Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. **14**, 053016 (2012)

Plasma parameters (Argon): n=2x10⁸ cm⁻³, T_e=2.585eV (30000K), T_e/T_i=30, ν_{in} =0.1 ω_{pi} , λ_{De} =0.845mm
Potential for Streaming Ions: M=1.00



Dynamically screened Coulomb potential: 'wake' potential (first peak height: 29.9mV @ z=0.97mm)

Mach number
$$M\equiv \frac{u_i}{c_s}$$
, Bohm speed $c_s\equiv \sqrt{\frac{k_{\rm B}T_e}{m_i}}$

P.Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. **14**, 053016 (2012)

Plasma parameters (Argon): $n=2x10^{8}$ cm⁻³, $T_{e}=2.585$ eV (30000K), $T_{e}/T_{i}=30$, $\upsilon_{in}=0.1\omega_{pi}$, $\lambda_{De}=0.845$ mm

N-particle simulations using effective potential

1



Mixed structure of Yukawa ball and Strings



Langevin dynamics scheme:

$$m_d \ddot{\mathbf{r}}_k = -\nabla V_k^{\text{eff}}(\mathbf{r}, t) - \omega_0^2 m_d \mathbf{r}_k - \nu_{dn} m_d \dot{\mathbf{r}}_k + \mathbf{f}_k(t)$$
$$V_k^{\text{eff}}(\mathbf{r}, t) = \sum_{l \neq k}^{N_d} q_d \Phi_l(\mathbf{r}, t)$$

friction coefficient, Gaussian random force, and plasma temperature are related by the fluctuation-dissipation theorem

$$\langle \mathbf{f}_i^{\alpha}(t)\mathbf{f}_j^{\beta}(t')\rangle = 2m\nu_{dn}k_BT\delta_{ij}\delta_{\alpha\beta}\delta(t-t'), \ \alpha,\beta\in\{x,y,z\}$$

Accurate nonequilibrium multi-sclae simulation

Benchmark against full nonlinear PIC simulations Ludwig et al., New J. Phys. **14**, 053016 (2012)

Pioneered by G. Joyce, M. Lampe, See also: Murillo, Jenko et al. 1. Correlation effects in plasmas: liquids and crystals
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Strongly correlated plasmas in strong B-field

 $B = 10^3 \dots 10^7 T$



? Effect of magnetic field on plasma? when is a field strong/relevant

$$B = 10^6 \dots 10^{11} T$$



Figures: D. Schneider, LLNL, Coleman , UMD

B-field: Larmor precession of charged particles → reduced mobility across field

Known behavior of diffusion coefficient:

 $\mathsf{D}_{\!\scriptscriptstyle \perp} \left(\mathsf{B}\right) \sim 1/\mathsf{B}^2\,$, weak field

 \sim 1/B , strong field (Bohm diffusion)

 $D_{\parallel}(B) \sim const$

Behavior at strong coupling?

T. Ott and M. Bonitz, Phys. Rev. Lett. **107**, 135003 (2011)

Trajectories in a correlated plasma (B=0)

Moderate coupling, $\Gamma=2$



Coupling parameter

$$\Gamma = Q^2 / (4 \pi \epsilon_0 a k_B T)$$

Thermal velocity, plasma frequency, mean distance: v_T , ω_0 , a

2D one-component plasma during 5 plasma periods, MD simulation by T. Ott

Trajectories in a correlated plasma (B=0)



Strong coupling, Γ=100



Coupling parameter

$$\Gamma = Q^2 / (4 \pi \epsilon_0 a k_B T)$$

²D one-component plasma during 5 (50) plasma periods, MD simulation by T. Ott

Moderate magnetic field

Moderate coupling, $\Gamma=2$



Strong coupling, Γ=100



β=0.0

Cyclotron frequency:

Larmor radius:

$$\omega_c = QB/mc$$

 $r_L = v_T/\omega_c$

$$\beta = \omega_c / \omega_0$$
$$\delta = r_L / a \propto 1 / \Gamma^{0.5}$$

2D one-component plasma during 5 (50) plasma periods, MD simulation by T. Ott

Strong magnetic field

Moderate coupling, $\Gamma=2$



Strong coupling, Γ=100



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2D one-component plasma during 5 (50) plasma periods, MD simulation by T. Ott

Diffusion in a magnetized 3D complex plasma

First-principle MD simulations: T. Ott and M. Bonitz, Phys. Rev. Lett. **107**, 135003 (2011) (One-component plasma model)



Large B: Cohen, Suttorp (1984): for any coupling saturation of D______ (not confirmed)

Simulation result: large coupling: Bohm diffusion small coupling: slower algebraic decay

Magnetic field effects in correlated plasmas

Superposition of Coulomb correlations and B-field leads to new effects:

- \rightarrow radically altered transport properties (diffusion, heat conduction, viscosity etc.)
- \rightarrow strongly modified collective excitation spectrum,
 - Shear modes (Kalman, Golden)
 - "correlation-dressed" Bernstein modes:
 2D: M. Bonitz, Z. Donkó, T. Ott, H. Kählert, P. Hartmann, PRL 105, 055002 (2010)

3D: T. Ott, H. Kählert, A. Reynolds, M. Bonitz, PRL 108, 255002 (2012)

- inhibition of crystallization: T. Ott, H. Löwen, and M. Bonitz, PRL (2013)

Questions

1. Experimental verification in real complex (dusty) plasmas?

2. Use of dusty plasmas as test system for magnetized correlated plasmas?

Magnetized strongly coupled Coulomb systems

Universality: plasmas with same Gamma and beta have same properties (equilibrium, OCP)





Dusty plasma experiments with superconducting magnets:

Recent results: G. Morfill (Garching), A. Piel (Kiel) New devices: E. Thomas (Auburn)...

Fully magnetized electrons, partially magnetized ions

But: dust un-magnetized because of large particle mass

$$\beta = \frac{\omega_c}{\omega_p} = B \sqrt{\frac{\epsilon_0}{\rho}} \approx 3 \cdot 10^{-6} \frac{B \,[\mathrm{T}]}{\sqrt{\rho \,[\mathrm{kg \ m}^{-3}]}}$$

Mass density $\rho = mn$

Examples (4T):

$$d = 20 \,\mu m \,, \rho = 1200 \, kgm^{-3} \,\rightarrow \beta = 3 \cdot 10^{-5}$$

$$d = 100 \,nm \,, \rho = 4 \cdot 10^{-8} \, kgm^{-3} \,\rightarrow \beta = 0.06, (but : no optical diagnostics)$$

Dust particles set into rotation by rotating neutral gas $u(r) = (\Omega \hat{e}_z) \times r$.

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

$$m\ddot{r}_i = -\nabla_i V(\rho_i, z_i) + \sum_{j \neq i}^N F_{ij}^{\text{int}} - \nu m \left[\dot{r}_i - u(r_i)\right] + f_i$$

H. Kählert, J. Carstensen, M. Bonitz, H Löwen, F. Greiner, and A. Piel., PRL 109, 155003 (2012).

Dust particles set into rotation by rotating neutral gas $u(r) = (\Omega \hat{e}_z) \times r$.

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Transform to frame rotating with the neutral gas

$$m\ddot{\bar{r}}_{i} = -\bar{\nabla}_{i}\bar{V}(\bar{\rho}_{i},\bar{z}_{i}) + \sum_{j\neq i}^{N}\bar{F}_{ij}^{\text{int}} + \bar{F}_{\text{Cor}}(\dot{\bar{r}}_{i}) - \nu m\dot{\bar{r}}_{i} + \bar{f}_{i},$$
$$\bar{F}_{\text{Cor}}(\dot{\bar{r}}) = m\dot{\bar{r}} \times (2\Omega\,\hat{e}_{z})$$

Coriolis force equivalent to Lorentz force:

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

Experimental verification



Experiment: J. Carstensen

P=0.4Pa, Argon, Ω =0...30 Hz 2D dust cluster

Typical trajectory (rest frame)



Kählert et al., PRL 109, 155003 (2012).

Theory-Experiment comparison



Video camera diagnostics Particles with d=21.8µm in horizontal plane

7 (of 8) Normal modes of 4 particles for different rotation speeds

Symbols: experiment Lines: theory

→ easily reach β =3 equivalent B-field (without rotation): 100,000T!

Kählert et al., PRL 109, 155003 (2012)

Extension to macroscopic 2D systems: M. Bonitz, H. Kählert, T. Ott, and H. Löwen, Plasma Sources Sci.Technol. **22**, 015007 (2013) 1. Correlation effects in plasmas: liquids and crystals
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Quantum plasmas in the Universe and in the Lab



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- neutron stars

Dense laboratory plasmas:

- laser plasmas
- ion beam produced plasmas
- Inertial confinement fusion

From Contemporary physics education project 2010 (NSF, DOE sponsored) http://www.cpepphysics.org/fusion.html

Correlations of quantum plasmas



Partially ionized 2-comp. plasma



Partially ionized dense plasma

Need "chemical" composition of plasma: fraction of free and bound electrons

Equilibrium: mass action law (Saha equation), including correlation and quantum effects, Mott effect

 \rightarrow chemical models break down

Alternative: first principle simulations: Path integral quantum Monte Carlo

Illustration of PIMC



Computer lab, text books:

"Introduction to Computational Methods for Many-Body Physics", Rinton Press 2006 "Introduction to Complex Plasmas", Springer 2010

Ultra-dense fully ionized two-component plasma



MB, V. Filinov, V. Fortov, P. Levashov, and H. H. Fehske, PRL **95**, 235006 (2005)

From atomic nuclei to quarks



Quantum plasmas in the Universe and in the Lab



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Idea of laser fusion (ICF)



Radiation

Blowoff



Laser beams or laser-produced x rays rapidly heat the surface of the fusion target, forming a surrounding plasma envelope.

Fuel is compressed by the rocketlike blowoff of the hot surface material.

Inward transported thermal energy



During the final part of the capsule implosion, the fuel core reaches 20 times the density of lead and ignites at 100,000,000°C.



Thermonuclear burn spreads rapidly through the compressed fuel, yielding many times the input energy.

Failure of NIF

ScienceInsider, News Reports 12 December 2012

Agency Tells Congress That NIF Is Not Working by Daniel Clery

Ignition scheduled by Oct 1 2012, but campaign unsuccessful

"At present, it is too early to assess whether or not ignition can be achieved at the National Ignition Facility," wrote Thomas P. D'Agostino, administrator of the National Nuclear Security Administration (NNSA) in a report requested by Congress that was submitted last week....

...Although the laser itself, the diagnostic instruments, and the target fabrication have all met or exceeded specifications, the physics of the implosions was unexpected. "Experimental data demonstrate that the **physics underlying ignition implosions are not predicted accurately by the simulation codes** that were used to design ignition targets and to predict their performance," the report says.

New theoretical / simulation efforts in dense quantum plasmas needed

National Research Council, Report, Feb 20 2103

Realistic dense quantum plasmas

Required: selfconsistent account of

- 1. Many-component system (mass-asymmetric)
- 2. Quantum degeneracy of light component (electrons)
- 3. Bound states of electrons and ions
- 4. Strong ion coupling
- 5. Strong magnetic field
- 6. Nonequilibrium:
 - streaming plasmas, ion beams
 - laser pulse or FEL excitation etc.

Current status: no solution of the quantum many-body problem Theoretical concepts for limiting cases Accurate computer simulations in TD equilibrium

Theoretical concepts for dense quantum plasmas



Regimes of equilibrium plasmas



Theory of dense plasmas: Methods

	Classical Systems	Quantum Systems
Theory	-Density functional theory -Fluid theory	-Density operator theory -Nonequilibrium Greens functions
1st principle simulations	-MC -MD -Langevin MD -Kinetic MC	-PIMC, CPIMC -QMD -DFT -TDSE, TDCI, MCTDHF -NEGF

Configuration PIMC



T. Schoof, MB, A. Filinov, D. Hochstuhl and J.W. Dufty, Contrib. Plasma Phys. **51**, 687 (2011) T. Schoof, Diplomarbeit, Uni Kiel 2011

Strongly correlated classical ions & weakly coupled quantum electrons

Dynamics, Transport \rightarrow new multi-scale approach*:

- ions treated exactly (MD)
- electrons give rise to *dynamically screened* ion pair potential, includes quantum dielectric function with correlations (Mermin DF) and external field effects
- includes nonequilibrium effects, such as wakes

$$\phi_{ij}(\vec{r}_i - \vec{r}_j) = \int d^3 \vec{k} \frac{Z^2 e^2}{(2\pi)^2 k^2} \frac{e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}}{\varepsilon(\vec{k}, -\vec{k} \cdot \vec{v}_0)}$$

Similar concept: "Kinetic theory MD" (F. Graziani, LLNL 2011)

*P. Ludwig, MB, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series **220**, 012003 (2010) Correlated dielectric function: N.H. Kwong, and MB, Phys. Rev. Lett. **84**, 1768 (2000)

Conclusions

Strongly correlated plasmas fluid and crystal structures

Complex plasmas

room temperature, direct optical diagnostics prototype for correlated plasmas

Magnetized strongly coupled plasmas

reduced transport realized in complex plasmas without magnetic field

Dense quantum plasmas

Partial ionization First principle PIMC simulations Multiscale simulations for electrons and ions

Review: Bonitz, Henning, Block, Rep. Prog. Phys.**73**, 066501 (2010) Further information: www.theo-physik.uni-kiel.de/~bonitz






Complex plasmas - outlook



Diagnostics with unprecedented single-particle resolution \rightarrow Unique opportunities for comparison experiment – simulation - theory

- Fundamental properties, interaction beyond linear response
- Many-particle properties: phase diagram collective oscillation spectrum
- Magnetic field effects: competition of correlations and magnetization shear instabilities
- Technological applications: nanoparticle growth in magnetron discharge nanocomposite formation





Review: Bonitz, Henning, Block, Rep. Prog. Phys.**73**, 066501 (2010) Further information: www.theo-physik.uni-kiel.de/~bonitz