

# Progress in strongly correlated Coulomb systems

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# Coulomb systems

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charged particles: electrons, ions, holes, positrons, quarks\* ...

Behavior dominated by Coulomb interaction  $U(r) = q^2 / r$

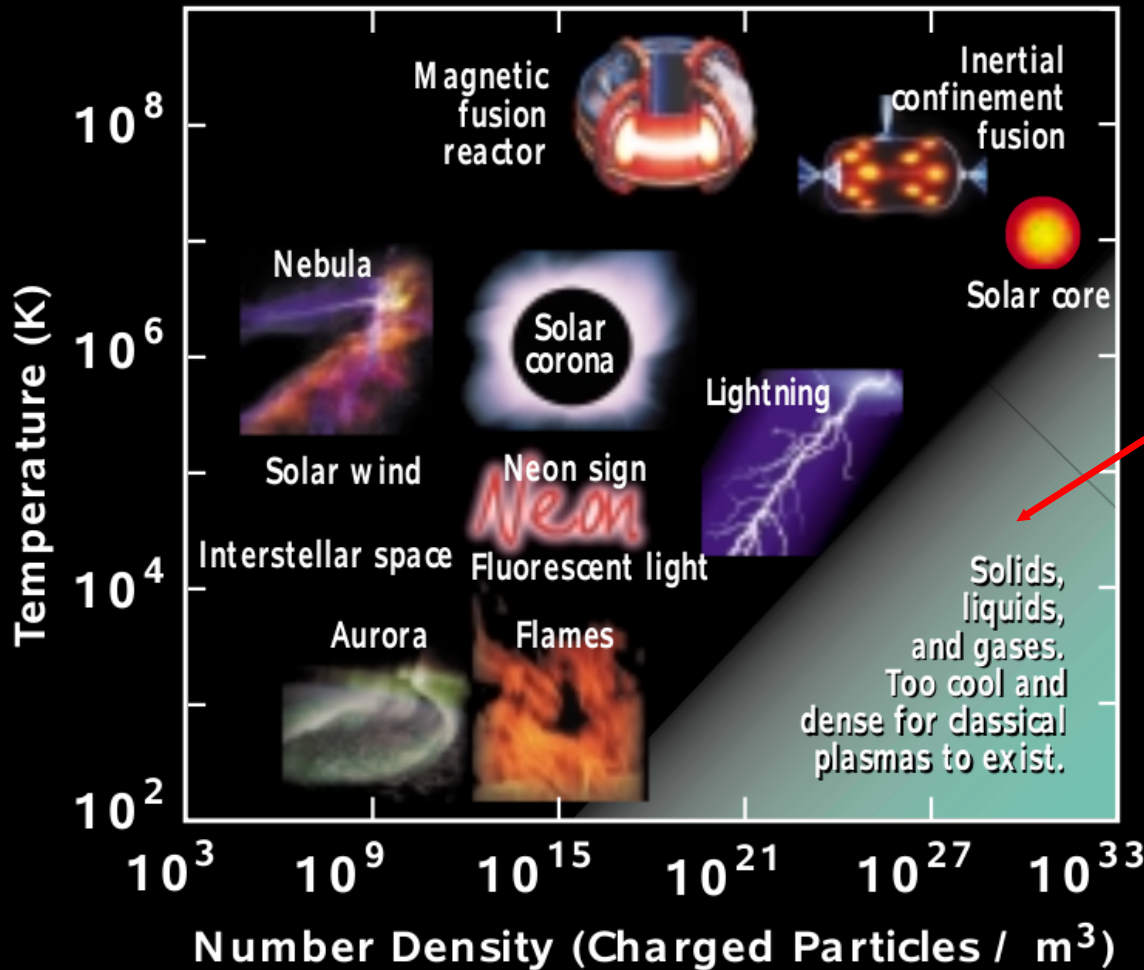
This interaction is strong and long range!

Wikipedia: „*More than 99 % of the visible matter in our universe is in the Plasma state*“

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also: Plasma of *magnetic* charges (monopoles) in spin ice:  
*MB, Nature Physics 7, 192 (2011)*

# Occurrences of plasmas\*

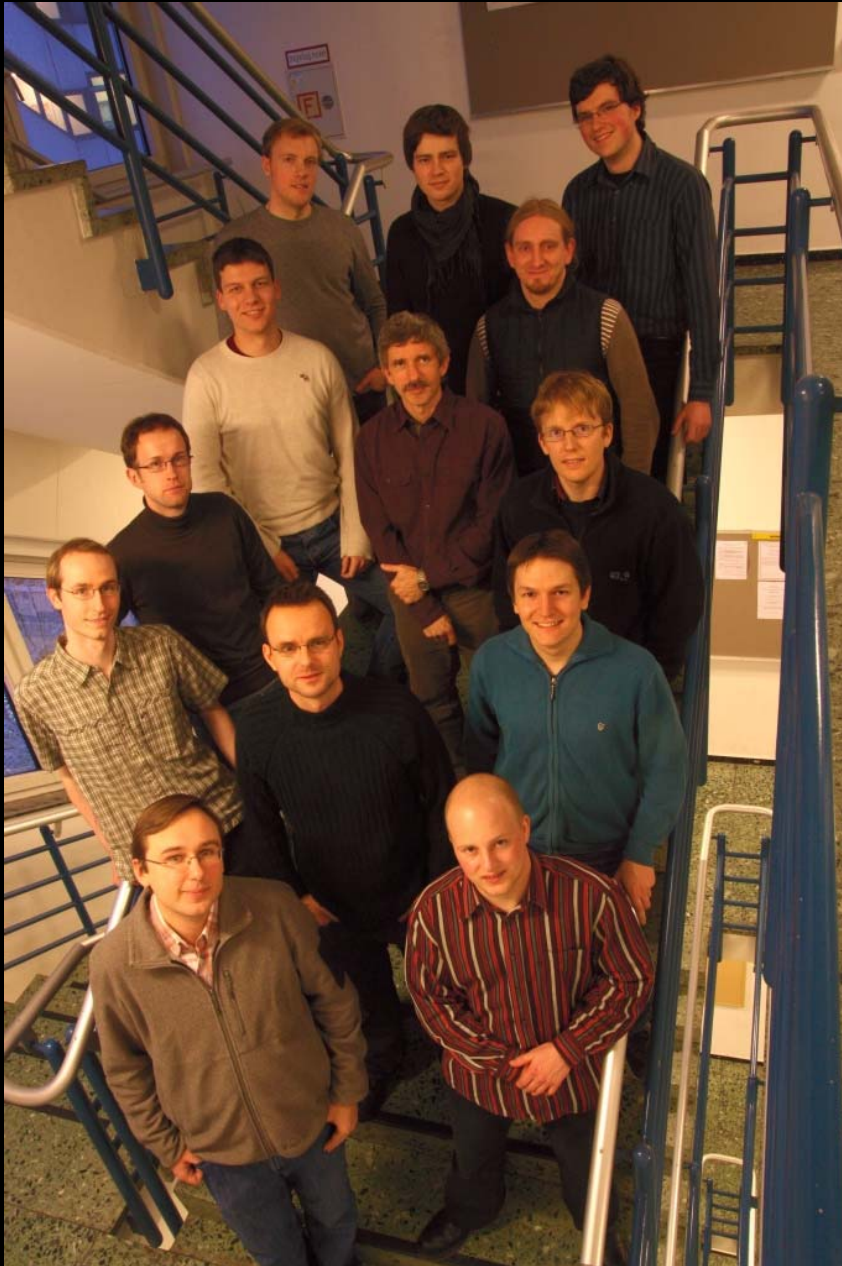


„unusual plasmas“

- astrophysical objects
- laser compression

*new states of matter*

# Acknowledgements 1: Group



Lasse Rosenthal , Torben Ott,

Sebastian Heerman

Karsten Balzer

Jens Böning, MB, Sebastian Bauch

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Tim Schoof, Patrick Ludwig, Kay Kobusch

Alexei Filinov, Hauke Thomsen

missing:

David Hochstuhl, Kenji Fujioka

Jan-Willem Abraham, Christopher Hinz

---

Master student, phd-student, postdoc

## Collaborations

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Yu. Lozovik, V. Filinov, V. Fortov (Moscow), S. Smolyansky (Saratov),

J.W. Dufty (Florida), G. Kalman (Boston),

P. Hartmann, Z. Donko (Budapest), R. Van Leeuwen (Jyväskylä),

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DFG

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## **1. Overview: strongly correlated plasmas**

- 1.1 One-component plasma (OCP) in TD equilibrium
- 1.2 Two-component plasma: partial ionization, compact stars, dense laboratory plasmas

## **2. Theory of strongly correlated plasmas**

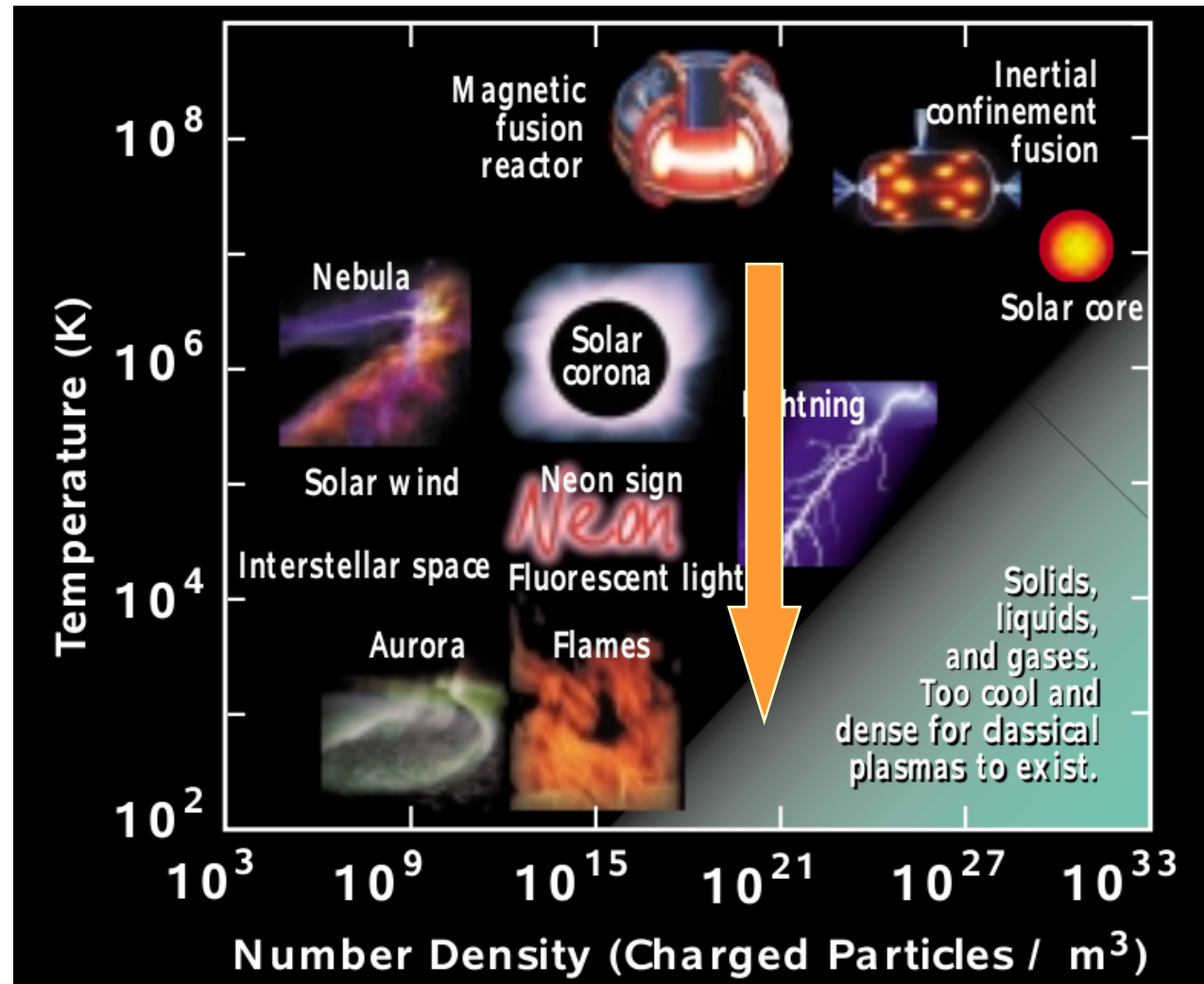
- 2.1 First-principle equilibrium simulations
- 2.2 Dense plasmas in nonequilibrium:
  - laser plasmas
  - photoionization

## **3. Outlook: Multiscale simulations of dense plasmas**

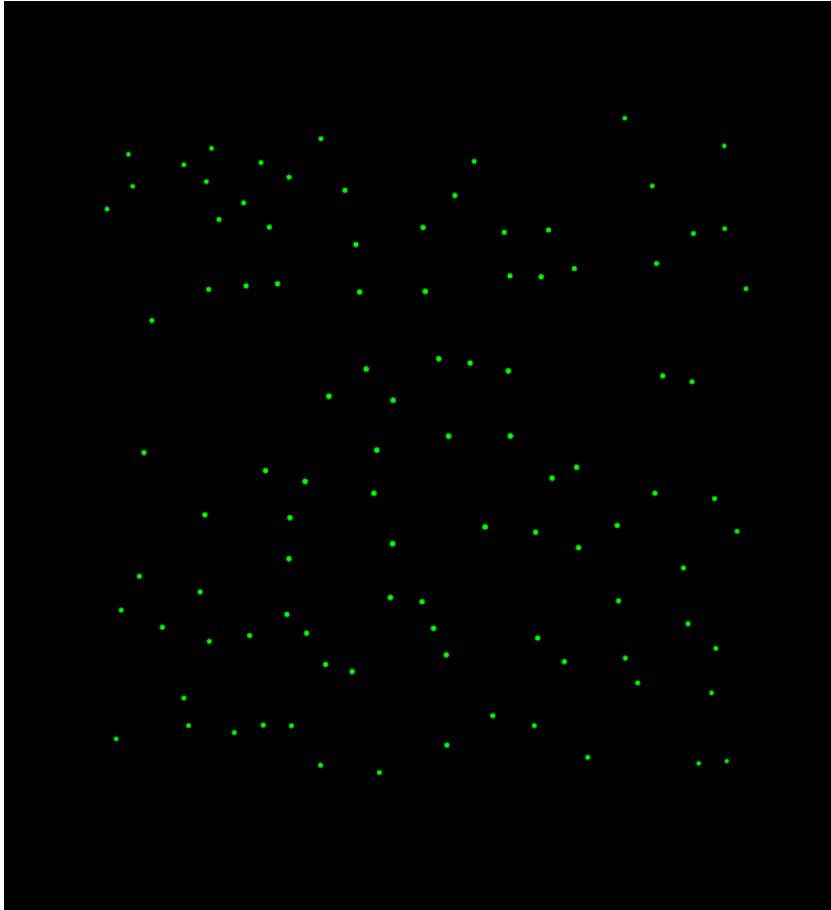
# One-component plasma model

- OCP: charged particles in neutralizing background (jellium)

1. Equilibrate
2. cool



# Thermodynamics of OCP



Classical „one-component plasma“ (OCP)

$$\Gamma = \frac{|\langle U \rangle|}{\langle E_{KIN} \rangle} = \frac{e^2}{k_B T \bar{r}}$$

**Liquid-solid transition** below critical temperature (above critical coupling strength).

$$\Gamma_{cr} \approx 175 \quad (2D : 137)$$

2D MD simulation of OCP cooling/heating,  
Periodic b.c., Torben Ott

Predicted by **Wigner** 1934 for the  
electron gas in metals.



# Plasma crystals in the laboratory

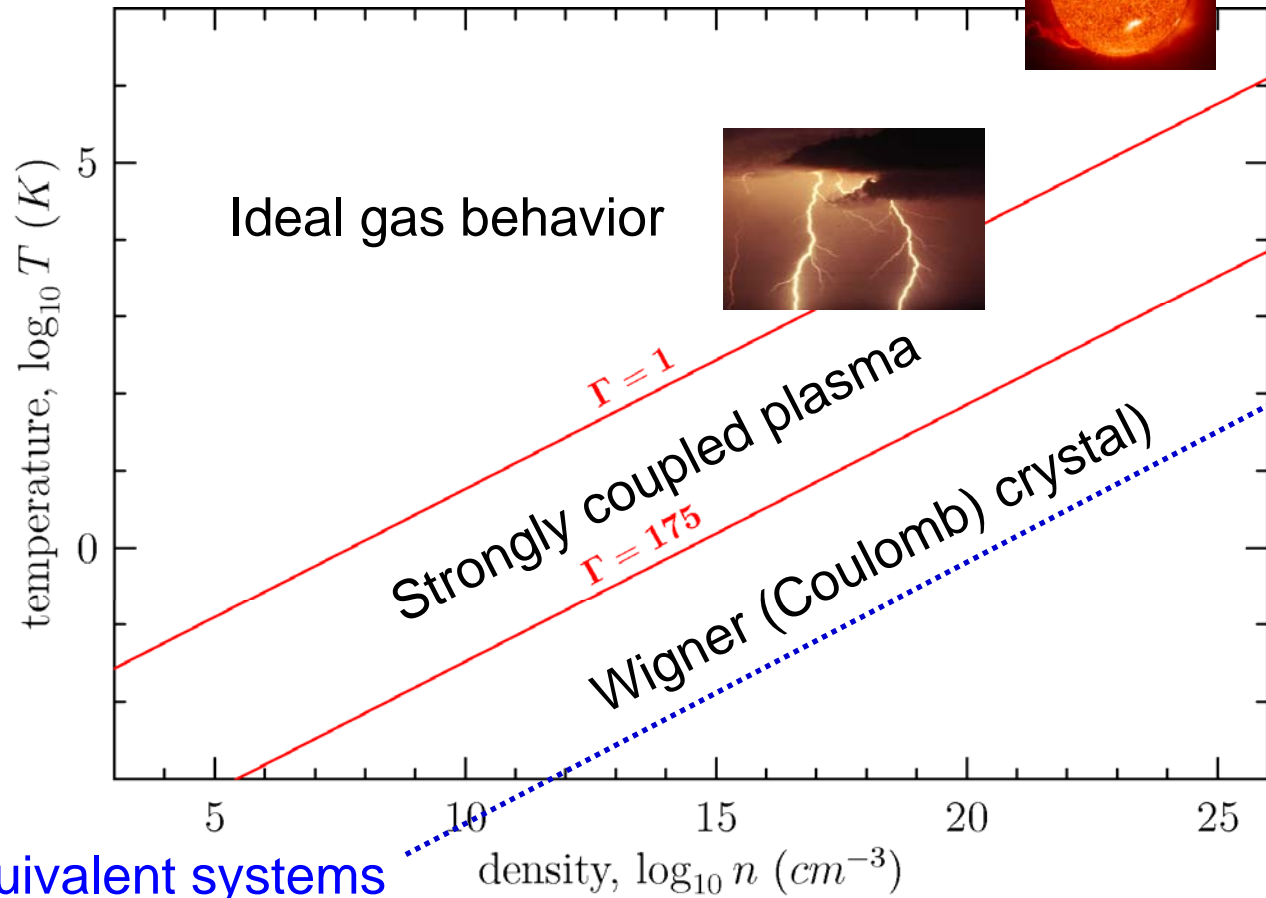
Need:  $\Gamma \geq \Gamma_{cr}$

$$\Gamma = \frac{|\langle U \rangle|}{\langle E_{KIN} \rangle} = \frac{e^2}{k_B T \bar{r}} \propto \frac{e^2 n^{1/3}}{T}$$



Ways to achieve:

1. cooling

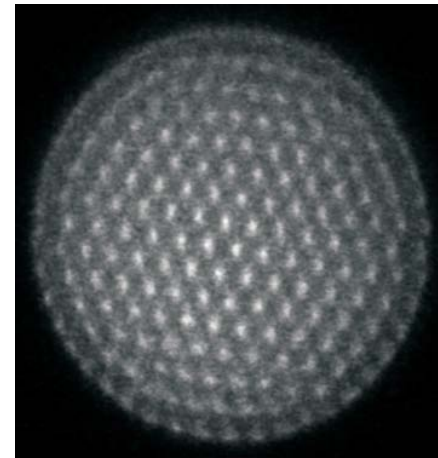
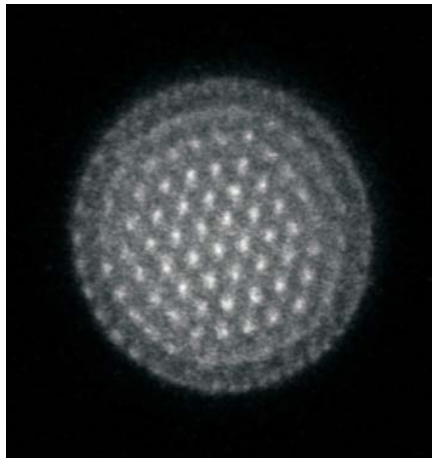


Physically equivalent systems

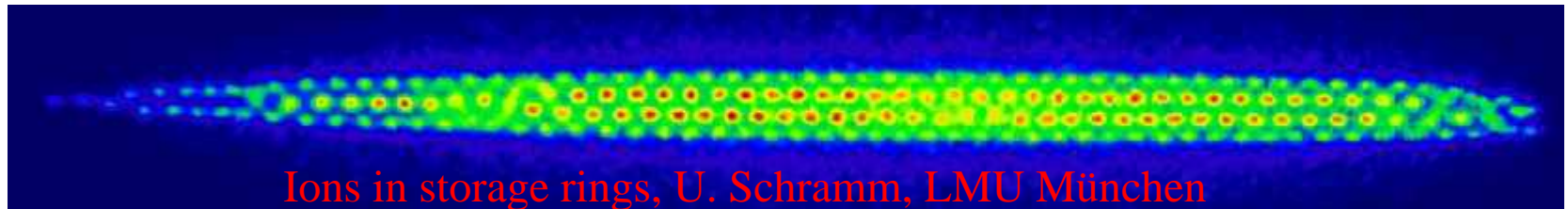
# Ion crystals in traps

1987 first realization in Paul trap and laser cooling (Ca, Mg,...)  
Bollinger et al. (NIST), Walther et al. (true 1-component plasma)

Today many active groups: Innsbruck (Blatt), Aarhus (Drewsen)...



Drewsen



Ions in storage rings, U. Schramm, LMU München

**Problem:** strong correlations require ultra-low temperatures (mK)

# Correlated plasmas – approach 2

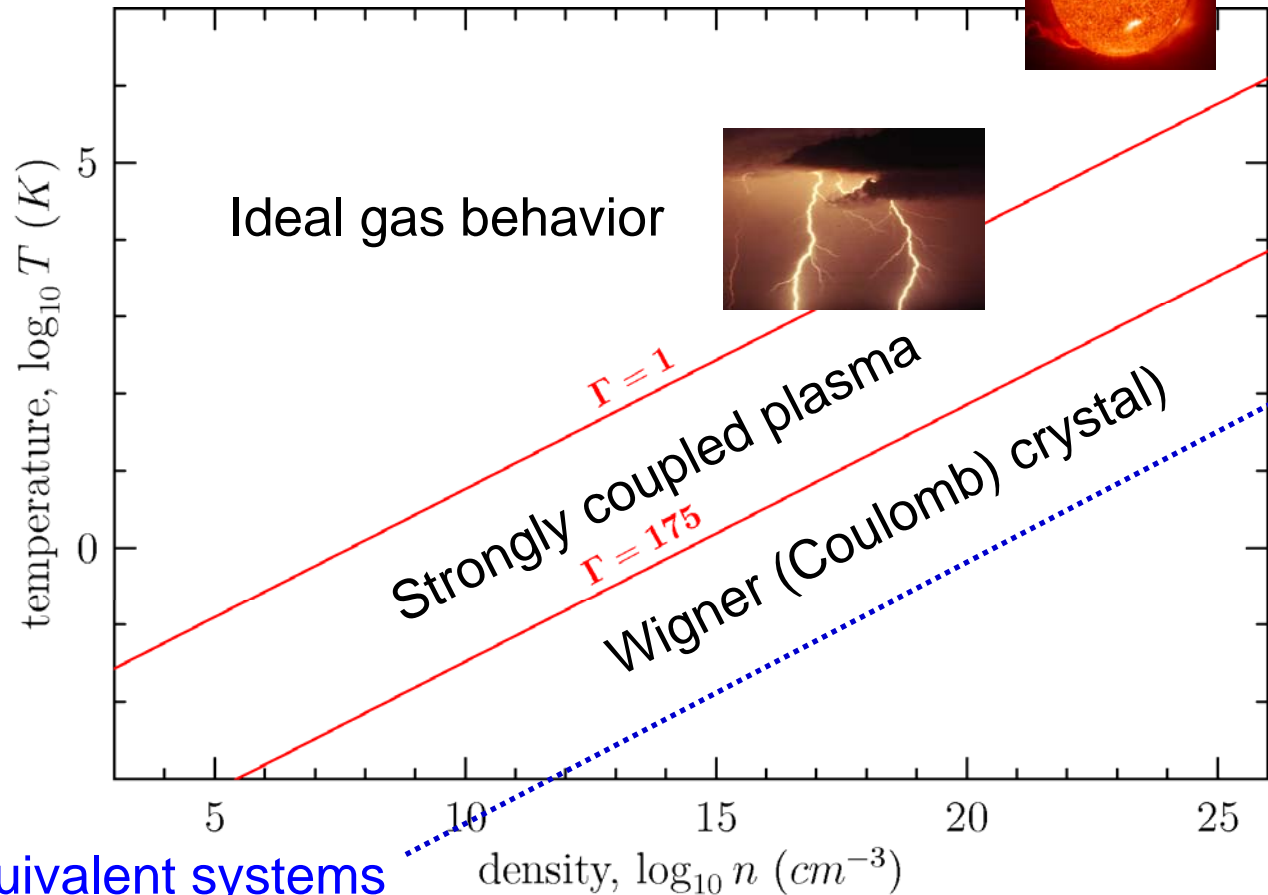
Need:  $\Gamma \geq \Gamma_{cr}$

$$\Gamma = \frac{|\langle U \rangle|}{\langle E_{KIN} \rangle} = \frac{e^2}{k_B T \bar{r}} \propto \frac{e^2 n^{1/3}}{T}$$



Ways to achieve:

1. cooling
2. Charge increase



Physically equivalent systems



Trapped ions

# Strongly correlated plasmas

Need:  $\Gamma \geq \Gamma_{cr}$

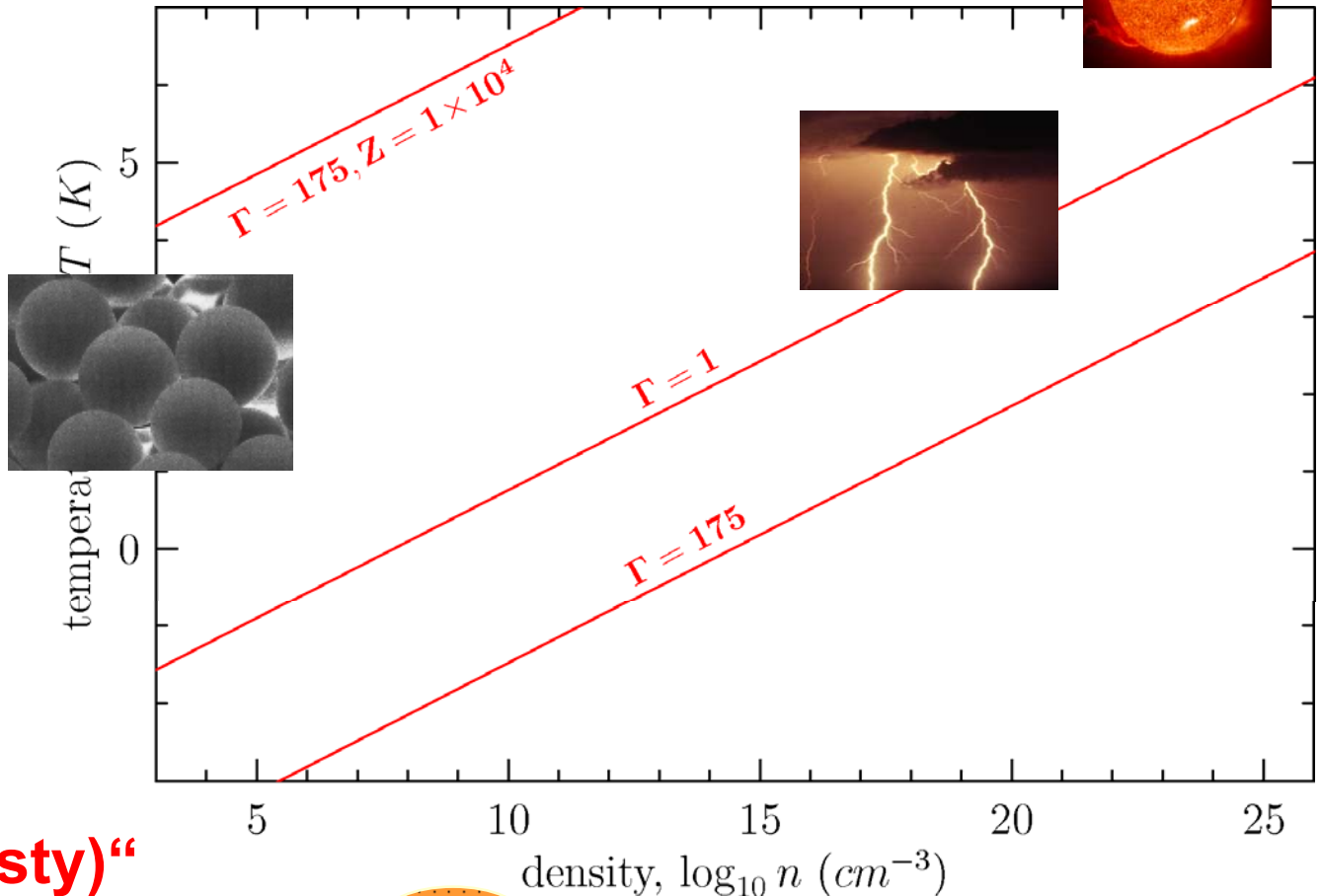
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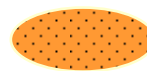
Ways to achieve:

1. cooling

2. Charge increase



„Complex (dusty)“  
plasma



Trapped ions

# Complex (dusty) plasmas\*

Experimental realization: 1994

Strongly correlated liquid and crystalline plasmas

Phase transitions

- prototype system to study charged particle correlations
- (virtually) exact computer simulations possible
- perfectly suited for development of theoretical concepts

→ Major progress in our understanding  
of strongly coupled Coulomb systems



Transregio-SFB „Fundamentals of complex plasmas“  
Greifswald/Kiel



\*M.B., C. Henning, D. Block, *Rep. Prog. Phys.* **73**, 066501 (2010)

„Introduction to Complex Plasmas“, MB, N. Horing and P. Ludwig (eds.), Springer 2010

# Correlated plasmas by compression

Need:  $\Gamma \geq \Gamma_{cr}$

$$\Gamma = \frac{|\langle U \rangle|}{\langle E_{KIN} \rangle} = \frac{e^2}{k_B T \bar{r}} \propto \frac{e^2 n^{1/3}}{T}$$

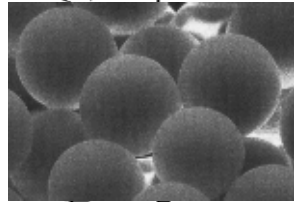
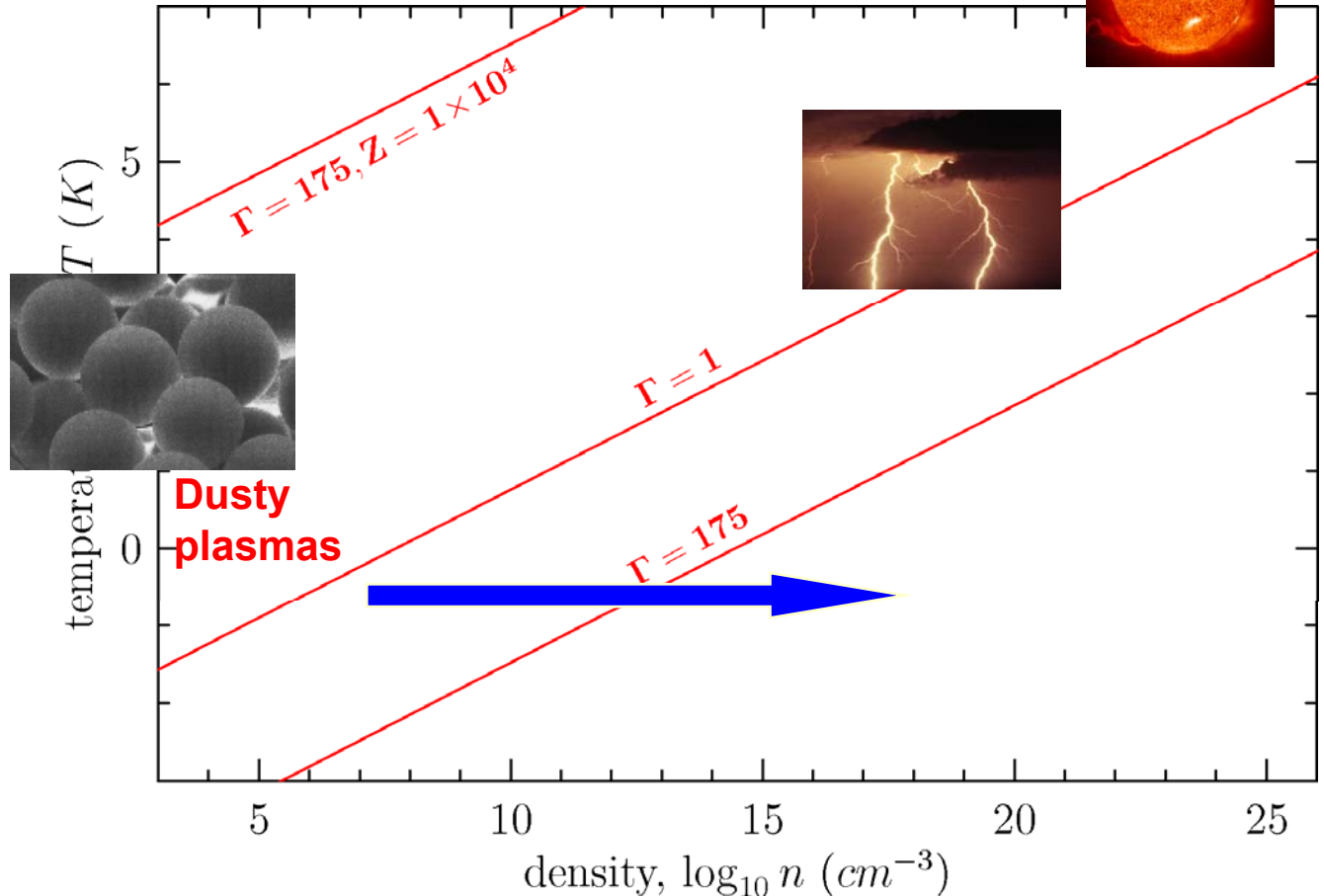


Ways to achieve:

1. cooling

2. Charge increase

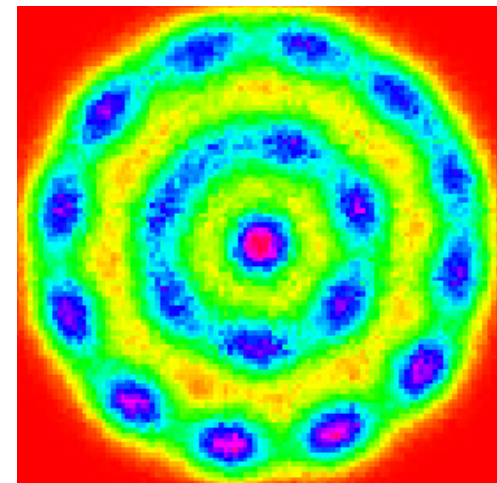
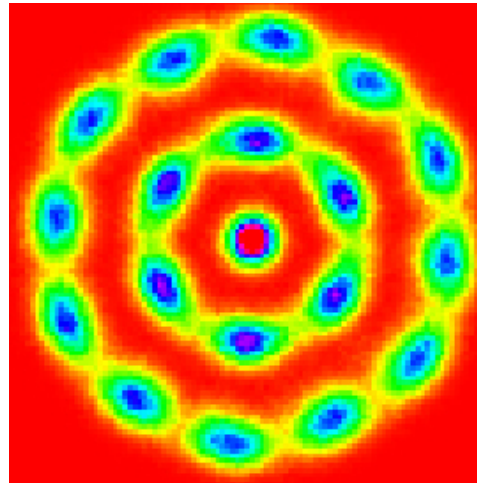
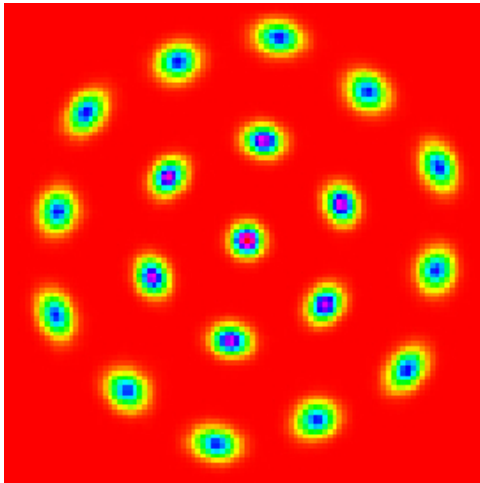
3. compression



Trapped ions

# Mesoscopic Coulomb crystal („artificial atom“\*)

compression  $\longrightarrow$



Density increase  $\rightarrow$  quantum („cold“) melting of „crystal“,  
despite increase of coupling parameter  $\Gamma$ ! Why?

$$\hat{H} = -\sum_{i=1}^N \frac{\hbar^2 \nabla_i^2}{2m_i^*} + \sum_{i=1}^N \frac{m_i^* \omega_0^2 r_i^2}{2} + \sum_{i < j}^N \frac{e^2}{\epsilon_b |\mathbf{r}_i - \mathbf{r}_j|}$$

\*R.C. Ashoori, Nature **379**, 413 (1996)

A.Filinov, MB, Yu. Lozovik, PRL **86**, 3851 (2001)

Phys. Rev. Focus (April 2001), Sciences et Avenir, Scientific American, FAZ 1.8. 2001...

# Correlations of quantum plasmas

crystal:  $\Gamma^Q = r_s \propto \frac{\bar{r}}{a_B} \geq r_s^{cr}$

$$\Gamma^Q = \frac{|\langle U \rangle|}{\langle E_{KIN} \rangle} \sim \frac{e^2}{E_F \bar{r}} \propto \frac{e^2 n^{1/3}}{n^{2/3}} \propto n^{-1/3}$$

## Quantum degeneracy

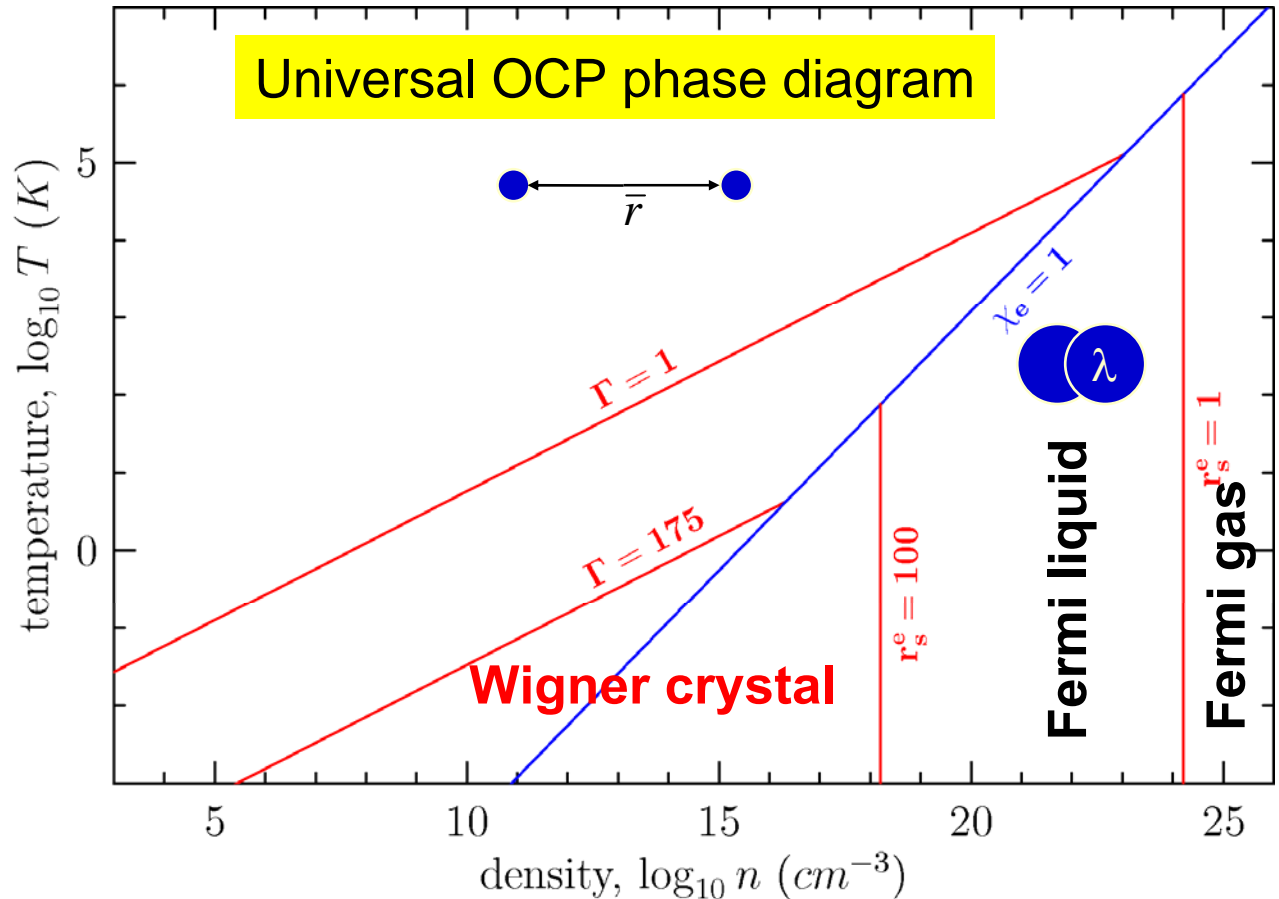
$$\chi = n\lambda^3$$

DeBroglie  
wave length

$$\lambda = h / \sqrt{2\pi m k_B T}$$

$$r_s^{cr} \approx 100/37 \text{ (3D/2D)}$$

Ceperley et al.,  
A. Filinov, MB





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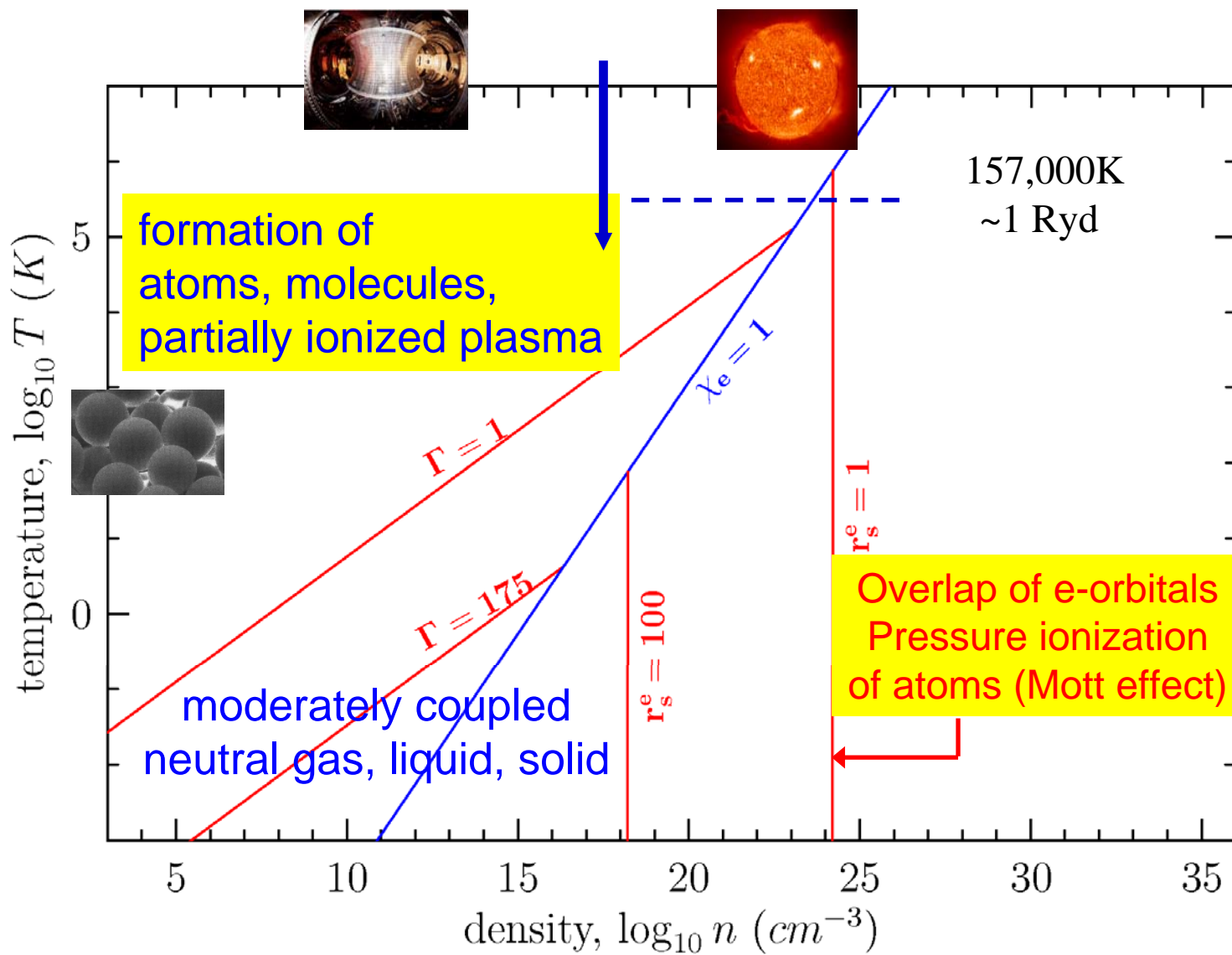
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- photoionization

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# Partially ionized 2-comp. plasma



# Ultra-dense fully ionized two-component plasma

$$\chi_a = n_a \Lambda_a^3$$

$$\sim \frac{n_a}{m_a^{3/2}}$$

$$r_{sa} = \bar{r}_a / a_{Ba}$$

$$\sim \bar{r}_a m_a Z_a^2$$

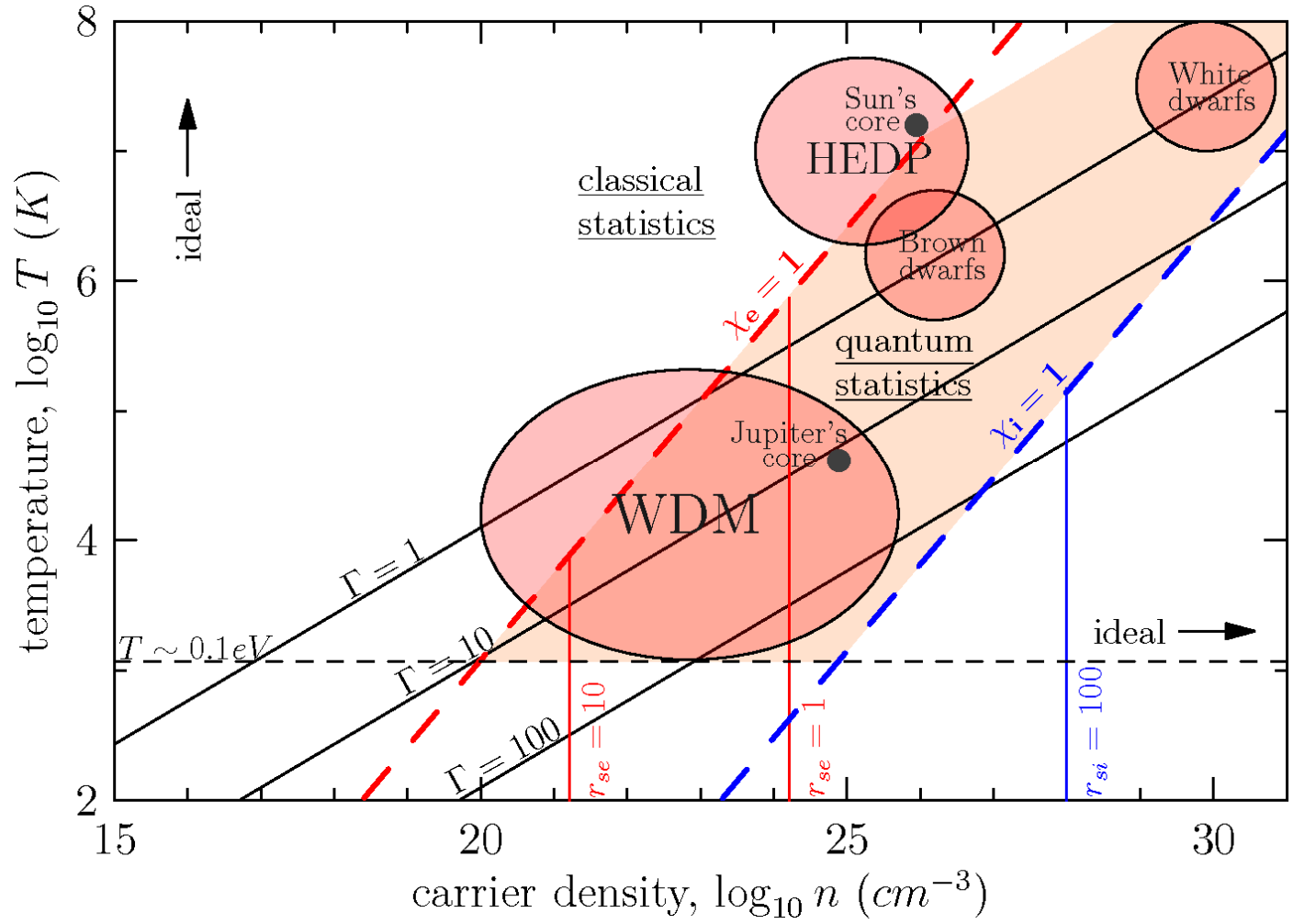
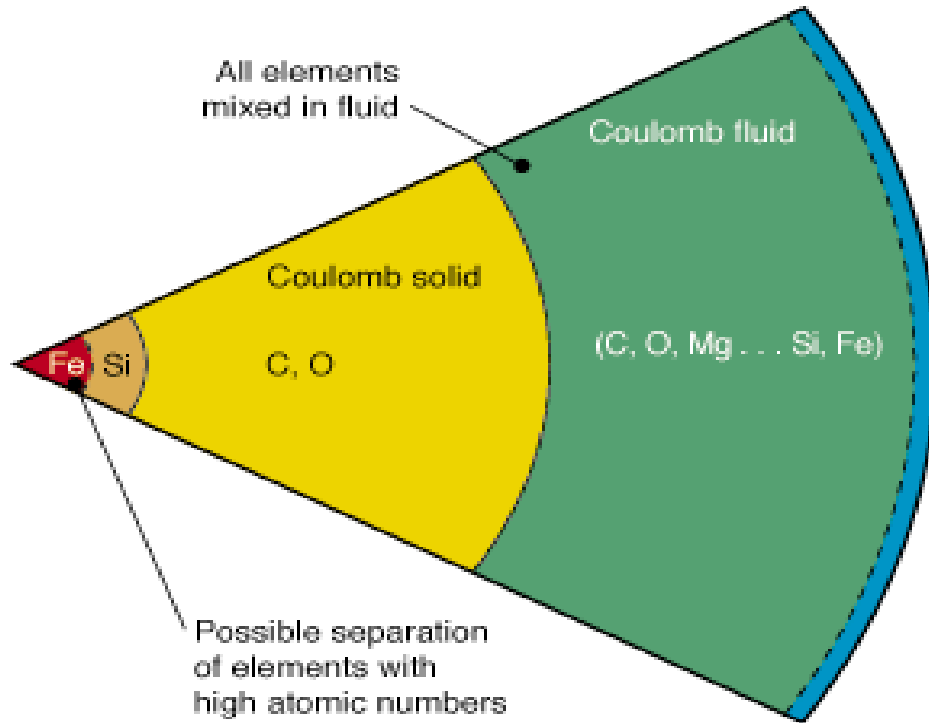


figure:  
Hydrogen

**WDM:** „warm dense matter“, **HEDP:** high energy density plasmas

# 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

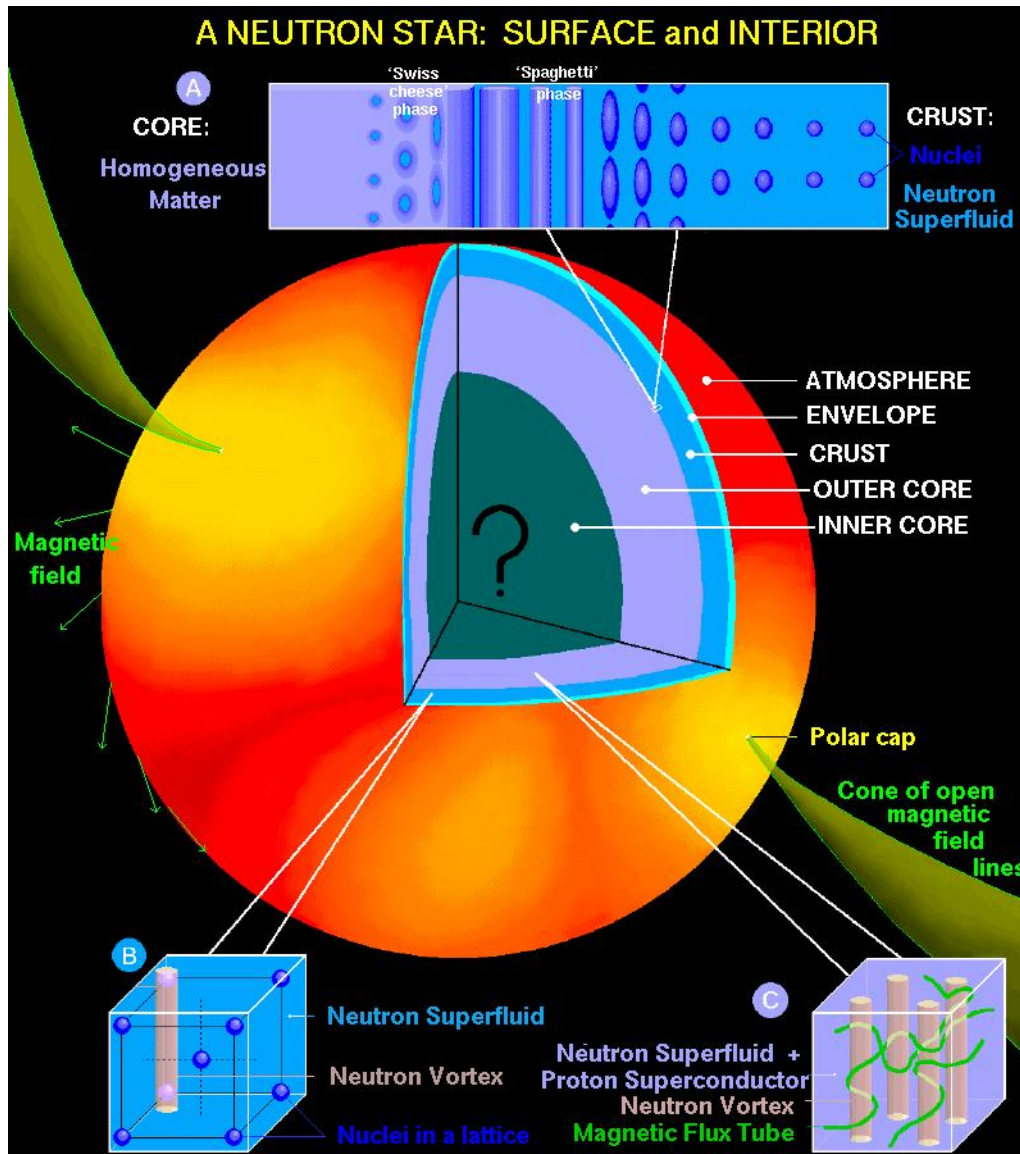
Size ~ our Earth  
Mass ~ our Sun  
→ density:

$$\rho \cong 10^6 \rho_{ERDE}$$

- classical fluid and crystal (**carbon, oxygen nuclei**) in „quantum sea“ of **nearly ideal electrons**
- Many observations



# Neutron star



Crust: crystal and quantum fluid of Fe-nuclei

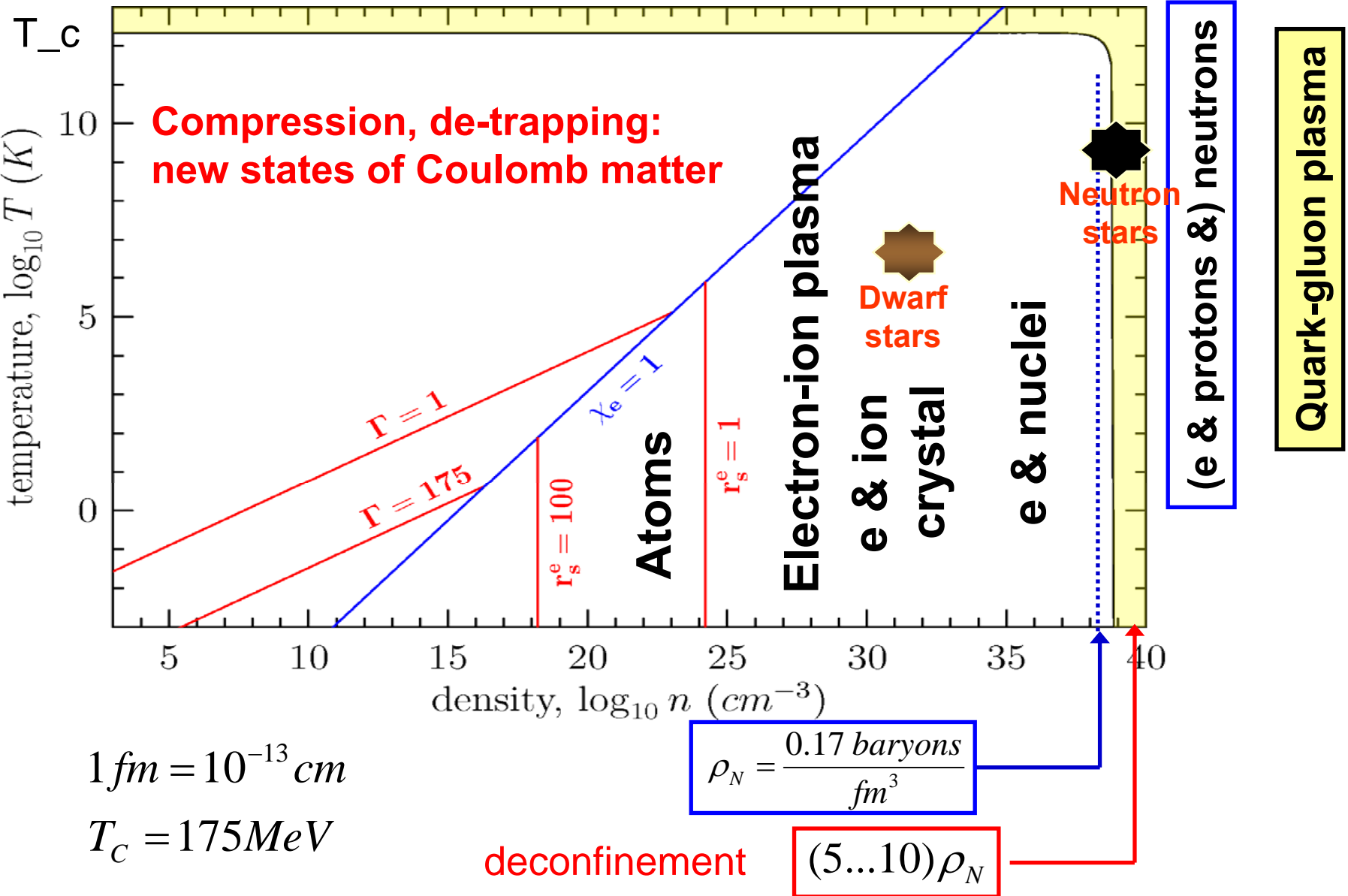
in „quantum sea“ of electrons

Radius ~ 10km  
Mass ~ our Sun

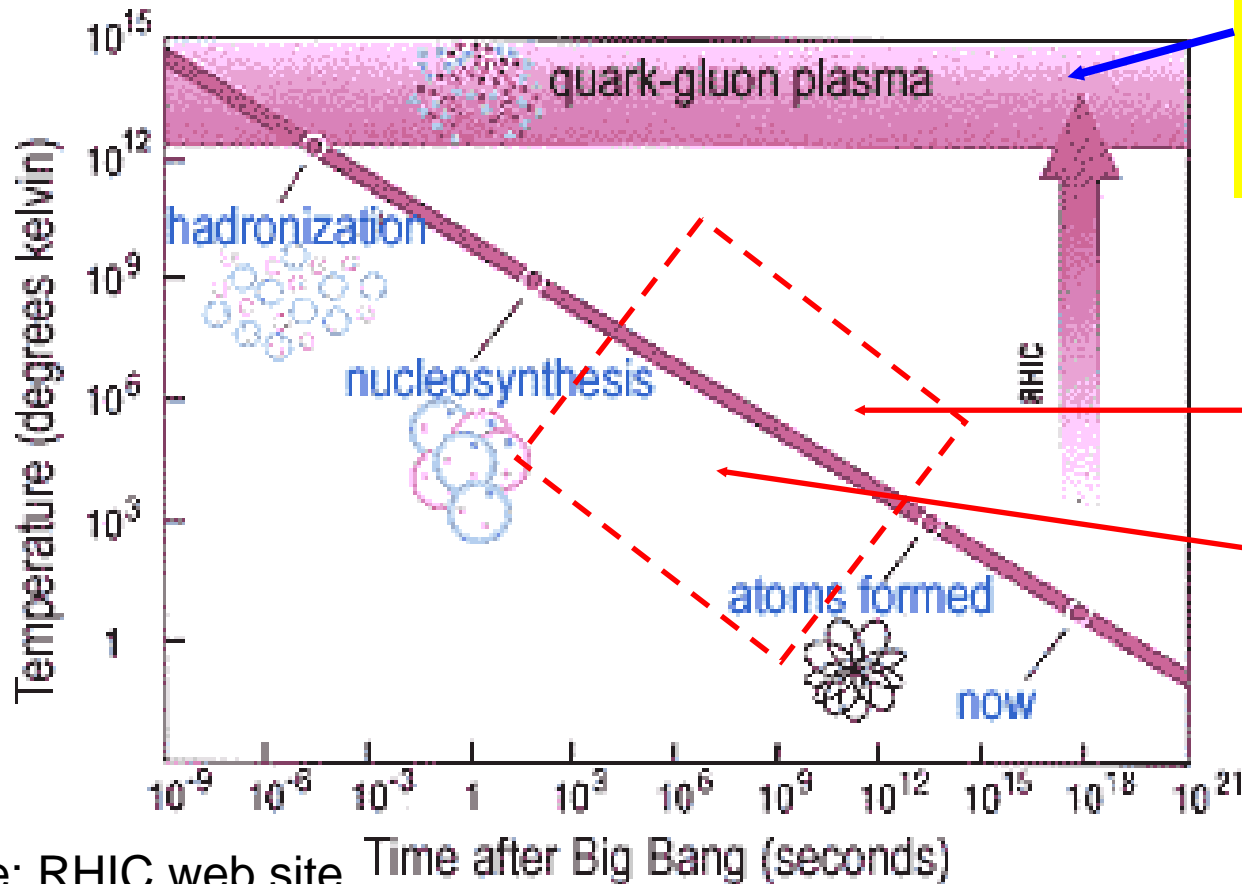
$$\rho \cong 10^{15} \text{ g cm}^{-3}$$

Source: Coleman, UMD

# From atomic nuclei to quarks



# Big bang: trapping of charged matter



**Plasma** with color  
Coulomb interaction,  
moderately coupled\*

**partially ionized  
plasma,  
ion recombination**

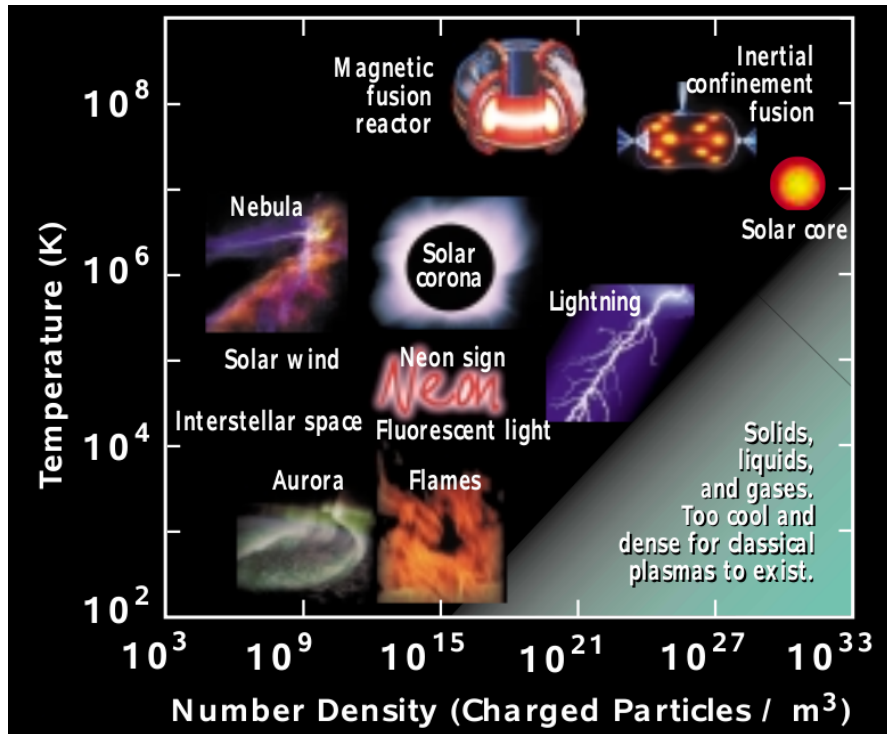
**liquid or crystal  
of nuclei, ions**

Source: RHIC web site

**Quark-gluon plasma** realized at: Relativistic Heavy ion collider, Brookhaven  
Large Hadron collider, CERN

\*V. Filinov, MB, Y.B. Ivanov, P.R. Levashov, and V.E. Fortov,  
*Contrib. Plasma Phys.* **49**, 536 (2009) and **51**, 322 (2011); *Phys. Particles and Nuclei Lett.* (2011)

# Summary 1: „white corner“



## Dense Coulomb systems

- Universal plasma properties (scaling from one plasma to another)
- Exciting forms of matter
- Fundamental questions: Early universe, dense astrophysical objects

Realization in laboratory experiments?

Technological applications?

**Theoretical plasma physics concepts?**



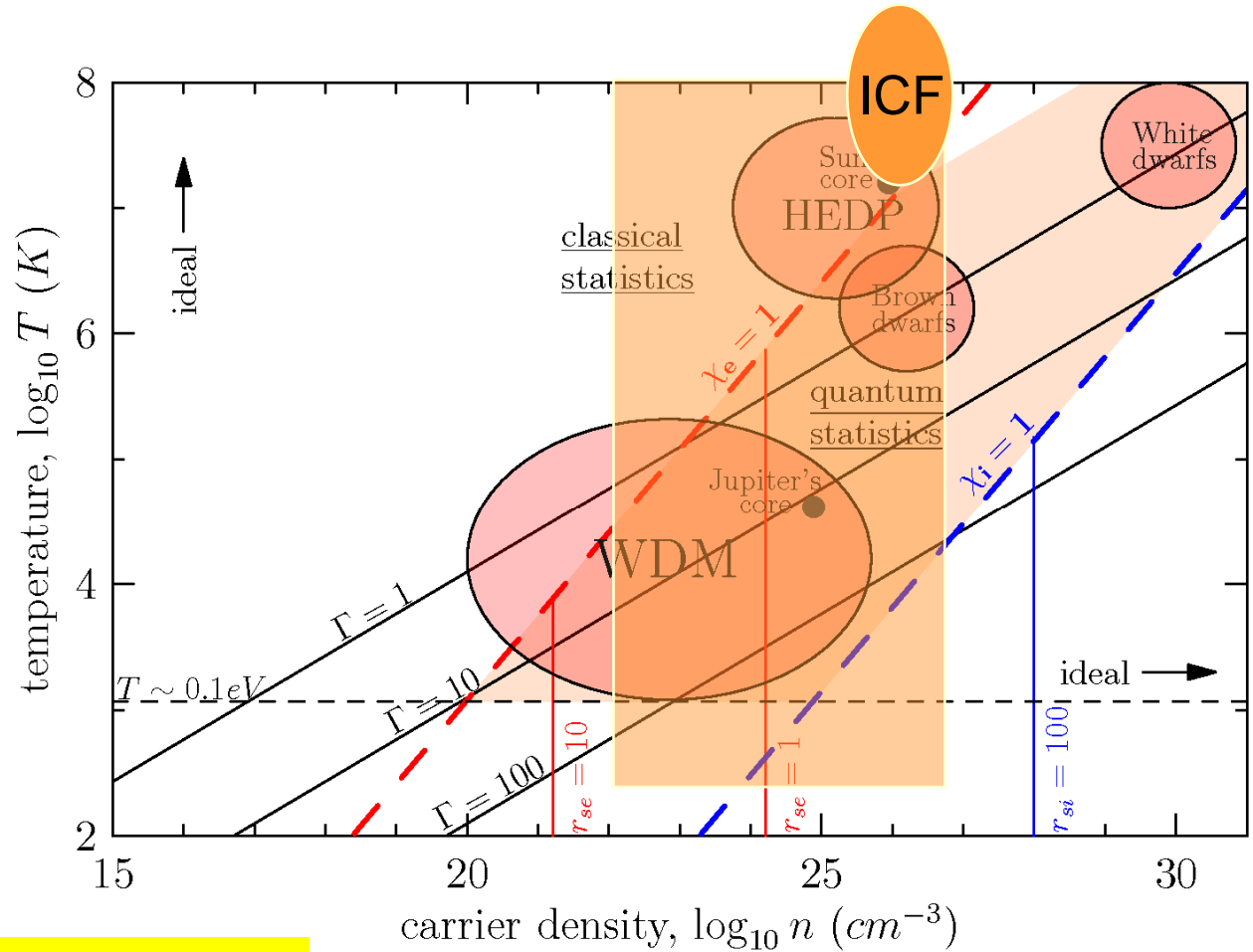
# Dense plasmas in the laboratory

Shock compression  
Z-pinch

**Lasers:** Omega,  
Vulcan, Jupiter...  
NIF (LLNL)  
ELI (Europe)

...

**Ion beams:**  
(NDCX\_II, FAIR...)



**Tremendeous progress  
in the next 10 years!**

**ICF:** Inertial confinement fusion

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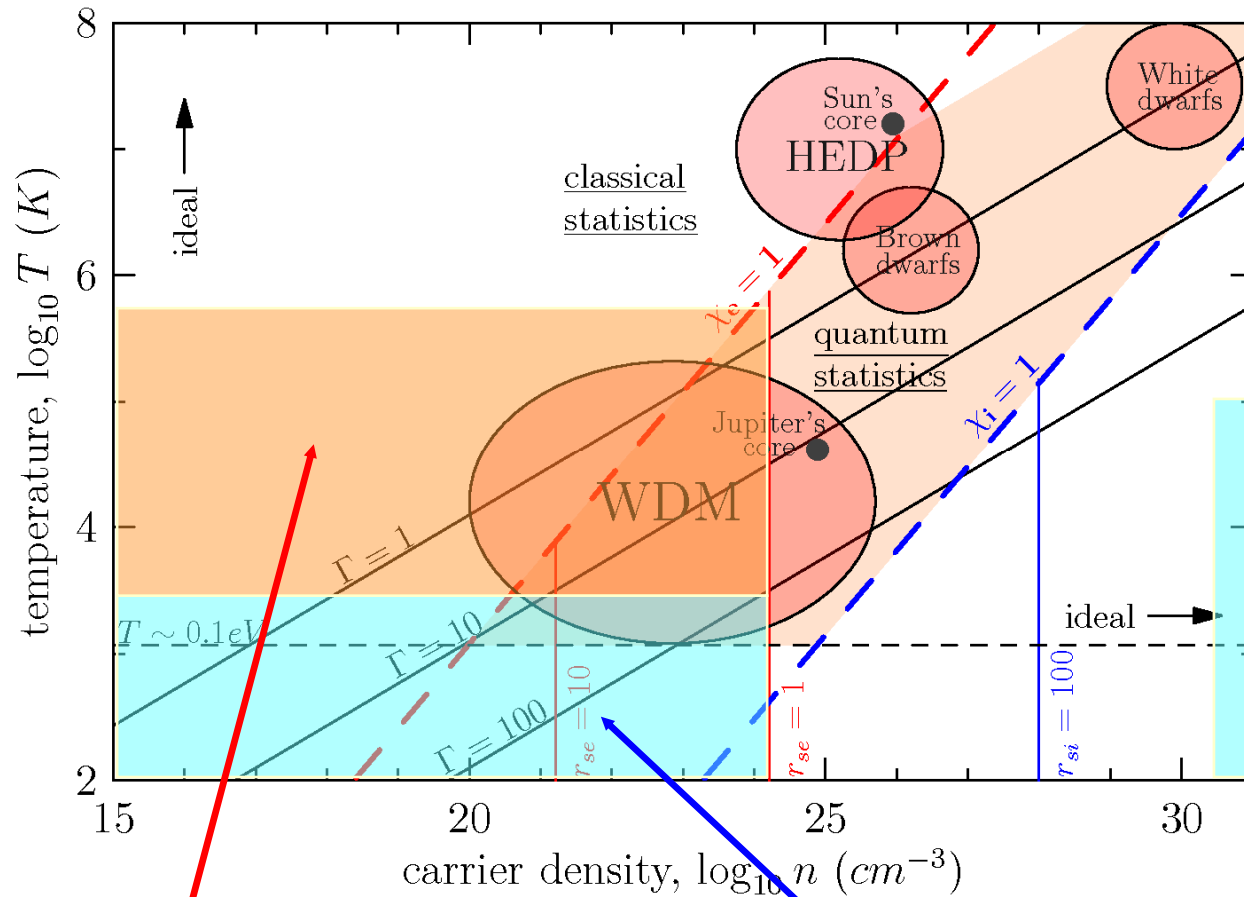
- 1.1 One-component plasma (OCP) in TD equilibrium
- 1.2 Two-component plasma: partial ionization, compact stars, dense laboratory plasmas

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- 2.1 First-principle equilibrium simulations
- 2.2 Dense plasmas in nonequilibrium:
  - laser plasmas
  - photoionization

## 3. Outlook: Multiscale simulations of dense plasmas

# Theoretical concepts for dense plasmas



**Overlap of  
plasma physics  
with other disciplines**

**Nuclear physics,  
High-energy physics**

## Atomic physics

- atoms, molecules
- ionization/recombination

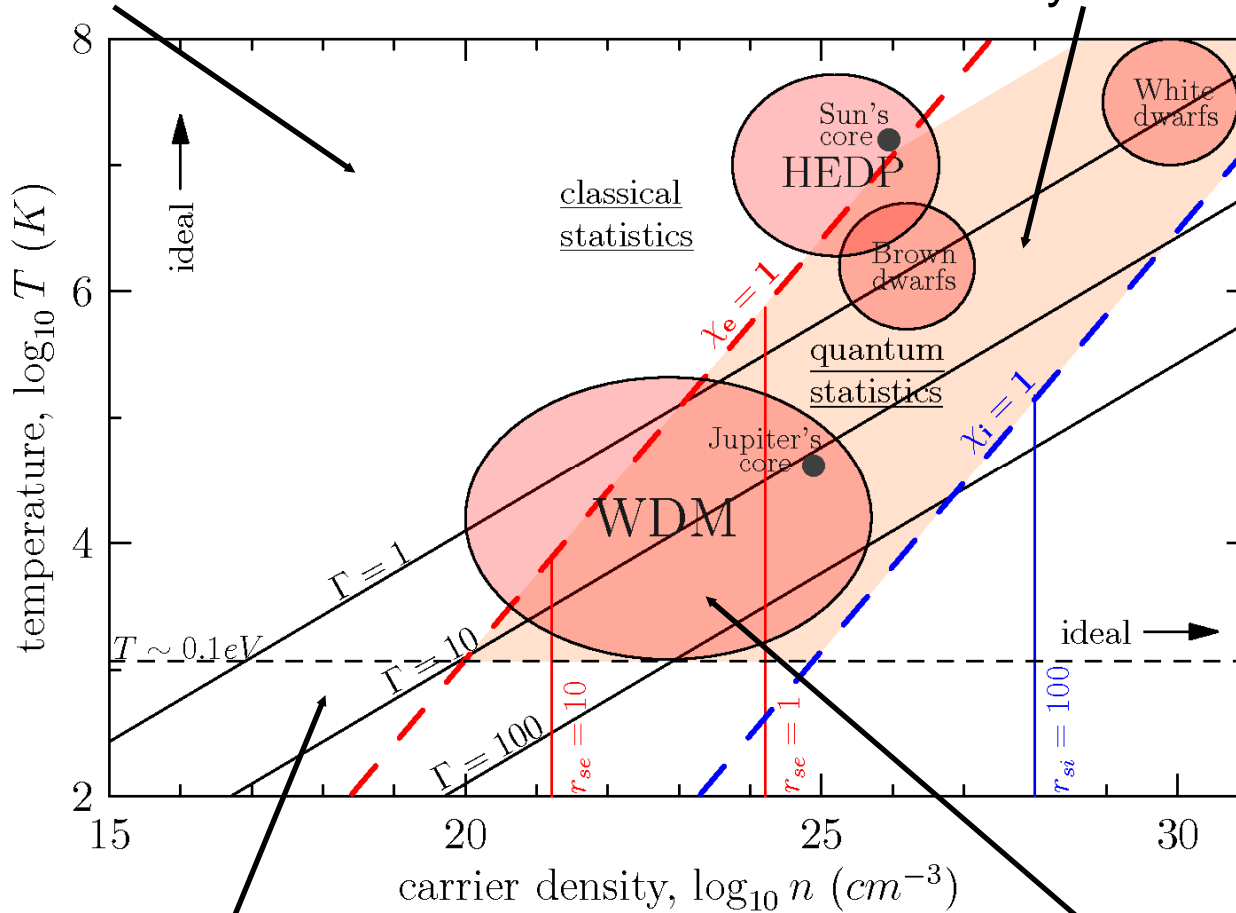
## Solid state physics

- molecular/atomic crystal
- targets for laser ionization

# Regimes of equilibrium plasmas

I. weakly nonideal plasma, perturbation theory

IV. strongly coupled classical ions, nearly ideal quantum electrons



Coupling grows with ion charge!

figure:  
Hydrogen

II. strongly coupled classical OCP

III. partially ionized plasma

# II. Strongly correlated classical OCP

1. **Spatially confined complex plasmas: plasma liquids, crystals („Yukawa balls“)**, close collaboration with experiments  
→ **first-principle MC and MD simulations:**
  - shell structure, metastable states
  - determination of effective pair interaction
  - plasma excitations, normal modes
  - melting behavior, crystallization dynamics
  - laser excitation and heating of plasma



Selected  
publications:

*Ludwig et al., PRE 71, 046403 (2005)*

*MB et al., PRL 96, 075001 (2006)*

*Block et al., Plasma Phys. Control. Fusion 49, B109 (2007)*

*Böning et al., PRL 100, 113401 (2008)*

*Henning et al. PRL 101, 045002 (2008)*

*Block et al., Phys. Plasmas 15, 040701 (2008)*

*Käding et al., Phys. Plasmas 15, 073710 (2008)*

*Baumgartner et al., New J. Phys. 10, 093019 (2008)*

*Kählert, MB, PRL 104, 015001 (2010)*

*MB et al., Rep. Prog. Phys. 73, 066501 (2010)*

# II. Strongly correlated classical OCP

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## 2. Spatially confined complex plasmas:

plasma liquids and crystals, „Yukawa balls“,

→ **Analytical theory**: benchmark tests with experiments and simulations

- statistical theory of metastable states
- average density profile (mean field plus LDA)
- shell structure (HNC plus bridge terms)
- collective excitations, normal modes

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Selected  
publications:

*Henning et al., PRE 74, 056403 (2006)*

*Henning et al., PRE 76, 036404 (2007)*

*Kählert et al., PRE 78, 036408 (2008)*

*Wrighton et al., PRE 80, 066405 (2009)*

*Kählert, MB., PRE 82, 036407 (2010)*

*Kählert, MB, PRE 83, 056401 (2011)*

# II. Strongly correlated classical OCP

## 3. Strongly coupled macroscopic 2D and 3D plasmas

→ **first-principle MD and Langevin simulations:**

- transport properties: diffusion, anomalous diffusion
- normal mode spectra, dynamic structure factor
- strongly coupled plasma in strong magnetic field
- transport, diffusion in strong B-field



**Basic understanding of correlations in classical equilibrium plasmas**

Selected  
publications:

*Ott et al., PRE 78, 026409 (2008)*

*Ott et al., PRL 103, 099501 (2009)*

*Ott, MB, PRL 103, 195001 (2009)*

*Ott, MB, Contrib. Plasma Phys. 49, 760 (2009)*

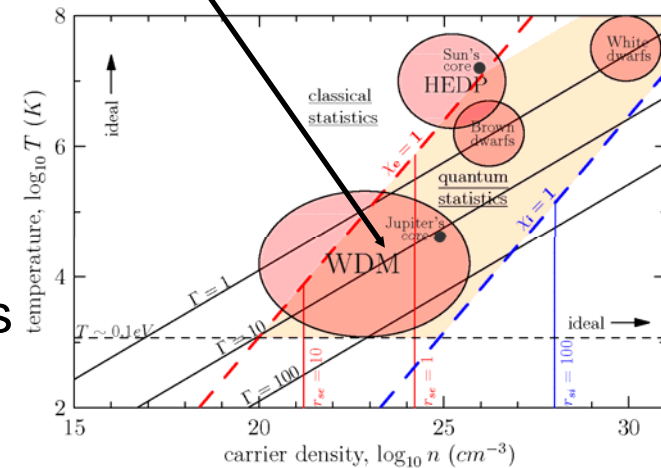
*MB et al., PRL 105, 055002 (2010)*

*Ott et al., PRE 83, 046503 (2011)*

*Ott et al., IEEE-TPS in press (2011)*

# III. Partially ionized dense plasma

- Examples:**
- laser plasmas
  - ion beam compressed plasmas
  - ionization of solid targets
  - plasmas containing highly charged ions



**First-principle path integral Monte Carlo simulations\*:** include

- strong Coulomb correlations
- quantum and spin effects of electrons
- Rigorous treatment of bound state formation  
(no artificial subdivision in free and bound particles)

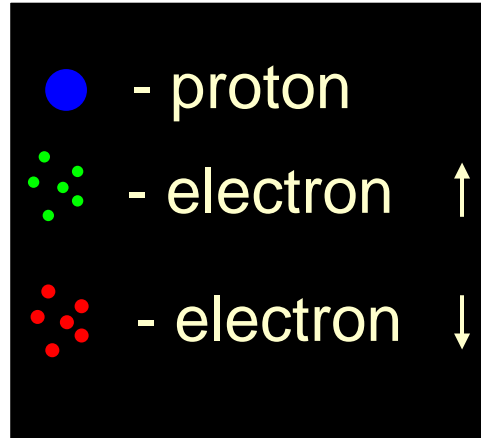
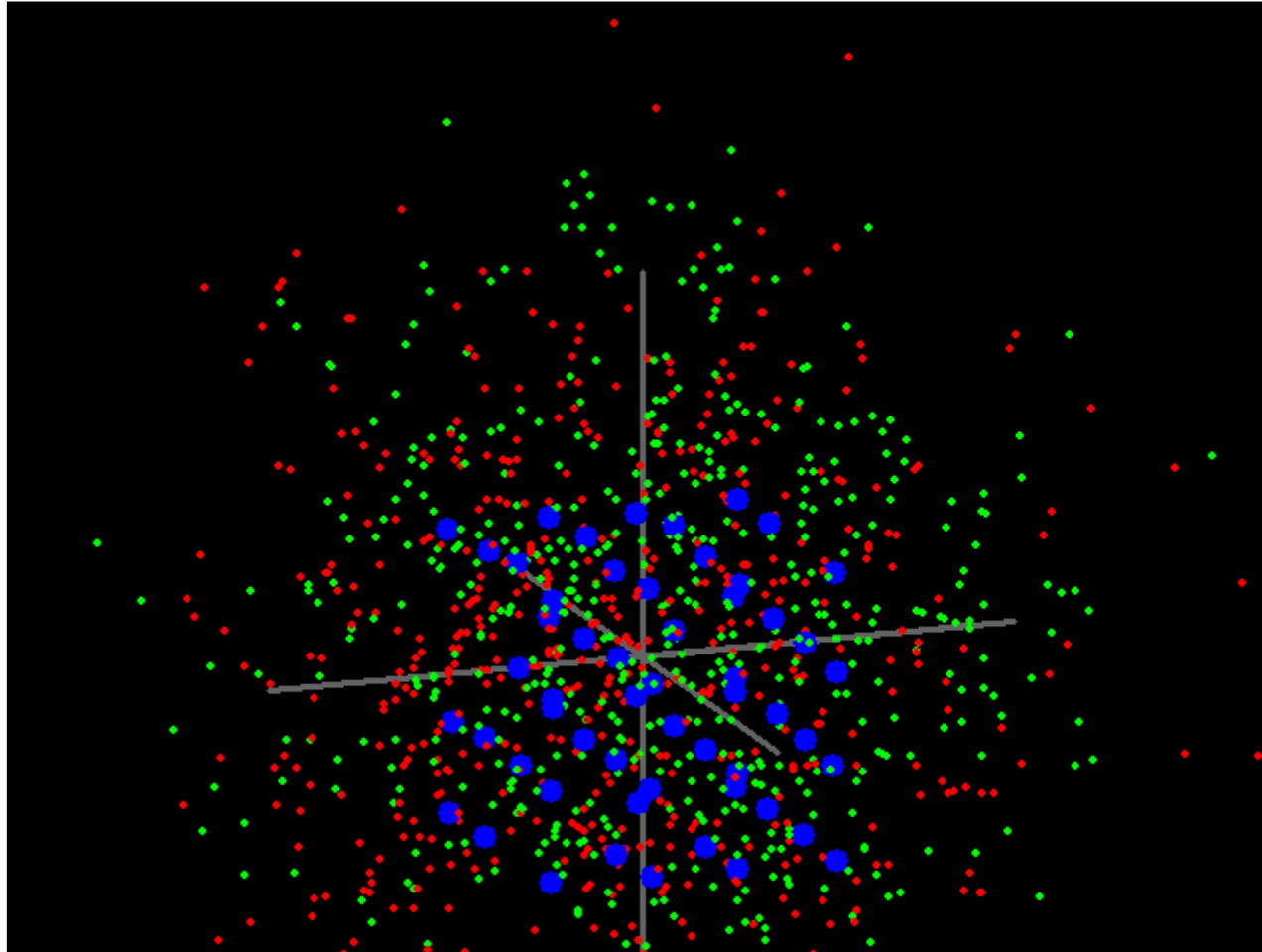


\*V. Filinov, MB, V. Fortov et al., *Plasma Phys. Control. Fusion* **43**, 743 (2001);  
*JETP Letters* **72**, 361 (2000), *JETP Letters* **74**, 384 (2001);  
MB, V. Filinov et al., *PRL* **95**, 235006 (2005), *JPA* **39**, 4717 (2006), *PRE* **75**, 036401 (2007)



# Proton crystallization in dense Hydrogen

$$T = 10,000 \text{ K}, n = 3 \cdot 10^{25} \text{ cm}^{-3}, \rho = 50.2 \text{ g/cm}^3$$



1<sup>st</sup>-principle  
Path integral  
Monte Carlo  
simulation

*Filinov, Bonitz, Fortov, JETP Letters 72, 245 (2000)*

# Quantum TCP Coulomb crystals

mass, charge and temperature asymmetry  $M = \frac{m_h}{m_e}$ ,  $Z = \frac{q_h}{q_e}$ ,  $\Theta = \frac{T_e}{T_h}$

## Analytical Results:

- Finite density range:

$$n^{Mott} \leq n_e \leq \left( \frac{M+1}{M^{cr}+1} \right)^3 n^{Mott}$$

- Critical mass ratio:

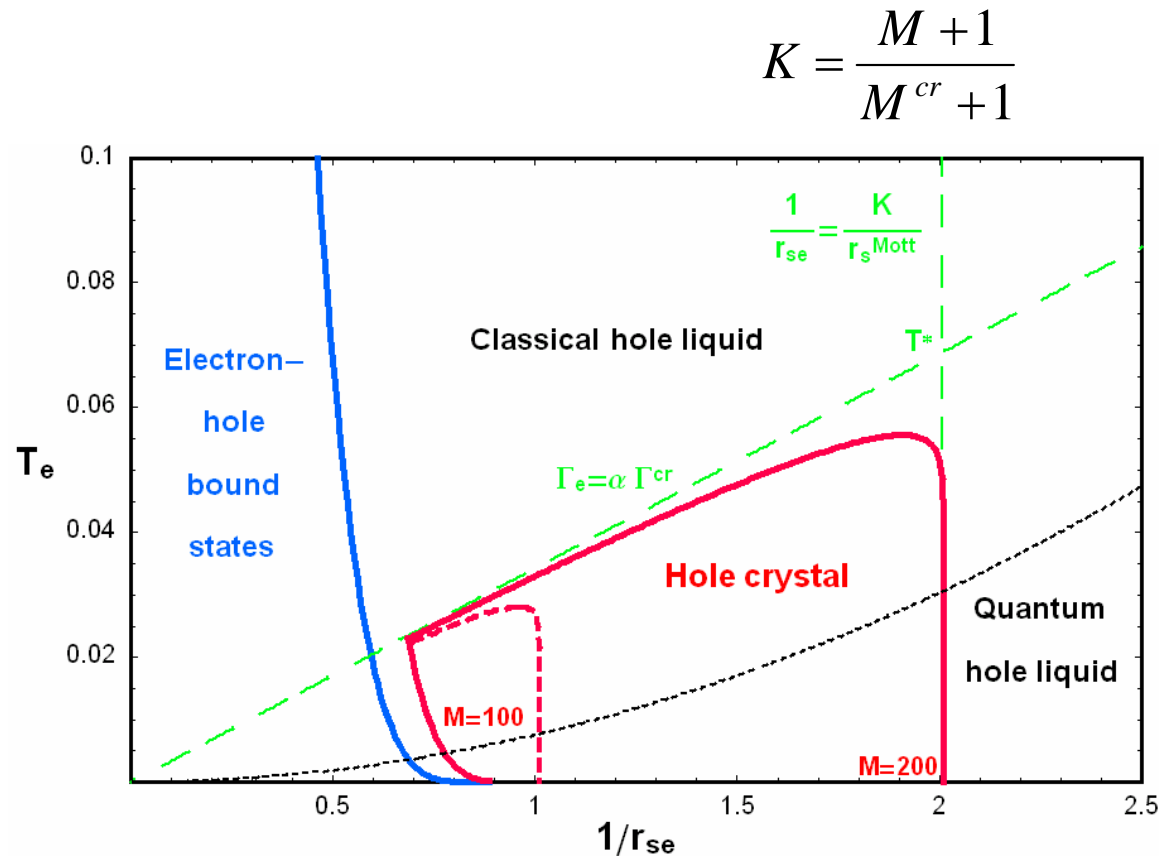
$$M \geq M^{cr}(T_e) = \frac{r_s^{cr}}{Z^{4/3} r_s^{Mott}(T_e)} - 1$$

- Maximum temperature:

$$\frac{k_B T_e}{E_B} = 4 \frac{Z^2 \Theta (M+1)}{\Gamma^{cr} r_s^{cr}}$$

# Phase diagram of ion (hole) crystal

$$T_e = \frac{3 kT}{2 E_R}$$



$$\alpha = \frac{1}{Z^2 \Theta}$$

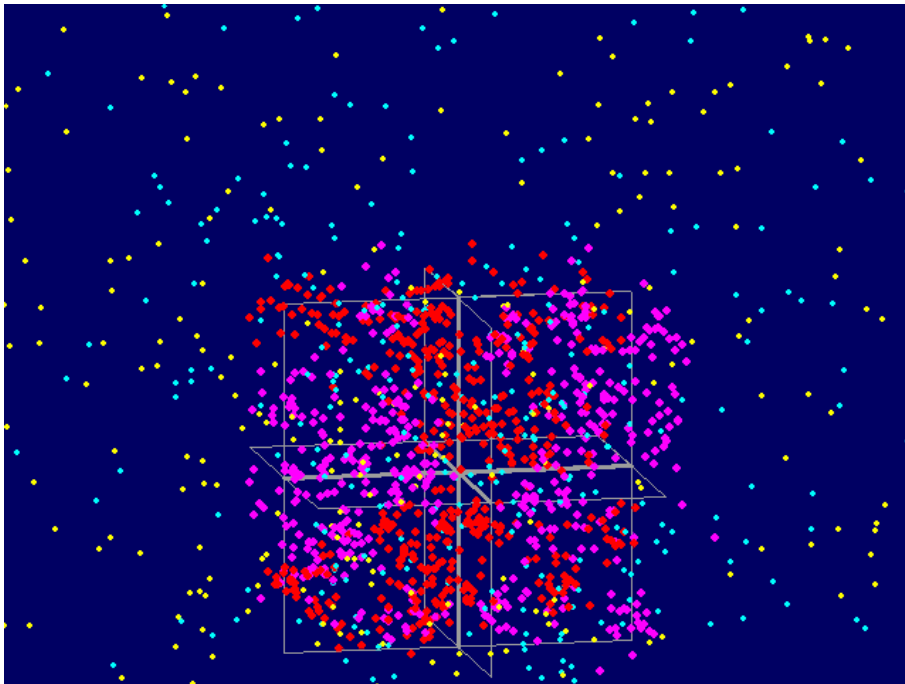
$$\frac{1}{r_{se}} = \frac{a_B}{\bar{r}_e} \propto n^{1/3}$$

- for  $Z=1$  (e.g. electron-hole plasma):  $M^{cr} = 83(3D), 60(2D)$

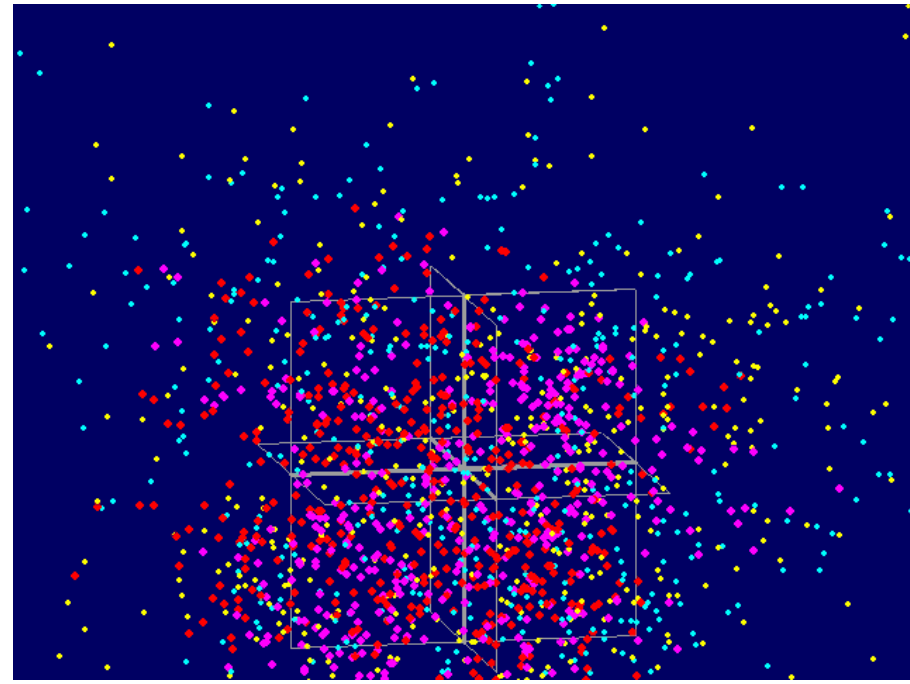
Bonitz, Filinov, Fortov, Levashov, and Fehske, *Phys. Rev. Lett.* **95**, 235006 (2005)

# Quantum melting of ion crystal

Reduce ion mass to  $M=25$  and  $M=5$   
to simulate density increase



**Ion liquid**



**Ion gas**

$$\chi = n\Lambda^3 \sim \frac{n}{m^{3/2}}$$

# TCP Coulomb crystals

	$n_{\min} [cm^{-3}]$	$n_{\max} [cm^{-3}]$	$T_{\max} [K]$
$C^{6+}$ Ions (white dwarfs)	$2 \cdot 10^{26}$	$3.6 \cdot 10^{33}$	$10^9$
Protons (hydrogen)	$5 \cdot 10^{24}$	$1.0 \cdot 10^{28}$	66,000

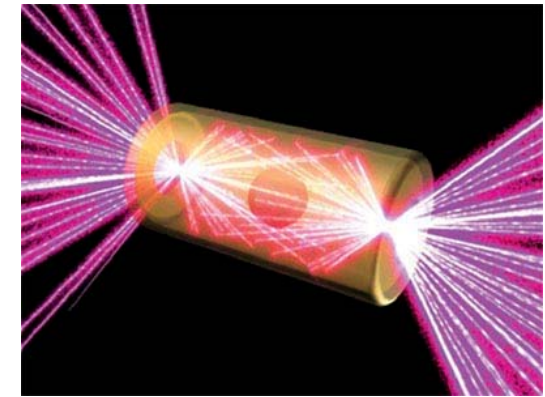
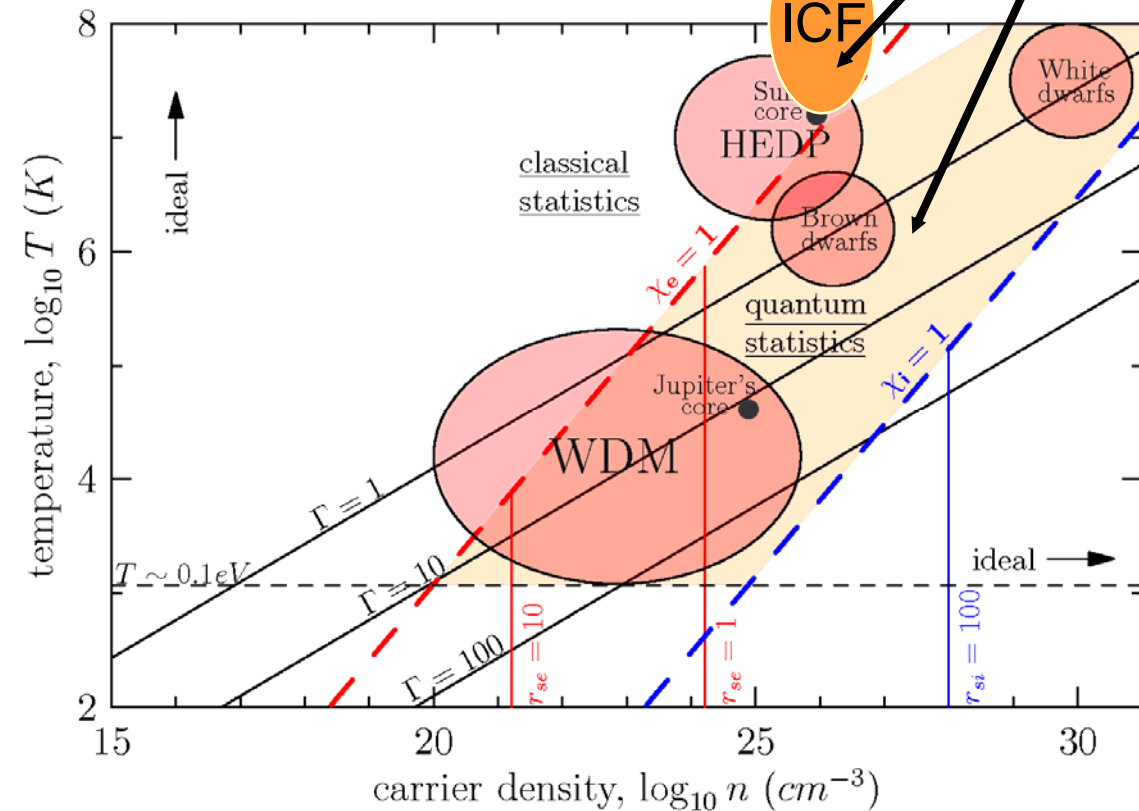
**Laser or ion beam compression experiments?**

Bonitz, Filinov, Fortov, Levashov, and Fehske, *Phys. Rev. Lett.* **95**, 235006 (2005)



# IV. Strongly correlated classical ions & weakly coupled quantum electrons

**Examples:** - laser compression  
- inertial confinement fusion (ICF):



Source: NIF web page, LLNL

$$\rho \propto 10^3 \text{ g cm}^{-3}, T = 10^3 \dots 10^5 \text{ eV}$$

# IV. Strongly correlated classical ions & weakly coupled quantum electrons

**Thermodynamics:** quantum Monte Carlo, quantum MD

**Dynamics, Transport** → 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

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

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)

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## 2. Theory of strongly correlated plasmas

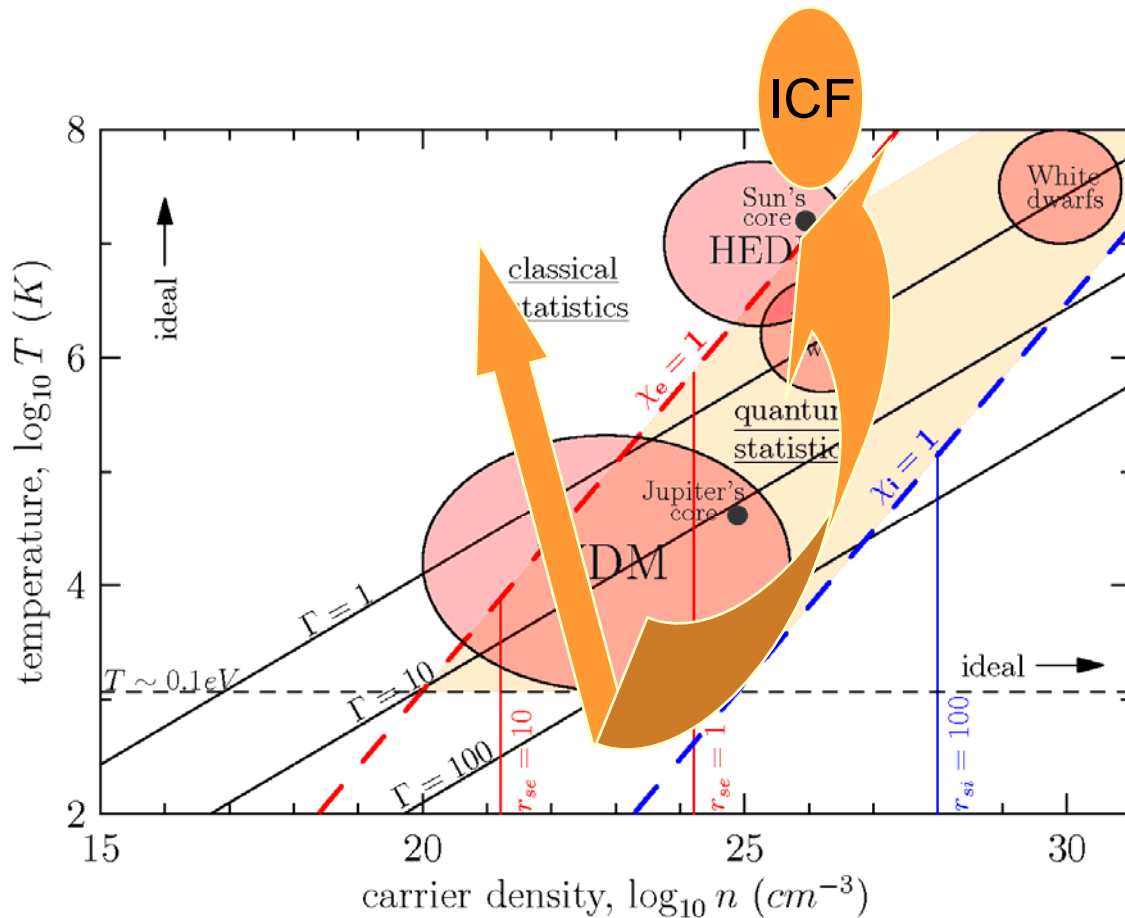
- 2.1 First-principle equilibrium simulations
- 2.2 Dense plasmas in nonequilibrium:
  - laser plasmas
  - photoionization

## 3. Outlook: Multiscale simulations of dense plasmas



# Dense plasmas in nonequilibrium

- Examples:**
1. interaction of strong laser pulse with plasma
  2. ionization of atoms, solid targets



excitation out of equilibrium and relaxation  
→ kinetic theory

# Dense plasmas in nonequilibrium

## Challenge:

1. thermalization requires collisions (beyond mean field, PIC)
2. collisions are modified by strong field
3. collisions have finite duration, comparable with pulse width, period  
→ nonlinear effects, photon absorption, harmonics generation
4. have to treat free and bound electrons (atoms), ionization
5. need to include quantum and spin effects of electrons, atoms

→ Requires to go beyond standard Boltzmann-type equations  
→ Development of generalized quantum kinetic theory:

- *M. Bonitz, „Quantum Kinetic Theory“, Teubner, Stuttgart, Leipzig (1998)*
- extension to gauge-invariant theory of field-matter interaction:  
*D. Kremp T. Bornath, MB, and M. Schlages, Phys. Rev. E **60**, 4725 (1999)*  
*H. Haberland, MB, and D. Kremp, Phys. Rev. E **64**, 026405 (2001)*

# Quantum kinetic theory\*

Electromagnetic field:  $\mathbf{A}(\mathbf{r}, t), \phi(\mathbf{r}, t)$ , external sources:  $\mathbf{A}^{\text{ext}}(t), \phi^{\text{ext}}(\mathbf{r})$

Maxwell's equations, classical field

Charged particles:  $\psi_a, \psi_a^\dagger$ , non-relativistic fermion fields

$a$  - carrier species (or energy band)

$$g_a^>(1, 1') = \frac{1}{i\hbar} \langle \psi_a(1) \psi_a^\dagger(1') \rangle, \quad g_a^<(1, 1') = -\frac{1}{i\hbar} \langle \psi_a^\dagger(1') \psi_a(1) \rangle$$

Carrier interaction: Mean field effects, exchange  $\rightarrow \Sigma_a^{\text{HF}}$

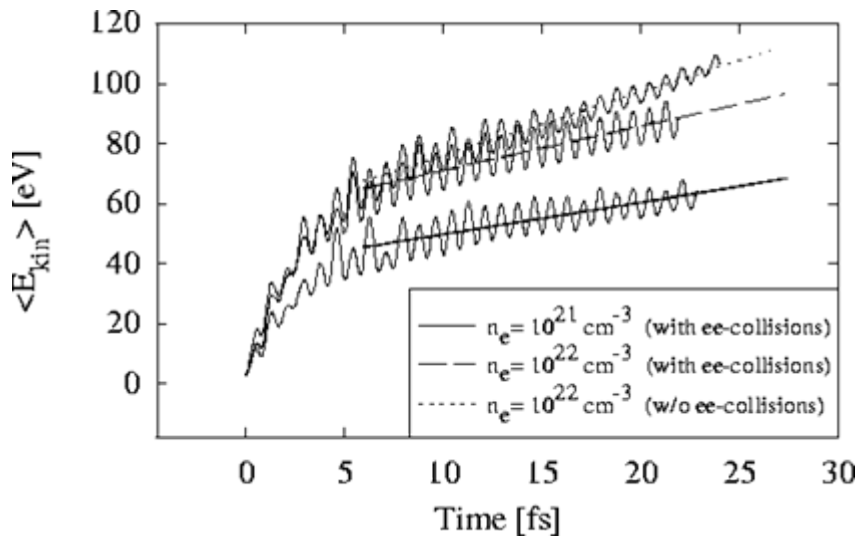
Correlations/Scattering  $\rightarrow \Sigma_a^{\cong}$

$$\left[ i\hbar \frac{\partial}{\partial t_1} - \frac{1}{2m_a} \left( \frac{\hbar}{i} \nabla_1 - \frac{e_a}{c} \mathbf{A}(1) \right)^2 - e_a \phi(1) \right] g_a^{\cong}(1, 1') - \int d\bar{\mathbf{r}}_1 \Sigma_a^{\text{HF}}(1, \bar{\mathbf{r}}_1 t_1) g_a^{\cong}(\bar{\mathbf{r}}_1 t_1, 1')$$
$$= \int_{t_0}^{t_1} d\bar{1} [\Sigma_a^>(1, \bar{1}) - \Sigma_a^<(1, \bar{1})] g_a^{\cong}(\bar{1}, 1') - \int_{t_0}^{t_1'} d\bar{1} \Sigma_a^{\cong}(1, \bar{1}) [g_a^>(\bar{1}, 1') - g_a^<(\bar{1}, 1')]$$

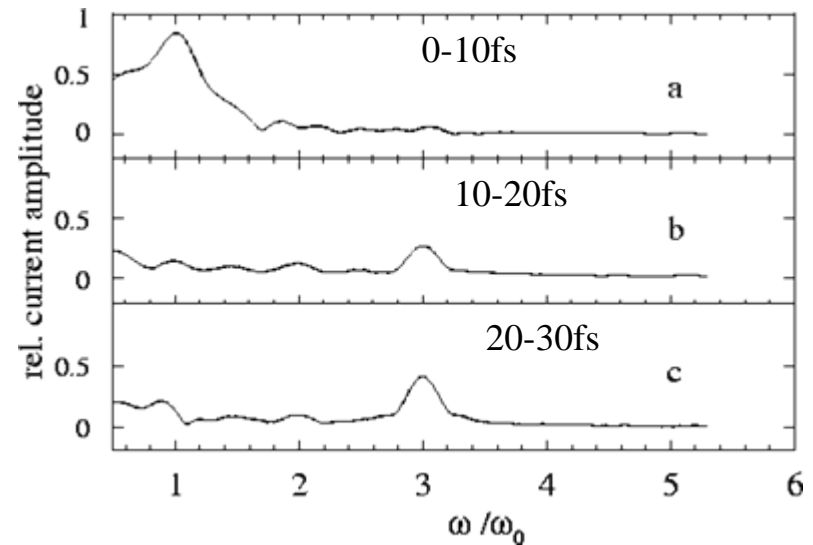
- M. Bonitz, „Quantum Kinetic Theory“, Teubner 1998
- „Introduction to Computational Methods for Many-Body Physics“, MB and D. Semkat (eds.), Rinton 2006
- N.H. Kwong, and MB, Phys. Rev. Lett. **84**, 1768 (2000)

# Collisional heating of laser plasmas

Plasma heating due to e-i collisions in strong field (inverse bremsstrahlung)



Nonlinear current spectrum: femtosecond time resolution



Fully ionized hydrogen plasma, monochromatic laser pulse  $I = 10^{14} \text{ Wcm}^{-2}$

Also developed: quantum kinetic theory for partially ionized plasma\*

H. Haberland, MB, and D. Kremp, *Phys. Rev. E* **64**, 026405 (2001)

\*Semkat et al., *J. Phys. Conf. Ser.* 2005 and 2006



# Dynamics of strong field ionization

- Examples:**
- interaction of strong uv...x-ray pulse with atoms, molecules:  
e.g. laser harmonics or FEL radiation\*
  - inner shell ionization, „hollow atoms“, Auger processes
  - many-electron dynamics on (sub-)femtosecond scale

## Theoretical approaches:

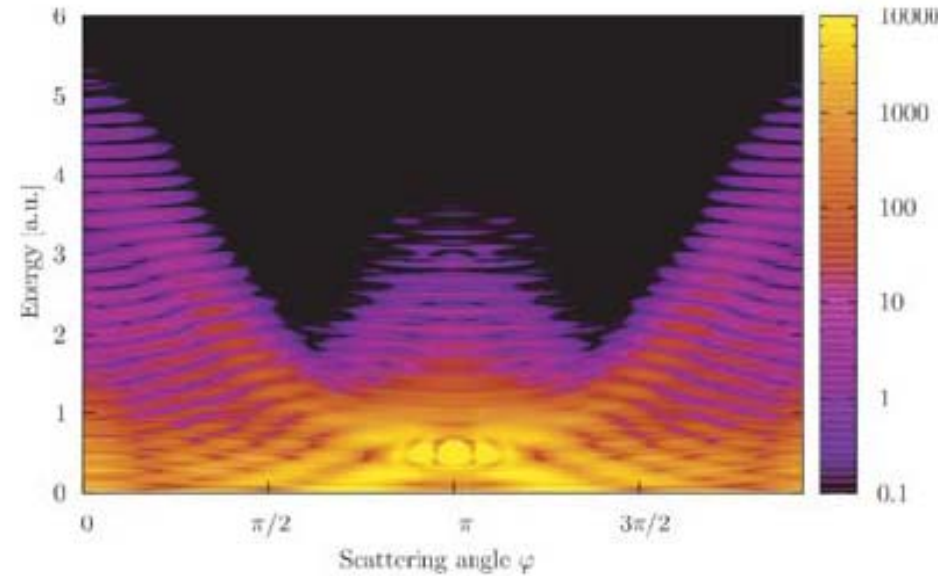
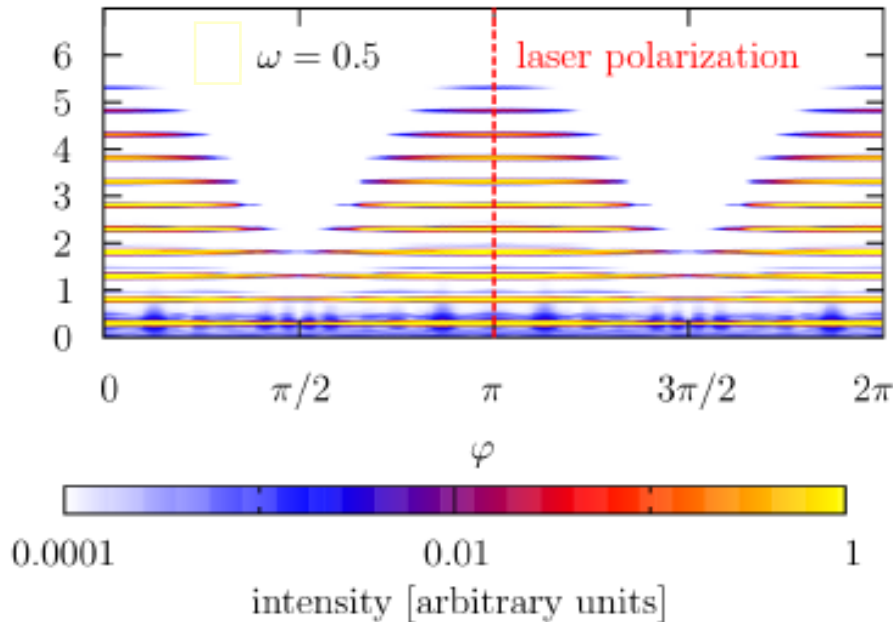
- 1.) time-dependent Schrödinger equation (TDSE, TDCI)
- 2.) time-dependent Hartree-Fock (TDHF)
- 3.) nonequilibrium Green's functions (NEGF), quantum kinetic theory
- 4.) Multiconfiguration time-dependent Hartree-Fock (MCTDHF)

- Problems:**
- 1. and 4.: exponential scaling with electron number
  - 2. pure mean field, no e-e correlations
  - 3. includes correlations, but memory-expensive
- required: combinations of methods, hybrid approaches

\*Collaboration with M. Drescher (DESY), BMBF-Verbund „Flash“

# Matter in strong UV field: solution of TDSE

1. **Photoionization**, energy spectrum in strong field,  $\omega=0.5$ ,  $E_0=0.1$
3. **Electron spectrum: e-i scattering** in strong field,  $\omega=0.2$ ,  $E_0=0.2$ ,  $k_0=1$



atomic units

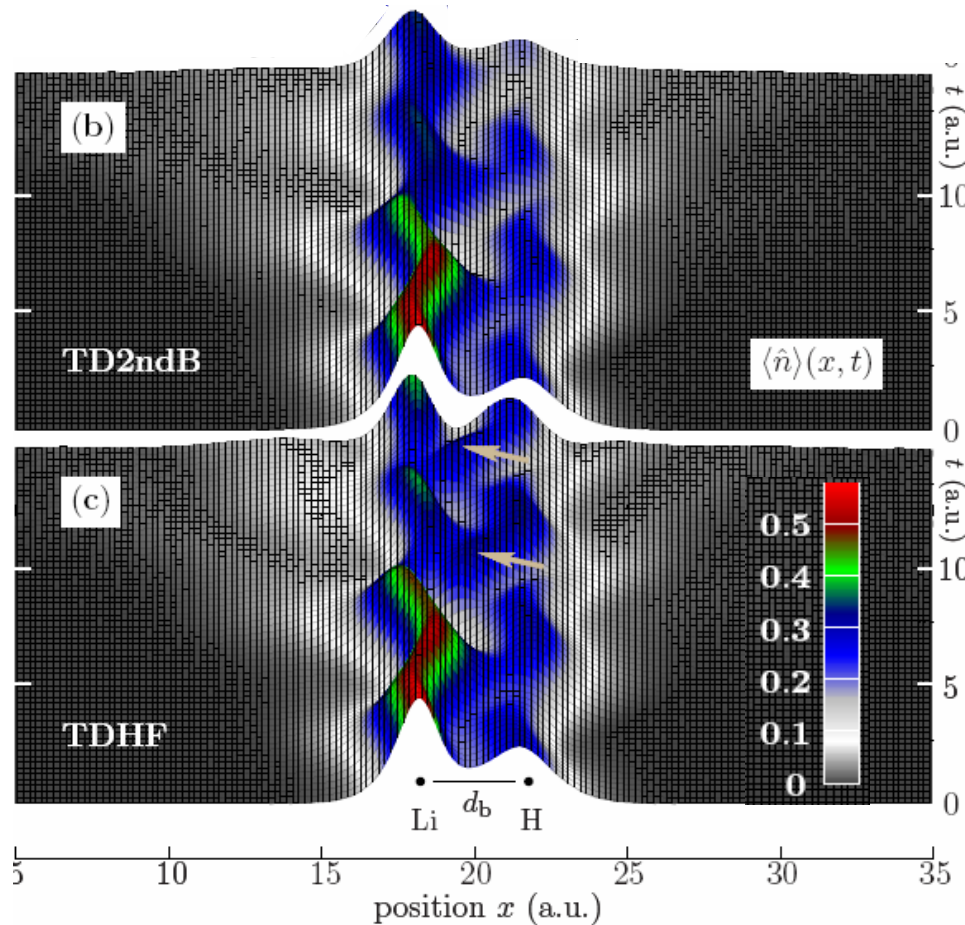
2. t-resolved **photoemission of solids**\* **Angle and energy resolved spectrum**

S. Bauch, and MB, *Phys. Rev. A* **78**, 043403 (2008); *Contrib. Plasma Phys.* **49**, 558 (2009)

S. Bauch et al., *Europ. Phys. Lett.* **91**, 53001 (2010)

\* E. Krasovskii, and MB, *Phys. Rev. Lett.* **99**, 247601 (2007); *Phys. Rev. A* **80**, 053421 (2009)

# Atoms and molecules in strong field



Attosecond dynamics of electron density (excitation, ionization)

4-electron molecule LiH  
Short-pulse laser excitation

NEGF (b, with e-e correlations) vs. TDHF (c, no correlations)

Inhomogeneous system treated via FEDVR basis. 1d model

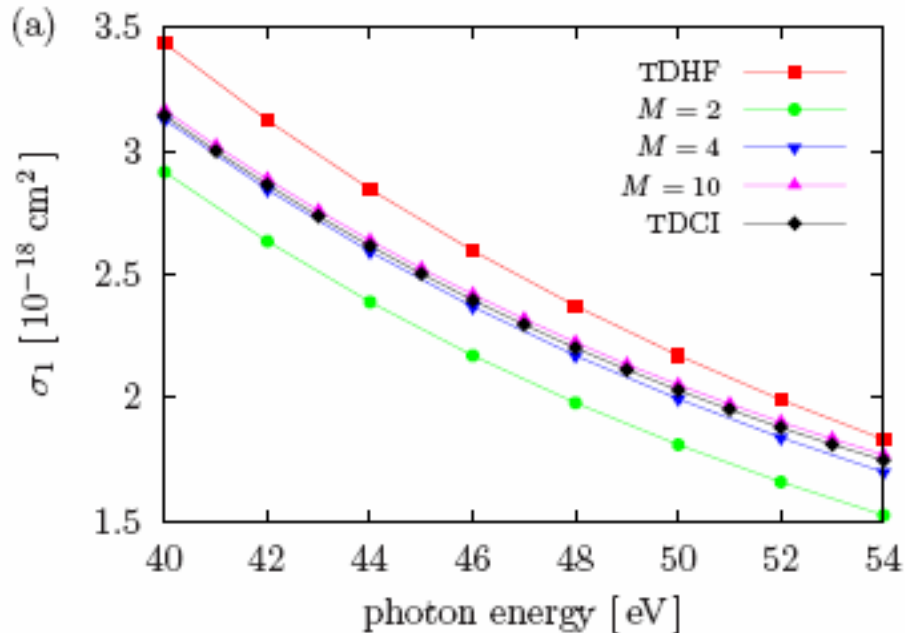
*M. Bonitz et al., Contrib. Plasma Phys. 50, 54(2010)*

*K. Balzer, S. Bauch, and MB, PRA 81, 022510 (2010)*

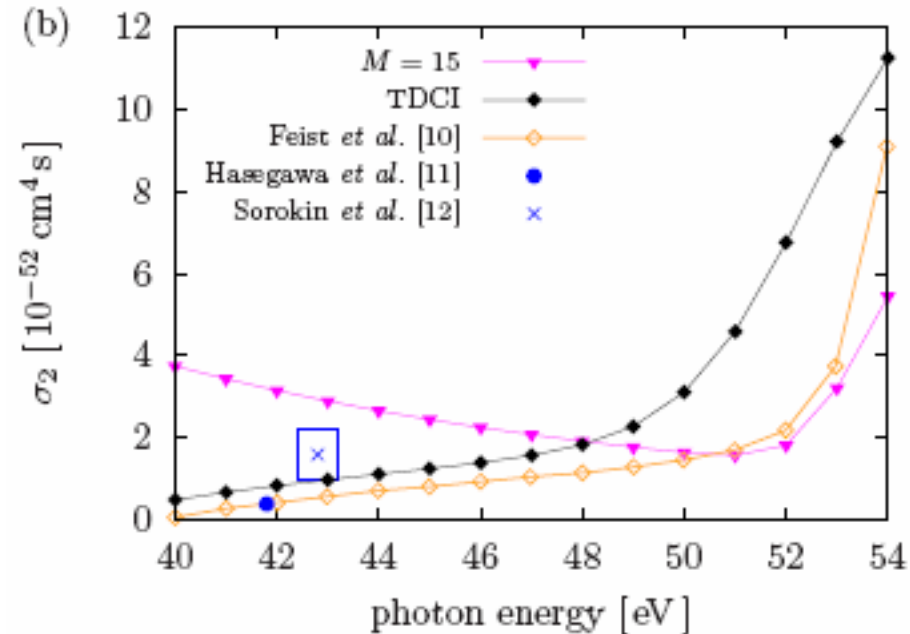
*K. Balzer, S. Bauch, and MB, PRA 82, 033427 (2010)*

# Two-photon ionization cross sections

Single ionization cross section



Double ionization cross section



**MCTDHF full 3D Helium**, radial FEDVR basis,  
different  $M$ , vs. exact results (**TDCI**) and experiments (symbols)

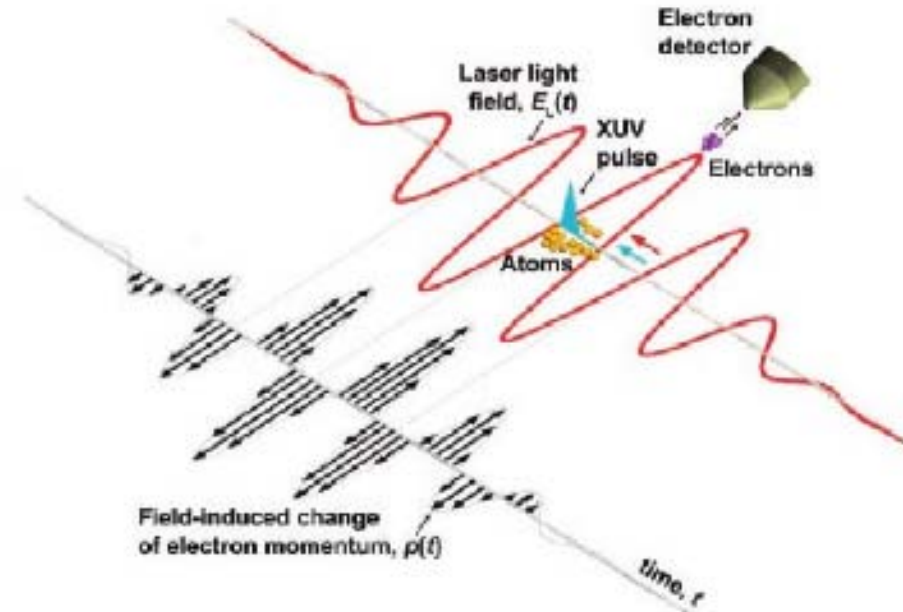
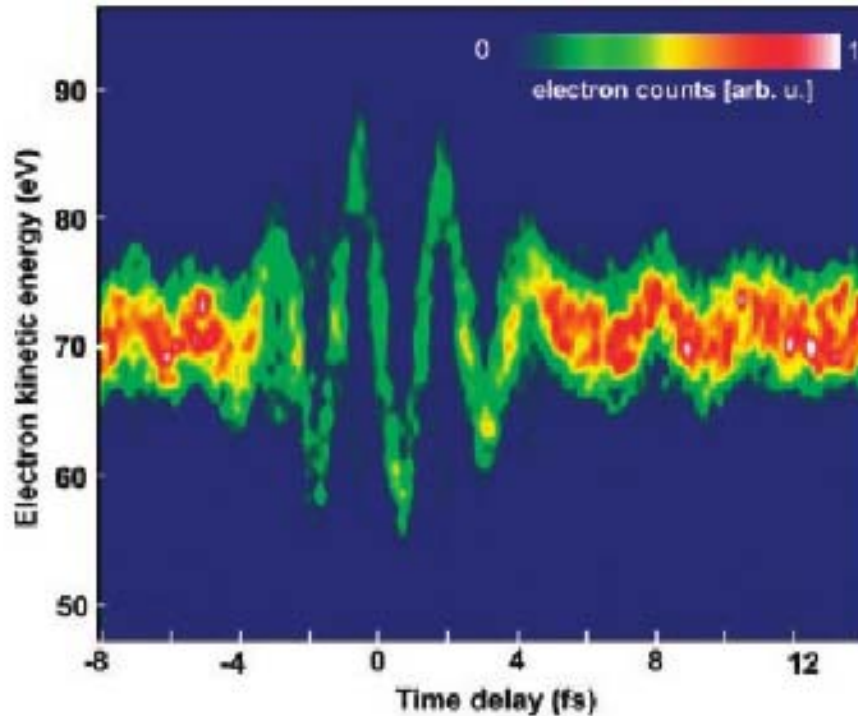
$$I = 10^{13} \text{Wcm}^{-2}$$

*D. Hochstuhl, and MB, J. Chem. Phys. 134, 084106 (2011)*



# Simulation of as-streaking experiments

Goal: angle, energy and **time**-resolved spectrum

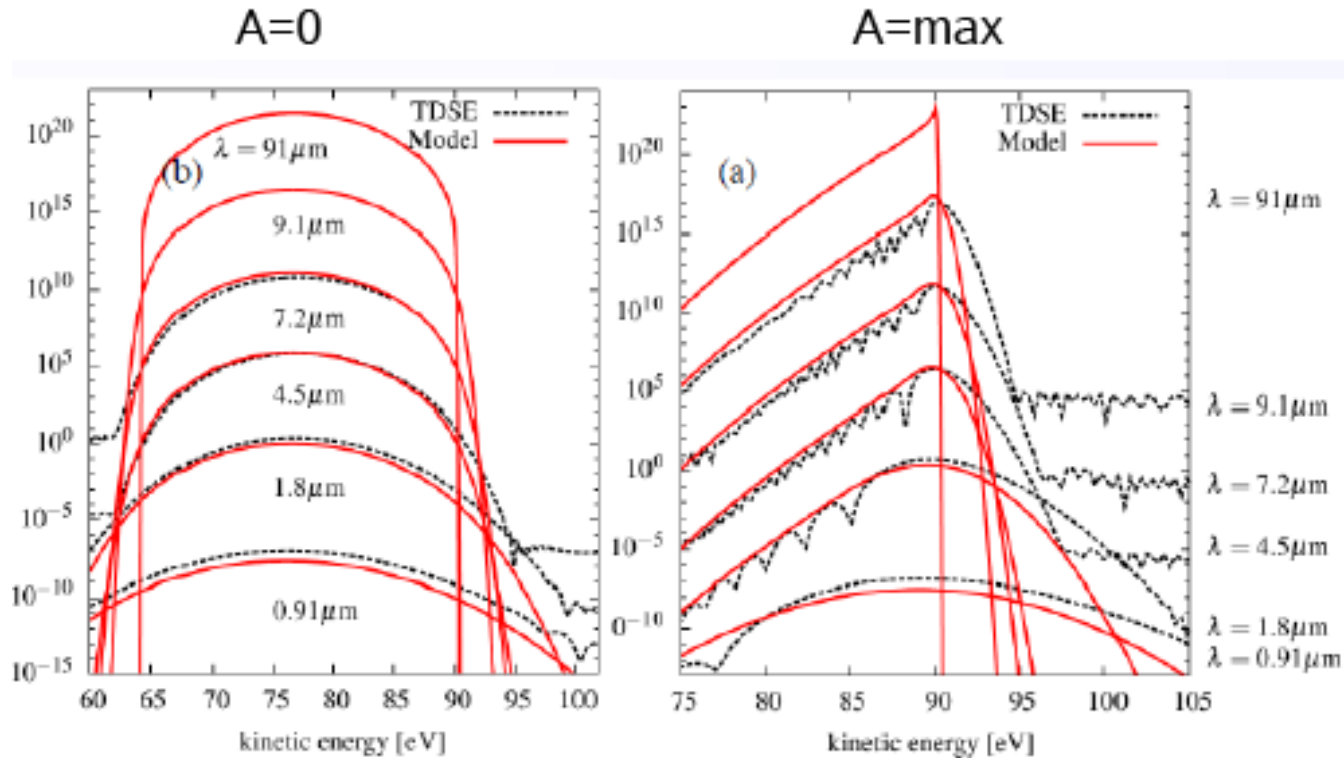


xuv/ir pump-probe measurement

Goulielmakis et al., Science **305**, 1267 (2004)

# Simulation of THz-streak camera\*

Extension to FEL radiation: xuv (5...60 fs pulses) + THz pulse



Solution of TDSE compared to semiclassical model\*\*

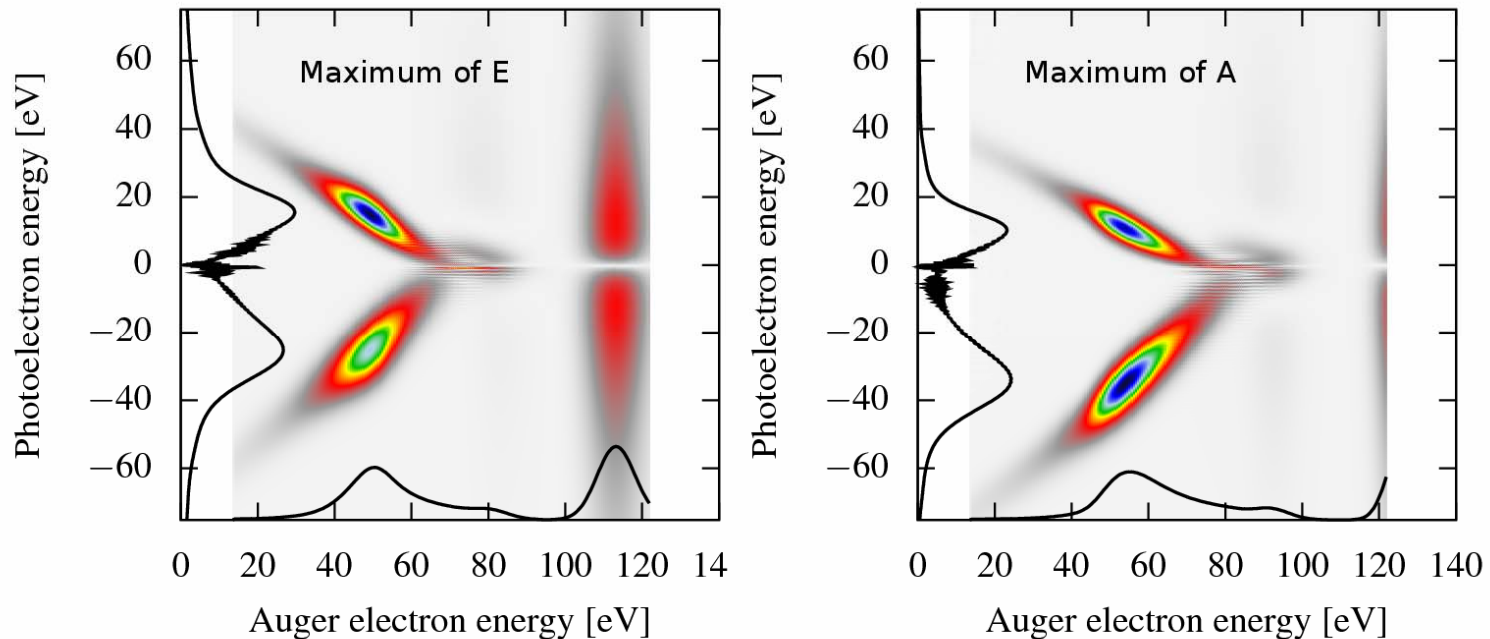
\*Frühling et al., Nature Photonics **3**, 523 (2009)

\*\* E. Krasovskii, and MB, Phys. Rev. Lett. **99**, 247601 (2007); Phys. Rev. A **80**, 053421 (2009)  
U. Frühling, S. Bauch, M. Drescher, and MB, to be published

# Correlated electron dynamics\*

- UV...x-rays: Ionization of inner shell electrons, Auger processes
- e-e, e-i coincidence experiments, e.g. Coltrims

→ diagnostics of laser pulse shape, sub-fs resolution of inneratomic electron dynamics, diagnostics of surrounding plasma



\*S. Bauch et al., *Europ. Phys. Lett.* **91**, 53001 (2010)

U. Fröhling, S. Bauch, M. Drescher, and MB, to be published



# Contents

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## **1. Overview: strongly correlated plasmas**

- 1.1 One-component plasma (OCP) in TD equilibrium
- 1.2 Two-component plasma: partial ionization, compact stars, dense laboratory plasmas

## **2. Theory of strongly correlated plasmas**

- 2.1 First-principle equilibrium simulations
- 2.2 Dense plasmas in nonequilibrium:
  - laser plasmas
  - photoionization

## **3. Outlook: Multiscale simulations of dense plasmas**

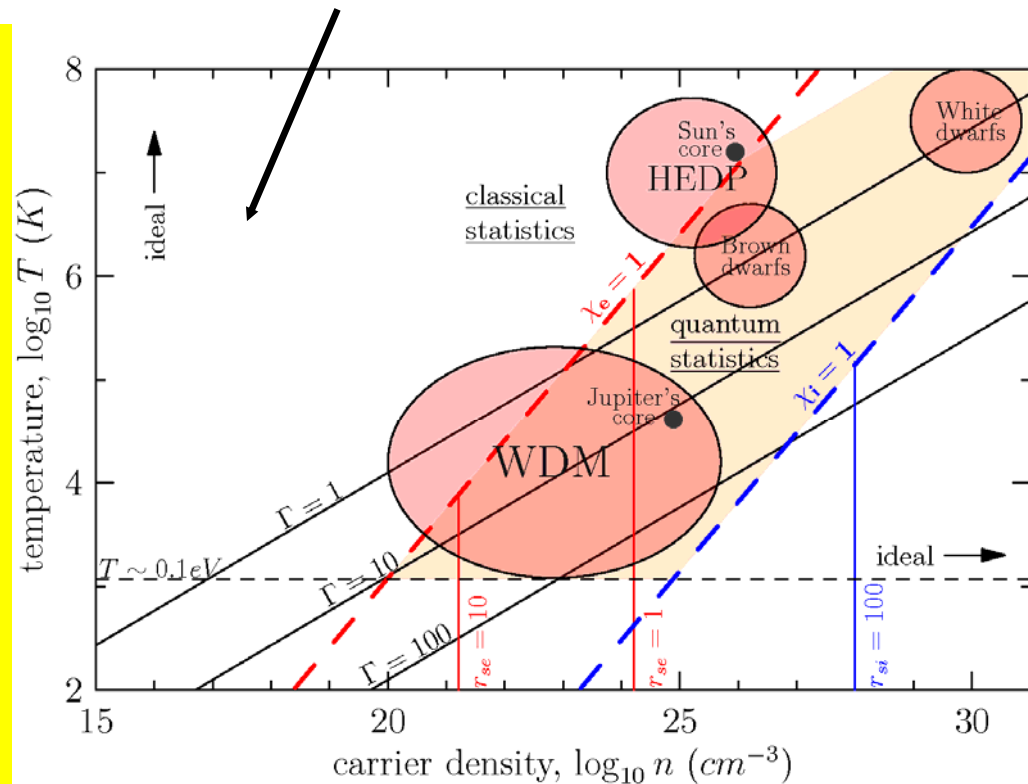
# Correlations in relativistic plasmas

Relativistic PIC simulations: mean field

## I. weakly nonideal plasma

### Correlation and quantum effects:

- e-i scattering effects in EMF (inverse bremsstrahlung [1,2])
- inner shell ionization, highly charged ions [3]
- pair creation in strong AC field, Gies et al. but: modification by quantum & plasma effects [1,4]



[1] M. Bonitz, „Quantum Kinetic Theory“

[2] D. Kremp et al., *Phys. Rev. E* **60**, 4725 (1999); MB et al. *Contrib. Plasma Phys.* **39**, 329 (1999)

[3] D. Hochstuhl, and MB, *J. Chem. Phys.* **134**, 084106 (2011)


[4] S. Smolyanski, MB et al. (2007-2010, Schwinger vs. Landau-Zener tunneling)



# Dense plasma simulations: perspectives

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## Towards multi-scale simulations from first principles:

1. Effective static i-i, e-i quantum pair potentials from equilibrium QMC   
Improvement of PIMC, dynamic and transport properties
2. First-principle ion MD with dynamically screened potentials  
Inclusion of nonequilibrium electrons, field effects
3. Combination of ion dynamics with electron quantum kinetics:  
TDHF, quantum kinetic equation or NEGF
4. Inclusion of inelastic processes in partially ionized plasmas:
  - ionization and recombination of atoms and (highly charged) ions
  - radiative processes
5. Modification of atomic processes by plasma and field

# Multi-scale simulations for dense plasmas (1)

**EM field**

Input:  $f_e$

**Electrons**



**Ions**

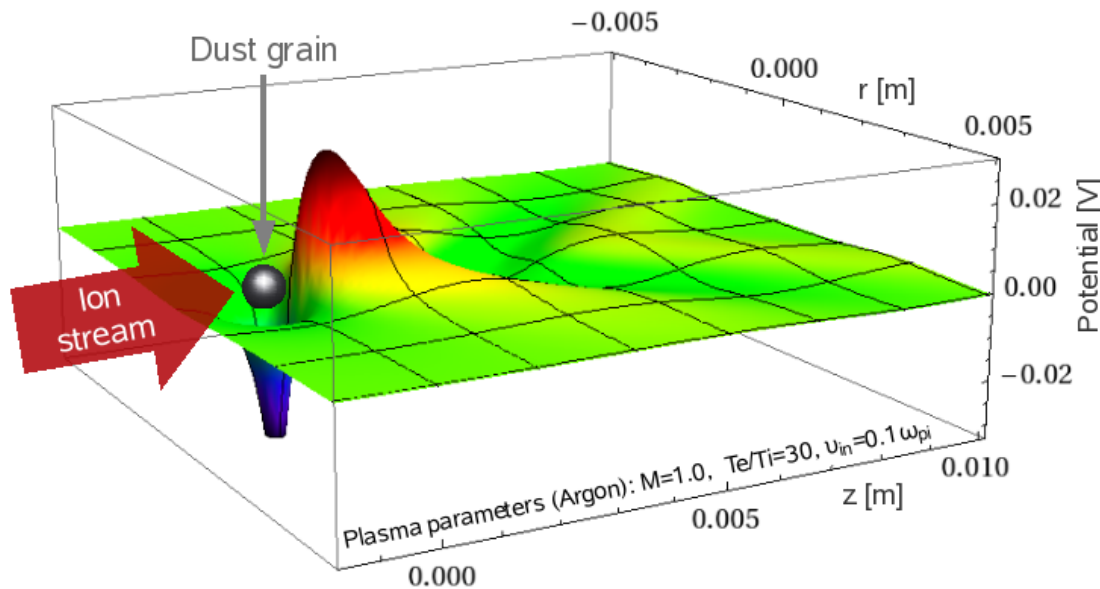
MD

*P. Ludwig, MB, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series **220**, 012003 (2010),  
P. Ludwig, W. Miloch, and MB, to be published*

# Ion dynamics dynamically screened by nonequilibrium quantum electrons

**Examples:** - laser compression

- inertial confinement fusion:  $\rho \propto 10^3 \text{ gcm}^{-3}$ ,  $T = 10^3 \dots 10^5 \text{ eV}$



**Electrons:**  
Mermin dielectric function (Lindhard plus collisions)

**Test system:**  
dust in streaming e-i plasma (experiments)

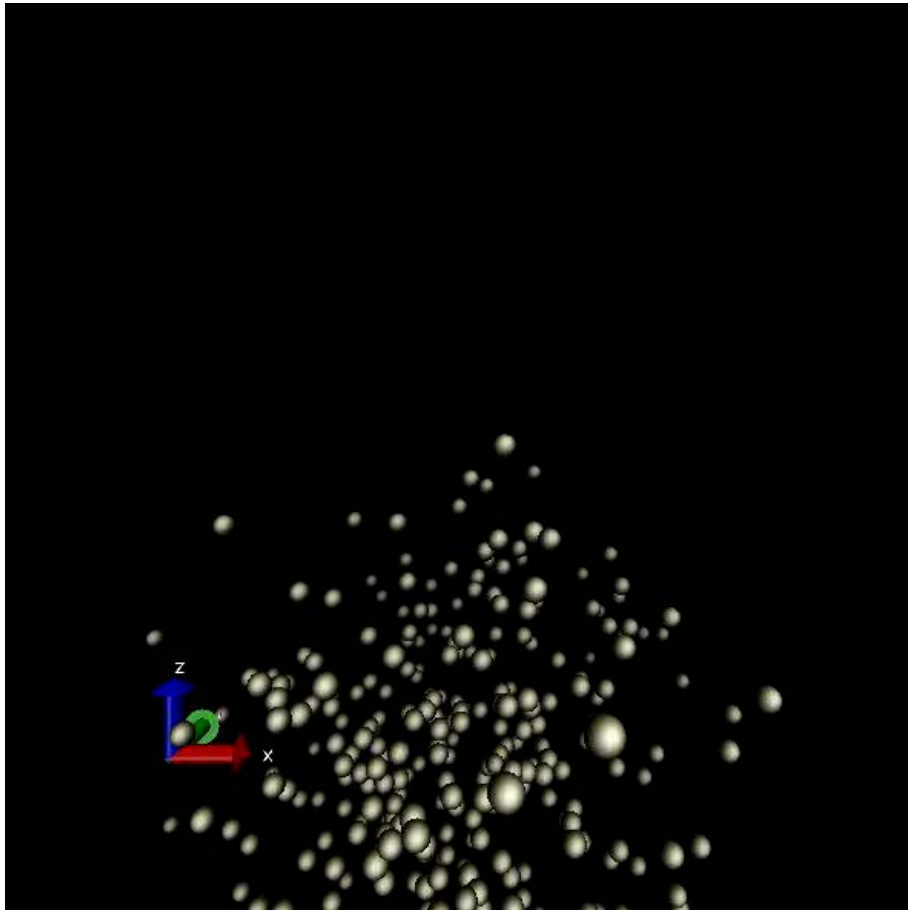
Wake field *attraction* of equally charged particles



*P. Ludwig, MB, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series 220, 012003 (2010),  
P. Ludwig, W. Miloch, and MB, to be published*



# Strongly correlated heavy particles in streaming flow of light particle



## Test system:

300 heavy particles

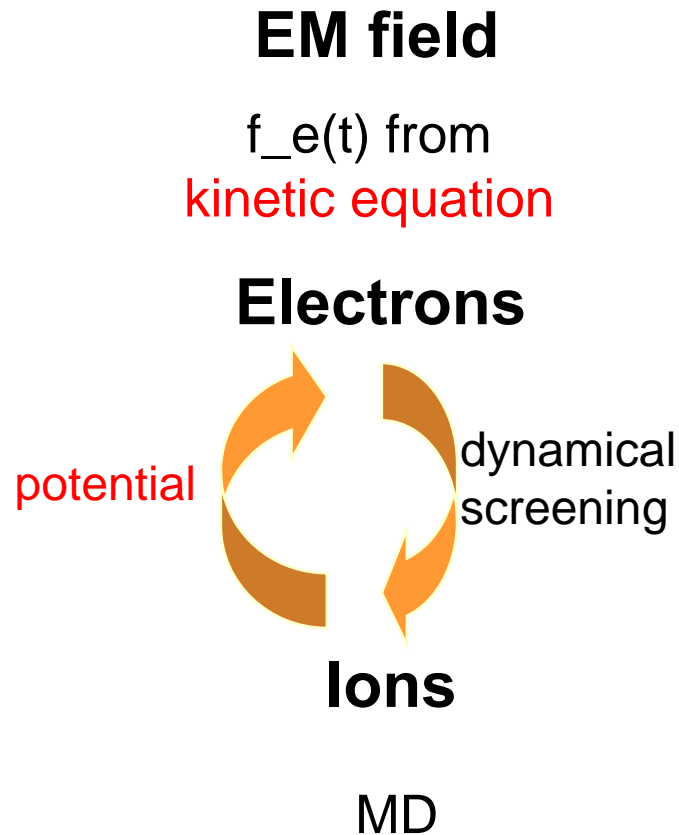
Plasma flow  
downward,  $M=0.8$

Non-hamiltonian system,  
collective modes,  
instabilities

MD Simulation:  
Patrick Ludwig

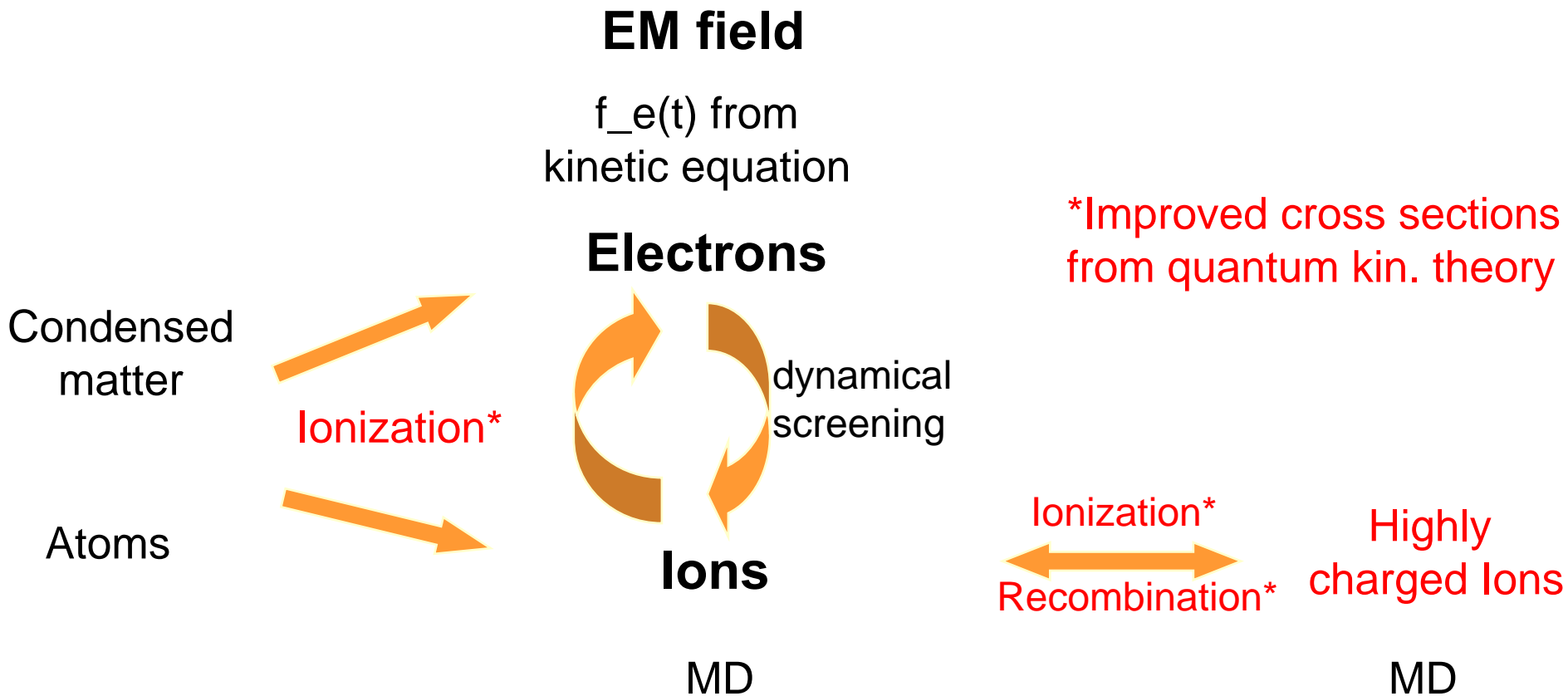
*P. Ludwig, MB, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series **220**, 012003 (2010),  
P. Ludwig, W. Miloch, and MB, to be published*

# Multi-scale simulations for dense plasmas (2)

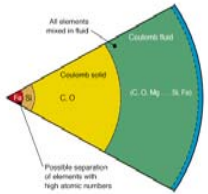


*P. Ludwig, MB, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series **220**, 012003 (2010),  
P. Ludwig, W. Miloch, and MB, to be published*

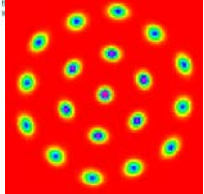
# Multi-scale simulations for dense plasmas (3)



# Summary



Structure of the interior of a white dwarf star, showing how the elements are distributed. ESI1-DITSIAP (revisited) 10/1

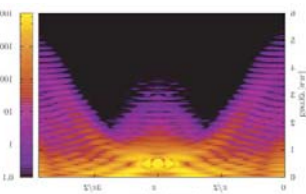
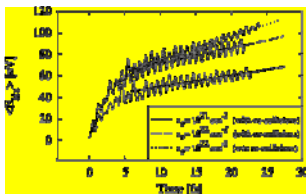


## 1. Correlated plasmas: new states of matter

- compact stars, quark-gluon plasma,
- lasers and ion beams: WDM, HEDP, ICF

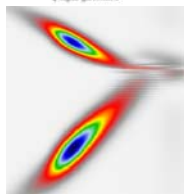
## 2. Theory of strongly correlated plasmas

- First-principle equilibrium simulations: QMC, QMD
- nonequilibrium: quantum kinetic theory
- atomic ionization dynamics



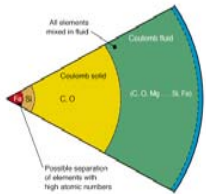
## 3. Outlook

- Correlations, quantum effects in relativistic plasmas
- Multiscale simulations of dense plasmas

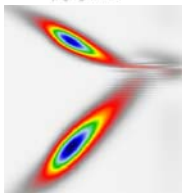
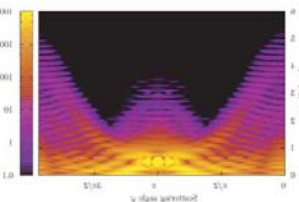
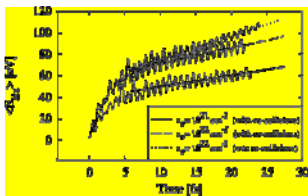
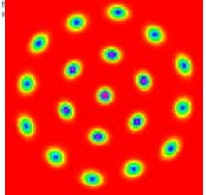


# Thank you

*good luck Helmholtz institute Jena!*



Structure of the interior of a white dwarf star, showing how the elements are distributed. EOST-DFTSDAP visualizes the



## Further information:

[www.theo-physik.uni-kiel.de/~bonitz](http://www.theo-physik.uni-kiel.de/~bonitz)

**APS/DPP meeting 2011:** mini-symposium  
„quantum plasmas in nonequilibrium“

**Network:** „time-dependent many-body systems  
out of equilibrium“