Quantum effects in plasmas

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With contributions from S. Hu, V. Karasiev (Rochester), H. Kersten (Kiel), T. Killian (Rice), D. Kraus (Rostock)

„APS/DPP Meeting“, Long Beach, November 2025

pdf of talk at https://www.itap.uni-kiel.de//theo-physik/bonitz/talks.html

2025

INTERNATIONAL YEAR OF
Quantum Science
and Technology

2025

unesco

INTERNATIONAL YEAR OF
Quantum Science
and Technology

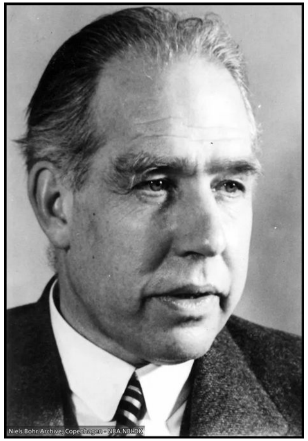
100 years of Heisenberg’s/Schrödinger’s equation

$$i\hbar\frac{\partial}{\partial t}\psi(\underline{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r})\right]\psi(\underline{r},t)$$

honoring the „fathers“ (and „mothers“) of quantum mechanics,
in particular: Bohr, Schrödinger, Heisenberg, Born, Pauli, Dirac, Fermi...

2025

INTERNATIONAL YEAR OF Quantum Science and Technology



Niels Bohr:
one „researcher who created the foundation on which we all work today“

Letter to Marga Planck, Oct 14 1947
https://doi.org/10.38071/2024-01159-0

Max Planck (*1858 Kiel – 1947 Göttingen)

Dec. 14 1900*: quantum hypothesis

- quantization of electromagnetic radiation
- elementary photon energy E=hf
- Planck constant h

striking contradiction to 19th century physics

*„birthday of quantum physics“, revolution of science and technology

In fact: long and difficult path, with many obstacles

Planck studies Physics in Munich and Berlin

Planck is excited by theoretical physics, wants to continue

Advise from Prof. Philipp von Jolly*, in Munich, 1877:

„Theoretical Physics is close to completion,
… similar as geometry is long complete….“

„...in some „corners“ there might be a few tiny „dust grains“ left to explore and categorize, but the system as a whole is well founded.“

*view of an experimentalist

Planck, Naturwiss. **13**, 52-59 (1925)

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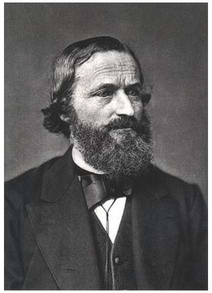
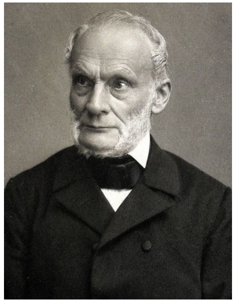
„…in some „corners“ there might be a few tiny „dust grains“ left to explore and categorize, but the system as a whole is well founded.“

Planck: „I do not desire to discover new ground, but only to understand the existing fundamentals of the physical science and, possibly, to deepen them.“

Planck, Naturwiss. **13**, 52-59 (1925)

First research results of Planck… ignored





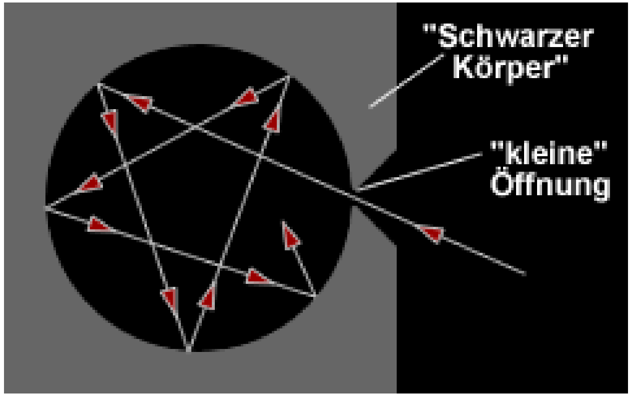
Lectures by Helmholtz, Kirchhoff, Weierstraß, Self-education: Clausius
strongly impressed by R. Clausius' thermodynamics, entropy

PhD thesis 1879, 1880 Habilitation: on 2nd law of thermodynamics
But: no response from the experts

1879-1885: Privatdozent (unpaid), 1885-89: professor in Kiel
Since 1889: professor in Berlin

Black-body radiation (EM spectrum in equilibrium)

1860 Kirchhoff: „black body“
(Gedanken-Experiment)



hohlraum at fixed T
confines radiation

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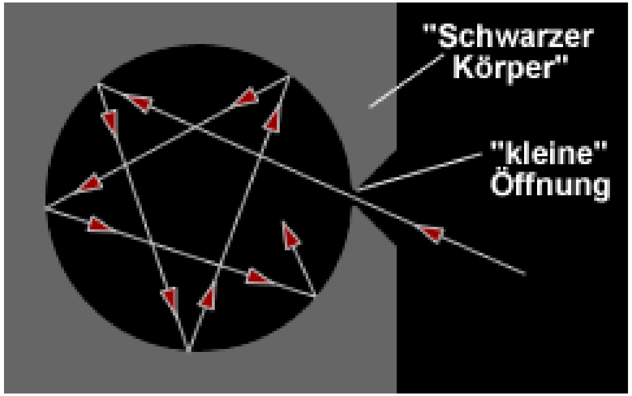
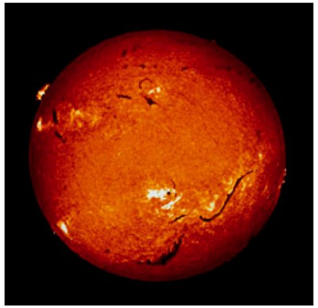
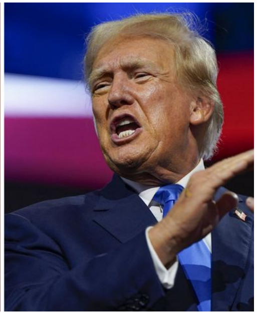


hohlraum at fixed T
confines radiation

Every body radiates! In TD equilibrium spectrum of EM waves universal, depends only on T


Black-body radiation spectrum: myths vs. facts

„**Ultraviolet catastrophe**“ (black: Rayleigh-Jeans) resolved by Planck*

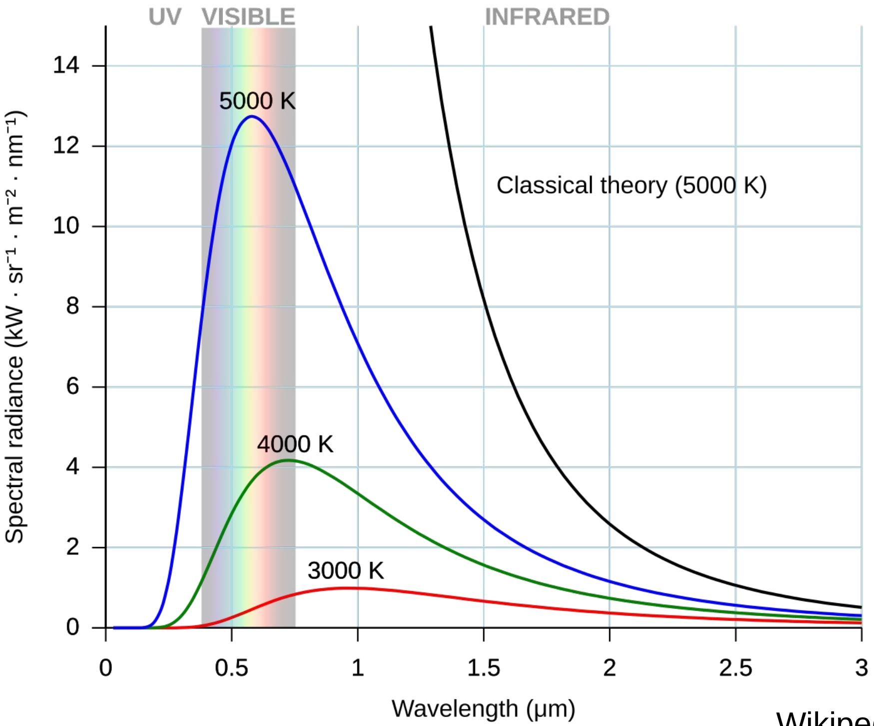
Radiation energy vs. wavelength/frequency at given temperature T

Planck’s result (Bose distribution)

$$\rho(\omega, T) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

$\omega = 2\pi f, \quad c = \lambda f$

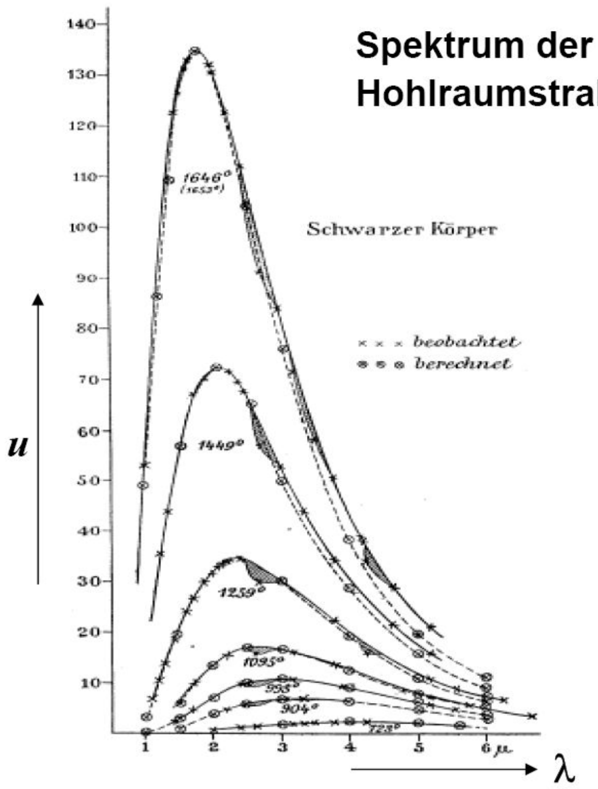
Planck identifies two constants: h, k_B
(„of universal importance“ for all cultures)



Wikipedia

*according to many text books

Black-body radiation spectrum: myths vs. facts



Messung von Lummer und Pringsheim (1900)

- 1896: Wien's radiation law
- 1897-1900: precision experiments by Lummer, Pringsheim, Rubens, Kurlbaum (PTR Berlin)
  → excellent agreement with Wien, small deviations at large wavelengths

M. Bonitz: https://doi.org/10.38071/2024-01159-0

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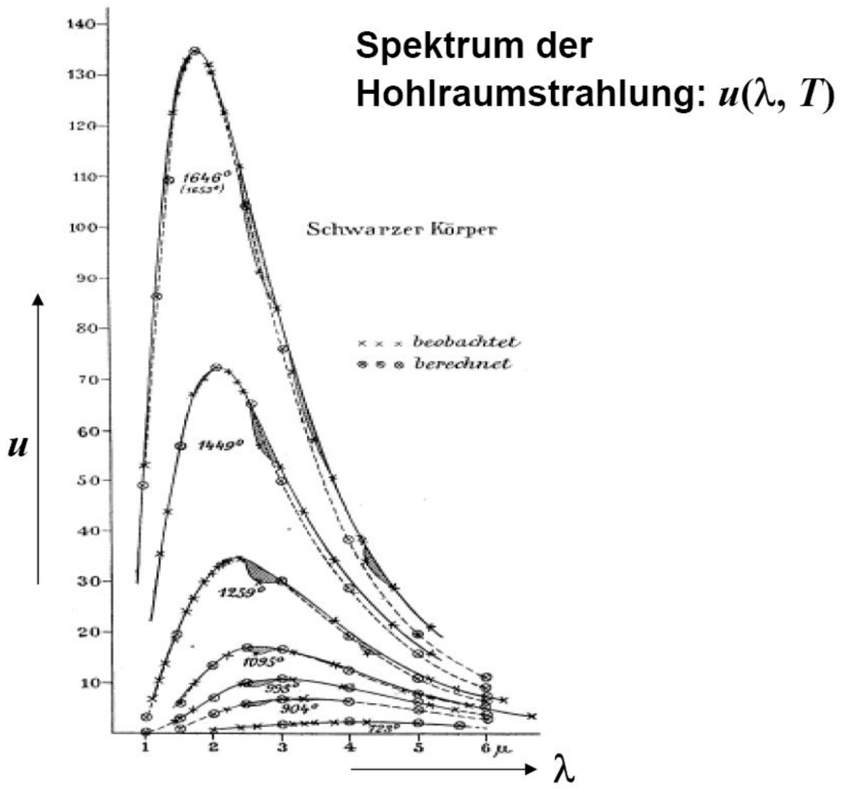

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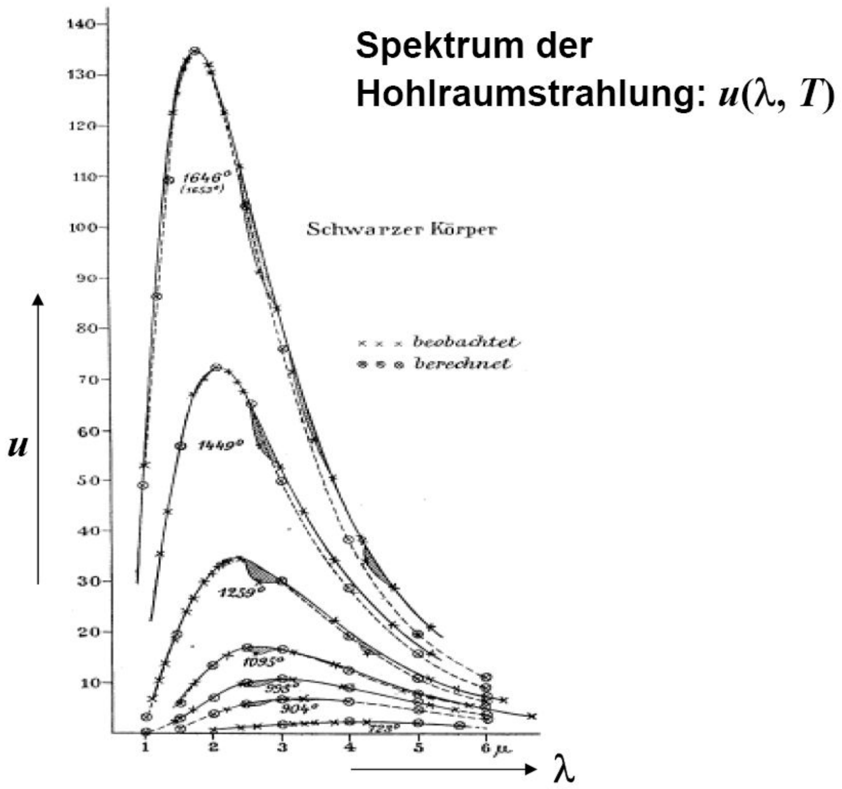
- Planck computes entropy S of radiation. He adds

Black-body radiation spectrum: myths vs. facts



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  $R_{WIEN} + R_{RAYLEIGH} = R_{PLANCK}$, where $R = \left(\frac{d^2 S}{dU^2} \right)^{-1}$

- Oct 19 1900: Planck presents his radiation law experimentalists confirm perfect agreement
- Dec 14 1900: Planck presents his derivation based on the quantization of energy $U_\nu = N_\nu \cdot \varepsilon_\nu = N_\nu \cdot h\nu$

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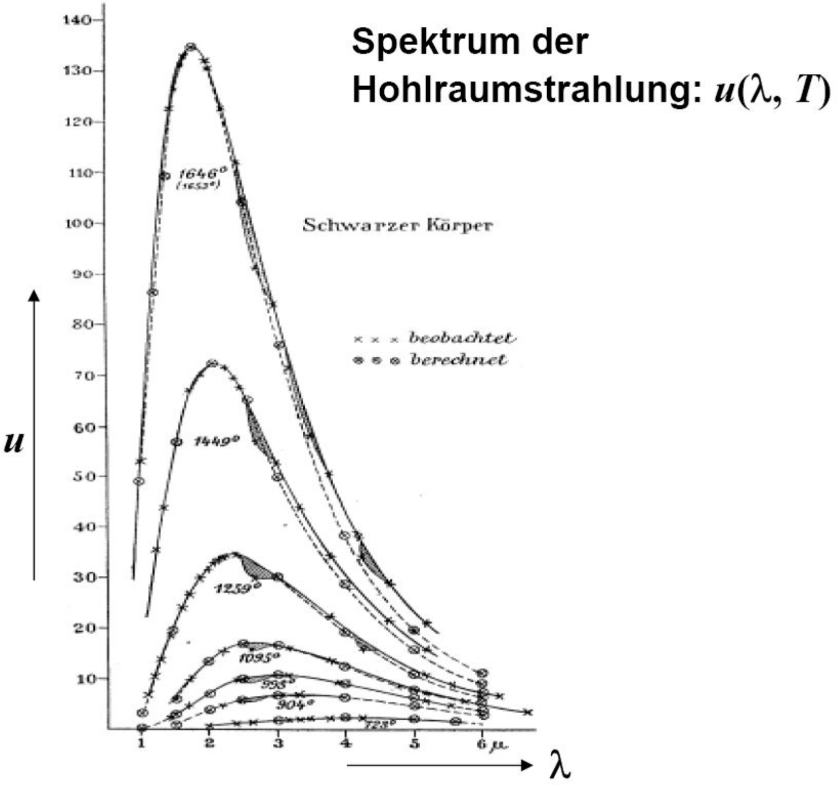

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1905: Rayleigh/Jeans (corrected equipartition)
1911: Nobel prize for Wien
1911: Ehrenfest „Ultraviolet catastrophe"
Today: many text books cultivate fiction

striking contradiction to 19th century physics
broad skepticism of leading physicists

Max Planck remains skeptical himself about interpretation of photon hypothesis, for many years

- 1905: Einstein applies hypothesis to photo effect
- 1913: Bohr uses h to quantize angular momentum of atom

very long and difficult path, contributions from many scientists

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very long and difficult path, contributions from many scientists

Nobel prize 1919 (for 1918)

„Planck's radiation theory is, in truth, the most significant lodestar for modern physical research, and it seems that it will be a long time before the treasures will be exhausted which have been unearthed as a result of Planck's genius."

A.G. Ekstrand, President of the Royal Swedish Academy of Sciences, 1. June 1920

More details in the Max Planck museum at the Kiel Physics department (link)

Quantum physics – a „gold mine“ in 20th, 21th centuries:
Recent Nobel prizes in physics

2025: macroscopic quantum tunneling: Clarke, Devoret, Martinis
2023: attosecond pulses (atomic physics): L’Huillier, Agostini, Krausz
2022: entangled photons: Aspect, Clauser, Zeilinger
(2020: black holes: Penrose, Glenzel, Ghez)
(2019: cosmology, exoplanets: Peebles, Mayor, Queloz)
2018: optical tweezer, High intensity lasers: Ashkin, Mourou, Strickland
2016: Topological phase transitions in 2D: Thouless, Kosterlitz, Haldane
2015: Neutrino Oscillations: Kajita, Mc Donald
2014: blue LEDs: Akasaki, Amano, Nakamura
2013: Higgs boson: Englert, Higgs
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Nearly all fields of physics. Also various chemistry nobel prizes. How about plasmas?

Outline

1. **Introduction**: why should plasma physicists care?

2. **Quantum effects in plasmas**
   2.1 Low pressure: classical electrons
   2.2 High pressure: quantum electrons
   2.3 Quantum effects of heavy particles
   2.4 Exotic quantum plasmas

3. **Methods for dense quantum plasmas/warm dense matter**
   3.1 Simulation methods
   3.2 Benchmarks: uniform electron gas, hydrogen

4. **Outlook**: toward precision modeling of quantum plasmas, ICF

1. Introduction: Quantum effects

Why should plasma physicists care?

1. Introduction: Quantum effects

Why should plasma physicists care?

What are quantum effects and where are they?

Single-particle quantum effects

Tunneling through potential barrier

Wave-like interference

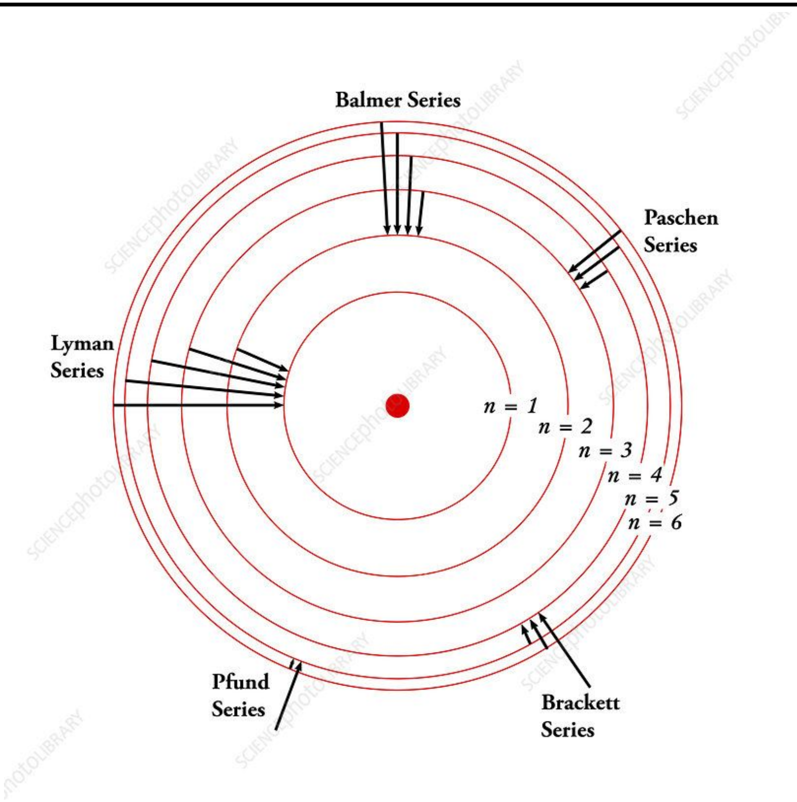
Wave-particle duality (?)

Single-particle quantum effects

Structure of atoms, molecules:

<u>pointlike</u> electrons on circular orbits
around nucleus, e.g. logo:

IAEA



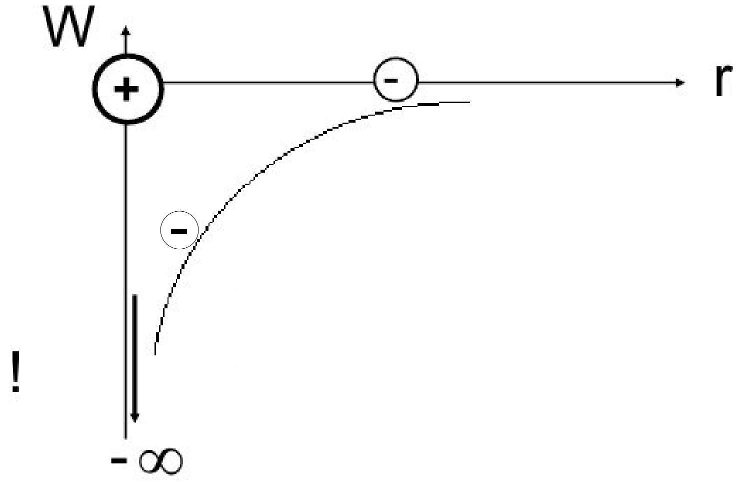
Bohr model of H-atom:
+ reproduces dipole radiation spectra
- but: unstable atom (radiation of electron)
- wrong, incomplete orbitals

Niels Bohr, 1913
pic: Wikipedia

Simple explanation of quantum effects

unstable atom:

1D model



Coulomb attraction
$W= - e^2/r$

electron „rolls down“ the hill to lower its energy without limit

Simple explanation of quantum effects

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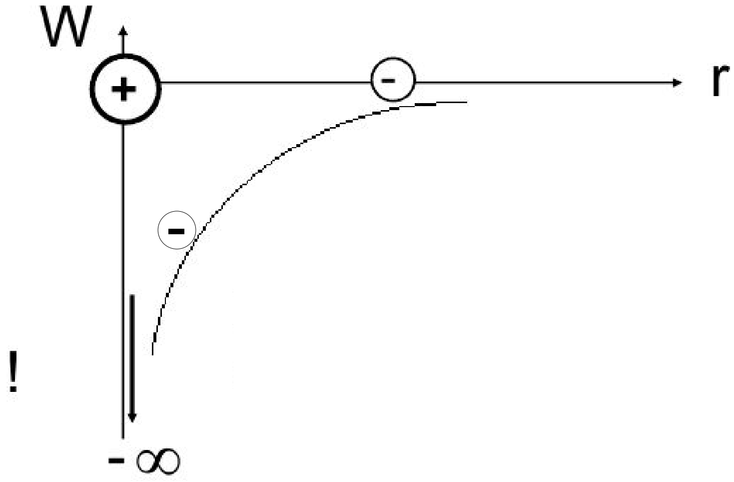

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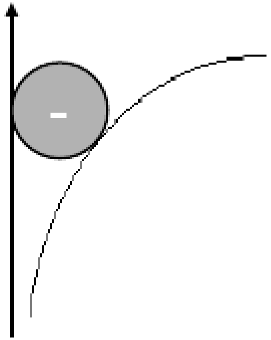
stable atom:

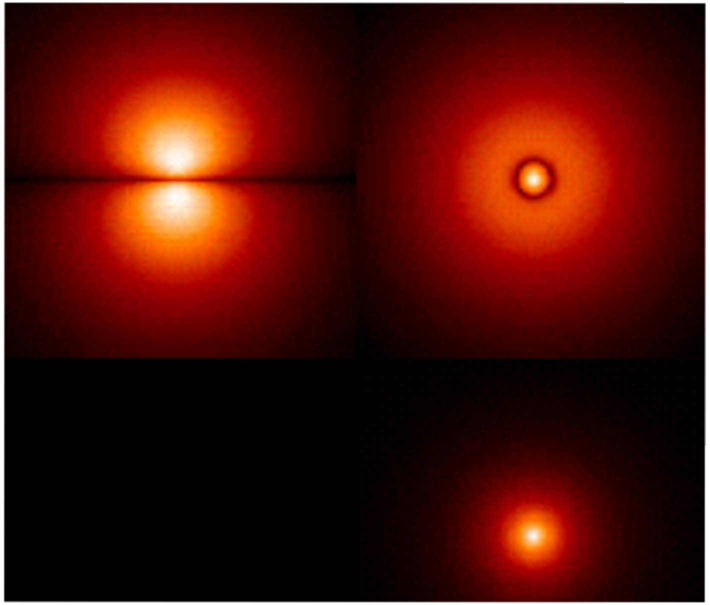


quantum electron „blows up“ to prevent collapse into nucleus

Interaction energy remains finite

Consequences of finite electron extension λ

Stable (stationary) atom
Quantum kintetic energy balances
Coulomb attraction
theory for all atoms, high precision



Hydrogen atom: 2p, 2s
1s
orbitals

Consequences of finite electron extension λ

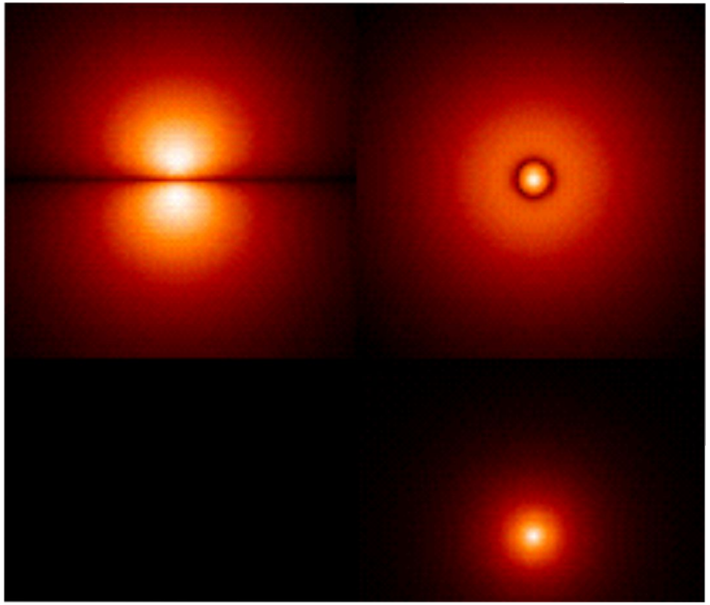
Stable (stationary) atom
Quantum kintetic energy balances
Coulomb attraction

Spreading of free wave packet

Tunneling through potential barrier

Wave-like interference

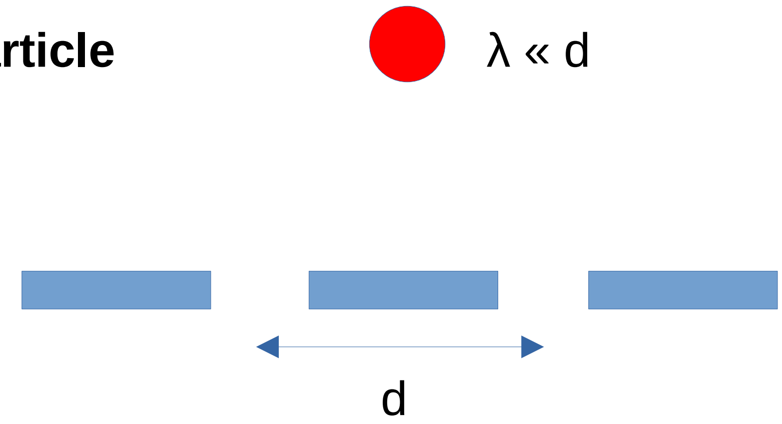
Wave-particle duality: trivial consequence of Fourier transform of wave packet



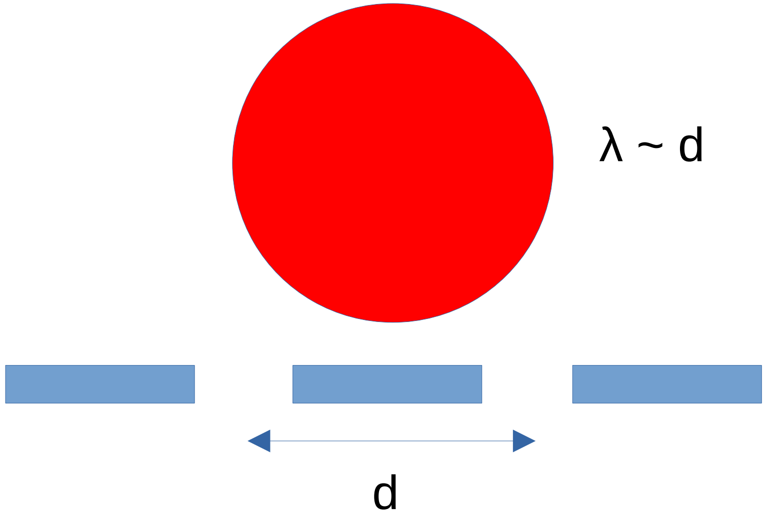
Hydrogen atom: 2p, 2s
1s
orbitals

When are quantum effects important (1)?

1 particle

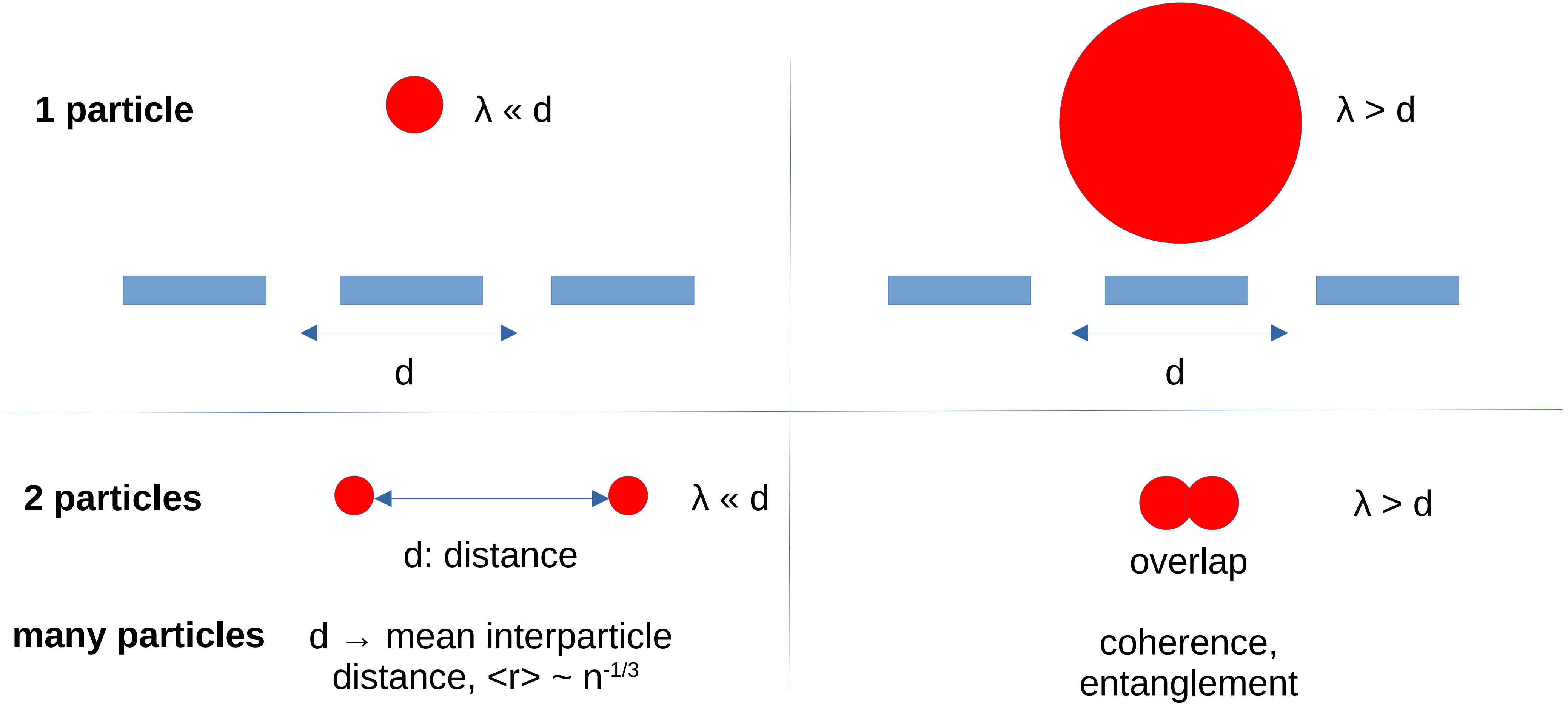


No interference



interference,
diffraction,
tunneling

When are quantum effects important (1)?



Dimensionless parameters of quantum plasmas

Strength of quantum effects: $\chi = n \Lambda^3$ or $\Theta = \frac{k_B T}{E_F}$ quantum degeneracy

In equilibrium: extension ~ thermal DeBroglie wave length: $\Lambda_a = \frac{h}{(2\pi m_a k_B T)^{1/2}}$

$r_s = \frac{d}{a_B}$ coupling (T=0)

Fermi energy: $E_F = (\hbar q_F)^2/2m$, $q_F = (3\pi^2 n)^{1/3}$

$$\Gamma = \frac{e^2}{d k_B T \frac{2\sigma+1}{n\Lambda^3} I_{3/2}(\beta\mu)}$$

generalized coupling par.

screening length: $r_D = \left(\frac{k_B T}{4\pi n e^2}\right)^{1/2}$,

plasma frequency unchanged: $\omega_p = \left(4\pi \frac{n e^2}{m}\right)^{1/2}$,

$$r_{TF} = \frac{\hbar}{2m^{1/2}}\left(\frac{\pi}{3n}\right)^{1/6}$$

M. Bonitz *et al.*, Phys. Plasmas 2024

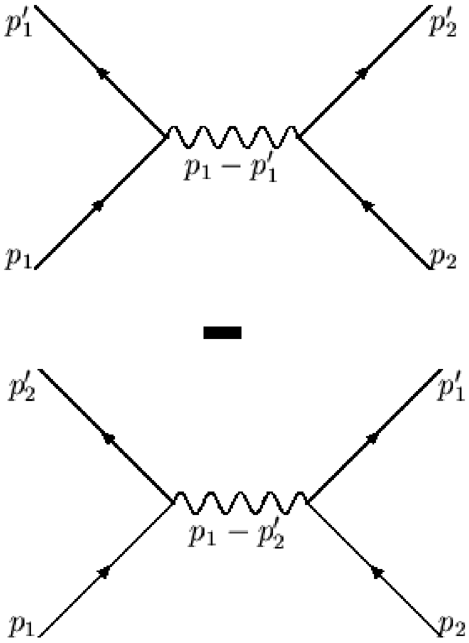
Many-particle (exchange) quantum effects (2)

Fermi energy (kinetic energy, T=0): $E_F \sim n^{2/3}$
Rapid increase with n,
plasma becomes *ideal upon compression*

Many-particle (exchange) quantum effects (2)

Fermi energy (kinetic energy, T=0): $E_F \sim n^{2/3}$
Rapid increase with n,
plasma becomes *ideal upon compression*

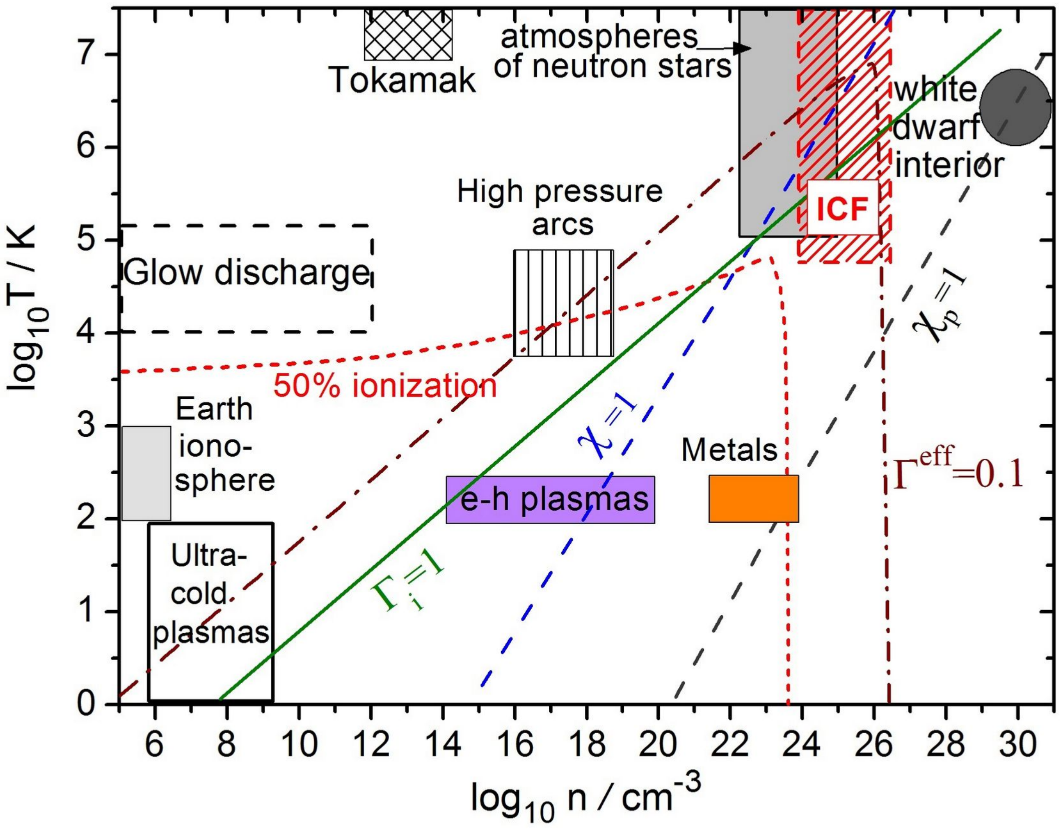
Quantum exchange
Example: e-e Coulomb scattering



Pauli blocking:
Reduced scattering rate **~** $[1-f(p'_1)][1-f(p'_2)]$

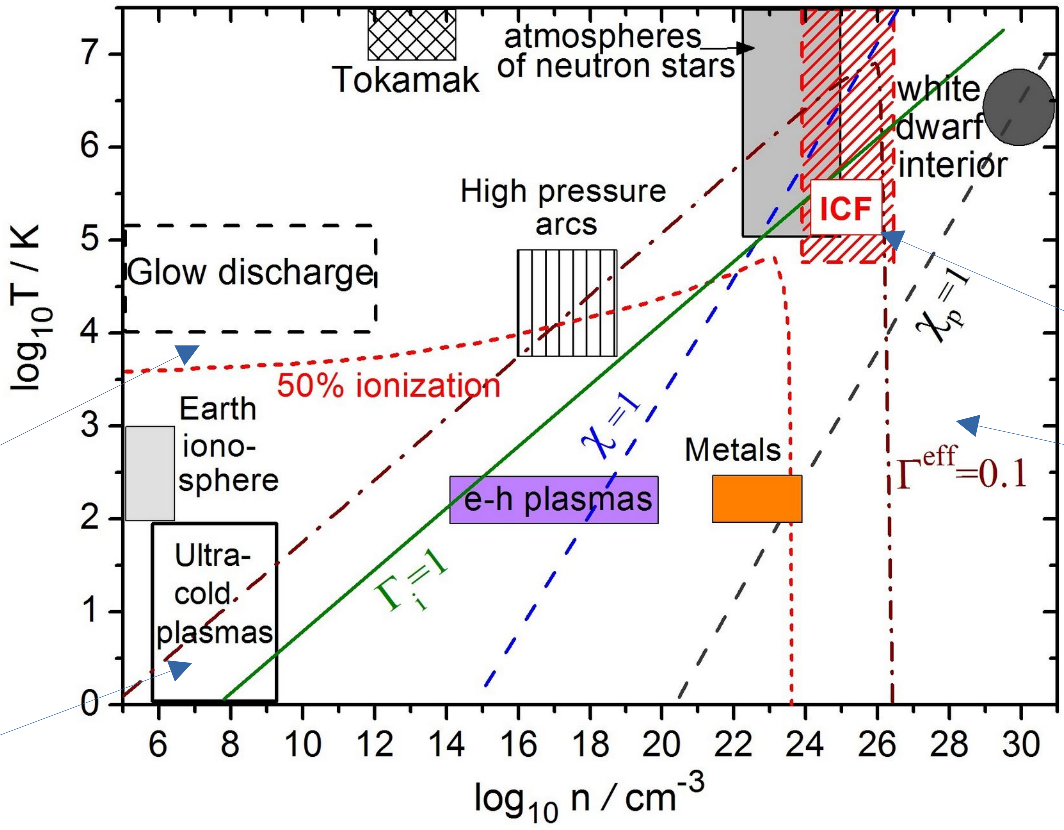
Properties of bosons relevant for photons (low intensity)
and atoms or ions (very high density)

Plasmas span huge parameter range



Bonitz *et al.*, Phys. Plasmas **27**, 042710 (2020)

Plasmas span huge parameter range



2.1 low-pressure

the coldest plasmas...

2.2. high pressure

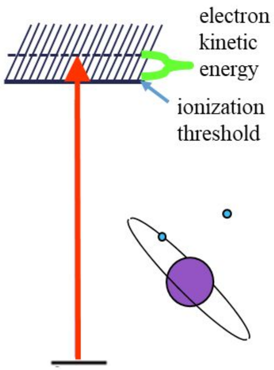
2.3. quantum protons

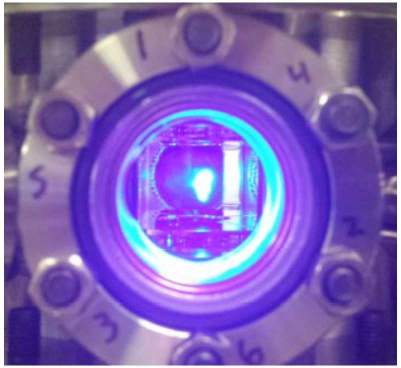
2.4. exotic quantum plasmas

Bonitz *et al*., Phys. Plasmas **27**, 042710 (2020)

Ultracold Neutral Plasmas

Killian research group at Rice University: ultracold.rice.edu

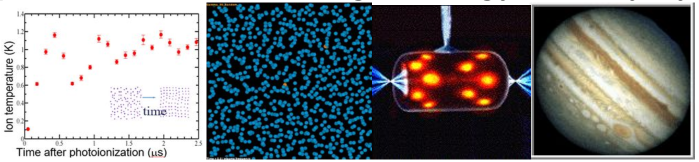




- created by photoionizing a laser cooled gas near the ionization threshold with a ~ns pulsed dye laser
- 10^8 ions, 1mm size, n~10^9 cm^{-3}
- electron temperature ~ 1K
- ion Coulomb coupling parameter: Γ_i ~ 2

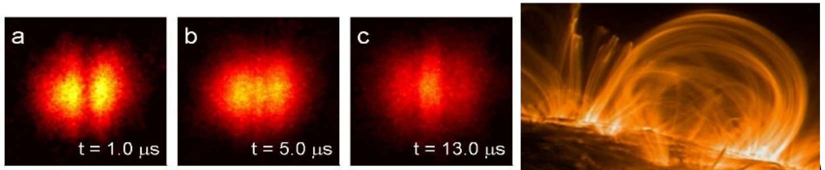
- Discovery plasma science

- Equilibration and transport of strongly coupled plasmas - simulate high-energy density systems



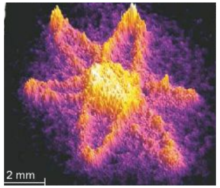
Phys. Plasmas **26**, 100501 (2019)

- Testbed for hydrodynamic and kinetic plasma models



- Technologies: Bright charged-particle beams for accelerators and ion/electron microscopes (not at Rice)

Nature Physics 7, 785 (2011)



U.S. DEPARTMENT OF ENERGY

NSF

RICE | RCQM Rice Center for Quantum Materials

2.1 Quantum effects in low pressure plasmas

2.1 Quantum effects in low pressure plasmas

→ Plasmas with classical electrons

A. Plasmas containing atoms, molecules
B. Interface of plasmas and solids
C. Fusion (magnetic)

2.1.A. Low-p plasmas containing atoms or molecules

Accurate plasma diagnostics possible exploiting quantum effects:

via spectroscopy of atoms, molecules

- absorption, emission, scattering, frequency combs etc.

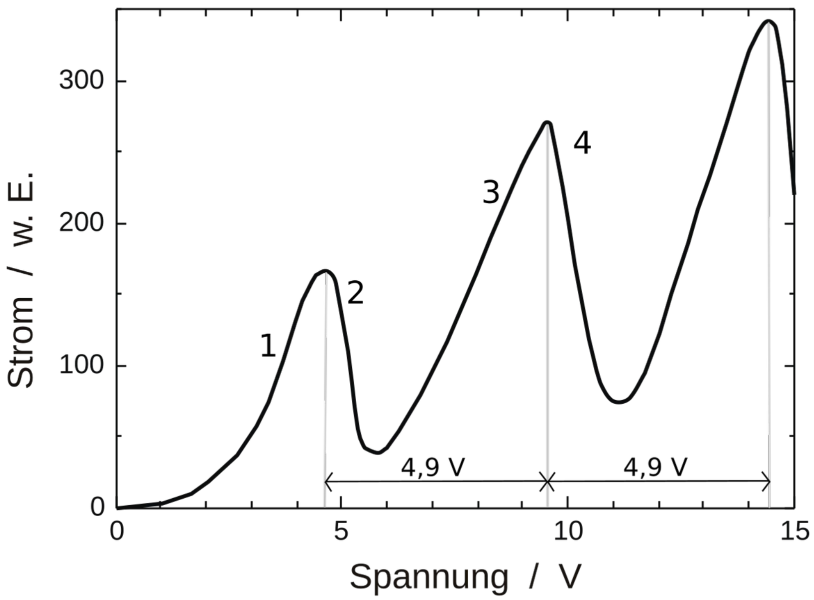
- models require atomic levels and cross sections
- plasma properties: transport, line broadening
  Saha equation

U. Fantz, PSST **15**, 137 (2006)
V.N. Ochkin, *Spectroscopy of Low Temperature Plasma*, Wiley 2009
I.H. Hutchinson, Principles of Plasma Diagnostics, Cambridge U Press 2009

Macroscopic quantum effects in low-p plasmas

Current vs voltage

Franck-Hertz experiment (1914)
(inelastic collisional excitation of atoms by electrons, existence of discrete excited states)
electron current vs voltage →



straightforward to demonstrate in low pressure plasma
(Holger Kersten, Kiel)

→ Video

Macroscopic quantum effects in low-p plasmas

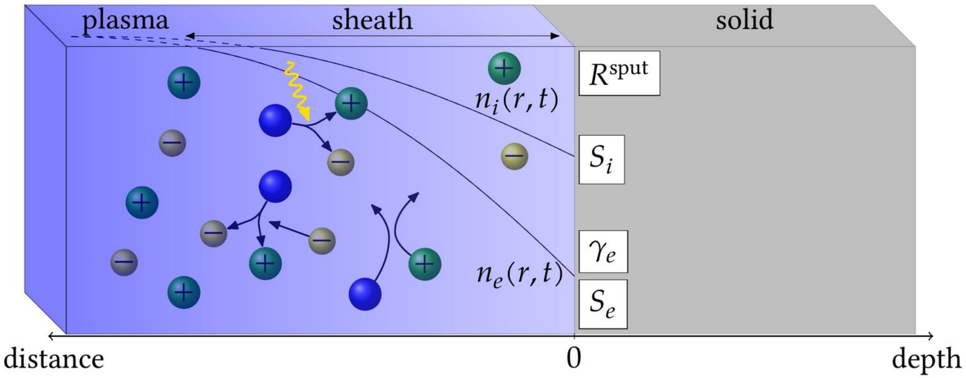
Standing striations in low pressure plasmas:

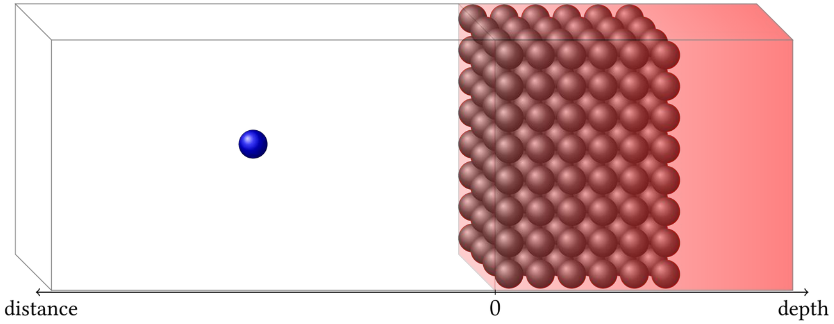
Franck-Hertz experiment (1914)
(inelastic collisional excitation of atoms by electrons,
existence of discrete excited states)

Demonstrated in low pressure H-plasma
(Holger Kersten, Kiel)

2.1.B. Plasma-surface interaction

Quantum effects in solid surface of plasma





plasma influenced by solid….

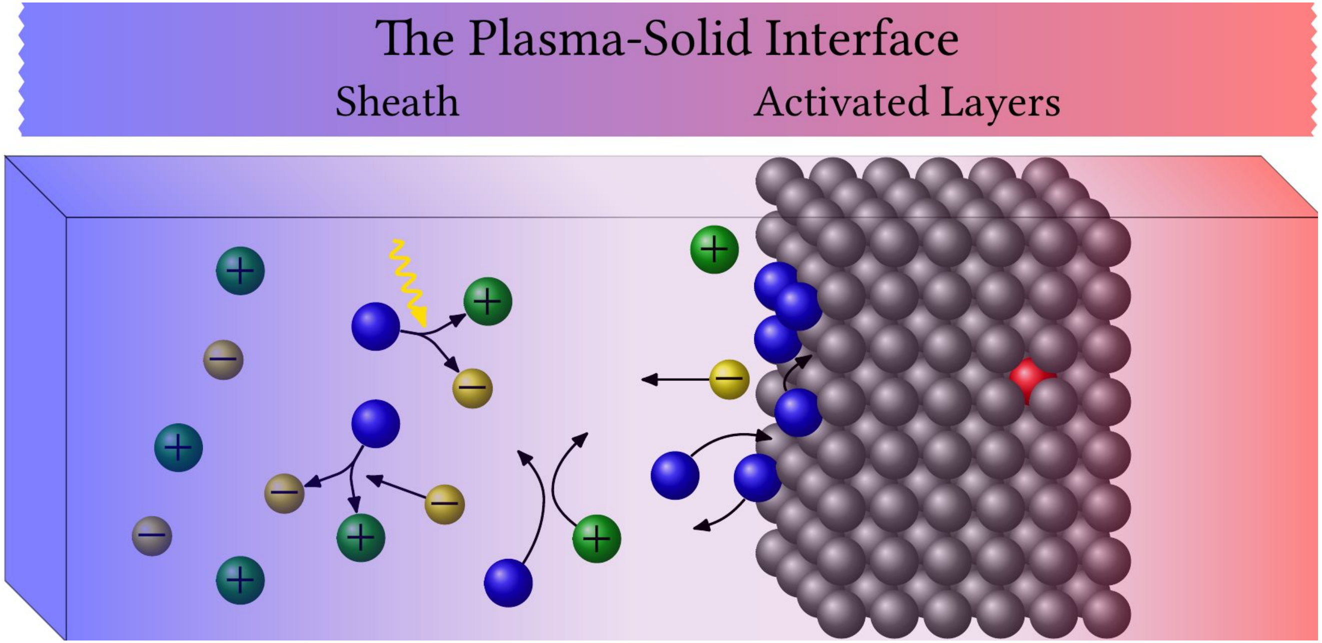
phenomenological coefficients

solid influenced by plasma….

results for single ion/atom impact

Selfconsistent modeling of plasma-surface interaction

Quantum effects in solid surface impact plasma properties

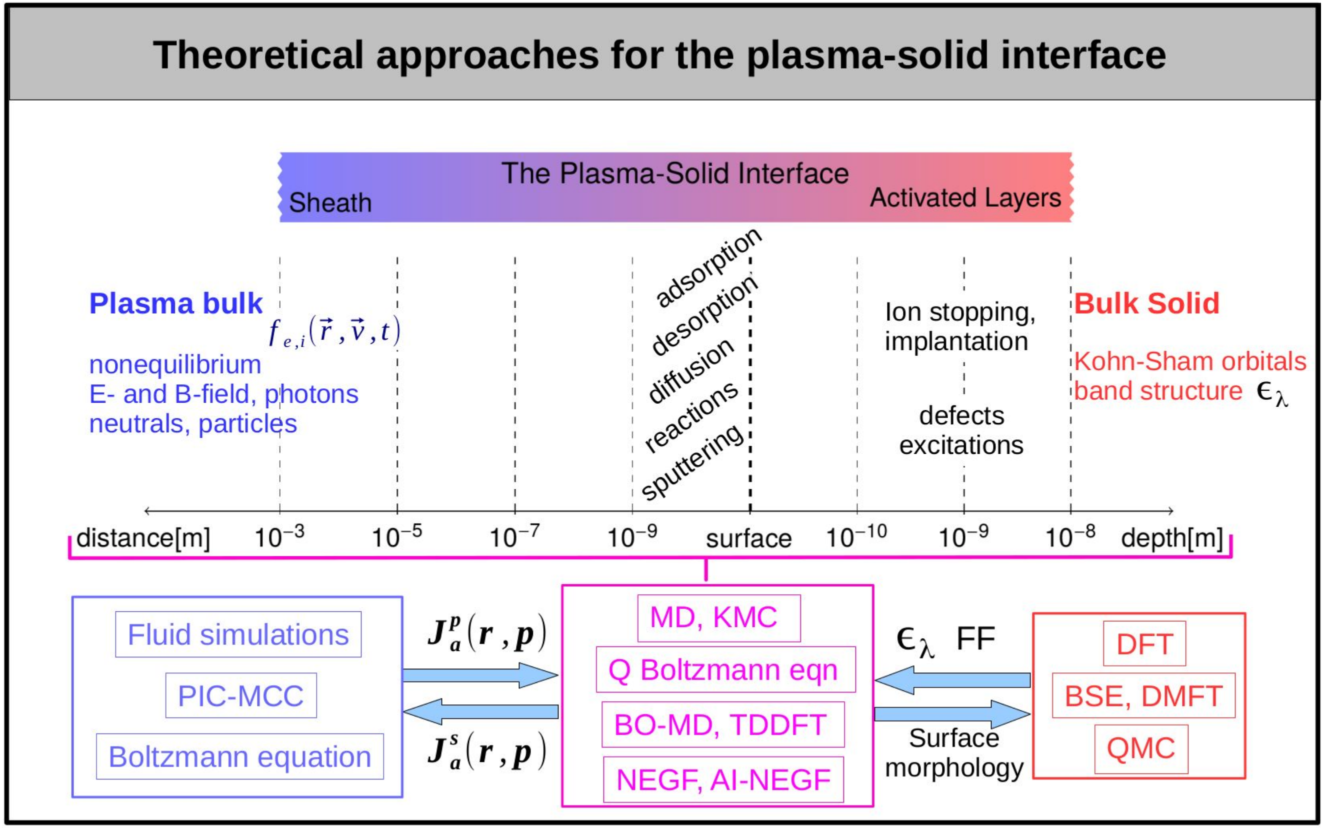


- <u>in situ/operando</u> **experiments** (TEM, X-rays)

- Invoke condensed matter **simulations** (DFT, NEGF, QMC), <u>modified</u> by plasma effects

Bonitz *et al.*, Front. Chem. Sc. Engin. **13**(2), 201-237 (2019)

Theoretical approaches for the plasma-solid interface



MD: molecular dynamics
KMC: kinetic Monte Carlo
BO-MD: Born-Oppenheimer MD

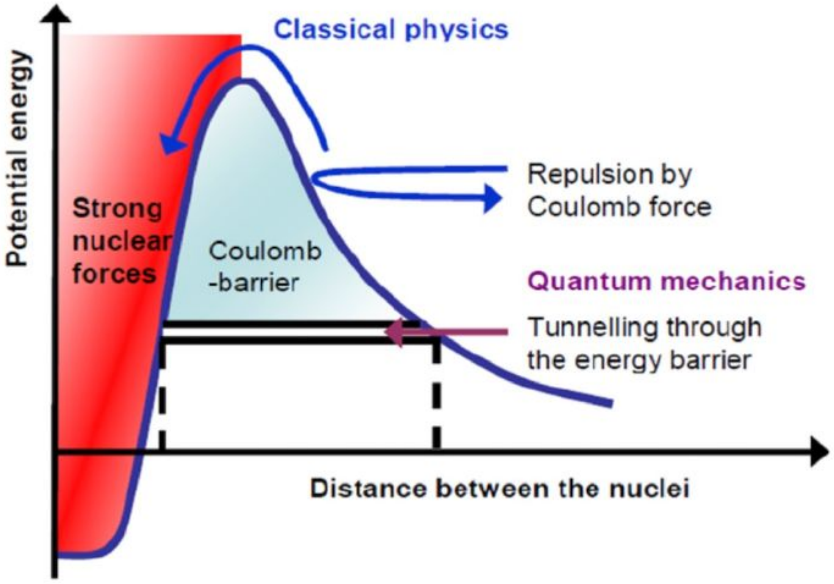
TDDFT: time-dependent DFT
NEGF: nonequilibrium Green fcts.
AI-NEGF: ab initio NEGF
DFT: density functional theory

BSE: Bethe Salpeter equation
DMFT: dynamical mean field theory
QMC: quantum Monte Carlo

Bonitz *et al.*, Front. Chem. Sc. Engin. **13**(2), 201-237 (2019)

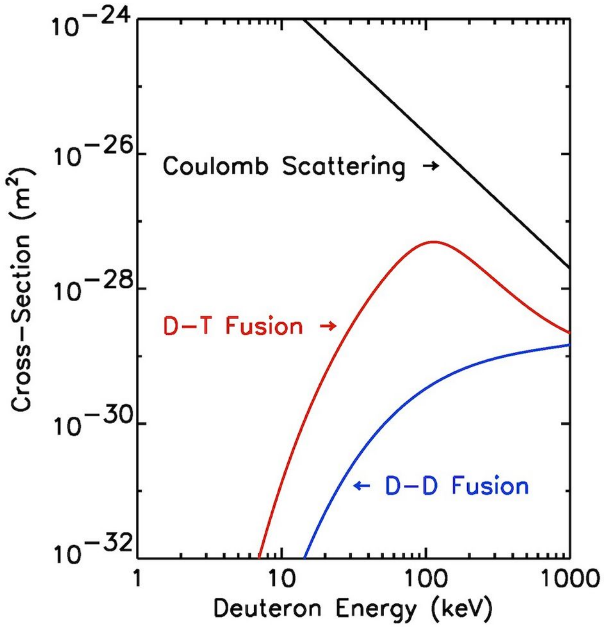
2.1.C. Quantum effects in Fusion

Quantum tunneling crucial



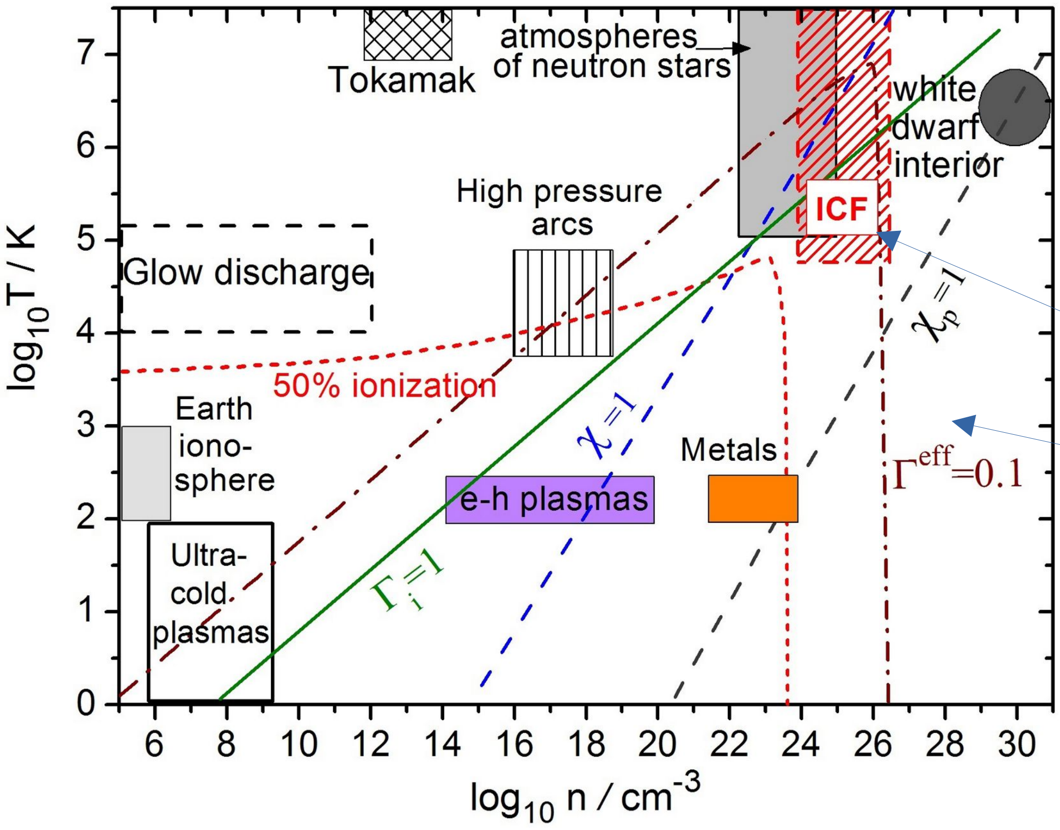
https://www6.lehigh.edu/~eus204/lab/PCL_fusion.php

D-D, D-T cross sections



Interaction with wall: requires advanced condensed matter (quantum) tools, see above

Plasmas span huge parameter range



Bonitz *et al.*, Phys. Plasmas **27**, 042710 (2020)

2.4. exotic quantum plasmas

2.2. high pressure

2.3. quantum protons

2.2 High pressure: quantum electrons

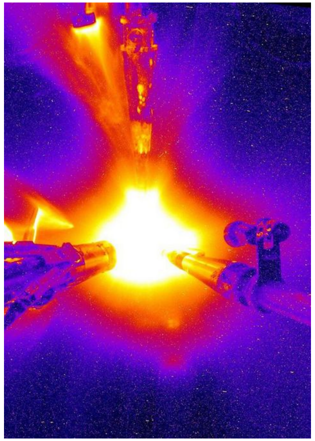
Astrophysics:

- gian planet interiors
- brown dwarfs
- newly discovered exoplanets
- Earth interior

Sci-News.com [Img4]

Lab experiments, shock compression:

- lasers, FELs, Z-pinch, ion beams
- basic high compression studies at the NIF
- ICF (see below)



Don Jedlovec, LLNL

2.2 High pressure: quantum electrons

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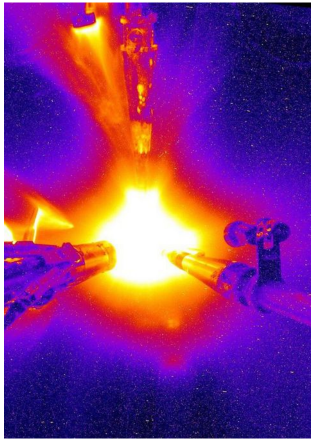
Sci-News.com [Img4]



Don Jedlovec, LLNL

Basic physics:

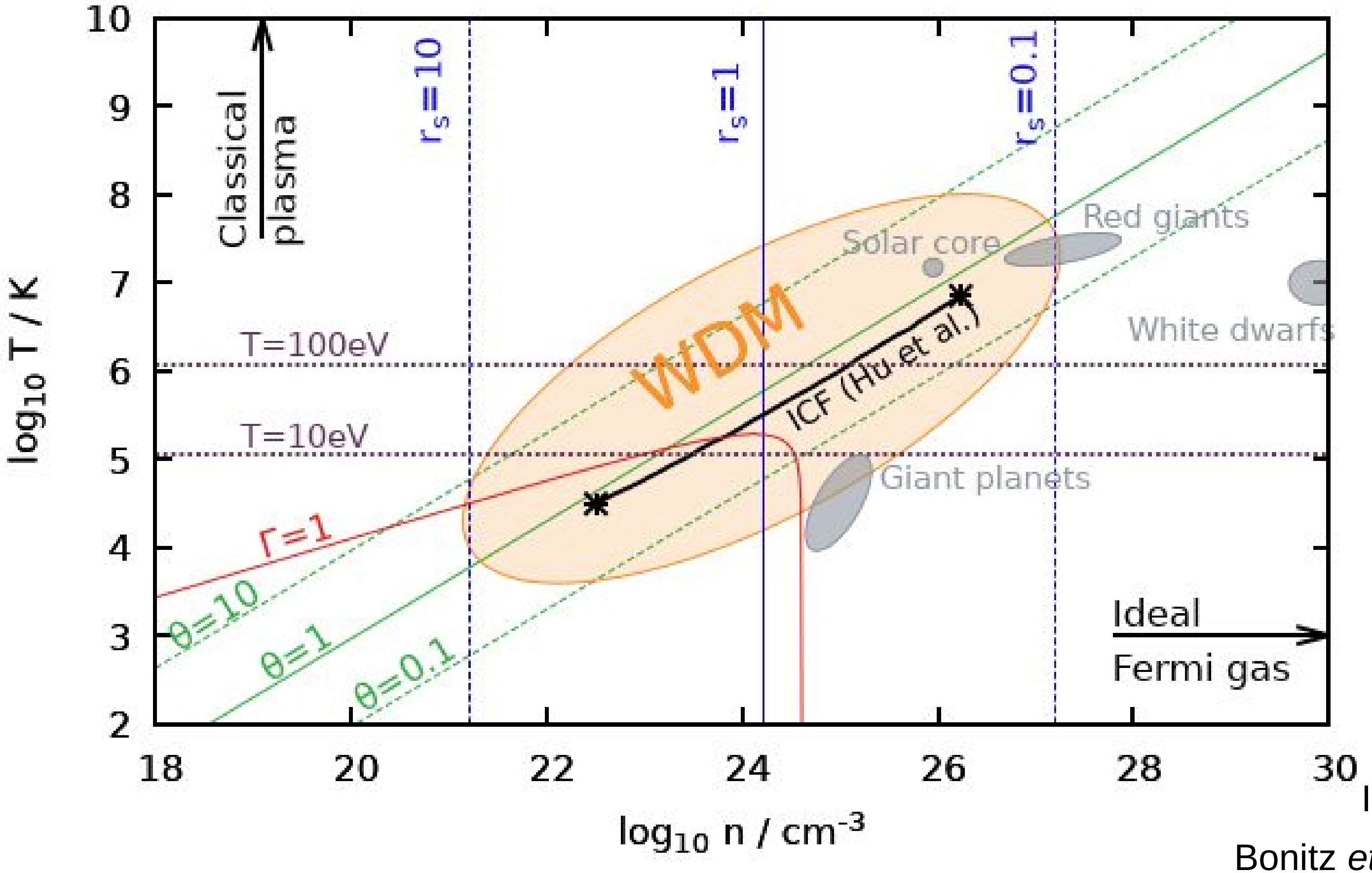
- behavior of matter under compression
- transition of condensed matter into plasma state
- properties under strong excitation

- behavior of atoms, molecules: Modification of bound states: IPD, continuum lowering

Simulation approaches:

- capture correlations, quantum and spin effects
- resolve relevant time scales

Quantum electrons: „Warm dense matter“ (WDM)*



$$\Theta = \frac{k_B T}{E_F}$$ quantum degeneracy

$$r_s = \frac{d}{a_B}$$ coupling (T=0)

$$\Gamma = \frac{e^2}{d k_B T \frac{2\sigma+1}{n\Lambda^3} I_{3/2}(\beta\mu)}$$

generalized coupling par.

ICF path: Hu *et al.* Phys. Plasmas 2015

Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

Main driver: recent breakthroughs in ICF a the NIF

H. Abu-Shawareb *et al*, “Lawson criterion for ignition exceeded in an inertial fusion experiment,” Phys. Rev. Lett. **129**, 075001 (2022). [August 8]

H. Abu-Shawareb *et al*, “Achievement of Target Gain Larger than Unity in an Inertial Fusion Experiment“, Phys. Rev. Lett. **132**, 065102 (2024) [subm. 27 Oct 2023, published Feb. 5 2024]

364 and 212 citations (Nov 13 2025)

2022 Dawson Award for Excellence in Plasma Physics Research for „NIF’s Burning Plasma Team“

DOE Press conference on Dec 13 2022 (quoting „historic shot“ of Dec 5): global news response

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Astonishing impact on politics and research world-wide: many startups + public investment

US: DOE Fusion Science & Technology Roadmap, > $ 9 B private investments, public infrastructure by mid 2030s (magnetic fusion and ICF)

Germany: novel „High-tech agenda“ lists fusion as one of 6 focus areas
Action plan of federal government „Germany on track towards a fusion power plant“
Goal: „build the first fusion power plant in Germany“ (demo)
Public Investment: € 1.7B until 2029
Focus on research (magnetic fusion and ICF)

2.3 Quantum effects of heavy particles

Astrophysics & lab

- q effects of nuclei important for properties of light atoms

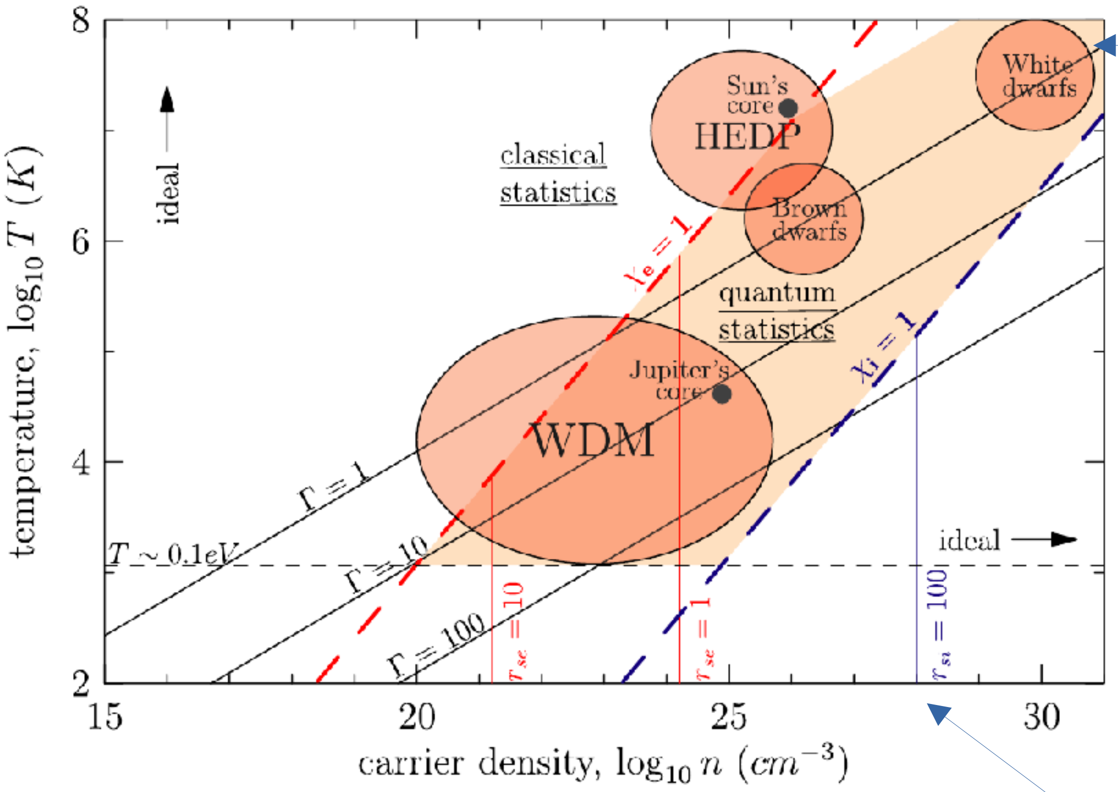
- at high density crystallization of ions

- still higher pressure: melting of ion crystal

- for ion crystal exists M_{cr}~80, mass ratio $M=m_i/m_e$
  prediction of hole crystallization

  In semiconductors

Bonitz et al. PRL **95**, 235006 (2005)



ion crystal in E-Fermi gas

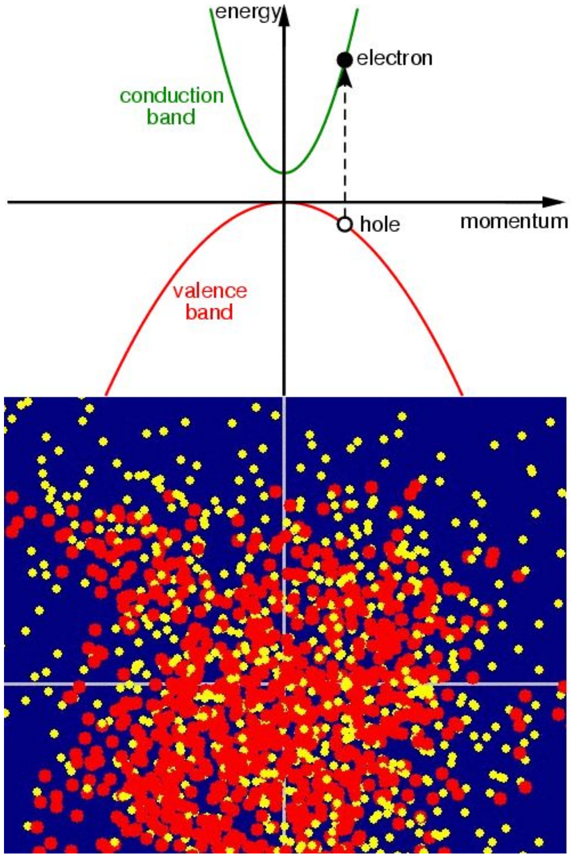
neutron star cores
(ion quantum liquid)

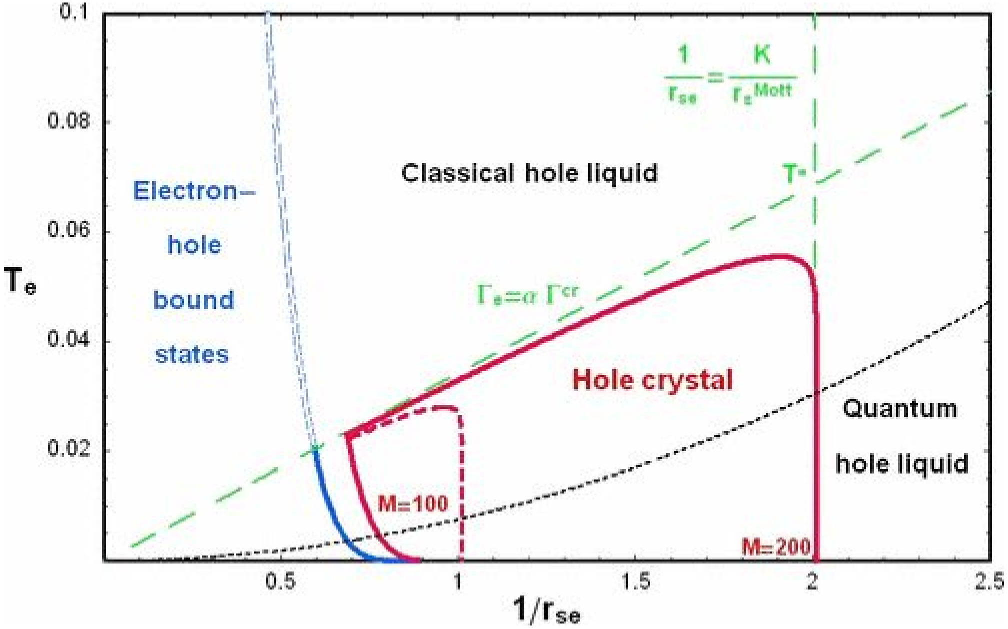
$\chi_i = \chi_e / M^{3/2}$

Quantum melting

The hole/ion crystal and its quantum melting

Link to video





density$^{1/3}$ →

Path integral MC simulations by V. Filinov
Bonitz et al. PRL **95**, 235006 (2005), Phys. Rev. Focus

Large hole mass in rare earth semiconductors, e.g. Tm[Se, Te], Wachter et al., PRB **69**, 094502 (2004)

2.4 Exotic quantum plasmas (A)

A. Condensed Matter

- electron gas in metals
- electron-hole plasma in semiconductors, including 2D quantum wells, 1D quantum wires, superlattices

1950s, 1960s: Strong impact of plasma physicists

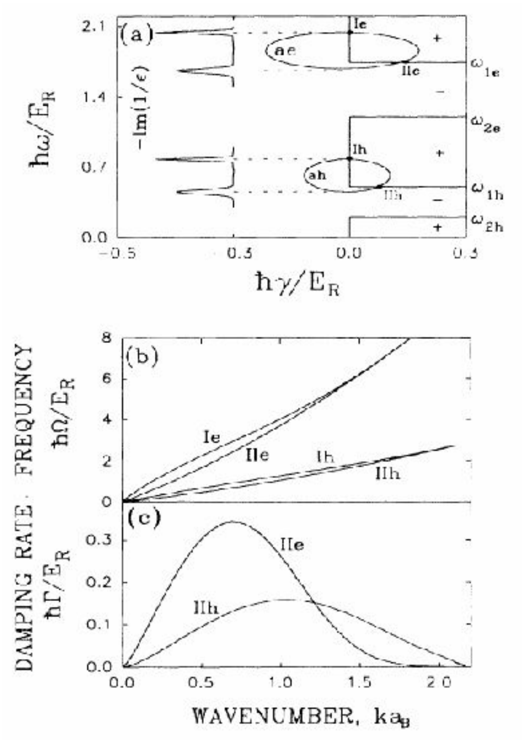
Examples:
- theory of fluctuations (Klimontovich)
- dielectric theory: quantum Vlasov / RPA dielectric function (Klimontovich, Silin, Rukhadse)
- plasmon dispersion
- Nonlinear plasma oscillations, instabilities (Bakshi *et al.*, 1990, Das Sarma *et al.*, Bonitz *et al.*)

- plasmon undamping in isotropic 3D semiconductors, accelerated thermalization (Lampin, MB *et al.* 1999)

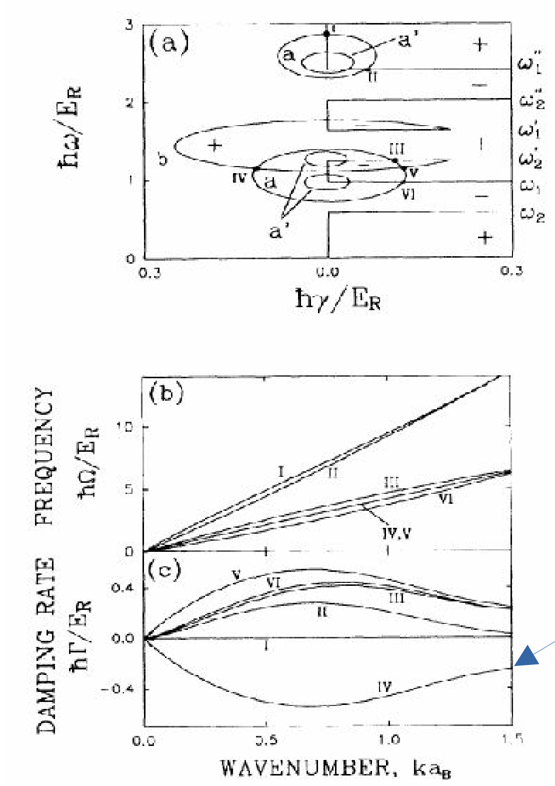
- plasmon instabilities in 1D quantum wires (Bonitz *et al.* 1993): create bump on tail instability using two laser pulses

Plasmon instability in a 1D quantum wire (Electron-hole plasma)

One laser pulse:
Only stable plasmons



two laser pulses:
one unstable plasmon



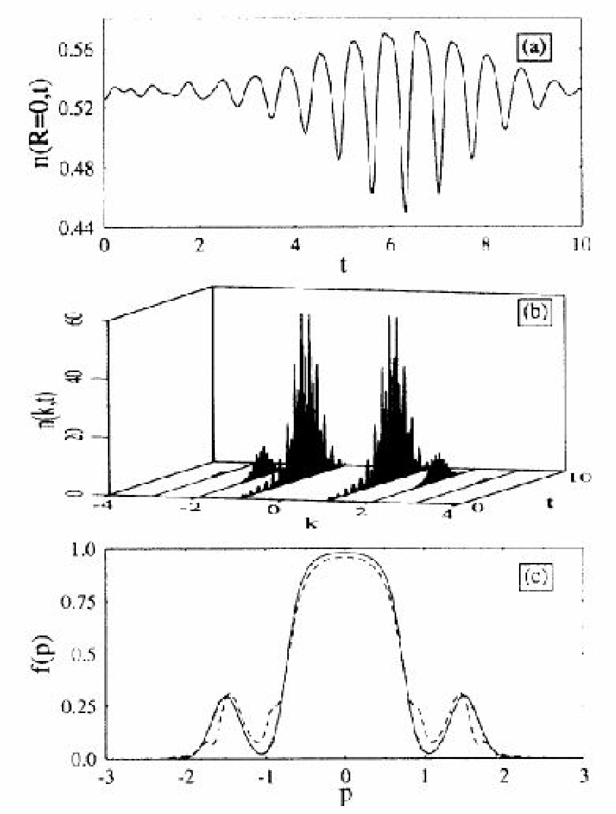
plasmon dispersion from
zeroes of ε in complex plane:
Re ε(ω,k) = Im ε(ω,k) = 0

Unstable plasmon

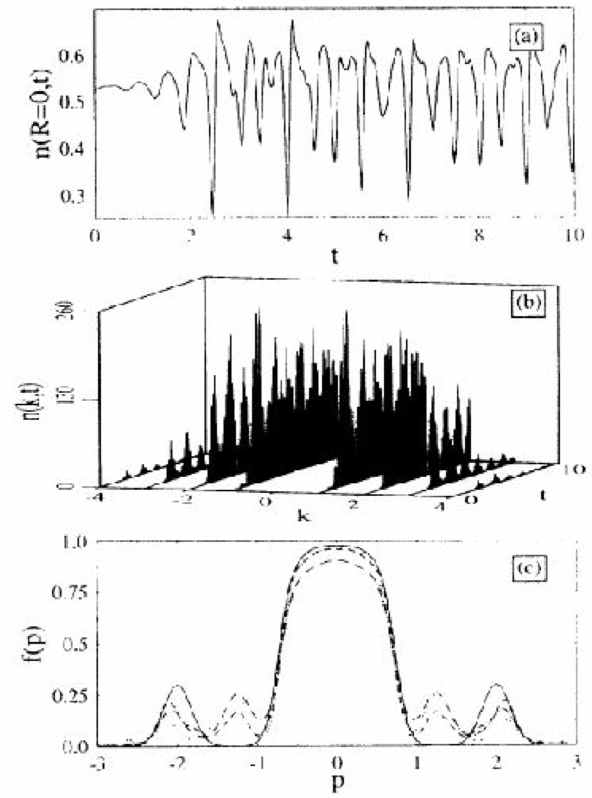
Bonitz *et al.*, PRL **70**, 3788 (1993)

Nonlinear stabilization of plasmon instability in a 1D quantum wire

Weak excitation



strong excitation



Solution of nonlinear Quantum Vlasov eq.

Bonitz *et al.*, PRB **20**, 15059 (1994)

Quantum plasmas in Condensed Matter: a word of caution

- electron gas in metals
- electron-hole plasma in semiconductors, including 2D quantum wells, 1D quantum wires, superlattices

Small impact of previous direct extensions of plasma physics results to e-h plasmas

Reason: standard plasma physics approaches/models are too simple/outdated

- model of parabolic dispersion has little to do with realistic semiconductor [band structure $E_a(p)$]
- finite carrier life time, phonon effects, excitons etc. cannot be neglected
- current approaches use condensed matter methods: DFT, quantum kinetic theory

Very often ignored. Typical example: from abstract of a paper in Phys. Plasmas 2024:

„ ...The applications extend to the stream instability in quantum charge transport in

metals, semiconductors, plasmonic devices…“

Bold unproven claims! Should be critically verified by referees, editors

2.4 Exotic quantum plasmas (B)

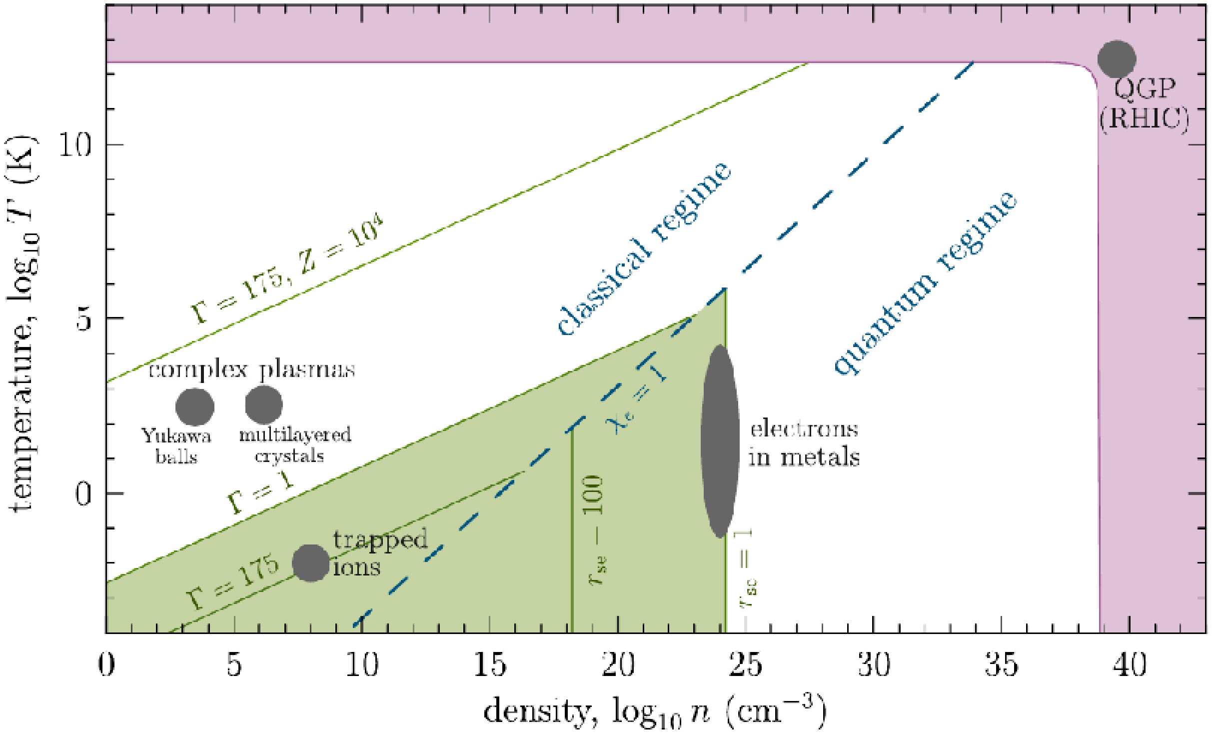
B. quark gluon plasma (QGP)
extreme T or p

Pink: range of QGP (qualitative)

Break up of hadrons similar to thermal or pressure ionization of plasmas, similar phase diagram

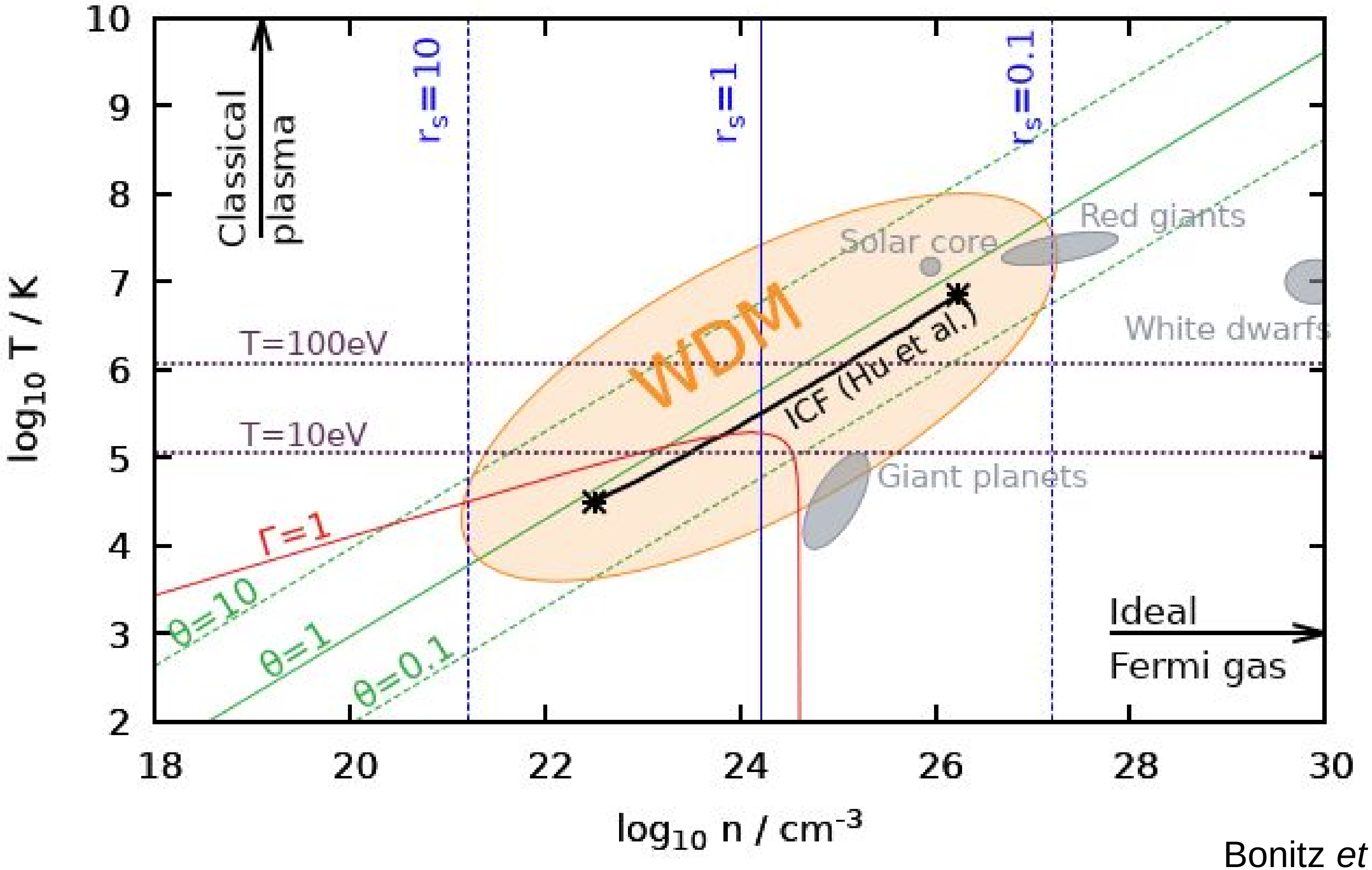
Similar simulation methods can be tried, e.g. „color path integral Monte Carlo Simulations“,
V. Filinov, MB *et al.* PRC **87**, 035207 (2013)

Good (qualitative) agreement with lattice QCD



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

3. Methods for Quantum plasmas/„Warm dense matter“*



$$\Theta = \frac{k_B T}{E_F}$$ quantum degeneracy

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generalized coupling par.

Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

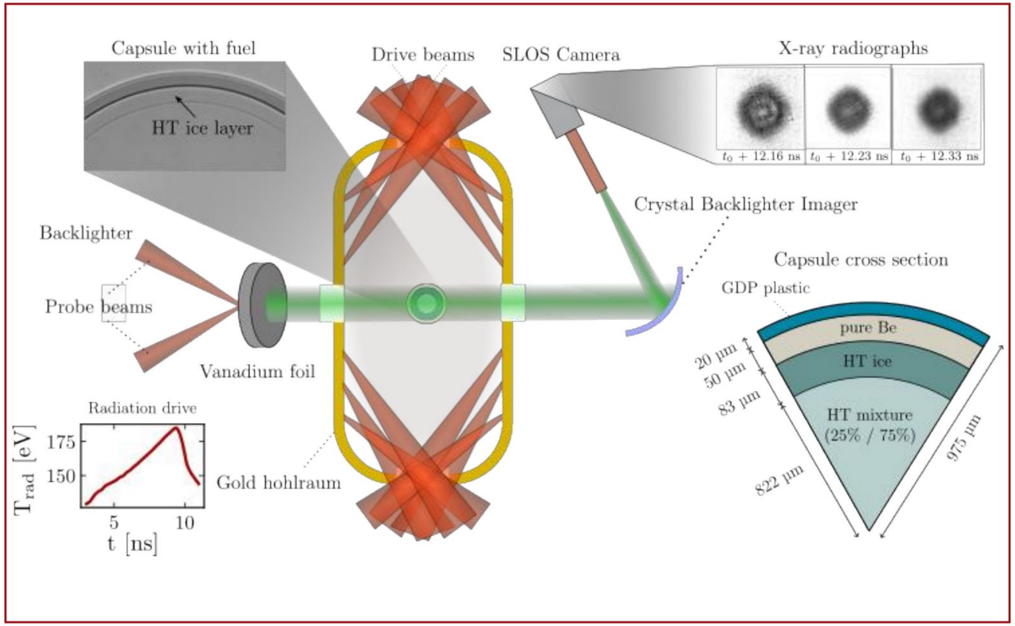
Warm dense matter: challenges and opportunities

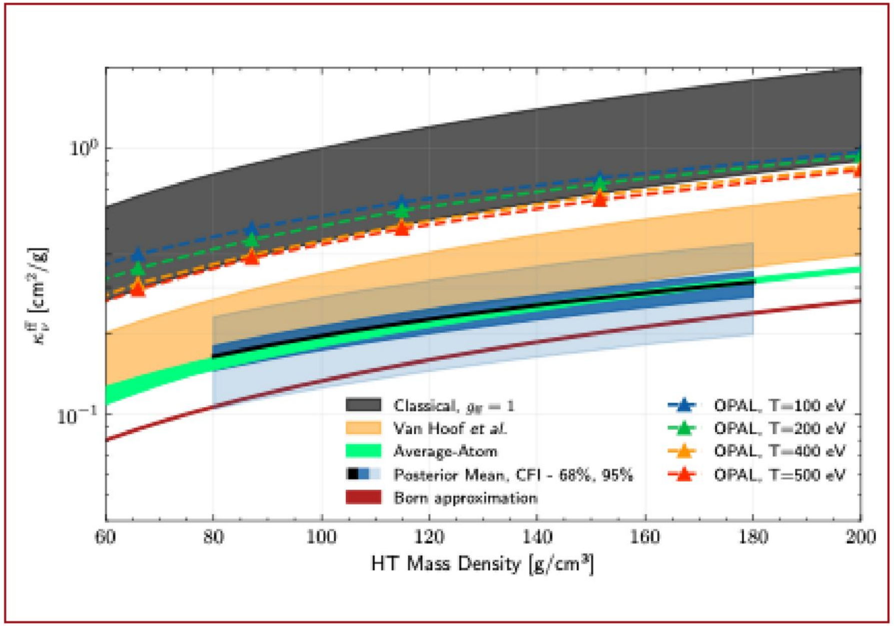
1. Challenges: - mix of condensed matter and plasma phases
- condensed matter at high temperature (not ground state)
- plasma partially ionized
- strong many-particle effects, quantum screening, bound state renormalization
- quantum and spin effects of electrons (delocalization, exchange, Pauli blocking)
- short life time of compressed states
- high density: short plasma period, plasma optically non transparent

2. Dramatic recent progress in **WDM experiments**, in particular, at the NIF

3. Progress in **WDM diagnostics**, accuracy, e.g., X-ray Thomson scattering (XRTS)

Measurement of the opacity of hydrogen at stellar conditions





Experiments at NIF determine the free free opacity of hydrogen at 800-1000ρ_{solid} and T~200 eV

Platform: J. Lütgert et al., Physics of Plasmas 29, 083301 (2022)
Theory: S. Schumacher et al., CTPP e70002 (2025)
Results: S. Schumacher, J. Lütgert, M. Bethkenhagen, T. Döppner, D. Kraus et al., in prep.

Talk Monday, 11:42, HED radiation physics, room 203

Warm dense matter: challenges and opportunities

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2. Dramatic recent progress in **WDM experiments**, in particular, at the NIF

3. Progress in **WDM diagnostics**, accuracy, e.g., X-ray Thomson scattering (XRTS)

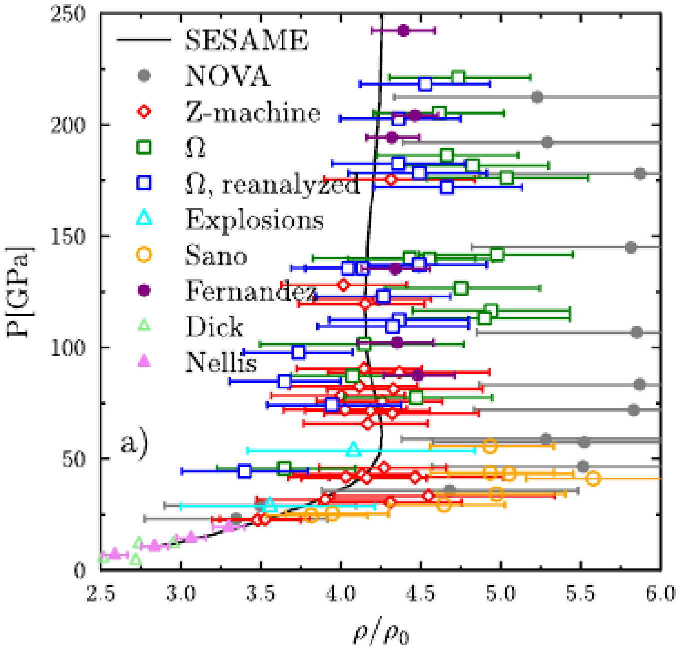
4. Model-free high precision analysis of XRTS data (temperature diagnostic)
T. Dornheim *et al.*, Nat. Comm. Phys. **13**, 7911 (2022), Phys. Plasmas **30**, 042707 (2023)

5. progress in theory and simulations: traditional (hydrodyamics, kinetic theory) and more recent methods: DFT, TDDFT, Green functions, quantum Monte Carlo

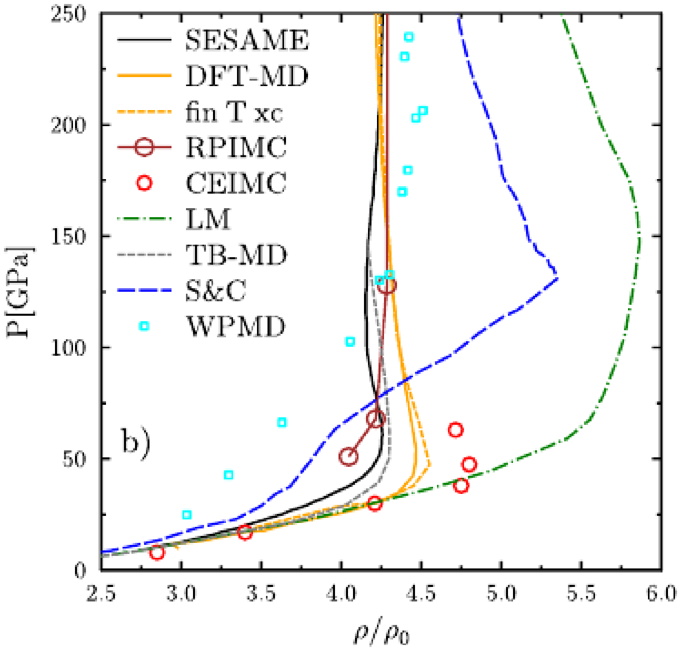
Difficult theory-experiment comparisons in WDM

Example: hydrogen hugoniot (1996-2000, unknown T, model input)

Experiment



Theory



Experiment:
- large scatter of data
- large statistical errors
- poorly known system. errors

Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Difficult theory-experiment comparisons in WDM

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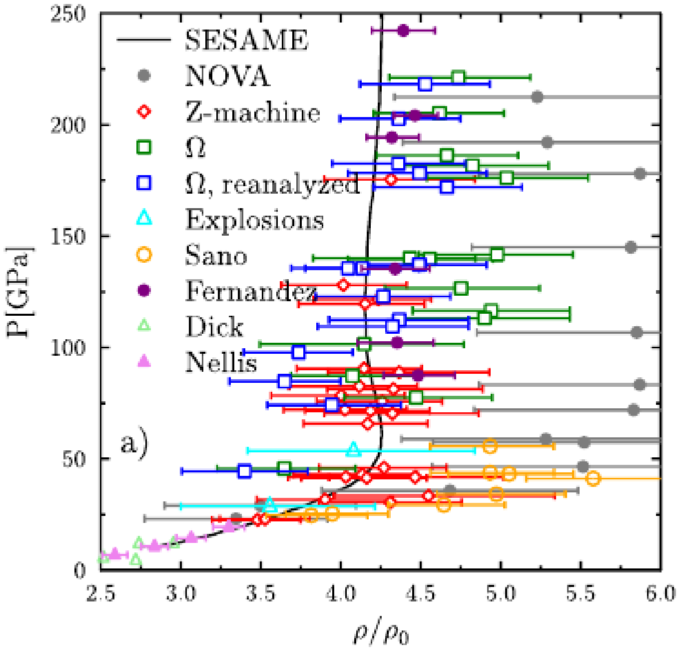

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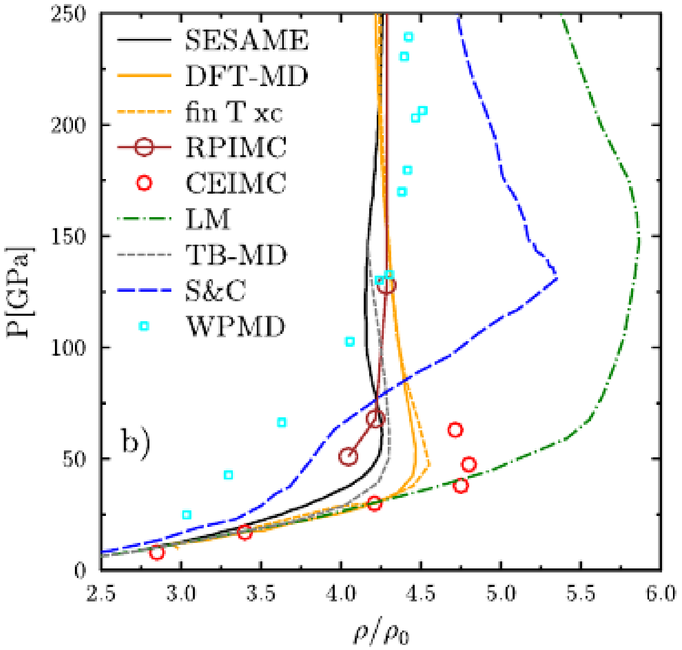

Experiment:
- large scatter of data
- large statistical errors
- poorly known system. errors

Theory:
- general goal (of course): agreement with experiment
- here: agreement does not mean that theory is correct

needed:
- independent, reliable results

Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

RPIMC, CEIMC: quantum MC; LM: linear mixing, S&C: Saumon/Chabrier
WPMD: wave packet MD

How accurate are the simulations?

How large are the statistical errors in the simulation?

How large are the systematic errors?
What are the assumptions being made?
What are the validity limits (parameter range) of the simulation?

In practice: accuracy of most simulation results not known. **No predictive capability**

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How large are the statistical errors in the simulation?

How large are the systematic errors?
What are the assumptions being made?
What are the validity limits (parameter range) of the simulation?

In practice: accuracy of most simulation results not known. **No predictive capability**

Choice of approximations based on experience, intuition

Examples: E_{xc} of DFT, selfenergy of Green functions, Coulomb logarithm, IPD,
screening parameters, hydrodynamic closures etc.

Novel opportunity: use accurate, predictive simulations as benchmark

Simulations with predictive capability

They exist!	**Even though, they have limitations**
- Solution of Schrödinger's equation (CI)	Only N=2...20, microcanonical ensemble
- DMRG simulations	Only 1D
- Quantum Monte Carlo simulations without nodal or other restrictions	only for parameters permitted by fermion sign problem, only WDM in equilibrium
Additionally: exact results for models: Ideal gas, uniform electron gas*, OCP etc.	No experimental realization, but useful special cases for simulations (match Θ, Γ, r_s)

Red: relevant for WDM, *Dornheim et al., Phys. Rep. **744**, 1-86 (2018)

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Computer experiments are source for benchmarks, complementing real experiments

Recent breakthroughs in first-principles/predictive QMC simulations for WDM in our group

Physics Reports **744**, 1-86 (2018)

The uniform electron gas at warm dense matter conditions

Tobias Dornheim [1], Simon Groth [1], Michael Bonitz *

Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, 24098 Kiel, Germany

PHYSICAL REVIEW LETTERS **121,** 255001 (2018)

***Ab initio* Path Integral Monte Carlo Results for the Dynamic Structure Factor of Correlated Electrons: From the Electron Liquid to Warm Dense Matter**

T. Dornheim,[1] S. Groth,[1] J. Vorberger,[2] and M. Bonitz[1]

[1]*Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstraße 15, D-24098 Kiel, Germany*

[2]*Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany*

PHYSICAL REVIEW E **108**, 055212 (2023)

Equation of state of partially ionized hydrogen and deuterium plasma revisited

A. V. Filinov * and M. Bonitz †

Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstraße 15, 24098 Kiel, Germany

The test case: the warm dense uniform electron gas

Exchange correlation energy at different temperatures vs. density parameter

← density

Restricted PIMC simulations
Brown *et al.*, PRL **110**, 148405 (2013)
unknown accuracy of nodes

No fermionic PIMC at high density
Due to fermion sign problem

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density

density

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unknown accuracy of nodes

No fermionic PIMC at high density
Due to fermion sign problem

Novel PIMC approach in Fock space (CPIMC): Schoof, MB et al., CPP (2012)
no sign problem at high density, no systematic error, very high accuracy

Schoof *et al.*, PRL **115**, 130402 (2015)

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no sign problem at high density, no systematic error, very high accuracy

Schoof *et al.*, PRL **115**, 130402 (2015)

Extend to low densities with novel PIMC approach (PB-PIMC):
Dornheim, MB et al., NJP (2015)

combination CPIMC-PB-PIMC yields exact results for Θ>0.5
Dornheim *et al.*, PRL **117**, 156403 (2016)

The test case: the warm dense uniform electron gas

- extension to thermodynamic properties
  over entire n-T range

- parametrization of xc free energy,
  Input for DFT simulations (LDA)

- rigorous benchmark for other methods

- extension to dynamic properties (dyn.
  Structure factor), Dornheim *et al.*, PRL (2018)

Review:
Dornheim, Groth, Bonitz, Phys. Rep. **744**, 1-86 (2018)

REVIEW ARTICLE | NOVEMBER 13 2024

Toward first principles-based simulations of dense hydrogen

Special Collection: Papers from the 65th Annual Meeting of the APS Division of Plasma Physics , Reviews and Tutorials in Inertially Confined Plasmas, High-Energy Density Plasma Science, and Warm Dense Matter

Michael Bonitz ; Jan Vorberger ; Mandy Bethkenhagen ; Maximilian P. Böhme ; David M. Ceperley ; Alexey Filinov ; Thomas Gawne ; Frank Graziani ; Gianluca Gregori ; Paul Hamann ; Stephanie B. Hansen ; Markus Holzmann ; S. X. Hu ; Hanno Kählert ; Valentin V. Karasiev ; Uwe Kleinschmidt ; Linda Kordts ; Christopher Makait ; Burkhard Militzer ; Zhandos A. Moldabekov ; Carlo Pierleoni ; Martin Preising ; Kushal Ramakrishna ; Ronald Redmer ; Sebastian Schwalbe ; Pontus Svensson ; Tobias Dornheim

Phys. Plasmas **31**, 110501 (2024)
(86 pages, 800 Refs.)

8 of the authors at PNP 2024 conference,
Oxford Univ, LMH (organizer: G. Gregori)

Simulations relevant for warm dense matter (1)*

TABLE III. First-principles simulation methods for dense hydrogen in thermodynamic equilibrium at finite temperature ordered by their expected accuracy. Numbers I.–V. in the column "Observables" refer to the list in Sec. III A 2. $G^M(q,\tau)$: Matsubara Green function of "imaginary time" τ. The column "benchmarks" lists available relevant benchmarks of pressure (p), interaction energy (V), degree of ionization (α). For new benchmarks provided in this paper, the relevant figures are indicated, for details see footnotes and main text. For a more complete list of observables, see Tab. VI.

Method	Observables	approximations	main limitations	benchmarks	Section
Fermionic PIMC (FPIMC)	I., II. $G^M(q,\tau)$ nonlinear response	number of particles N number of high-T factors P	fermion sign problem $\Theta \gtrsim 0.5$ statistical errors	N/A	III E 1
Restricted PIMC (RPIMC)	I.	fixed node approximation	$\Theta \gtrsim 0.1$	p, α based on FPIMC Figs. 14, 23	III E 4
CEIMC	I., IV. DOS, energy gap	BO approximation Electrons in ground state using VMC or RQMC	$\Theta \lesssim 0.1$	N/A	III F
Green functions	I., II., III., IV. $A(q,\omega)$ DOS	Selfenergy Σ	moderate coupling strength	interaction energy based on FPIMC[a] model systems	III H 3
Kohn-Sham-DFT-MD	I., V. III.[b]	BO approx., XC functional		p for LDA, PBE and KDT16 Fig. 15	III C
Linear-response TDDFT	II.	BO approx., XC functional XC-kernel	no reliable dynamic XC-kernel	N/A[c]	III H 4
Orbital free DFT-MD	I., V.	BO approx., XC functional non-interacting free-energy functional	accurate only for relatively high T due to free-energy functional	N/A	III C

[a] Benchmarks of potential energy of Ref. 117 for jellium.
[b] Optical properties can be computed from a set of KS-orbitals via the Kubo-Greenwood relation that does, however, not include electron-electron collision, see Sec. IV E.
[c] Note that LR-TDDFT results for different XC-functionals and XC-kernels can be benchmarked against PIMC results for the ITCF $F(\mathbf{q},\tau)$ [cf. Eq. (121)] in future studies.

Observables

I. TD properties: p, E, g(r), S(q)

II. e-dynamic properties: $S_{ee}(q,\omega)$, $F_{ee}(q,\tau)$

III. e-transport and opt. prop.s: $\sigma(\omega)$, $\lambda(\omega)$, $\kappa(\omega)$

IV. e-spectral properties: DOS, $A(q,\omega)$

V. Ion dynamic properties: $S_{ii}(q,\omega)$, $D_i(\omega)$

*Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

Quantum Monte Carlo simulations for dense H*

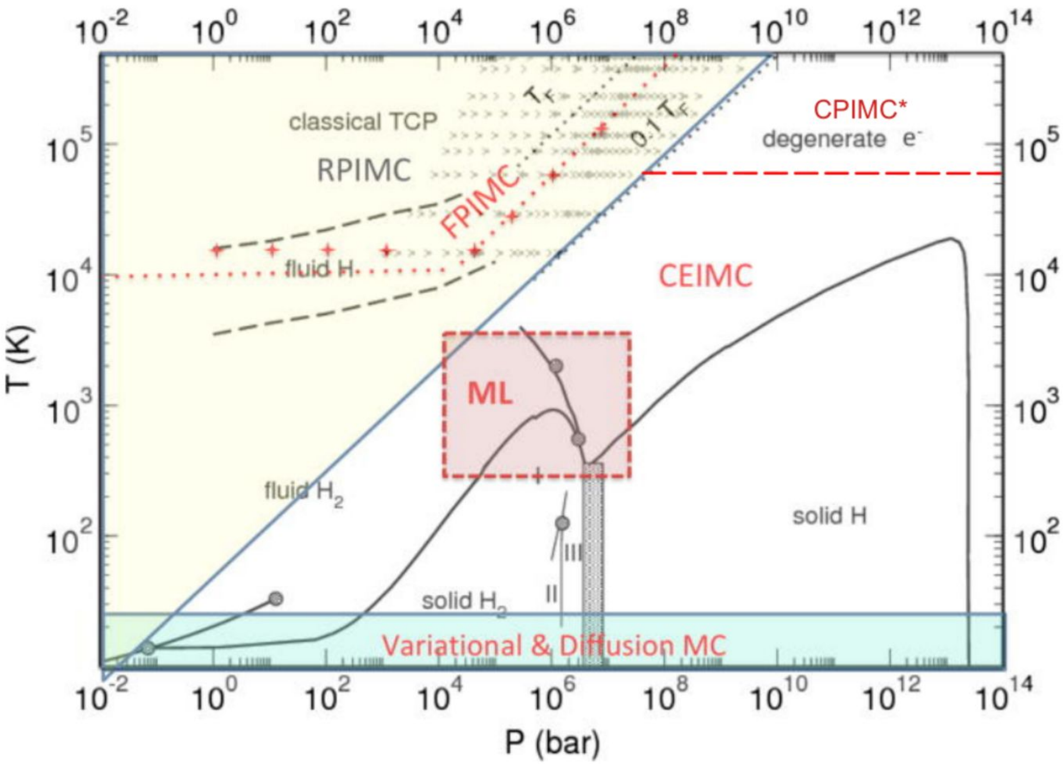


FIG. 8. Applicability range of different simulation methods across the hydrogen phase diagram. RPIMC: restricted PIMC, extends to about $0.1\,T_F$, Sec. III E 4, CEIMC: coupled electron-ion Monte Carlo, Sec. III F, FPIMC: fermionic PIMC, extends to about $0.5\,T_F$ and was applied to temperatures above 10 000 K, Sec. III E 5. ML denotes region fit by QMC-based machine learning force fields in Ref. 206 and also the region where CEIMC has been applied. Red pluses show FPIMC simulation points from Ref. 115 that mark the border of what is feasible today. Light black crosses show regions covered by the RPIMC database[114]. The other lines are introduced in Fig. 4.

CPIMC: high degeneracy, complementary to FPIMC

*M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Updated version from Vorberger *et al.*,
„Roadmap for Warm Dense Matter Physics“, 2025

Benchmarking RPIMC for dense H: Equation of state*

Average sign of fermionic PIMC

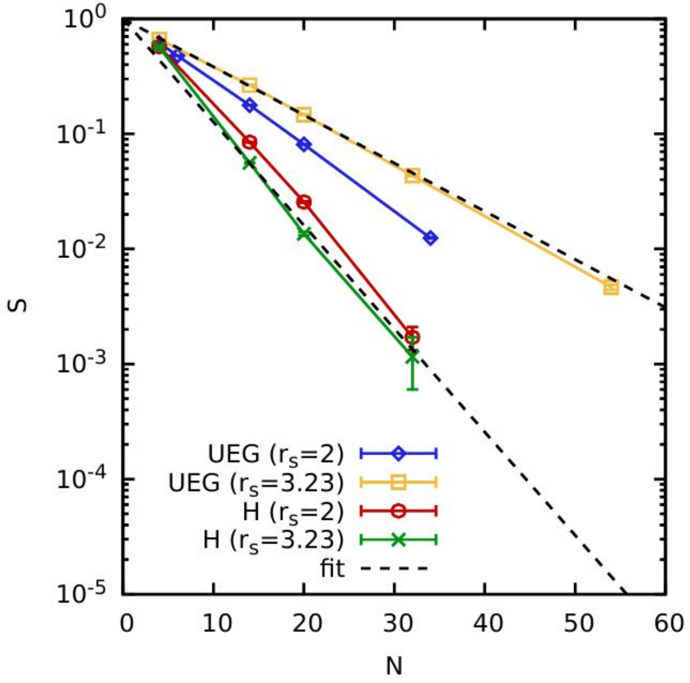
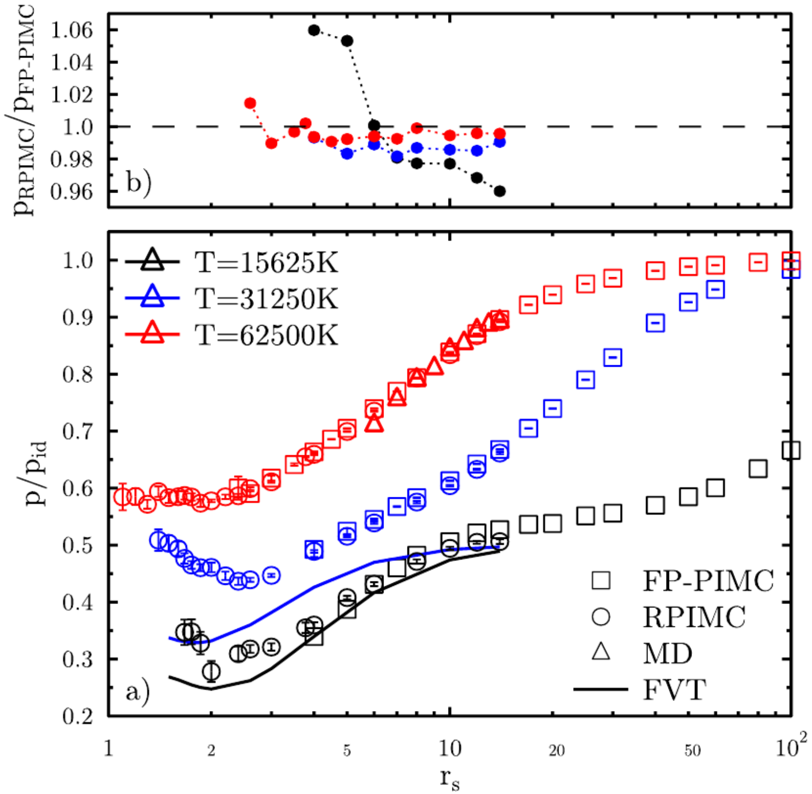


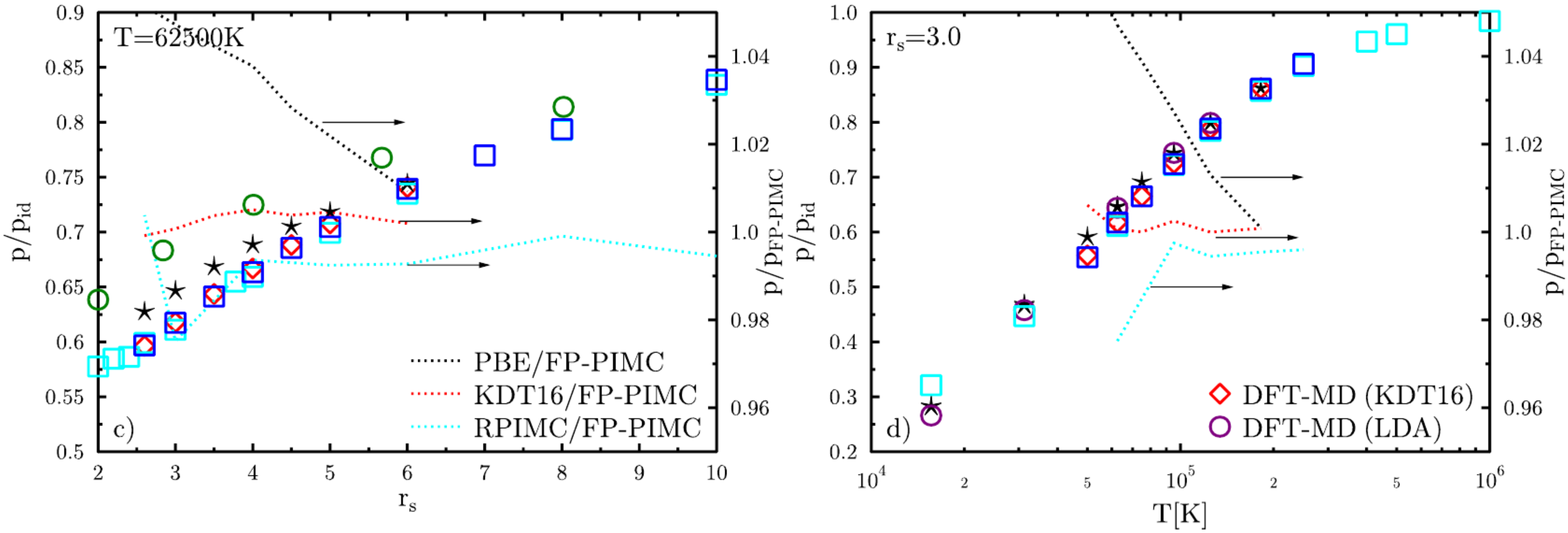
FIG. 10. Average sign S as a function of the number of electrons N at the electronic Fermi temperature $\Theta = 1$, for $r_s = 2$ ($\rho = 0.34\,\mathrm{g/cm^3}$, $T = 12.53\,\mathrm{eV}$) and $r_s = 3.23$ ($\rho = 0.08\,\mathrm{g/cm^3}$, $T = 4.80\,\mathrm{eV}$). The dashed black lines show exponential fits to the PIMC data, cf. Eq. (70). Reproduced from Ref. 149 with the permission of the authors.



RPIMC validated by fermionic PIMC

*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)
M. Bonitz *et al.*, Phys. Plasmas 2024

Benchmarking DFT, Average atom simulations for dense H*

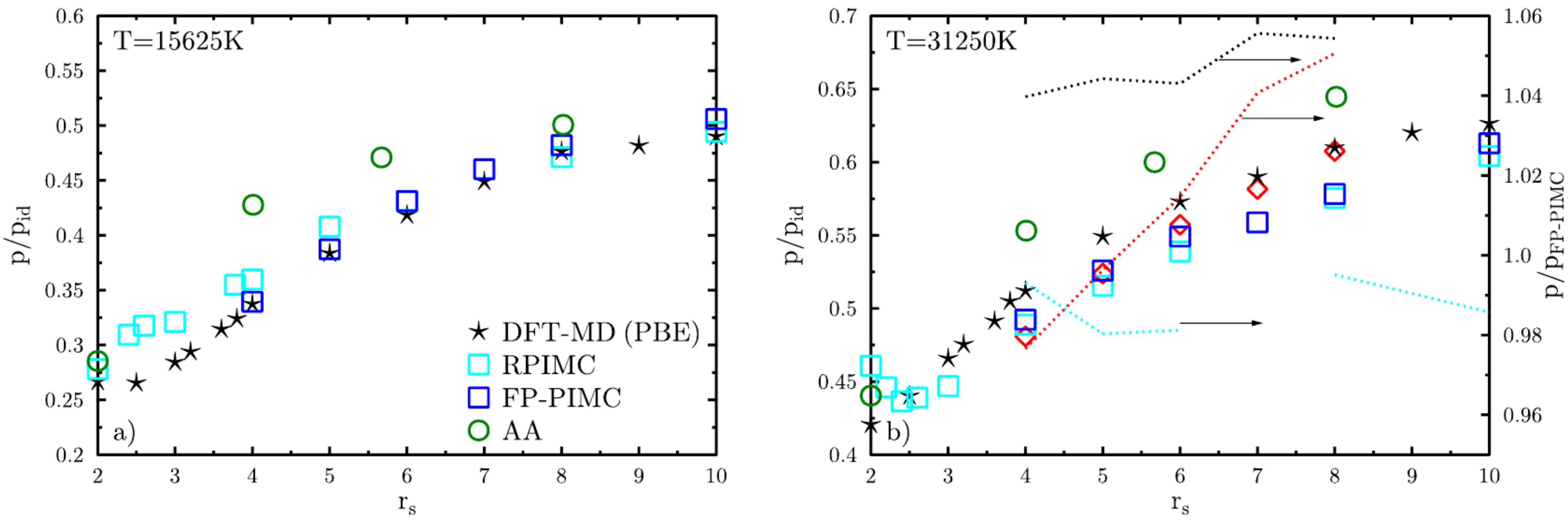


Dotted lines with arrows (right axes): relative error compared to FPIMC

*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)

Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

Benchmarking DFT, Average atom simulations for dense H*



*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)
Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

Dotted lines with arrows (right axes): relative error compared to FPIMC

4. Outlook: Toward precision modeling of quantum plasmas and ICF

Which method to choose? There is no „silver bullet“*

- There is no single simulation that can reliably predict all relevant properties of warm dense matter, including ICF.

- first principles/predictive approaches do not reach the scales of interest

- simulations that do extend to large length / time scales (quick and cheap) have untested accuracy, no predictive power

*Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

Which method to choose? There is no „silver bullet“*

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The alternative: development of set of different methods and their combination.
Preserve predictive capability as much as possible

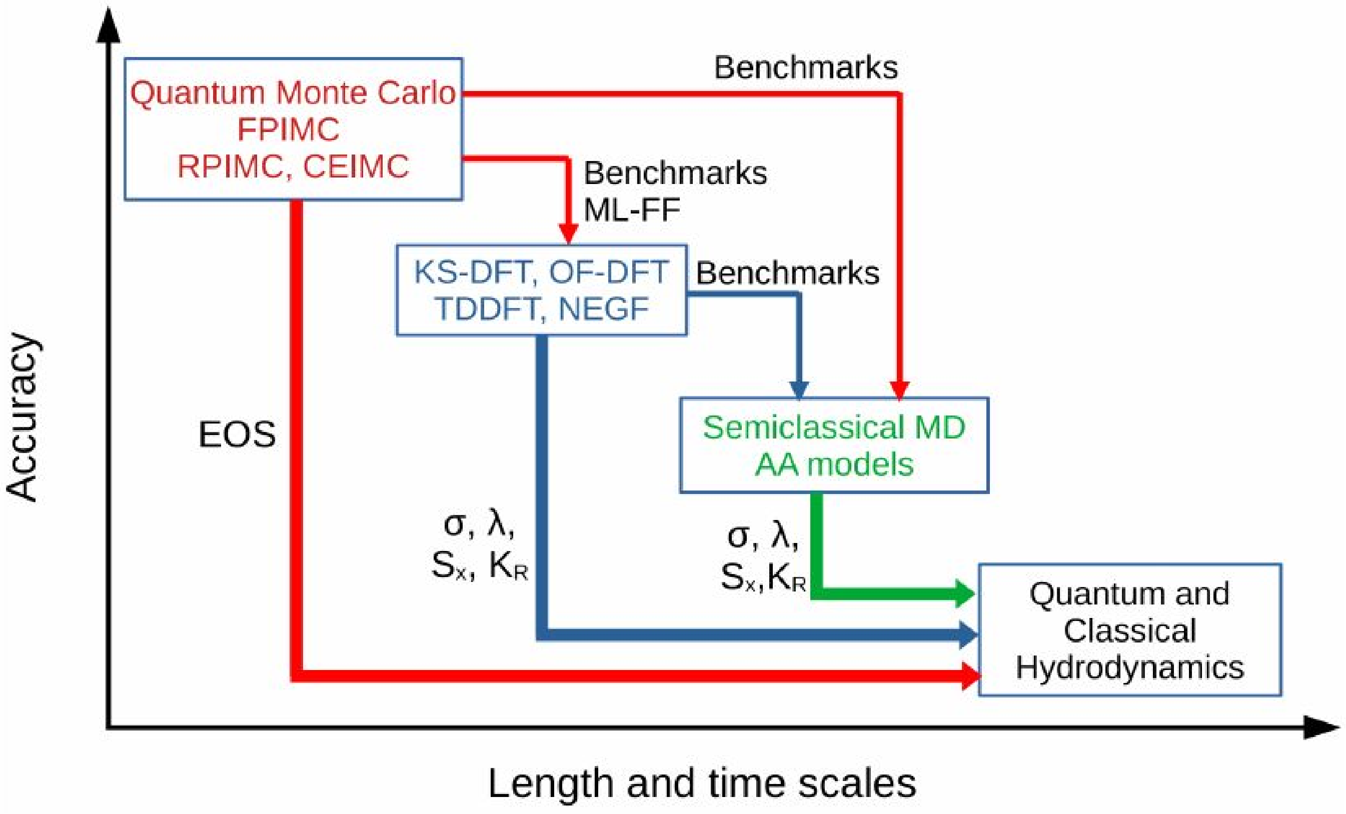
*Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

FPIMC „downfolding": smart combination of methods

Starting from predictive simulations (Fermionic PIMC)

→ selection of most accurate approximations of lower level models

→ reduction of resolution + increase of accessible r- and t-scales + preservation of acceptable accuracy



Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

FPIMC downfolding: Kohn-Sham-DFT

Exact theory

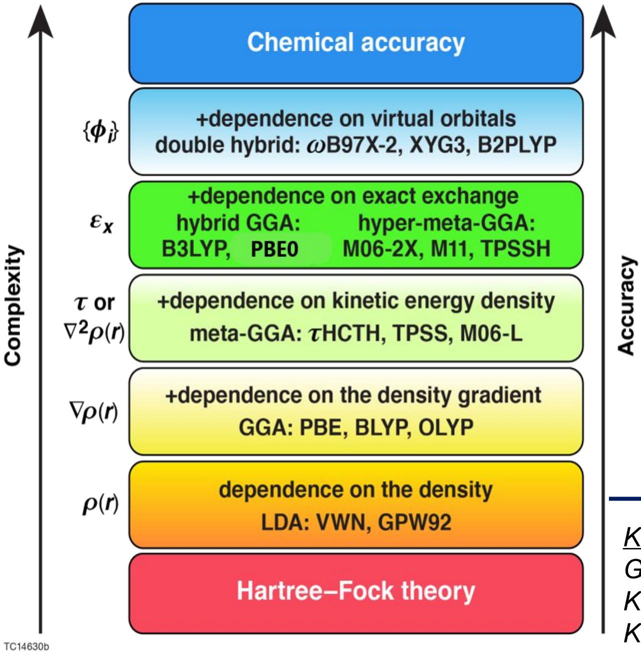
	Path integral	Density functional
Two exact Formulations W different resolution	Path integral representation	Density functional representation*, exact E_{xc}
Practical implementation	MC integration still exact, with statistical errors	Approximation: choice of approximate E_{xc}
„Measurement" microscopic observable [e.g., **g(r), S(k)**] for identical parameters	Simulation result (**function**) as exact benchmark	

* Hohenberg-Kohn theorems

S.X. Hu and V. Karasiev (U Rochester): Development of T-dependent XC functionals

LABORATORY FOR LASER ENERGETICS | University of Rochester

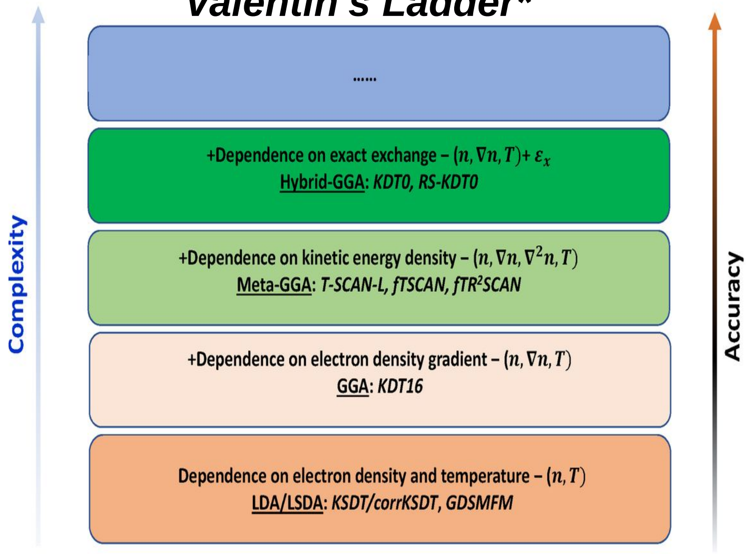
XC-functionals @ T=0 (cond. Matt. physics & Q chemistry)

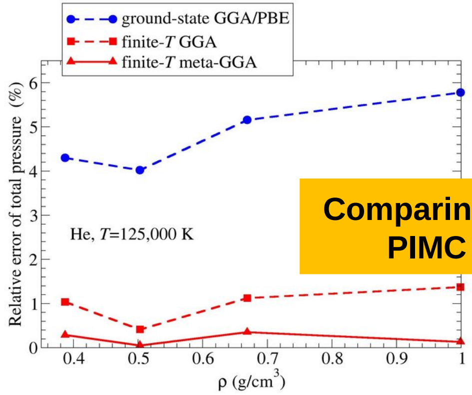


"Jacob's Ladder"

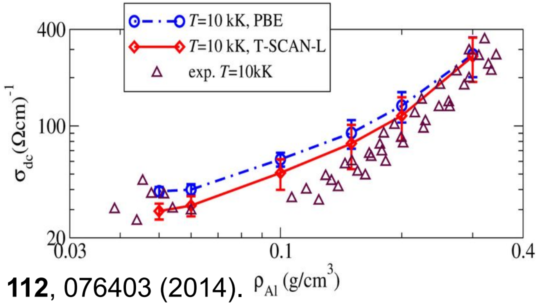
XC-functionals @ WDM

"Valentin's Ladder*"





Comparing to PIMC



KSDT: V. V. Karasiev, T. Sjostrom, J. Dufty, and S. B. Trickey, PRL **112**, 076403 (2014).
GDSMFM: T. Dornheim, S. Groth, T. Sjostrom, F. D. Malone, W. M. C. Foulkes, and M. Bonitz, PRL **117**, 156403 (2016).
KDT16: V. V. Karasiev, J. W. Dufty, and S. B. Trickey, PRL **120**, 076401 (2018).
KDT0: D. I. Mihaylov, V. V. Karasiev, and S. X. Hu, PRB **101**, 245141 (2020).
T-SCAN-L: V. V. Karasiev, D. I. Mihaylov, and S. X. Hu, PRB **105**, L081109 (2022).
fTSCAN: K. P. Hilleke, V. V. Karasiev, S. B. Trickey, R. M. N. Goshadze, S. X. Hu, PR Materials **9**, L050801 (2025).
RS-KDT0: A. A. Ellaboudy, V. V. Karasiev, D. I. Mihaylov, K. P. Hilleke, S. X. Hu, PRB **112**, 10xxxx (2025).

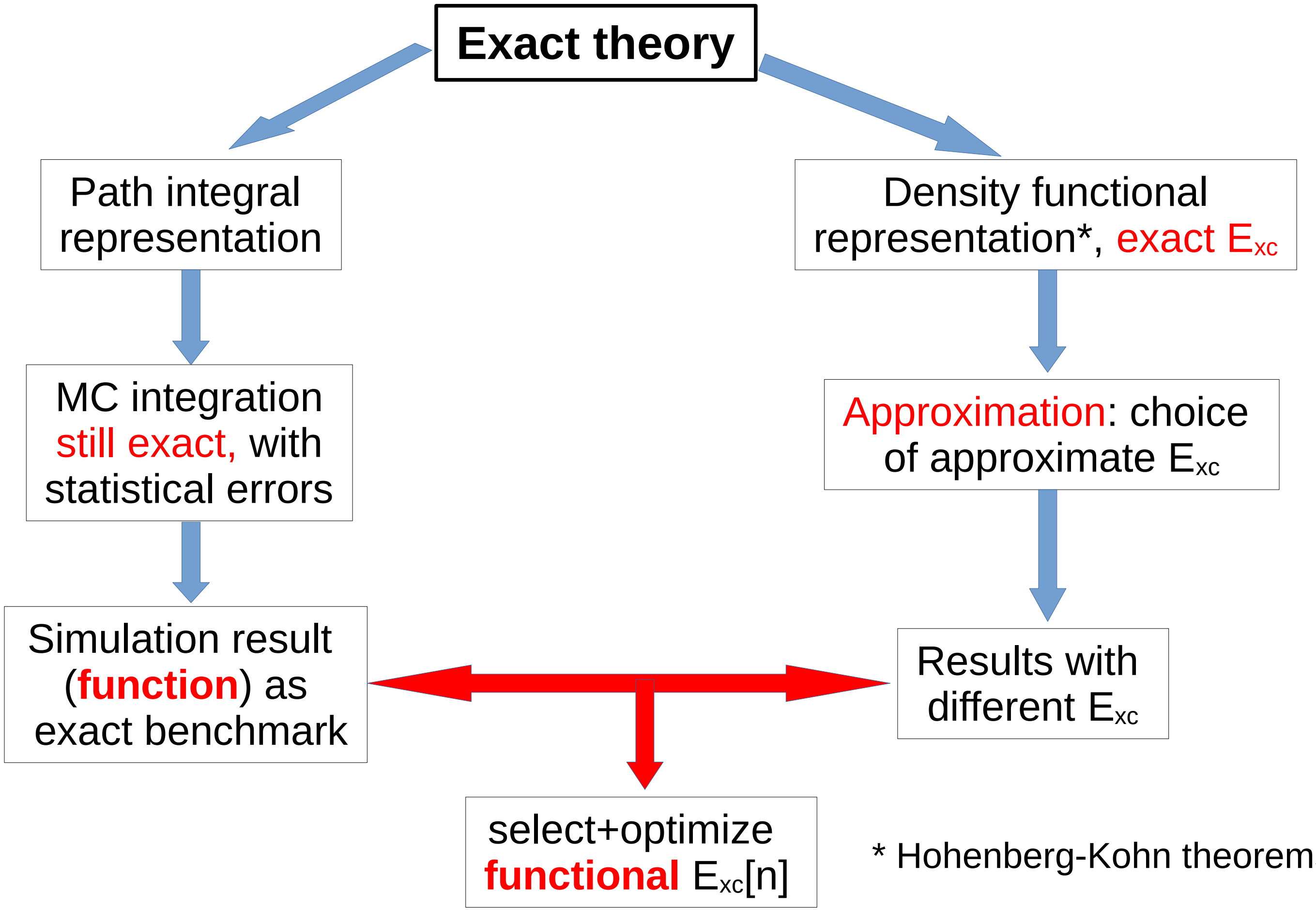
* S. X. Hu, "***Computational Methods for Quantum High-Energy-Density Physics***", (Oxford Univ Press, July (2026).

FPIMC downfolding: Kohn-Sham-DFT

Two exact
Formulations
W different resolution

Practical
implementation

„Measurement“
microscopic observable
[e.g., **g(r), S(k)**] for
identical parameters



* Hohenberg-Kohn theorems

FPIMC downfolding: Saha equation, IPD

Exact theory

Exact formulations

chemical picture

nonideal Saha equation
fractions α, x_A ↔ exact I^{eff}_{nl}

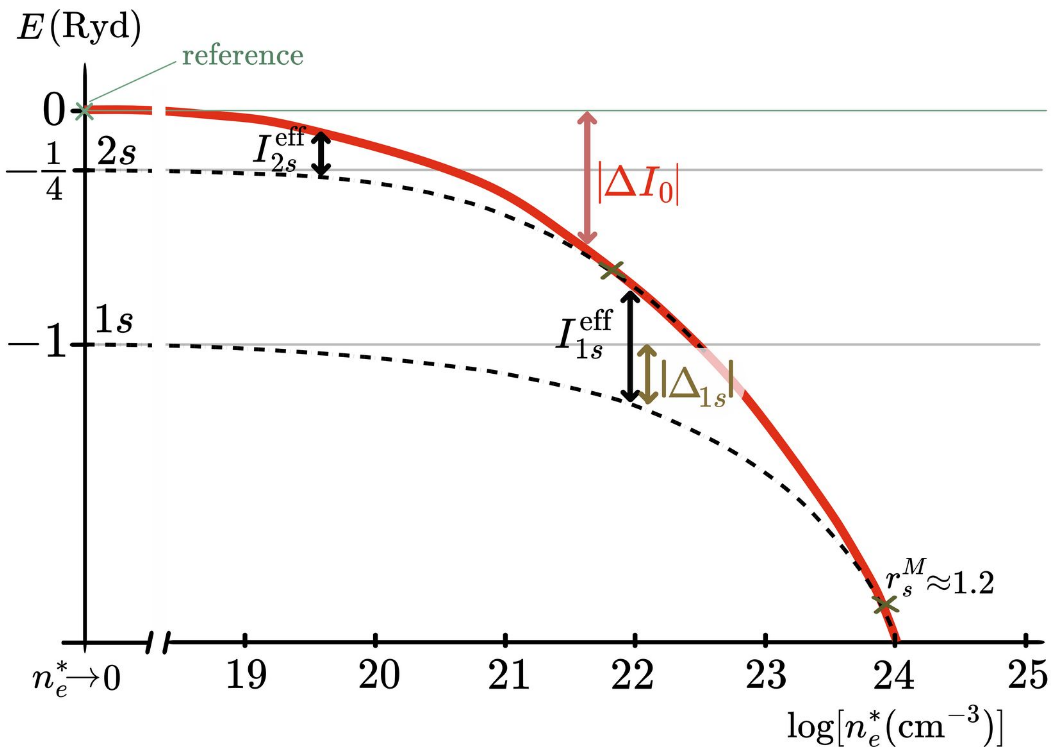
Practical implementation

Approximation: choice of approximate I^{eff}_{nl}

Measurement „fractions“ α, x_A

Compute approximate α, x_A

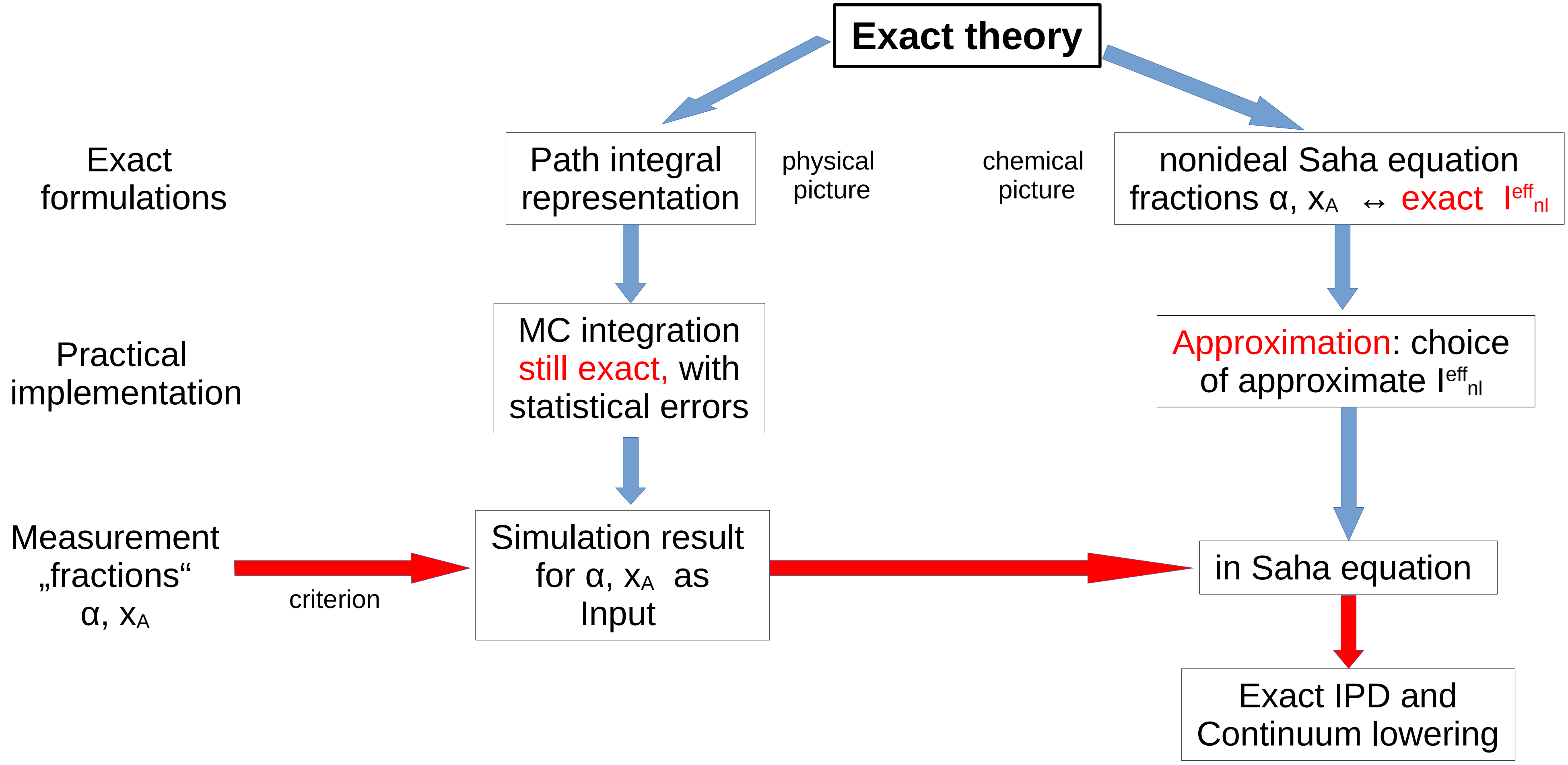
Standard picture of continuum lowering and Ionization potential depression (IPD)*



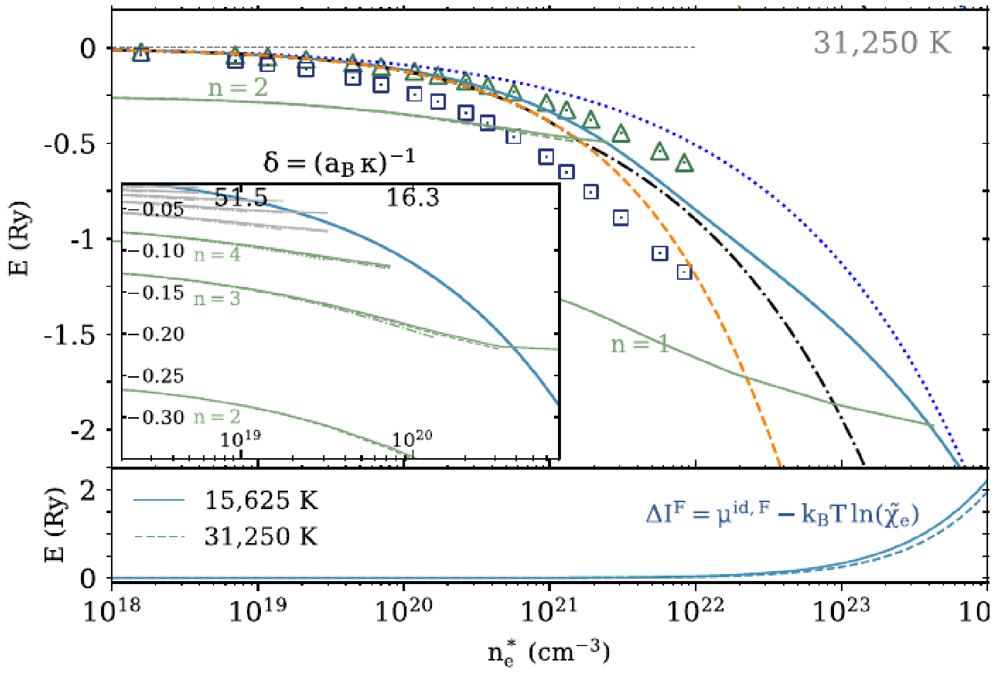
Model input for interaction contributions, yields IPD, Δ_{1s}
Solution of Saha equation yields α, x_A

*M. Bonitz and L. Kordts, CPP **65**, e70001 (2025)

FPIMC downfolding: Saha equation, IPD



FPIMC downfolding result for hydrogen continuum lowering*



△ FPIMC continuum w/o level shifts

□ FPIMC continuum with level shifts (from Rogers et al., PRA 1970)

Lines:
Debye model (dashes)
Stewart Pyatt (dots)
Ecker/Kröll (dash-dot)

ΔI^F: Fermi barrier
generalizes „Fermi surface rising"
S.X. Hu, PRL **120**, 119502 (2018)

use FPIMC results for α as input to obtain continuum lowering

* M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)
M. Bonitz and L. Kordts, CPP **65**, e70001(2025)

S.X. Hu (U Rochester): DFT results for warm dense carbon - Density of states and absorption

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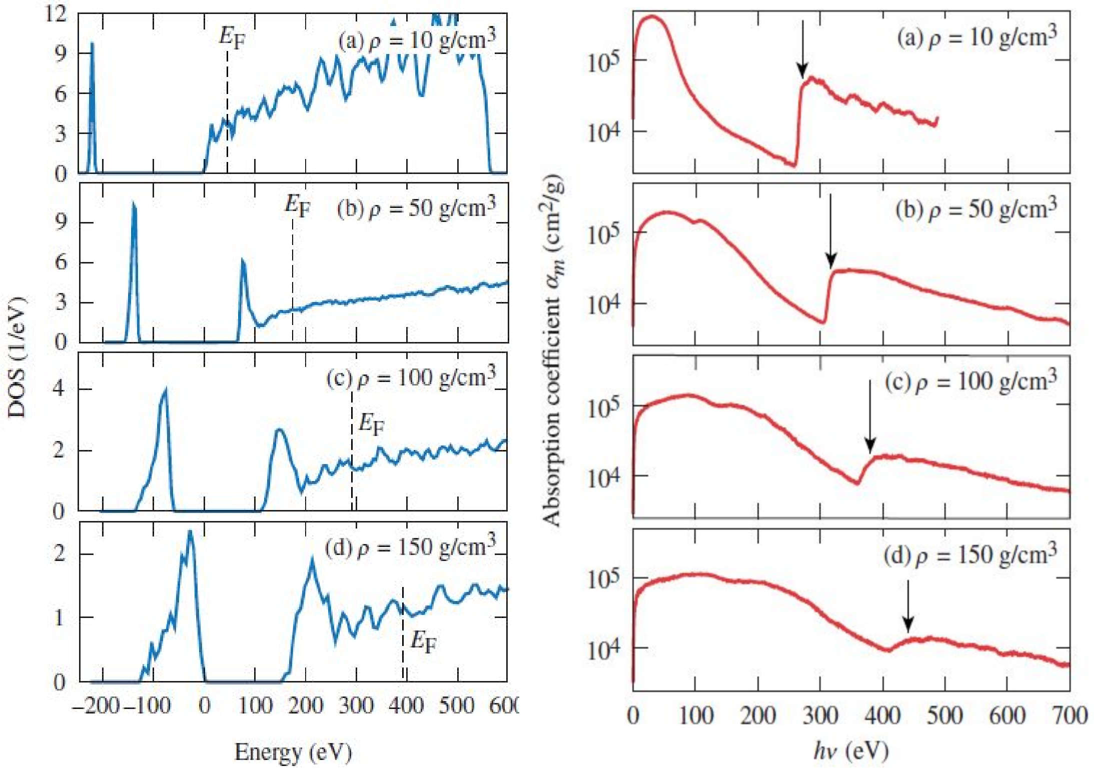
C at T = 1.35 eV



The quantum nature of plasma electrons causes significant **K-edge upshifting** in warm-dense or super-dense plasmas,

due to "*Fermi-surface rising**", "*Pauli blocking***", or "*Fermi barrier****"

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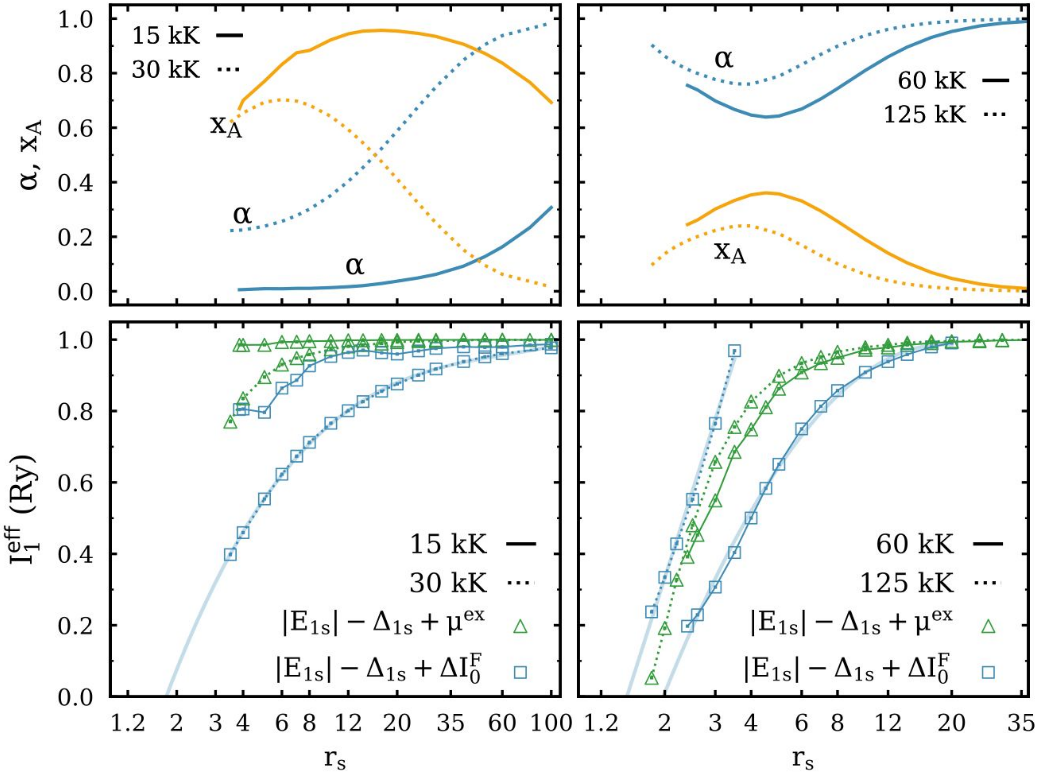
*   S. X. Hu, PRL **119**, 065001 (2017).

**   C. A. Iglesias and P. A. Sterne, PRL **120**, 119501 (2018);
S. X. Hu, PRL **120**, 119502 (2018).

***   M. Bonitz and L. Kordts, Contr. Plasma Phys. **65**, e70001 (2025).

FPIMC downfolding result for hydrogen ground state ionization potential*



* M. Bonitz and L. Kordts, CPP 65, e70001 (2025)

use FPIMC results for continuum lowering and fraction α

→ obtain effective ionization energy I^{eff}_{1s}

□ FPIMC with level shifts

△ Analytical model (Pade formula)

Extrapolation yields Mott density

Sensitivity to criteria for α and x_A: 3...5%

QMC-based benchmarks: benefit for ICF

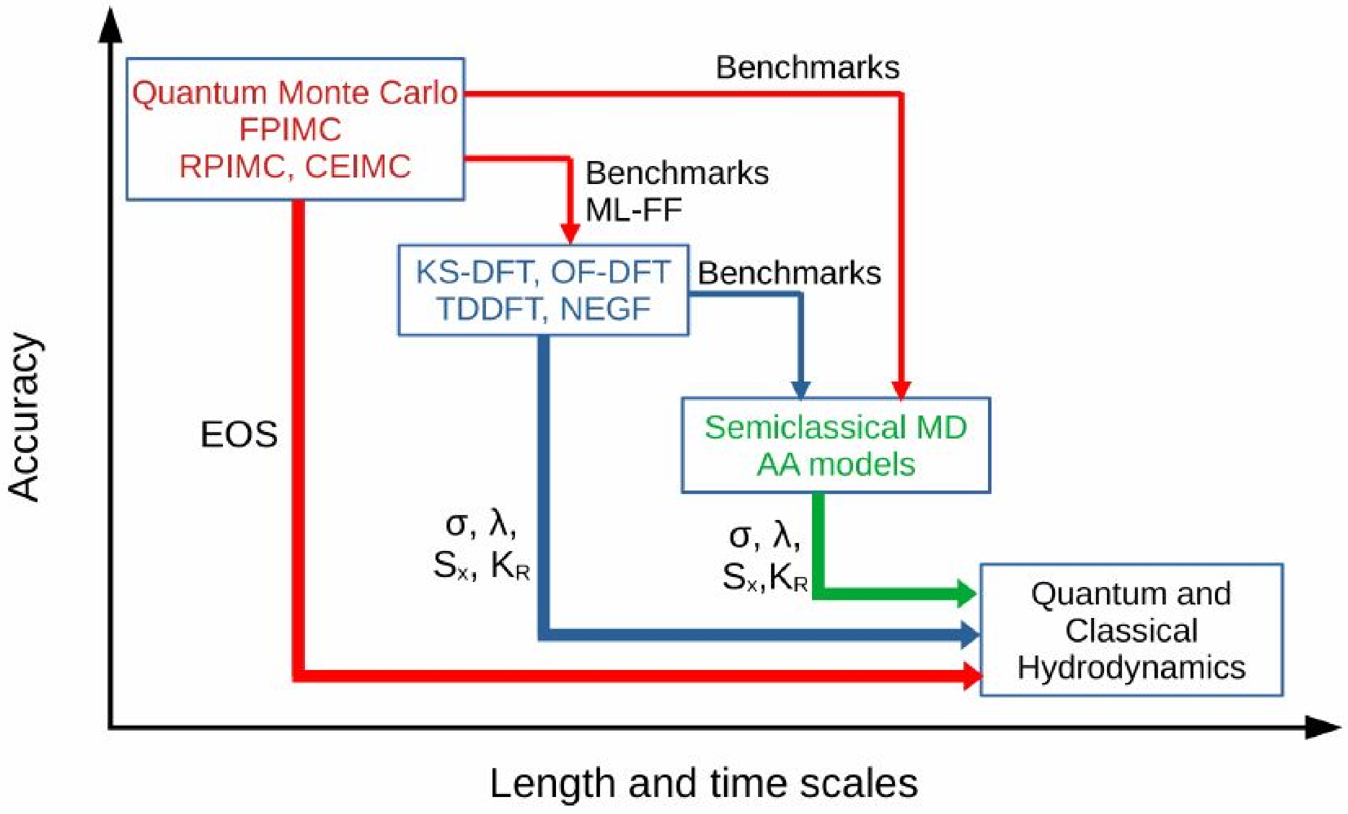
Hydro simulations indispensible to cover relevant scales and complexity

with present approach:

- needed input can be improved substantially

- limitations can be better quantified.

- **predictive simulations will become possible**



* M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Further benchmarks for WDM at equilibrium

- exact benchmarks provided by fermionic PIMC
  results beyond hydrogen (e.g. Be): Dornheim et al., Böhme et al,
  Allow for novel benchmarks of RPIMC, DFT etc.

- Militzer *et al.* (FPEOS): wide range equation of state tables for many materials:
  Successful combination of RPIMC and DFT (LDA)
  PRL **114**, 176403 (2015), PRE **103**, 013203 (2021)

Using FPIMC data, accuracy of these tables can be improved (better nodes and better xc functionals)

Towards benchmarks for nonequilibrium plasmas

Starting point: NEGF/quantum kinetic theory*
Recent breakthroughs: time linear G1-G2 scheme, quantum fluctuations approach
Schlünzen, Joost, MB, PRL **124**, 076601 (2020); Schroedter, Joost, MB, Cond. Matt. Phys. **25**, 23401 (2022)

Excellent agreement with cold atom experiments
Schlünzen *et al.*, PRB **93**, 035107 (2016)
Plasma applications in progress (C. Makait *et al.*)

Quantum Hydrodynamics (corrected): promising approach for ICF plasmas:
Graziani, Moldabekov, Olson, and Bonitz, Contrib. Plasma Phys. **62**, e202100170 (2022)
Require benchmarks/input from quantum kinetic theory/DFT
Moldabekov, Bonitz, and Ramazanov, Phys. Plasmas **25**, 031903 (2018)
Moldabekov *et al.* SciPost Phys. **12**, 062 (2022)
Correlated hydrodynamics (classical): D. Krimans *et al.* (PoP 2024), extension to quantum plasma in progress

* M. Bonitz, „Quantum Kinetic Theory“, 2nd ed. Springer 2016
M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Summary and Outlook

Quantum Physics has had a tremendous success since Planck, 1900

Crucial for future success of many areas of plasma physics
- Low pressure plasmas: spectroscopy of atoms, molecules, ions, macroparticles etc.
- magnetic fusion: interaction with wall

Quantum effects crucial for dense plasmas/Warm dense matter, ICF

- quantum effects of electrons determine the properties
- classical simulation approaches (MD, kinetic theory, hydrodynamics etc.) fail
  Plasma physics needs to learn and apply advanced quantum theory tools

New era of high-precision research in WDM via FPIMC benchmarks and downfolding

basis: first principles predictive fermionic PIMC simulations. Can be used
- for benchmarking other methods and optimizing choice of approximations (E_{xc}, F_{xc}, Σ etc.)
- needed: smart combination of methods, in particular RPIMC, DFT, Green functions, Hydrodynamics, average atom, semiclassical MD

2025

INTERNATIONAL YEAR OF
Quantum Science
and Technology

Quantum physics – a „gold mine“ in 21th century:
Recent Nobel prizes in physics

2010: Graphene: Geim, Novoselov

2023: attosecond pulses (atomic physics): L’Huillier, Agostini, Krausz

2025: macroscopic quantum tunneling: Clarke, Devoret, Martinis

Quantum physics – a „gold mine“ in 21th century:

Recent **and upcoming** Nobel prizes in physics

2010: Graphene: Geim, Novoselov

2023: attosecond pulses (atomic physics): L’Huillier, Agostini, Krausz

2025: macroscopic quantum tunneling: Clarke, Devoret, Martinis

2035: demonstration of large scale energy gain in ICF: xxx

2039: development of a magnetic fusion power plant: yyy

Thank you for your attention