Quantum effects in plasmas and how to simulate them

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pdf of talk @ https://www.itap.uni-kiel.de//theo-physik/bonitz/talks.html
Related preprint: arXiv:2604.03757

2025

INTERNATIONAL YEAR OF
Quantum Science
and Technology

2025

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INTERNATIONAL YEAR OF
Quantum Science
and Technology

100 years of Heisenberg’s/Schrödinger’s equations

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

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

2025

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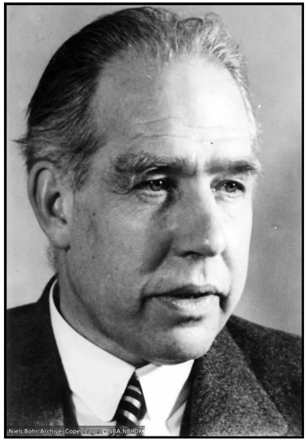
INTERNATIONAL YEAR OF
Quantum Science
and Technology


Niels Bohr Archive, Copenhagen - NBA.NBI.DK

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

Brief summary of Planck’s discovery

Max Planck

*1858 **Kiel** – 1947 Göttingen

- Dec. 14 1900*: quantum hypothesis

- quantization of electromagnetic radiation
- elementary photon energy E=hf
- Planck constant h (universal importance)
- universal EM radiation law (Bose distribution)

*„birthday of quantum physics“

- Starting point for revolution of science and technology

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This is the very short version – reality is much more complex
- long and difficult path, with many obstacles
- result was in striking contradiction to 19th century physics
- plasma physicists played an important role in early quantum theory
- interesting lessons to learn

Outline

1. **Introduction**: Max Planck, energy quanta – myths and facts
   Low pressure plasmas and quantum effects

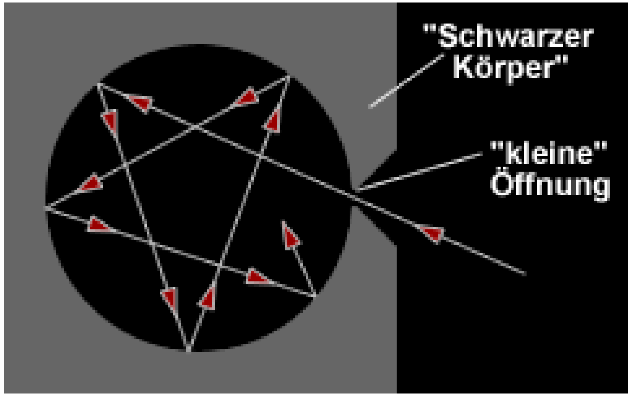
2. **Quantum effects in plasmas**
   - 2.1 Low pressure: classical electrons
   - 2.2 High pressure: quantum electrons
   - 2.3 Quantum effects of heavy particles
   - 2.4 Exotic quantum plasmas

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

4. **Summary and Outlook**

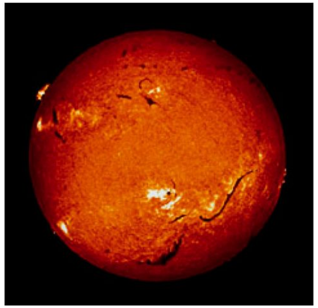
Black-body radiation (EM spectrum in equilibrium)

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



hohlraum at fixed T confines radiation

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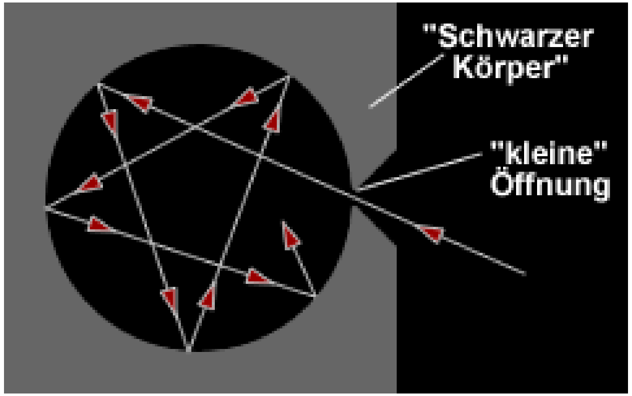

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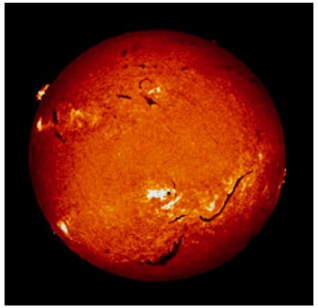
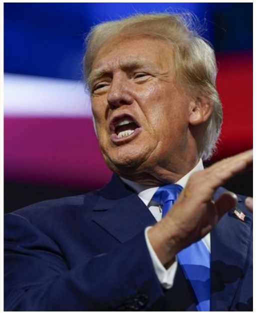
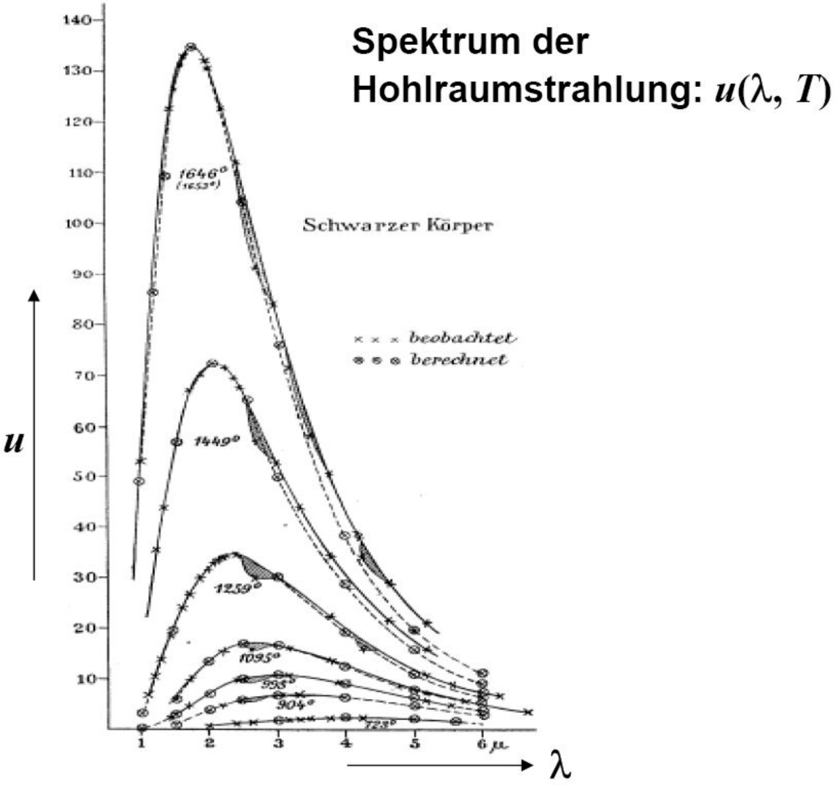



Black-body radiation spectrum

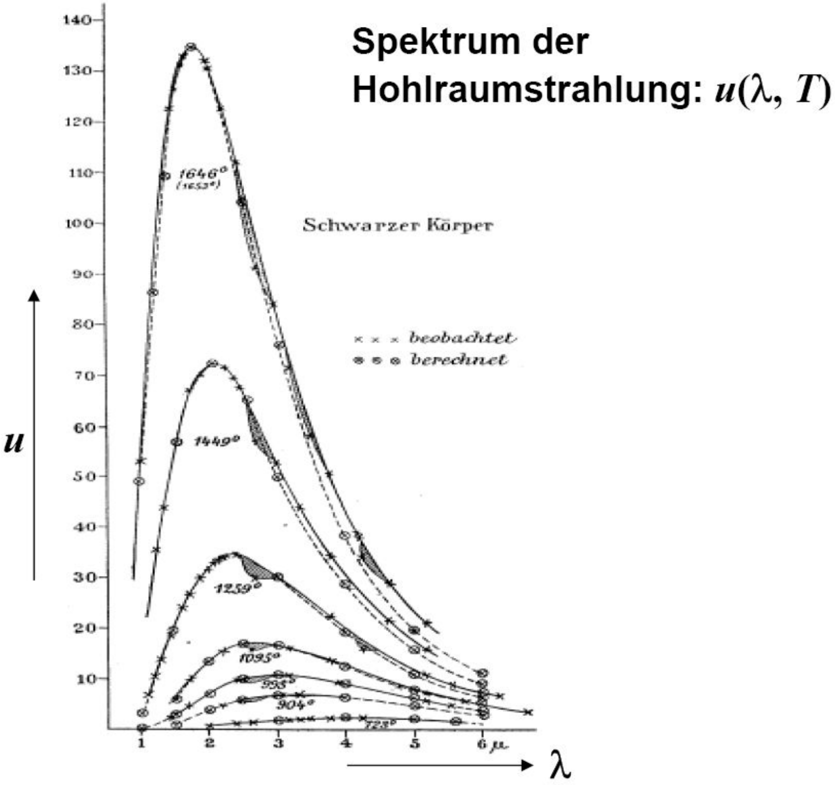

Spektrum der Hohlraumstrahlung: $u(\lambda, T)$

Messung von Lummer und Pringsheim (1900)

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

- 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

Black-body radiation spectrum



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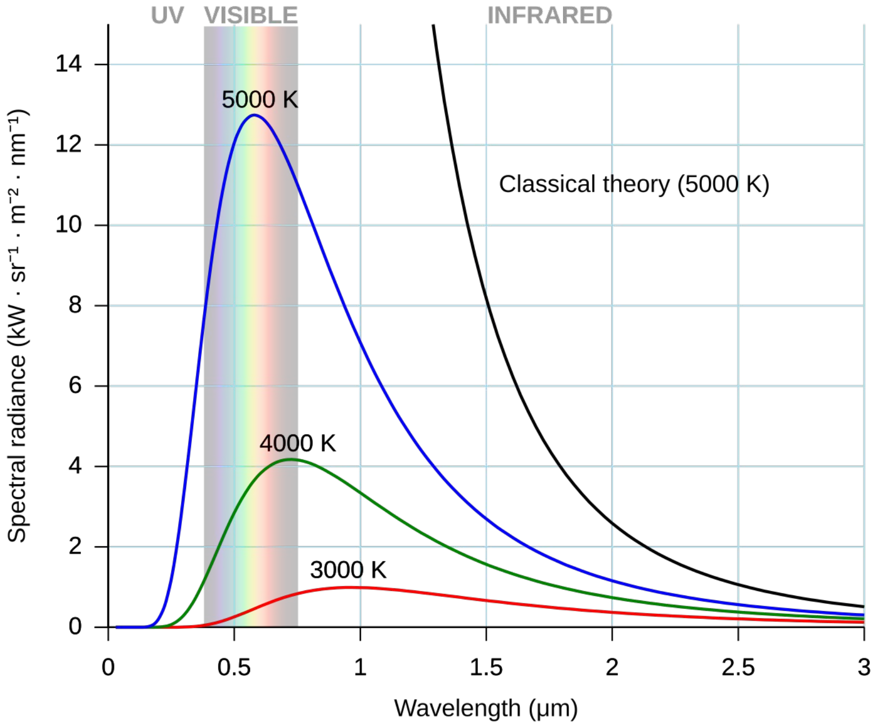
Black-body radiation spectrum



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

Planck's result
(Bose distribution)
$\omega = 2\pi\nu$, $c = \lambda\nu$

$$S^{\mathrm{P}}(U)=k_B\left[\left(\frac{U}{h\nu}+1\right)\ln\left(\frac{U}{h\nu}+1\right)-\frac{U}{h\nu}\ln\frac{U}{h\nu}\right]$$

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- 1897-1900: precision experiments by Lummer, Pringsheim, Rubens, Kurlbaum (PTR Berlin)
  → excellent agreement with Wien,
  small deviations at large wavelengths
- Oct 7 1900 Rubens informs Planck about Rayleigh's result (equipartition, Philos. Magaz. 1900)
- Planck computes entropy S of radiation. He adds

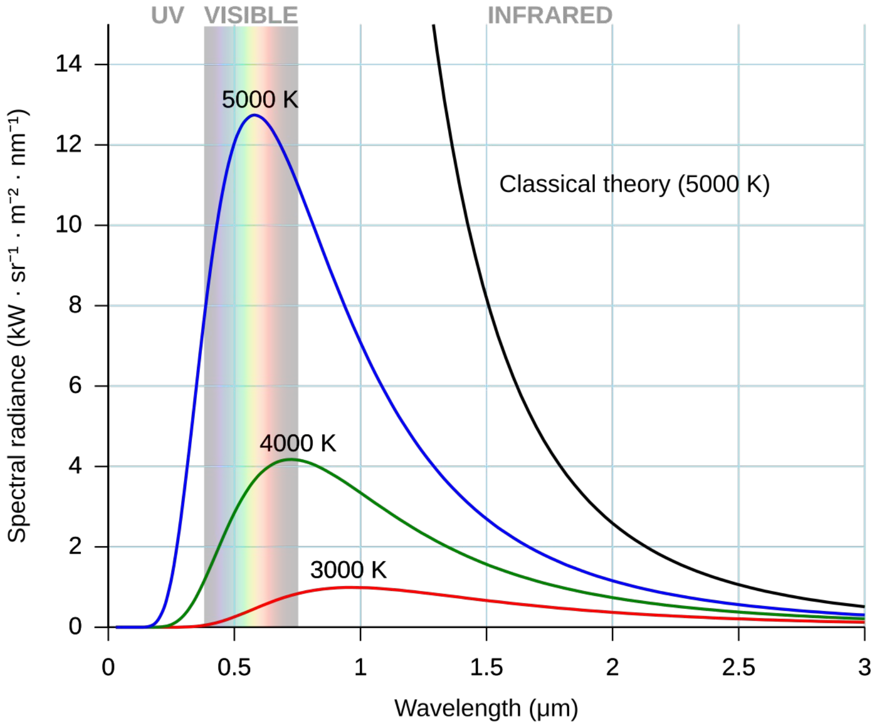
$R_{\mathrm{WIEN}} + R_{\mathrm{RAYLEIGH}} = R_{\mathrm{PLANCK}}$, where $R=\left(\frac{d^2S}{dU^2}\right)^{-1}$

- Oct 19 1900: Planck presents his radiation law experimentalists confirm perfect agreement

- Planck identifies two fundamental constants: k_B, h
  h: Elementary quantum of action is at the heart of all quantum theory today

  h is the basis for the novel international system of units (as of May 20 2019)

Black-body radiation spectrum



- Oct 19 1900: Planck presents his radiation law experimentalists confirm perfect agreement

- Dec 14 1900: Planck presents his new derivation based on the quantization of energy

$$U_\nu = N_\nu \cdot \varepsilon_\nu = N_\nu \cdot h\nu$$

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

Planck's result
(Bose distribution)
$\omega = 2\pi\nu$, $c = \lambda\nu$

Black-body radiation spectrum: myths

The common story told in many text books (including plasma physics):

Planck saved us from „ultraviolet catastrophe“
Planck interpolated between Wien and Rayleigh/Jeans

History:

1905: Rayleigh/Jeans (corrected equipartition)
1911: Ehrenfest „Ultraviolet catastrophe“

For details:
M. Bonitz et al., Phys. Plasmas (2026), arXiv: 2604.03757

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

Max Planck remains skeptical himself about interpretation of photon hypothesis, for more than 10 years

- 1905: Einstein applies hypothesis to photoelectric effect
- 1911: Nobel prize for Wien
- 1913: Bohr uses h to quantize angular momentum of atom
- 1914: Franck and Hertz prove discrete electronic structure of atom

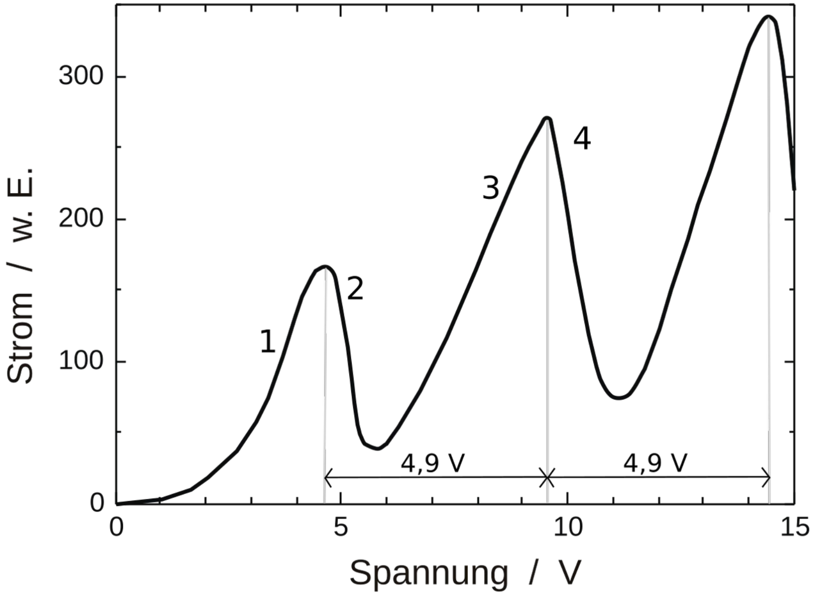
very long and difficult path, contributions from many scientists, including plasma (gas discharge) physicists

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

Macroscopic quantum effects in low-p plasmas

space-resolved
Franck-Hertz experiment

Standing striations in low
pressure plasmas:

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

first reported by W.H.T. Meyer 1858

Bonitz et al., Phys. Plasmas (2026)
arXiv:2604.03757

Nobel prize for Max Planck 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
2012: Manipulation of quantum systems: Haroche, Wineland
2010: Graphene: Geim, Novoselov

Nearly all fields of physics. Also various chemistry nobel prizes. How about plasmas?

Quantum effects

What are quantum effects and where are they?

Why should plasma physicists care?

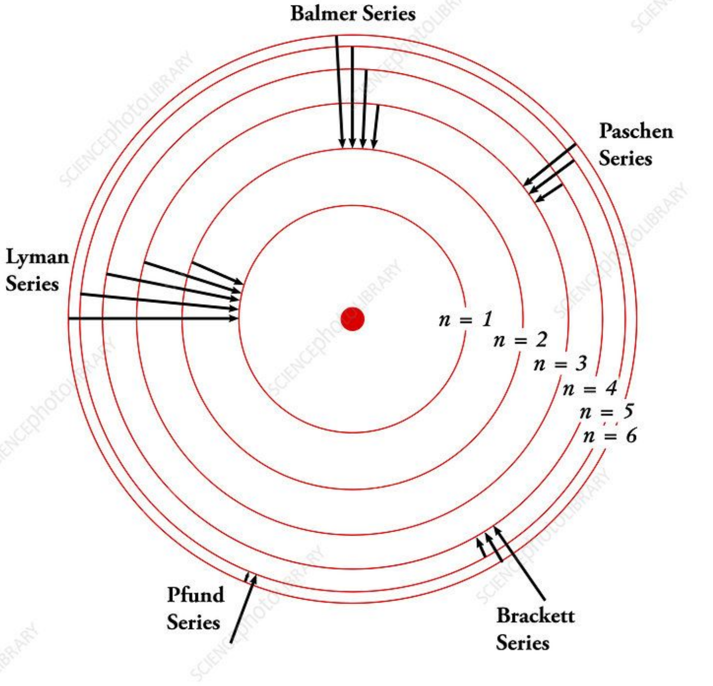
Single-particle quantum effects

Structure of atoms: „standard“ model

pointlike 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)
- orbitals incomplete, have wrong shape

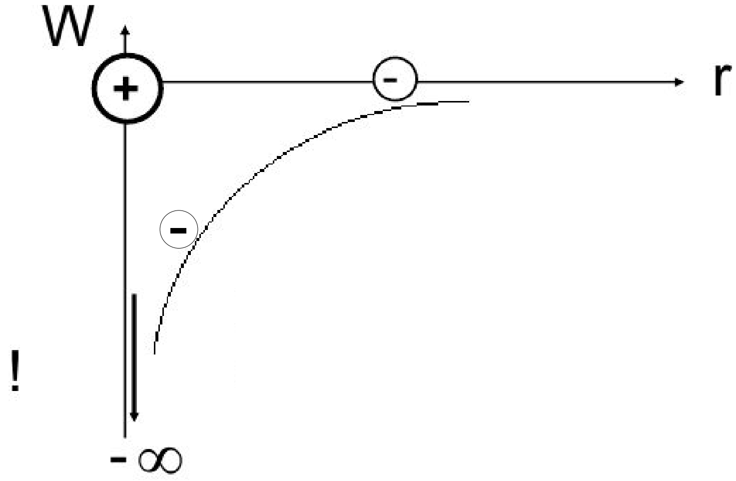


Niels Bohr, 1913
pic: Wikipedia

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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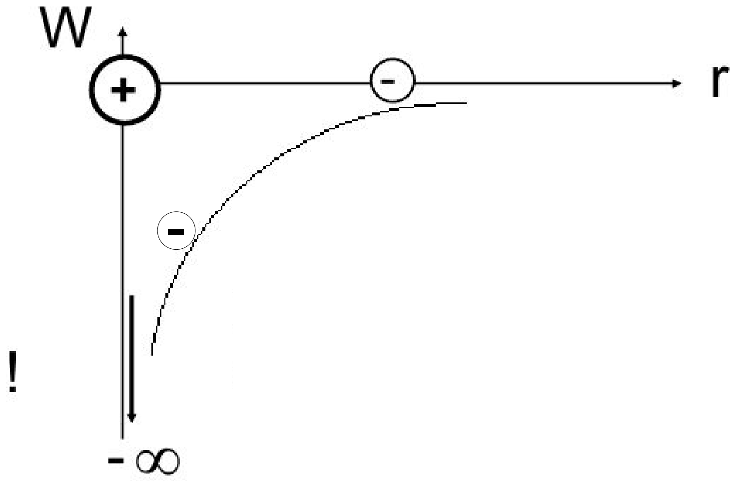
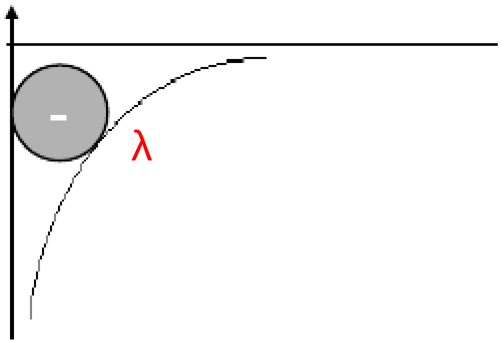


Coulomb attraction
$W = -e^2/r$

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

stable atom:

(schematic)



quantum electron „blows up“
to prevent collapse into nucleus

Interaction energy remains finite

Mathematical basis of quantum effects

Heisenberg 1925, Schrödinger 1926, Born, Jordan, Bohr, Dirac, von Neumann and others

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

Schrödinger equation

$$1 = \int d^3r\, \underline{|\psi(\mathbf{r},t)|^2}$$

normalization

probability density

Consequences of finite spatial extension λ

- Spreading of a free wave packet
- Tunneling through a barrier
- Selfinterference (wave behavior)

Heisenberg uncertainty relation:
$[x, p_x] \neq 0$, not measurable simultaneously
σ: standard deviation

$$\sigma(x)\big|_\psi \cdot \sigma(p_x)\big|_\psi \geq \frac{\hbar}{2}$$

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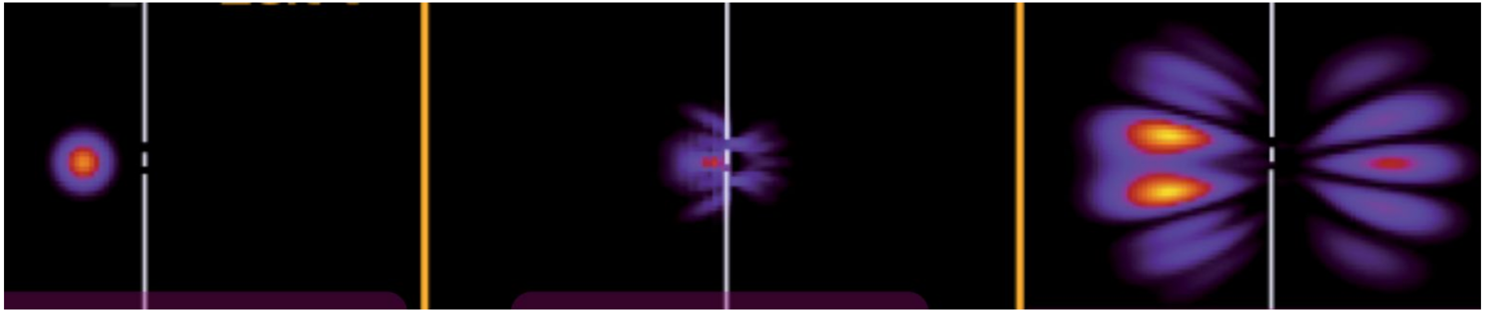
$$1 = \int d^3r\,|\psi(\mathbf{r},t)|^2$$

normalization

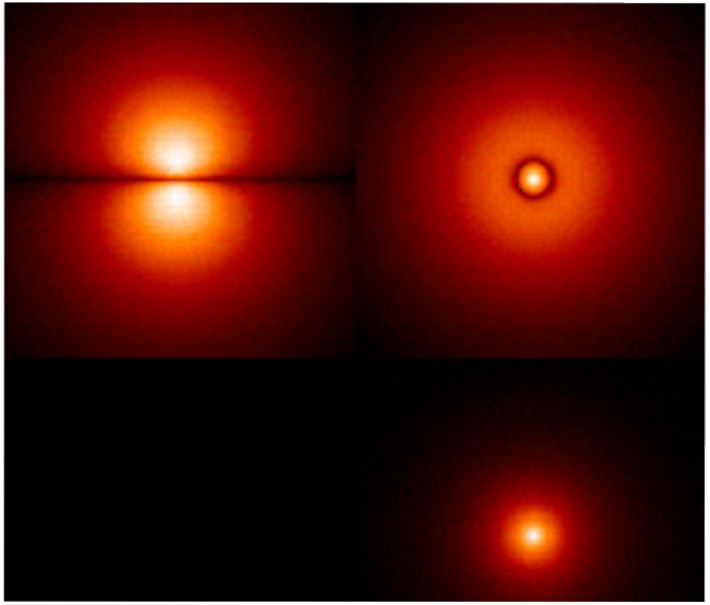
probability density

Electron selfinterference at double slit (snapshots at 3 time points)



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

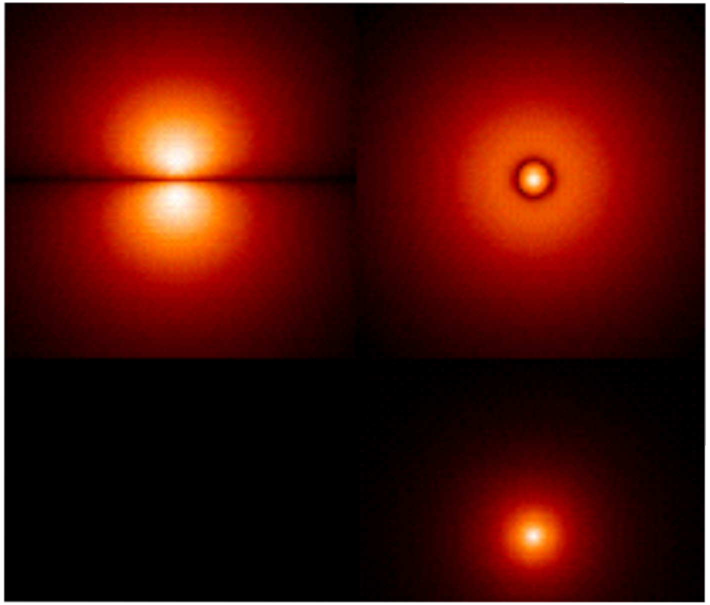
Stable (stationary) atom
Quantum kintetic energy balances
Coulomb attraction

Spreading of free wave packet

Tunneling through potential barrier

Wave-like interference (at CAU)

„wave-particle duality“: trivial consequence of
Fourier transform of
wave packet

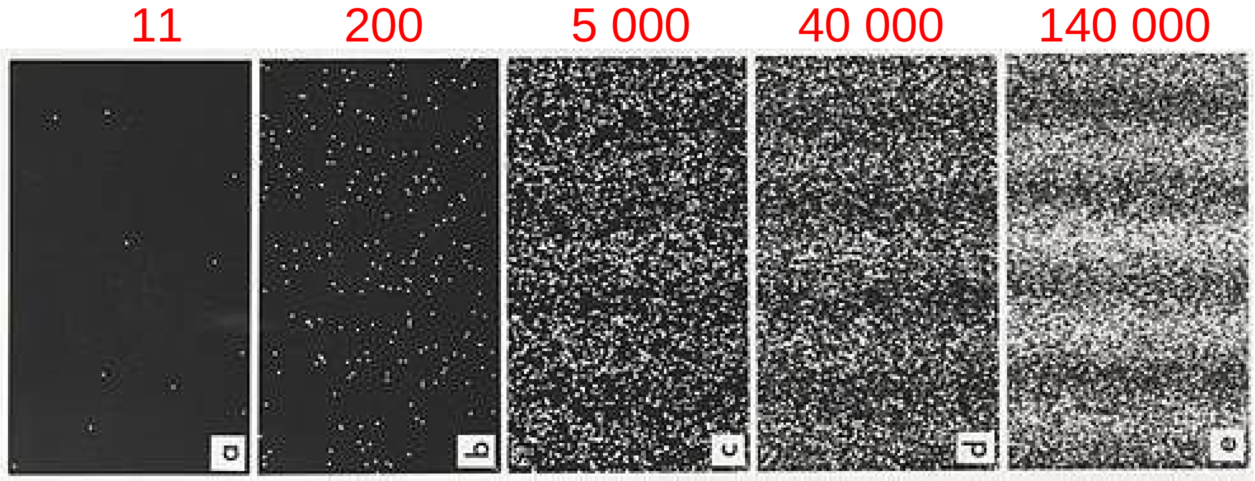


Hydrogen atom: 2p, 2s
1s

orbitals

Statistical interpretation of quantum mechanics

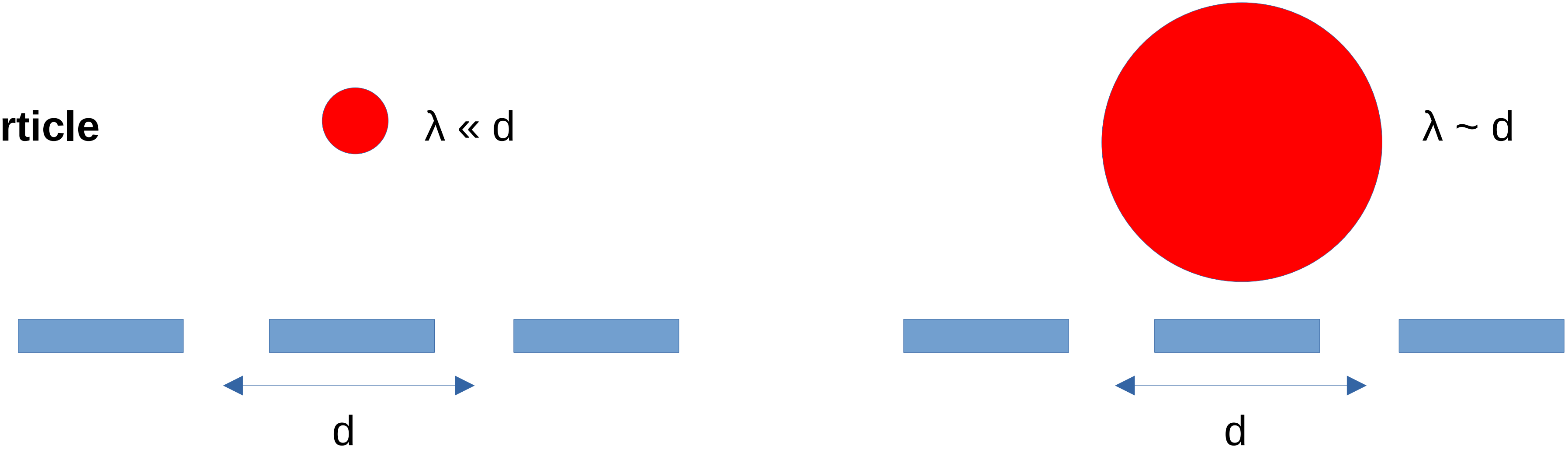
Experiment: electrons at double slit
Chamber contains only single electron
Selfinterference emerges statistically, but each event random



A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki, and
H. Ezawa, American Journal of Physics 57, 117 (1989)

When are quantum effects important (1)?

1 particle



λ « d

d

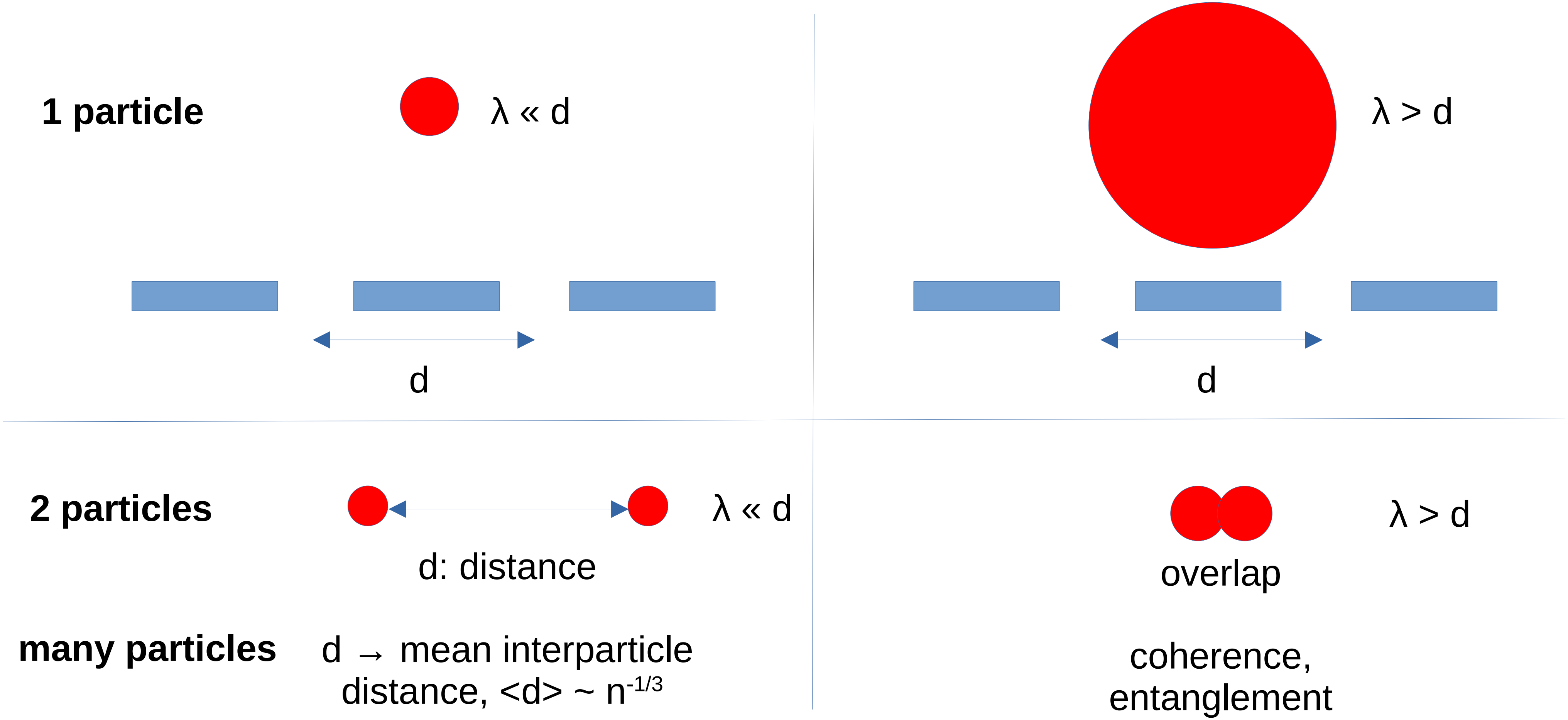
λ ~ d

d

No interference

interference,
diffraction,
tunneling

When are quantum effects important (1)?



1 particle

λ « d

d

λ > d

d

2 particles

λ « d

d: distance

λ > d

overlap

many particles

d → mean interparticle distance, <d> ~ $n^{-1/3}$

coherence, entanglement

Dimensionless parameters of quantum plasmas

Strength of quantum effects: $\chi = n\,\Lambda^3$ or

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

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

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

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

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

$$\Theta = \frac{k_B T}{E_F}$$ 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.

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

Many-particle (exchange) quantum effects

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

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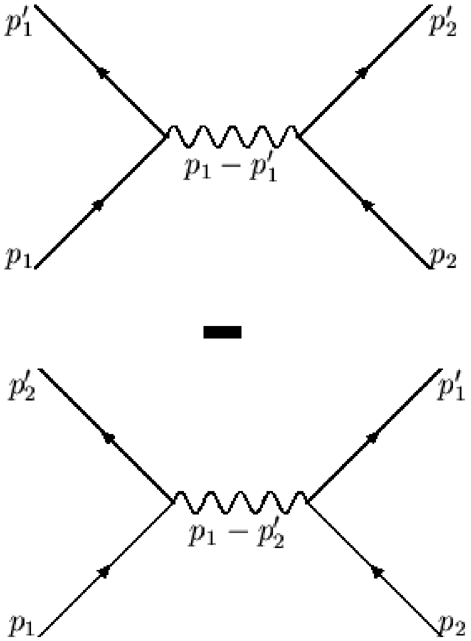
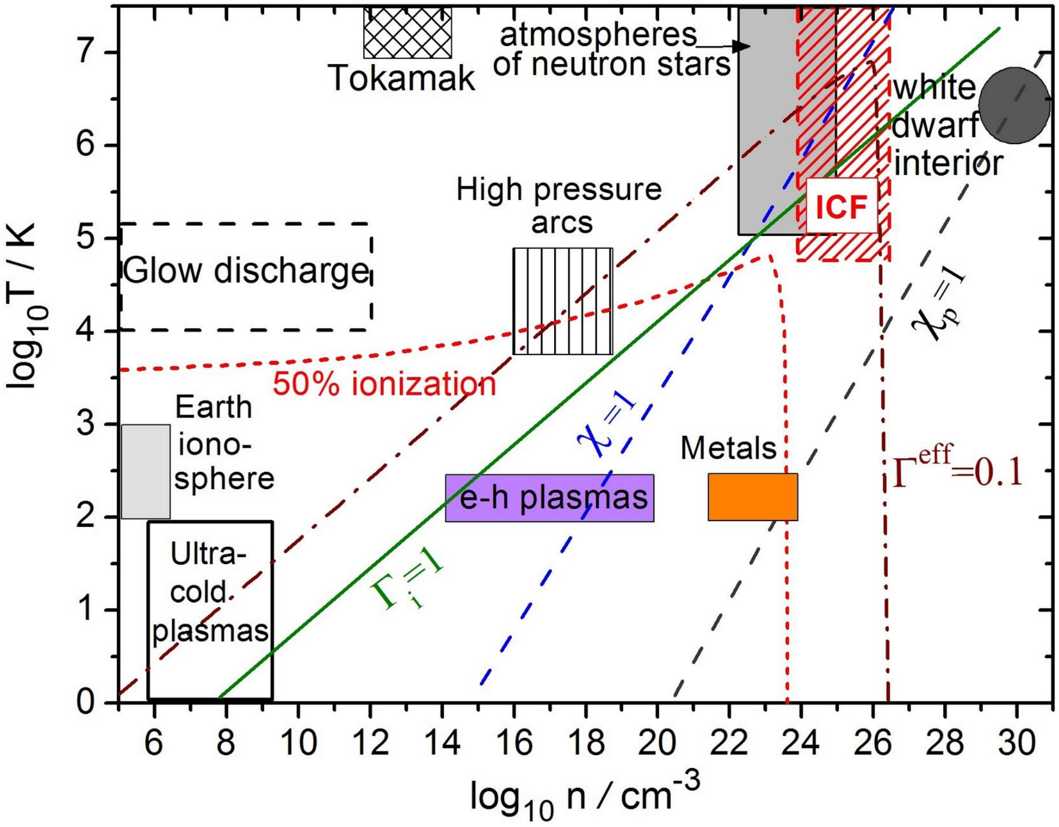


Quantum exchange
Example: e-e Coulomb scattering

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

Plasmas span huge parameter range



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

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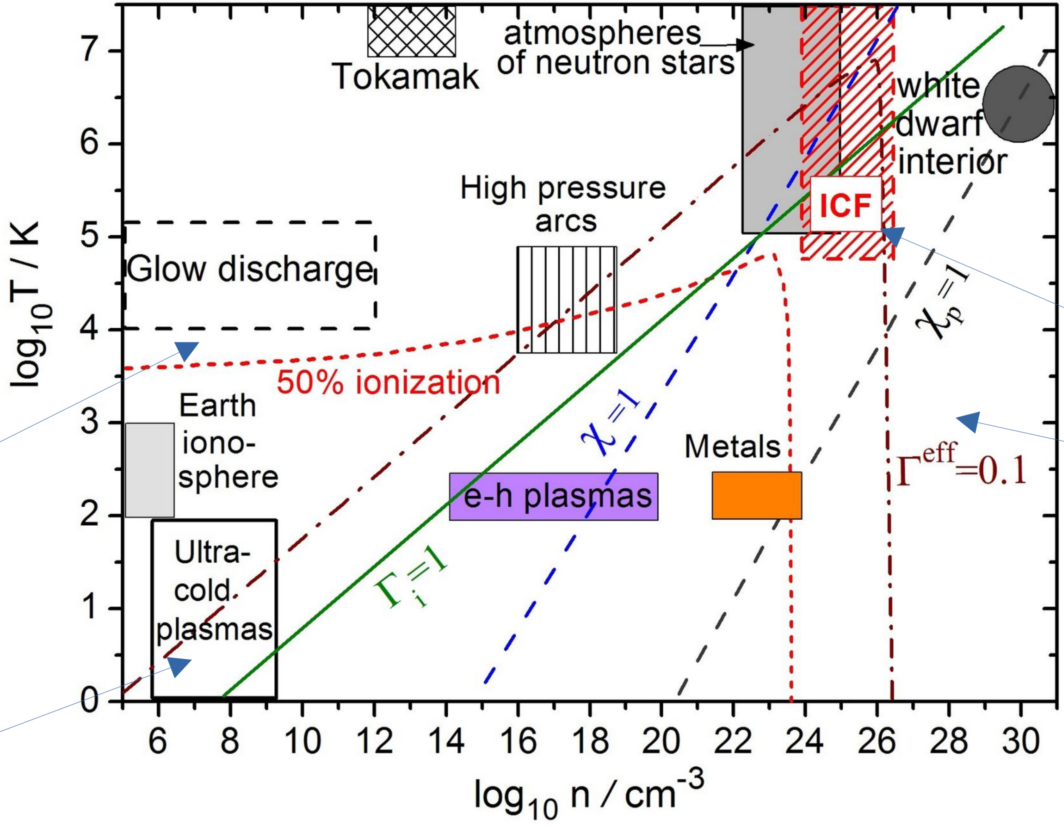


2.4. exotic quantum plasmas

2.2. high pressure

2.1 low-pressure

2.3. quantum protons

the coldest plasmas… are classical

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

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

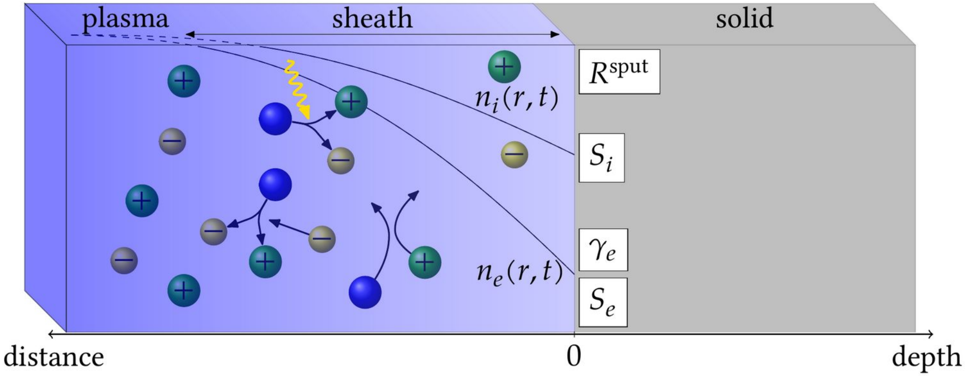
- absorption, emission, scattering, frequency combs etc.

- 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

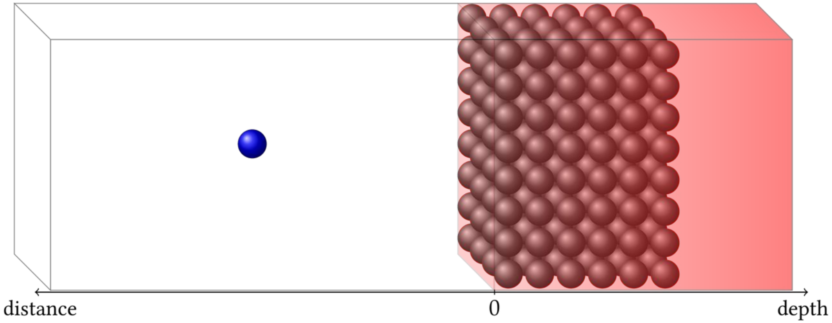
2.1.B. Plasma-surface interaction

Quantum effects in solid surface of plasma



plasma influenced by solid….

phenomenological coefficients

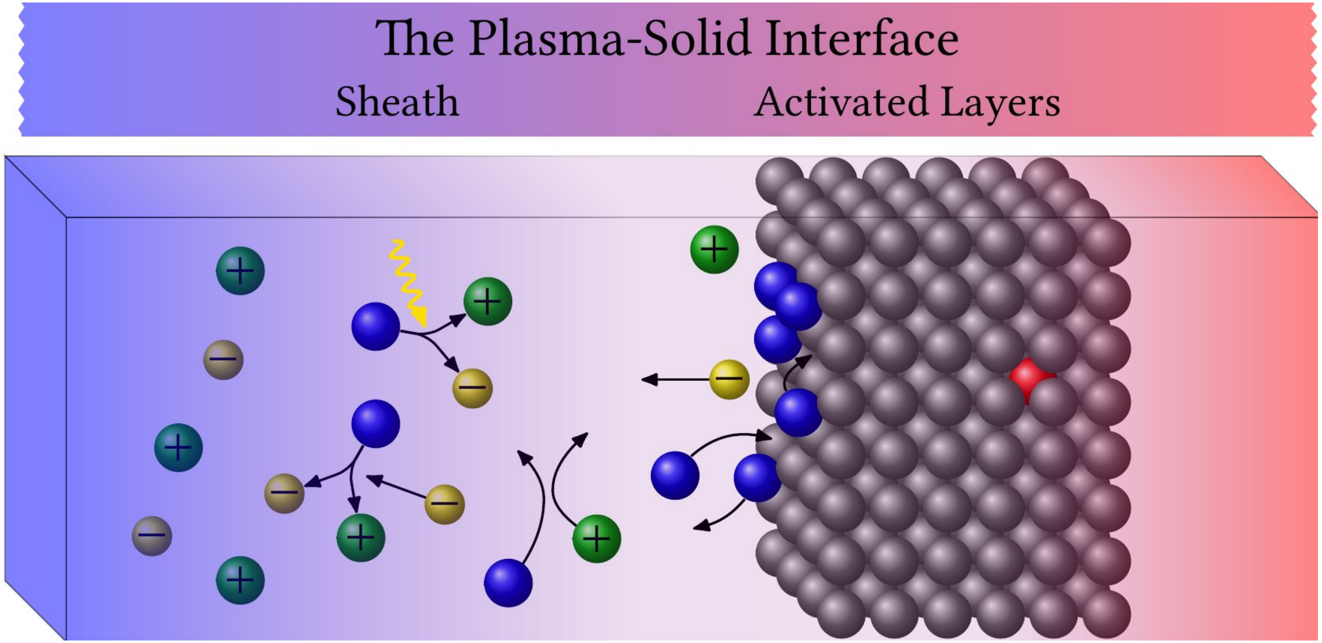


solid influenced by plasma….

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)

Talks at this EPS conference:

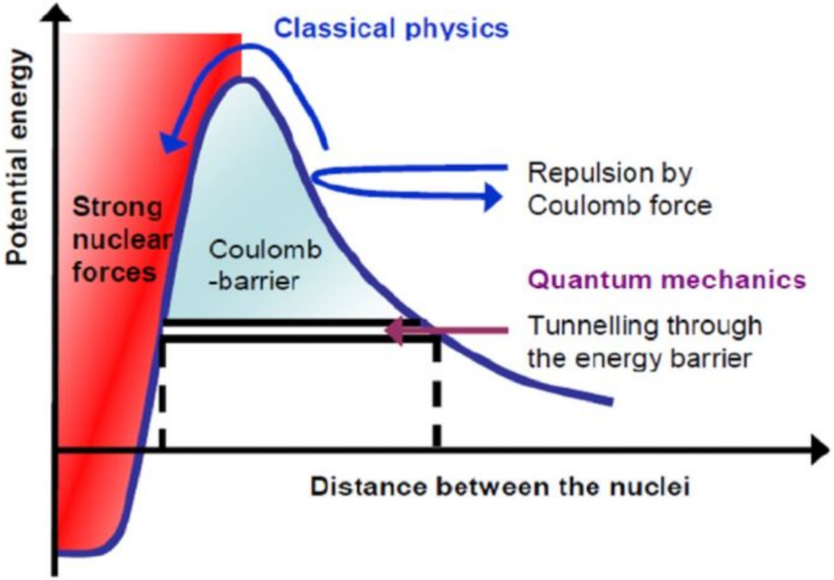
Dan Sun, Queen’s University, „Functional Nanocomposites Synthesized through Atmospheric Pressure Plasma…“
José Muñoz Espadero, University of Cordoba, „... Maximizing Graphene Production in a Microwave Plasma Torch“

2.1.C. Quantum effects in Fusion

Quantum tunneling crucial [1]

Coulomb barrier (DT) ~ 0.44 MeV

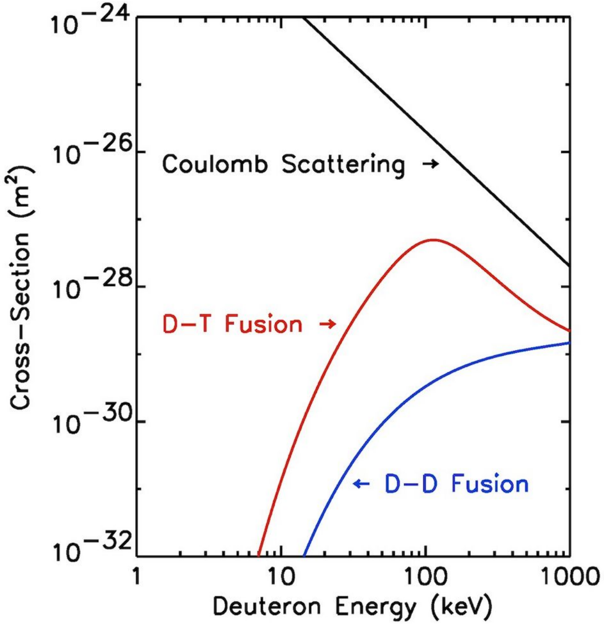
3/2 k_bT ~ 15 keV (at 10^8K)



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

[1] Gamov, Z. Phys. 1928

D-D, D-T cross sections



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

2.2 High pressure: quantum electrons

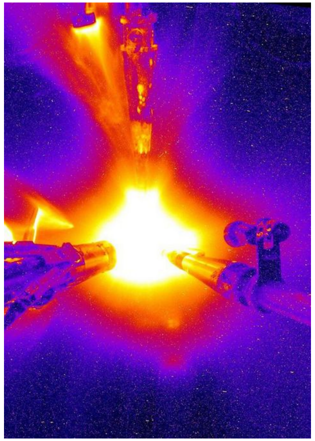
Astrophysics:

- 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



Don Jedlovec, LLNL

2.2 High pressure: quantum electrons

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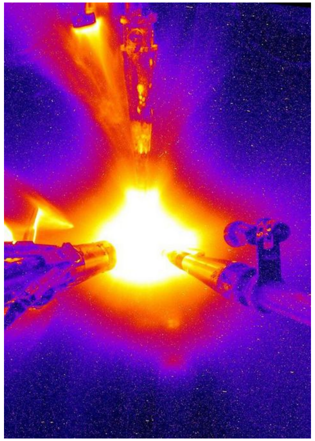


Don Jedlovec, LLNL

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

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]

472 and 367 citations (June 20 2026)

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

Main driver: recent breakthroughs in ICF a the NIF

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 (magnetic fusion and ICF)

Many talks at this EPS conference:

Matthew Khan, STFC/RAL/CLF, „The Shock Augmented Ignition route to high gain inertial fusion energy"
Nuno Lemos, LLNL, „Advancing the understanding of laser-plasma interaction in new scales of hohlraums"
Sam O'Neill, University of York, UK, „Non-local preheat in direct drive ICF implosions"
Micahel Tatarakis, Hellenic Mediterranean University, „The HiPER+ Initiative: Advancing Direct-Drive Inertial Confinement Fusion: Past, Present, and Future"
Wolfgang Theobald, Focused Energy, „Developing a Self-Consistent Target Design for Laser Direct Drive Inertial Fusion Energy"

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

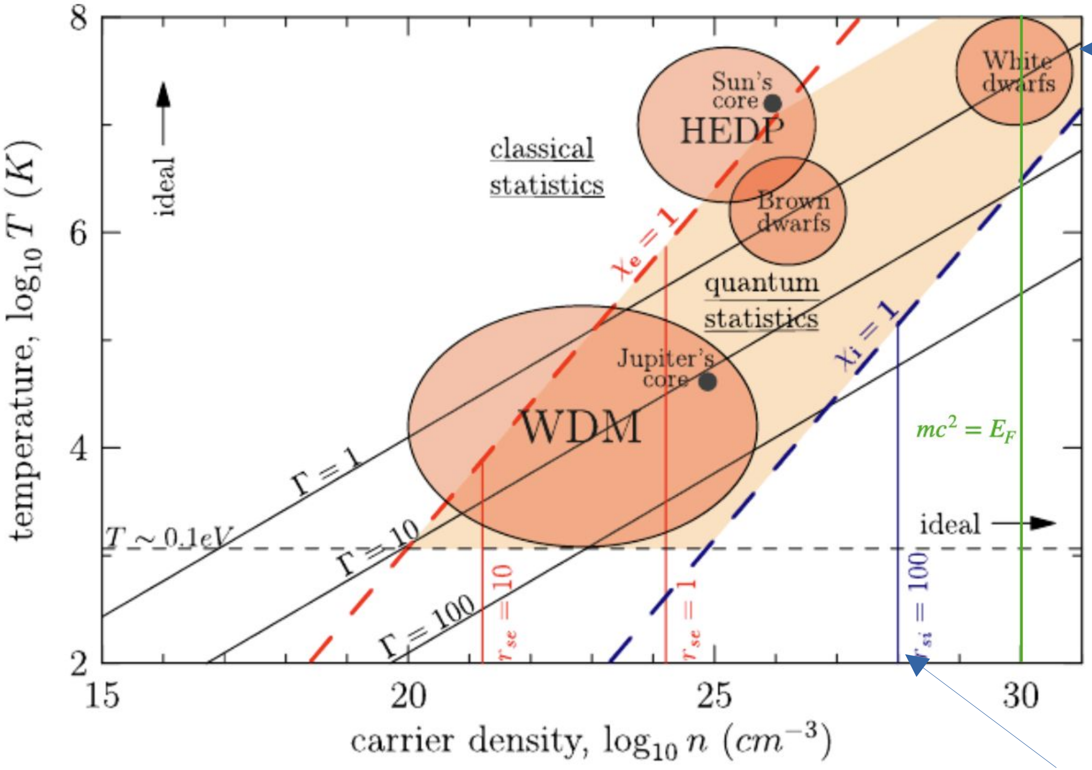
Bonitz *et al*., Phys. Plasmas (2026), arXiv:2604.03757

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: e.g. white dwarf stars only for $M < 1.4\, M_{SUN}$ (Chandrasekhar 1931)
- 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

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 on condensed matter theory

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

Quantum plasmas in Condensed Matter: a word of caution

Today: condensed matter theory advanced, novel specialized methods

standard plasma physics approaches/models are too simple/outdated to make an impact
- 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 in plasma physics.

A. 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…“

B. Prediction of „novel forces“, „novel band structures“, novel „kinetic equations“

based on inappropriate plasma physics models. Should be critically verified by referees, editors

2.4 Exotic quantum plasmas (B)

B. quark gluon plasma (QGP)

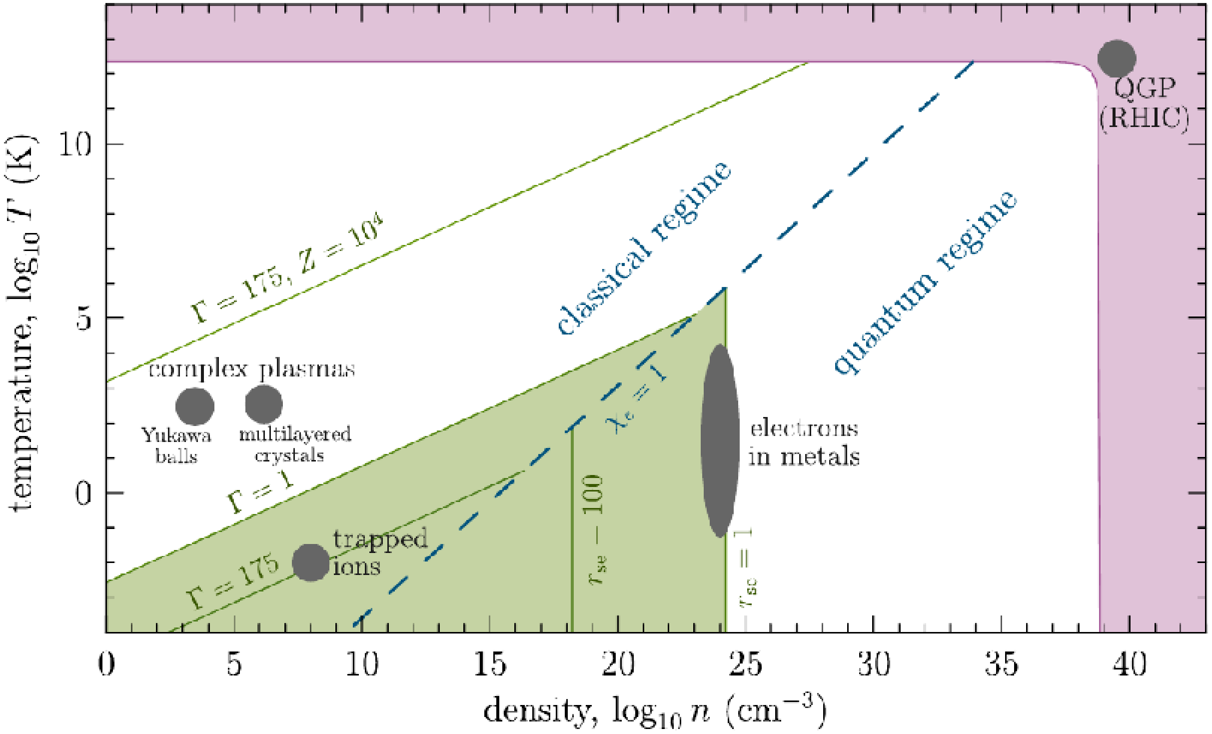
extreme T or p

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)

2.4 Exotic quantum plasmas (C)

C. Laser plasmas

Strong laser excitation creates extreme particle energies: relativistic effects, nonperturbative QED effects possible

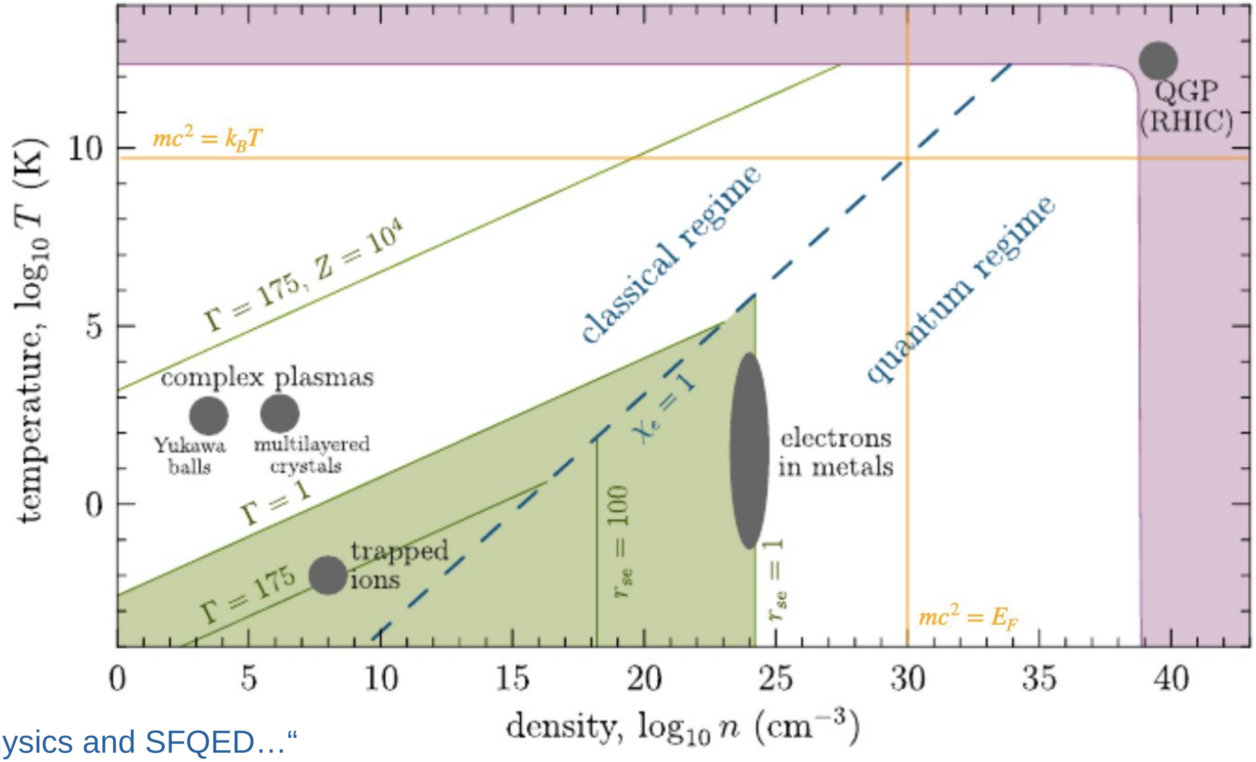
Beyond critical intensity

$$I_S = \frac{c\varepsilon_0 E_S^2}{2} \approx 4.65 \times 10^{29}\,\mathrm{W\,cm^{-2}}.$$

Schwinger field is reached:

$$E_S = \frac{m_e^2 c^3}{e\hbar} \approx 1.32 \times 10^{18}\,\mathrm{V\,m^{-1}}$$

Electron-positron pairs created



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

EPS talks 2026:

Sebastien Corde, LOA, „Plasma acceleration, astrophysics and SFQED…“
Zheng Gong, ITP, Chin. Ac of Sc, „Ultrarelativistic radiative spin-polarized plasmas“
Diana Gorlova, U of York, „Spin polarisation preservation in Direct Laser Acceleration“
Mohammad Mirzaie, Institute for Basic Science, Gwangju, „Strong-Field QED Studies…“
Yanfei Li, Xi'an Jiaotong University, „... Spin-Resolved Dynamics for Polarized Particle Generation...“

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

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

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.

Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024);
Phys. Plasmas (2026), arXiv: 2604.03757

Warm dense matter: challenges and opportunities (1)

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**, increased accuracy, e.g., X-ray Thomson scattering (XRTS)

Warm dense matter: challenges and opportunities (2)

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

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 advanced simulations: density functional theory (DFT), time-dependent DFT, Quantum kinetic theory*, Nonequilibrium Green functions (NEGF), quantum Monte Carlo

Novel opportunity: use accurate, predictive simulations as benchmark

*M. Bonitz, „Quantum Kinetic Theory“, 2nd ed. Springer 2016

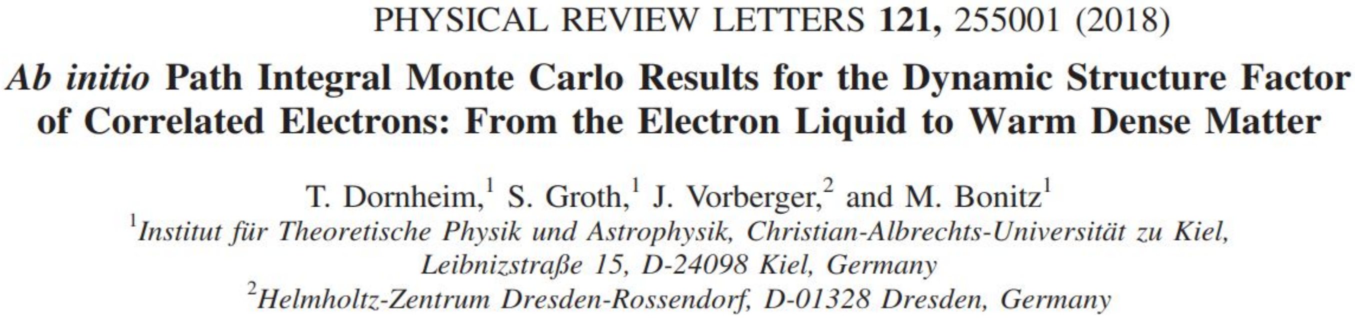
Recent breakthroughs in first-principles/predictive QMC simulations for WDM in our group

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

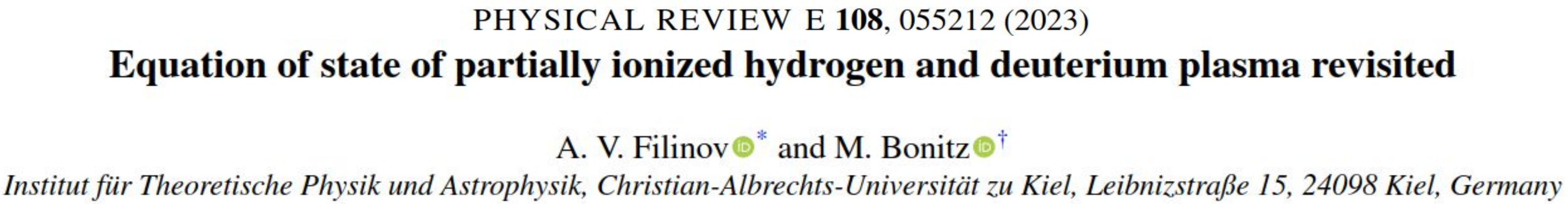


PHYSICAL REVIEW LETTERS **121,** 255001 (2018)

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

First-principles QMC (PIMC) simulations

Use Feynman’s path integral representation
of quantum mechanics

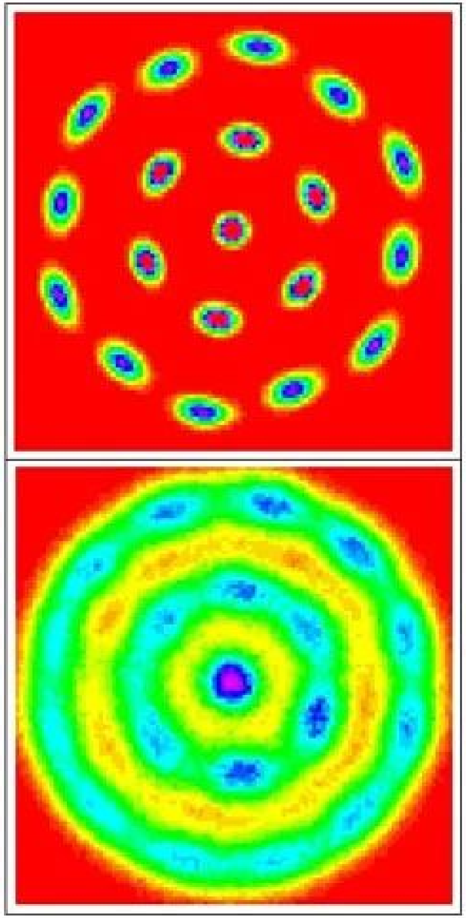
High-dimensional integrals (partition function)
efficiently evaluated with MC techniques

Natural representation of quantum extension (probability
density) of particles.

Simulations in principle achieve arbitrary accuracy,
(governed by statistical errors), hampered by fermion sign problem

Example:
Top: Wigner crystallization of electrons in spherical confinement
Bottom: density increase leads to overlap, quantum melting

A. Filinov, M. Bonitz, Yu. Lozovik, Phys. Rev. Lett. **86**, 3851 (2001)
Featured in Phys. Rev. Focus



Quantum Monte Carlo simulations for dense H*

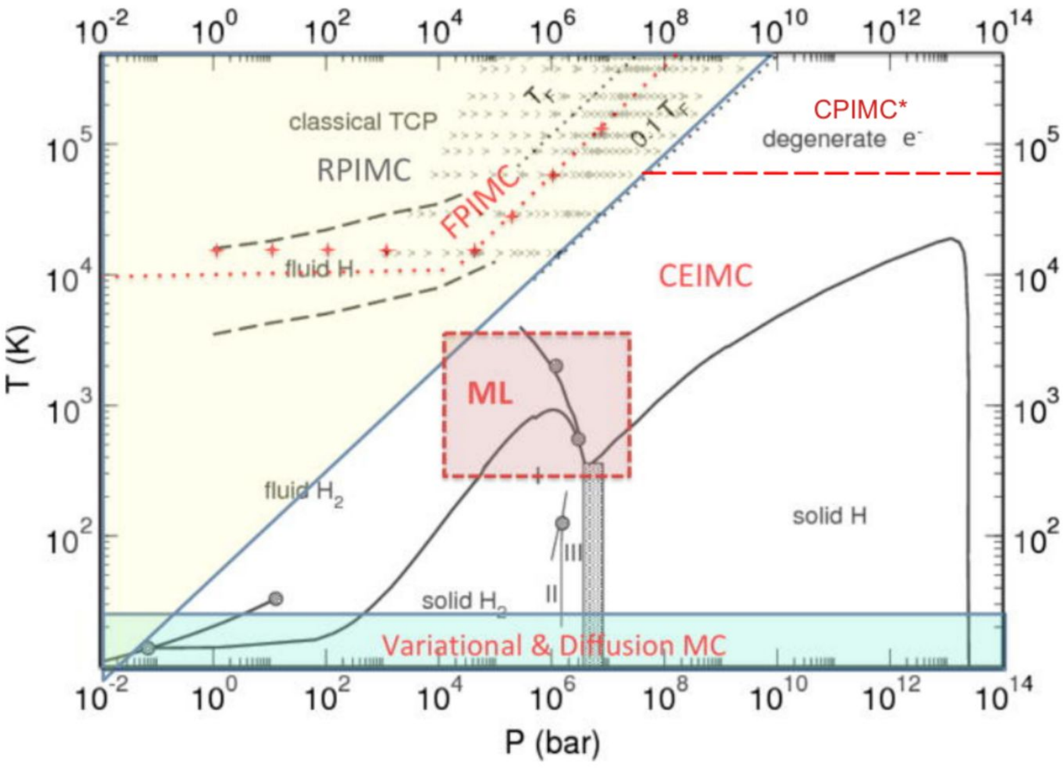


FIG. 8. Applicability range of different simulation methods across the hydrogen phase diagram. RPIMC: restricted PIMC, extends to about $0.1\,T_F$, Sec. III E 4, CEIMC: coupled electron-ion Monte Carlo, Sec. III F, FPIMC: fermionic PIMC, extends to about $0.5\,T_F$ and was applied to temperatures above 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“, 2026

Equation of state of dense Hydrogen (FPIMC)*

fermionic PIMC simulations validate

- restricted PIMC (top)

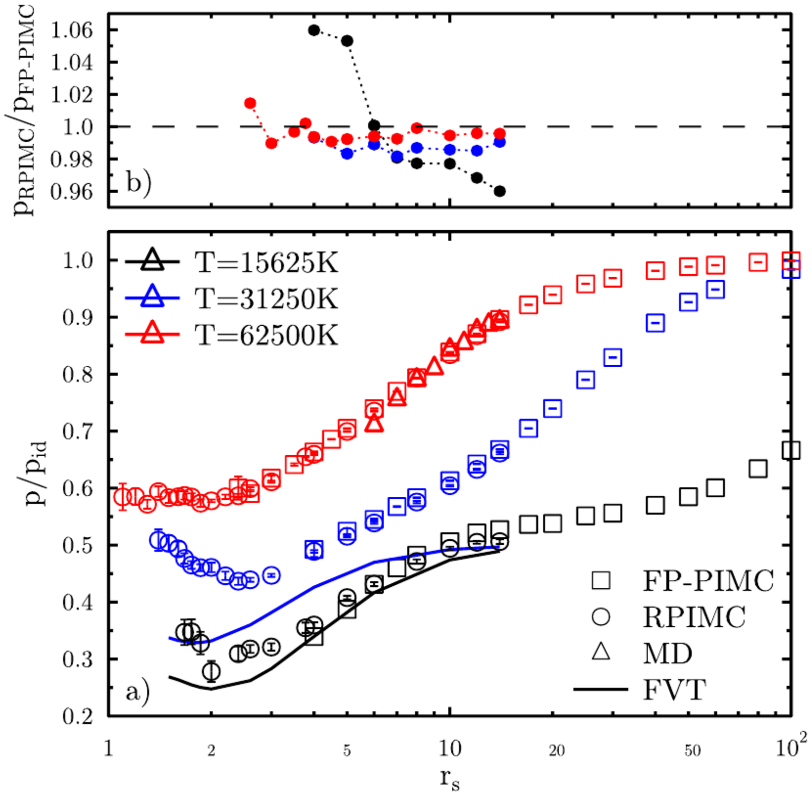
- chemical models (FVT)
- Semiclassical MD with
  Improved Kelbg potential
  [A. Filinov *et al.*, PRE 2004]

Accurate equation of state for
T > 60 000K

Results of Hanno Kähler

extendable to other materials
ML pair potentials

„cheap“ approach



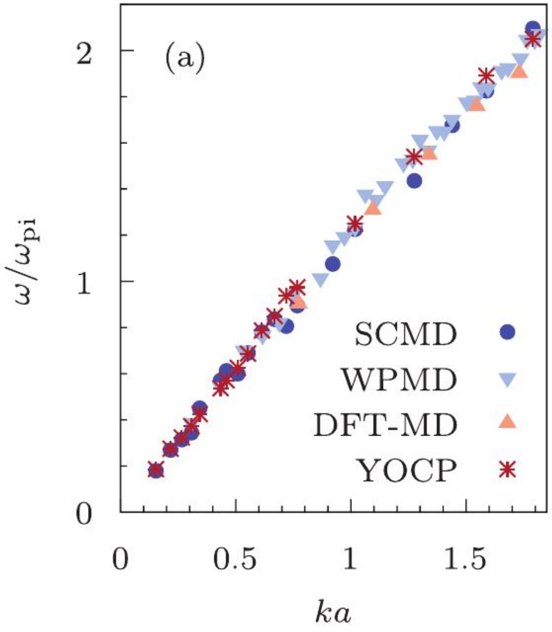
*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)
Accuracy of order 0.1% possible
M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Semiclassical MD: dynamic properties of dense H

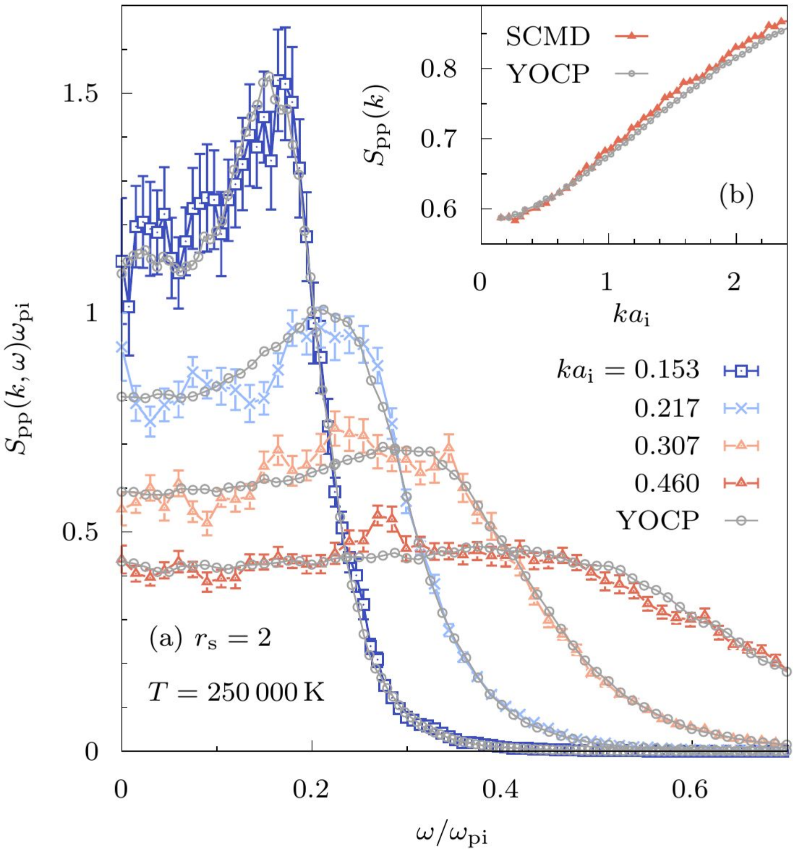
Ion-ion dynamic structure factor

ion-acoustic mode at small k

- good agreement for sound speed with WPMD / DFT-MD [1]
- well reproduced by Yukawa OCP with adjusted screening



[1] Svensson *et al.*, Phys. Rev. E **110**, 055204 (2024)



adapted from H. Kählert, Phys. Plasmas **33**, 022701 (2026)

Density Functional Theory

- Developed in 1960s by Kohn, Sham, Hohenberg, Mermin and many others
- main observable: electron density (ground state and finite T)
- Interacting problem mapped on non-interacting problem in external potential

- single approximation: exchange correlation potential, uses QMC data as an input
- choice of functional open question

- Natural representation of quantum extension (probability density) of particles.
- extension to time evolution: time-dependent DFT (TD-DFT, Runge, Gross)

DFT+MD for ions: main „work horse“ in WDM simulations

Recent overviews on WDM applications:
M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)
M. Bonitz *et al*., Phys. Plasmas (2026), arXiv: 2604.03757

Benchmarking DFT xc-functionals for dense H eq of state*

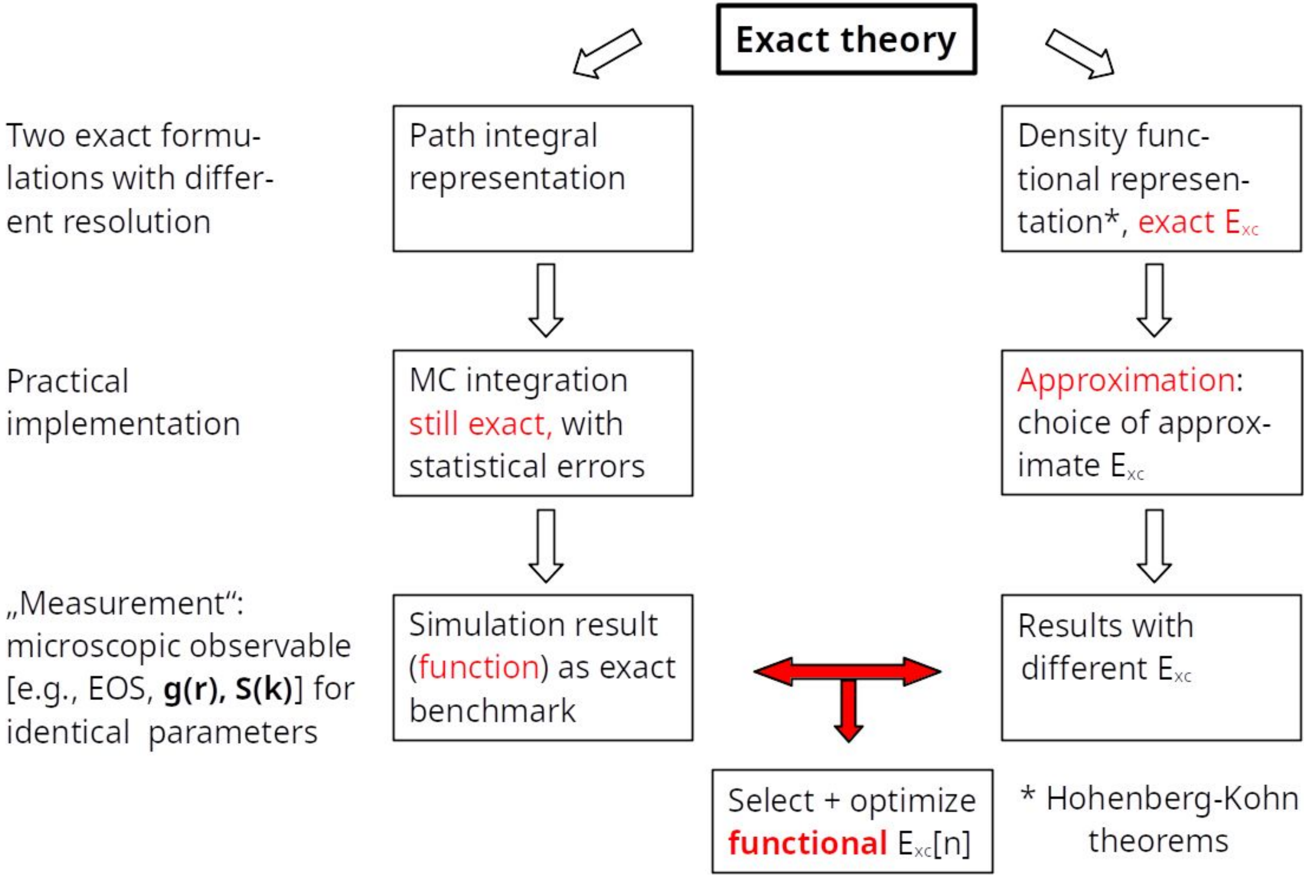
Relative error DFT vs fermionic PIMC

*FPIMC data: A.Filinov and M. Bonitz, PRE **108**, 055212 (2023);   DFT results: V. Karasiev, SX. Hu,

Bonitz *et al*., Phys. Plasmas (2026), arXiv: 2604.03757

The next step:

FPIMC downfolding: Kohn-Sham-DFT



Exact theory

Two exact formulations with 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., EOS, **g(r), S(k)**] for identical parameters

Simulation result (function) as exact benchmark

Results with different E_{xc}

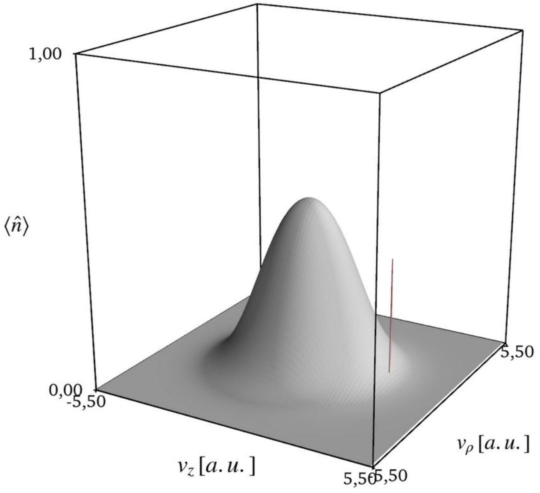
Select + optimize **functional** $E_{xc}[n]$

* Hohenberg-Kohn theorems

Similar applications to Green functions, Saha equation

Bonitz *et al*., Phys. Plasmas (2026), arXiv:2604.03757

Nonequilibrium quantum benchmarks: stopping power



- Obtain time-dependent distribution function f(p,t) and observables from solution of a quantum kinetic equation – potentially nonlinear effects
- Test case: relaxation of a monochromatic ‚beam‘ of protons or electrons
- **NEGF as benchmarks for nonequilibrium dynamics** (TDDFT, hydro)

M. Bonitz, „Quantum Kinetic Theory“ 2nd ed. 2015

Kiel: new developments in NEGF,:
G1-G2 scheme, Schlünzen et al., PRL **124**, 076601 (2020)
Quantum fluctuations approach, arXiv:2606.10773

Results of Christopher Maikait

Yellow: full beam relaxation (spreading)

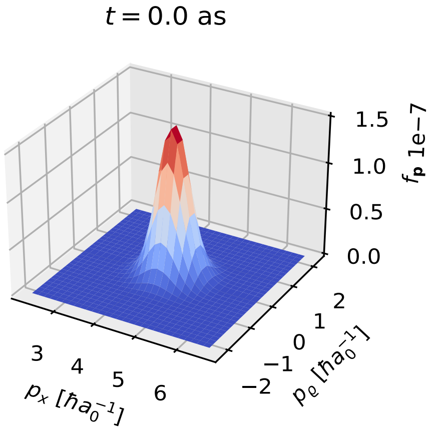
Proton stopping power: quantum kinetics vs. RPA

proton
beam
relaxation

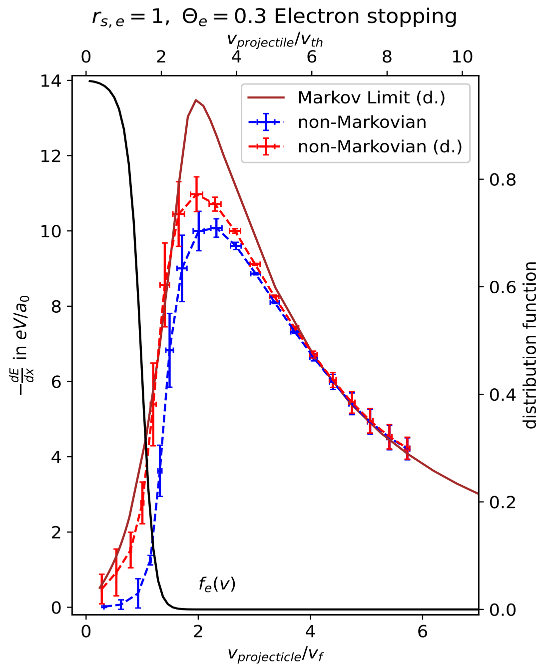
Dynamic stopping of proton projectiles agrees well with static RPA formula, confirming static assumption.

$$\frac{\mathrm{d}E_{\mathrm{kin}}}{\mathrm{d}t} = \frac{2Z_b^2e^2}{\pi v^2}\int_0^\infty \frac{\mathrm{d}k}{k}\int_{\hbar k^2/2m_b-kv}^{\hbar k^2/2m_b+kv} \mathrm{d}\omega \left[\omega - \frac{\hbar k^2}{2m_b}\right] \mathrm{Im}\,\varepsilon_{\mathrm{RPA}}^{-1}(k,\omega)\, n_B(\omega)\,,$$

Electron stopping: quantum kinetics vs. Balescu-Lenard („Markov“)



electron beam relaxation



stopping power reduced due to non-Markovian (correlation) effects (red) and Pauli-blocking (blue)

Relevant to hot-electron cooling (e.g., thermalization after X-ray flashes / laser excitation)

Results of Christopher Maikait

Strategy for WDM/quantum plasma/ICF simulations

Needed:

Combine radiation hydro with
more advanced simulations
on different scales

Needed: joined effort of different
groups, including Kiel, HZDR, HEDI
and beyond

Achieve predictive capability
for ICF simulations

from M. Bonitz, T. Dornheim and R. Redmer,
the Innovation Platform ISSUE 25 (2026)

Bonitz *et al*., Phys. Plasmas (2026), arXiv:2604.03757

Towards improved (rad-)hydrodynamics (1): correlations*

Standard hydrodynamic approach:

$$\rho\left(\frac{\partial\vec{v}}{\partial t}+\left(\vec{v}\cdot\vec{\nabla}\right)\vec{v}\right)=-\vec{\nabla}p+\eta\left(\vec{\nabla}^2\vec{v}+\frac{1}{3}\vec{\nabla}\left(\vec{\nabla}\cdot\vec{v}\right)\right)$$

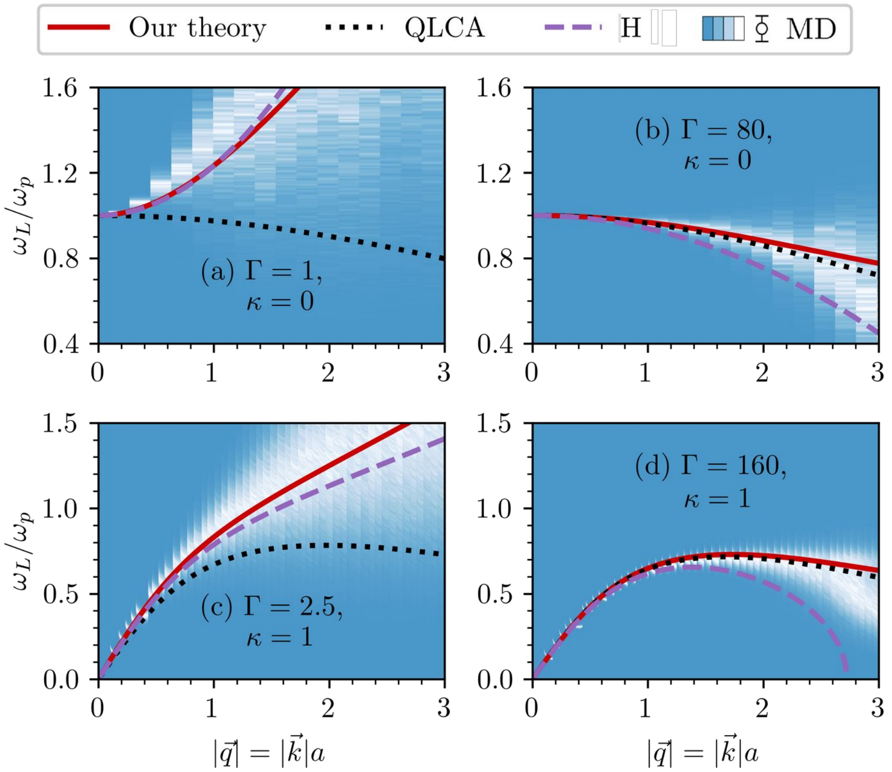
Input from WDM simulations (PIMC, DFT, MD)

Novel macroscopic variational principle:

$$L=K-U=\int\left(\frac{1}{2}m\vec{v}^2-\frac{3}{2}k_BT\right)n(\vec{x})\mathrm{d}\vec{x}$$

$$-\frac{1}{2}\iint\phi(|\vec{x}-\vec{x}'|)n(\vec{x})n(\vec{x}')\underline{g(n_0,T,|\vec{x}_0-\vec{x}_0'|)}\mathrm{d}\vec{x}\mathrm{d}\vec{x}'$$

Pair distribution, input from (PIMC, DFT, MD)



D. Krimans and S. Putterman, Phys. Fluids 36, 037131 (2024),
D. Krimans and H. Kählert, " Phys. Rev. E 113, 025201 (2026),
Plots: plasmon dispersion of Yukawa OCP

*D. Krimans, Marie-Curie project, part of Verbundprojekt „spearhed“ (M. Bussmann)

Towards improved (rad-)hydrodynamics (2): quantum effects*

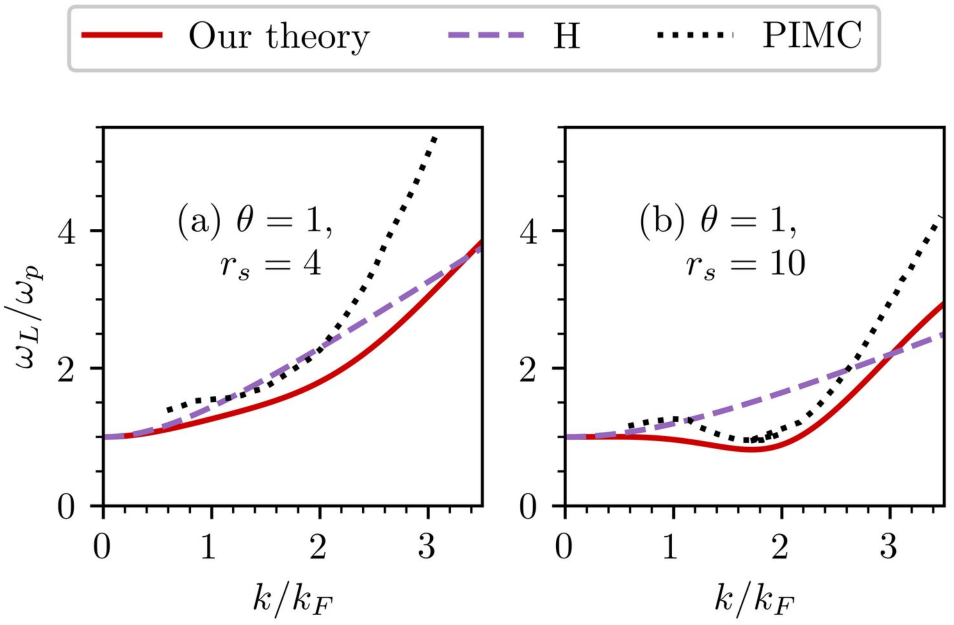
Variational principle for jellium

Pair correlations and kin. energy modified by quantum effects, combination with orbital-free DFT

$$\varepsilon(n,T) = \varepsilon_{\mathrm{id}} + \varepsilon_{\mathrm{xc}}$$

$$L = K - U = \int \left(\frac{1}{2}m\vec{v}^2 - \underline{\frac{3}{2}k_B T}\right) n(\vec{x})\,\mathrm{d}\vec{x}$$

$$- \frac{1}{2}\iint \phi(|\vec{x}-\vec{x}'|)\,n(\vec{x})\,n(\vec{x}')\,\underline{g(n_0,T,|\vec{x}_0-\vec{x}'_0|)}\,\mathrm{d}\vec{x}\,\mathrm{d}\vec{x}'$$



Plasmon dispersion of strongly correlated electrons:

D. Krimans, H. Kählert, M. Bonitz, to be published (2026),

PIMC data: T. Dornheim *et al.,* PRL **121,** 255001 (2018).

*D. Krimans, Marie-Curie project,
part of BMFTR laser fusion hub

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: fusion cross sections, accurate understanding of 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 physicists need 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