Dense quantum plasmas – failures of quantum hydrodynamic models

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Dense quantum plasmas

Space plasmas: - planet interiors
- dwarf stars, neutron stars ...

Laboratory systems: - electron gas in metals
- electron-hole plasma in semiconductors
- laser plasmas, „warm dense matter“

Theory: correlations, quantum and spin effects (Fermi statistics)
- quantum statistics, quantum kinetic theory
- first principle simulation (QMC, QMD)
- density functional theory (DFT)

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Models: Thomas-Fermi, quantum hydrodynamics (QHD), limited validity
spectacular predictions:
- „novel“attraction between protons in dense hydrogen
- quantum dusty plasmas
- giant spin polarization „spin-gradient driven laser“

published in leading plasma journals, very highly cited
growing popularity, but ignored by community

PRL 108, 165007 (2012) PHYSICAL REVIEW LETTERS week ending 20 APRIL 2012

Novel Attractive Force between Ions in Quantum Plasmas

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(Received 18 December 2011; published 20 April 2012)

In summary, we have discovered a new attractive force between two ions that are shielded by degenerate electrons in an unmagnetized quantum plasma. There are several

formation of ion clusters or ion atoms will emerge as new features that are attributed to the new electric potential

attractive force, we can have the formation of Coulombic ion lattices (Coulomb ion crystallization) and ion lattice

vealed the new physics of collective electron interactions at nanoscales, will open a new window for research in one of the modern areas of physics dealing with strongly coupled degenerate electrons and nondegenerate mildly coupled ions in dense plasmas that share knowledge with

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?

The Shukla-Eliasson potential

Screened potential of a proton

attractive minimum for α>0.25

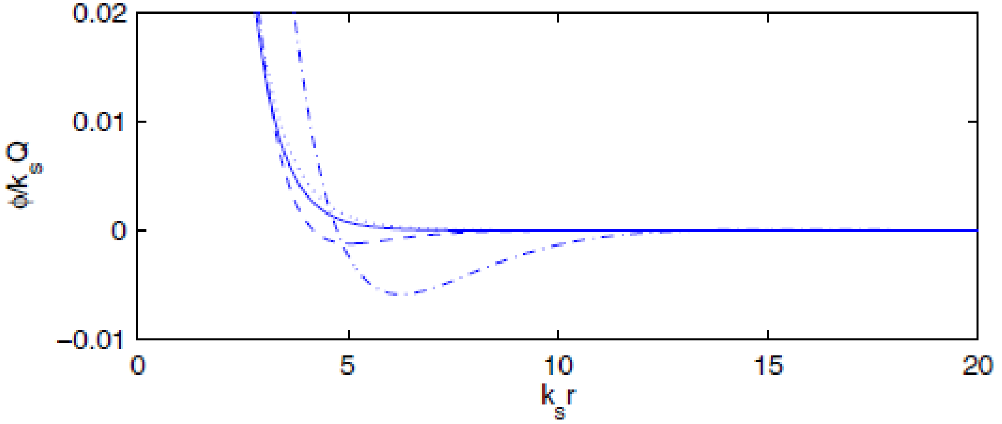


FIG. 1 (color online). The electric potential ϕ as a function of r for $\alpha = 10$ (dash-dotted curve), $\alpha = 1$ (dashed curve), $\alpha = 1/4$ (solid curve), and $\alpha = 0$ (dotted curve).

Problem: data cannot be reproduced,
no plasmas exist with these
Parameters
- information sent to authors

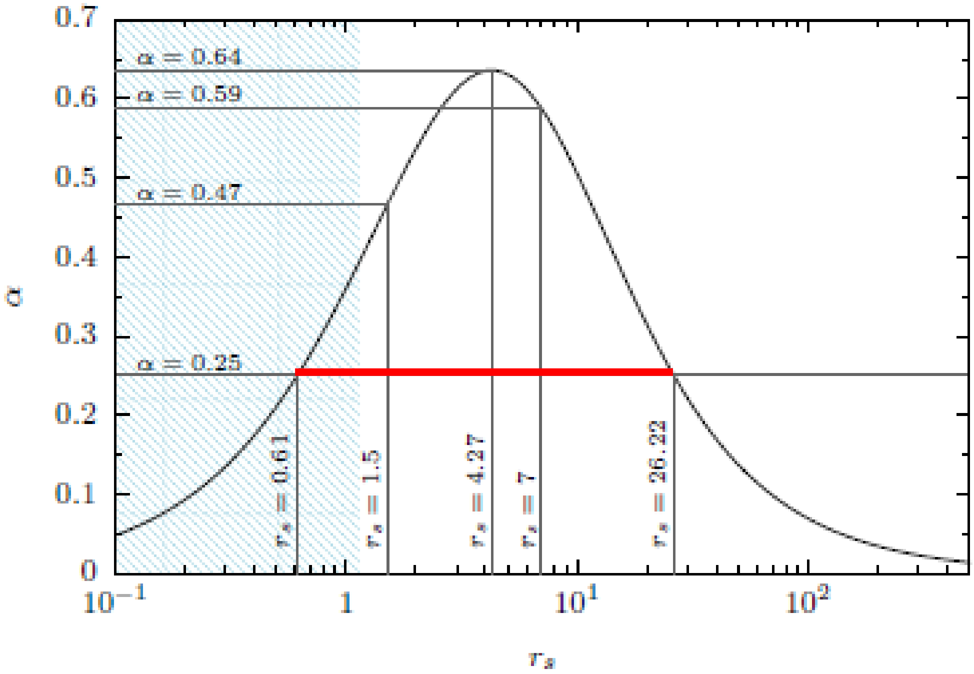
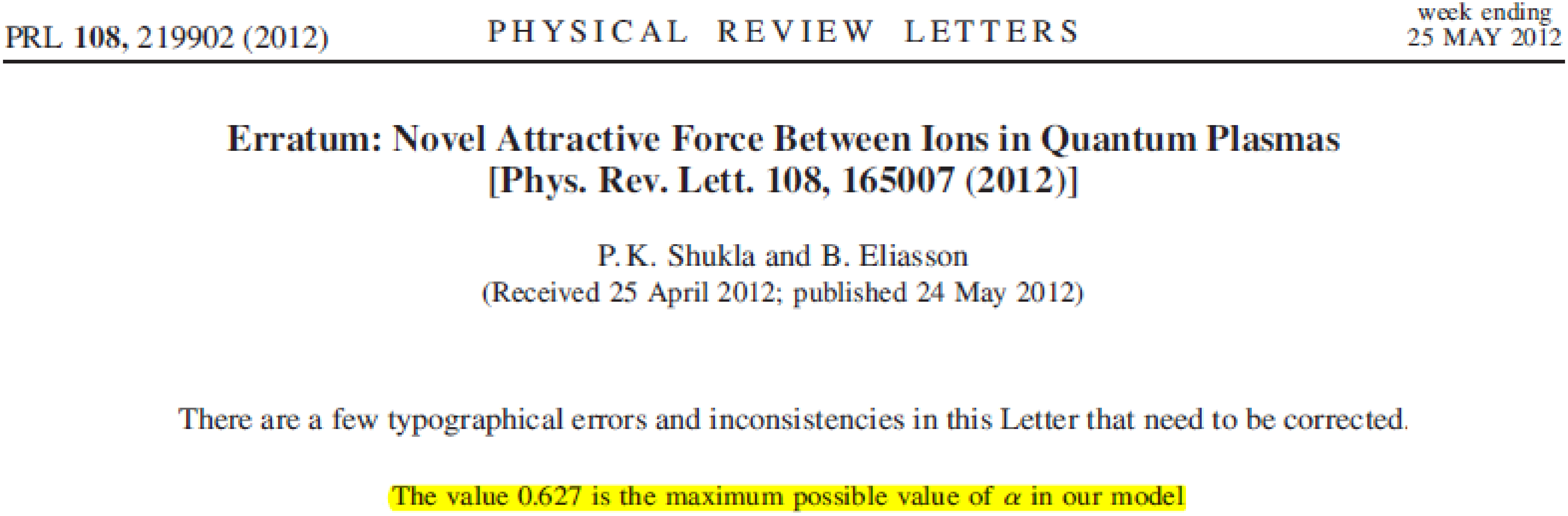


FIG. 1. Coupling parameter α versus Brueckner parameter r_s. An attractive proton potential is predicted in the density interval $26.22 \geq r_s \geq 0.61$ at zero temperature. The shaded area denotes the range of r_s where the plasmon energy is smaller than the Fermi energy, $\hbar\omega_{\mathrm{pe}} < k_B T_F$ (weak coupling).

Quantum coupling parameter: $r_s = \bar{r}/a_B$

Bonitz, Pehlke, Schoof,
PRE **87**, 033105 (2013) and 037101 (2013)

The Shukla-Eliasson potential (E1)



PRL 108, 219902 (2012) PHYSICAL REVIEW LETTERS week ending 25 MAY 2012

Erratum: Novel Attractive Force Between Ions in Quantum Plasmas [Phys. Rev. Lett. 108, 165007 (2012)]

P. K. Shukla and B. Eliasson

(Received 25 April 2012; published 24 May 2012)

There are a few typographical errors and inconsistencies in this Letter that need to be corrected.

The value 0.627 is the maximum possible value of α in our model

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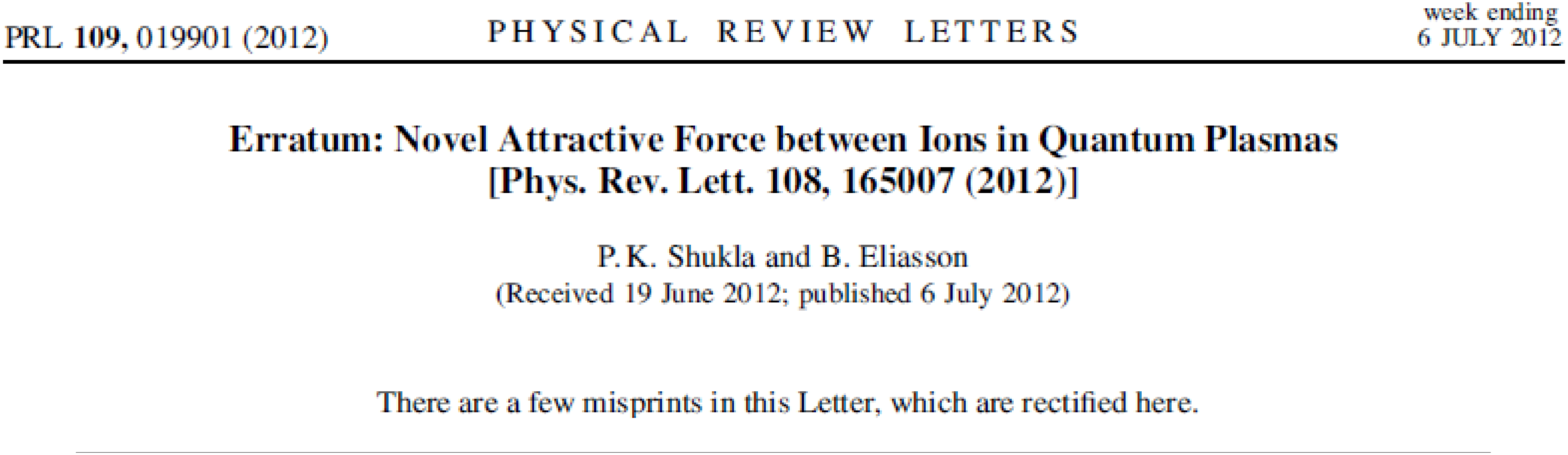
No source of the correction indicated.

Still results cannot be reproduced. Errors remain

The Shukla-Eliasson potential (E2)



PRL **109,** 019901 (2012) PHYSICAL REVIEW LETTERS week ending 6 JULY 2012

Erratum: Novel Attractive Force between Ions in Quantum Plasmas [Phys. Rev. Lett. 108, 165007 (2012)]

P. K. Shukla and B. Eliasson

(Received 19 June 2012; published 6 July 2012)

There are a few misprints in this Letter, which are rectified here.

Finally most equations are *formally* correct
But: still many errors

Problems: Bold claims without scientific justification
No comparison with earlier results, key references ignored
No discussion of applicability limits of SE-potential
No discussion of relevant plasma parameters
No critical test of proton crystal formation

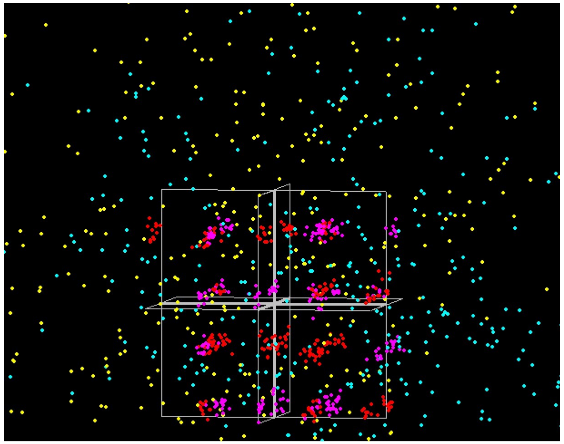
Phase diagram of dense hydrogen

PRL 95, 235006 (2005) PHYSICAL REVIEW LETTERS week ending 2 DECEMBER 2005

Crystallization in Two-Component Coulomb Systems

M. Bonitz,[1] V. S. Filinov,[1,2] V. E. Fortov,[2] P. R. Levashov,[2] and H. Fehske[3]

proton crystal formation in dense hydrogen plasma, analytical prediction confirmed by PIMC simulations



Phase diagram of dense hydrogen
well studied by first-principle simulations: quantum Monte Carlo, DFT

Recent overview:
Ceperley et al. RMP (2012)

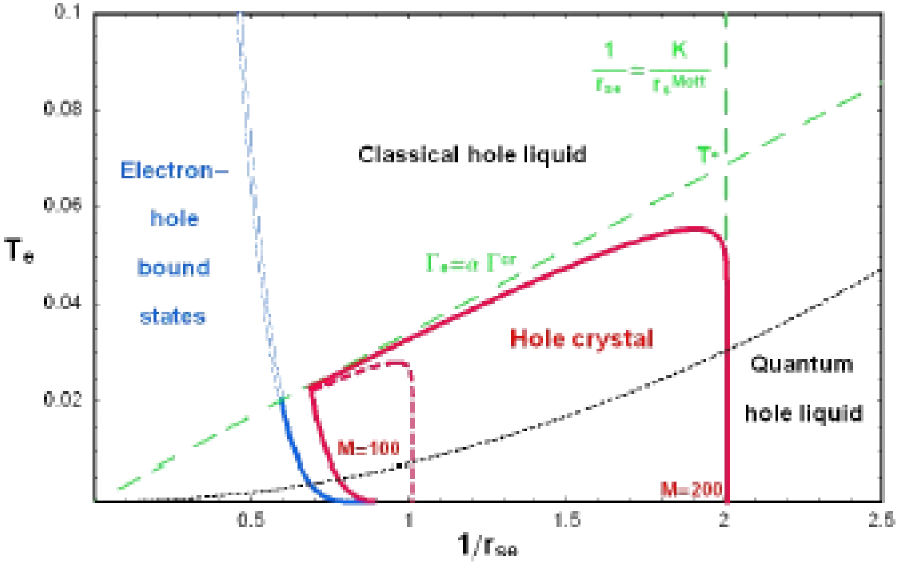
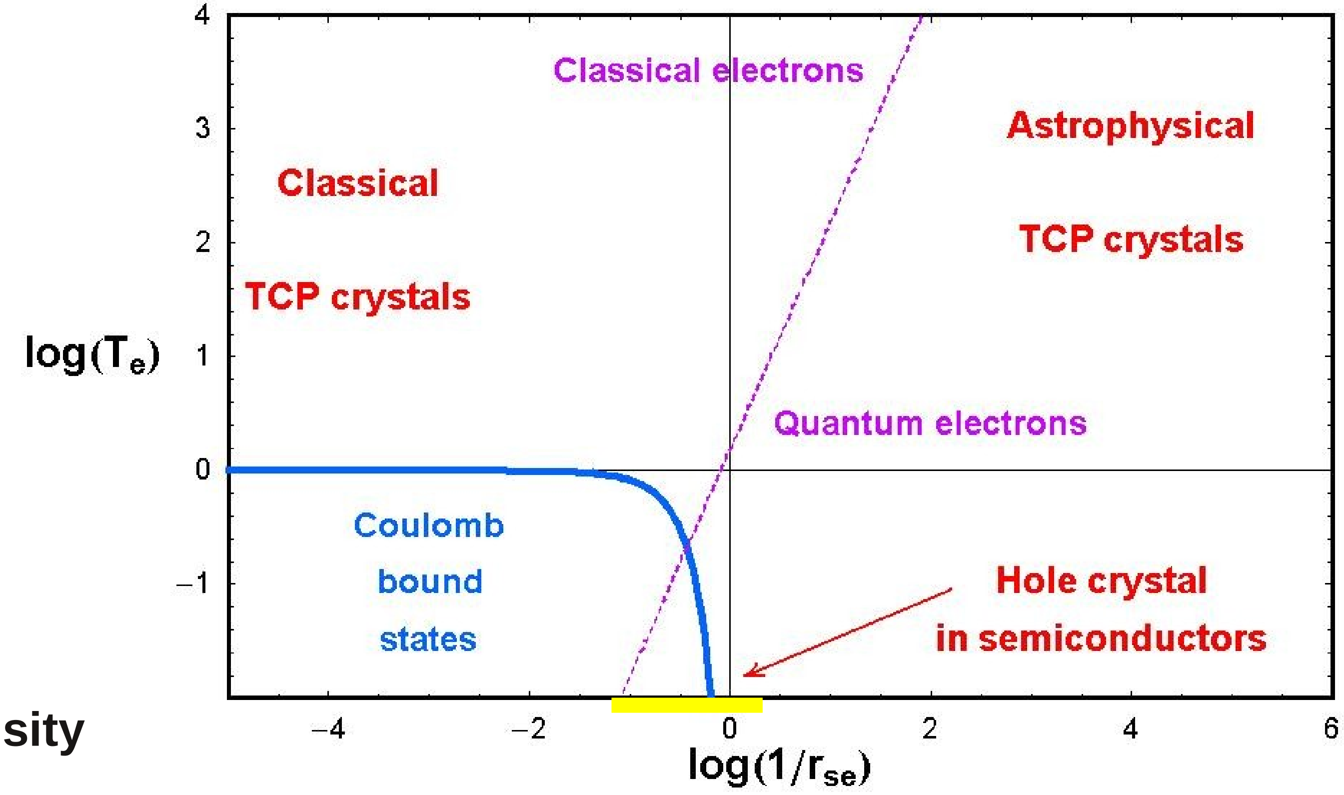


FIG. 3 (color online). Phase diagram of a two-component plasma in the plane of dimensionless electron temperature T_e and density parameter $1/r_{se}$. The boundary of the Coulomb bound state phase is given by $r_s^{\mathrm{Mott}}(T_e)$. Above (below) the dotted black line, holes are classical (degenerate). The red full (dashed) line is the boundary of the hole crystal for $\Theta = Z = 1$

Attractive potentials in dense hydrogen *in equilibrium*



Bonitz et al.,
J. Phys. A **39**, 4717 (2006)

Fermi gas
Friedel oscillations

low density

High density

$$26.22 \geq r_s \geq 0.61$$

T=0

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1. low density: H-H attraction (electron pairing) → H_2 molecules
2. high-density: Fermi edge singularity (Friedel oscillations)

the **Shukla-Eliasson model** does neither reproduce bound states nor Friedel oscillations

SE proton potential in atomic units

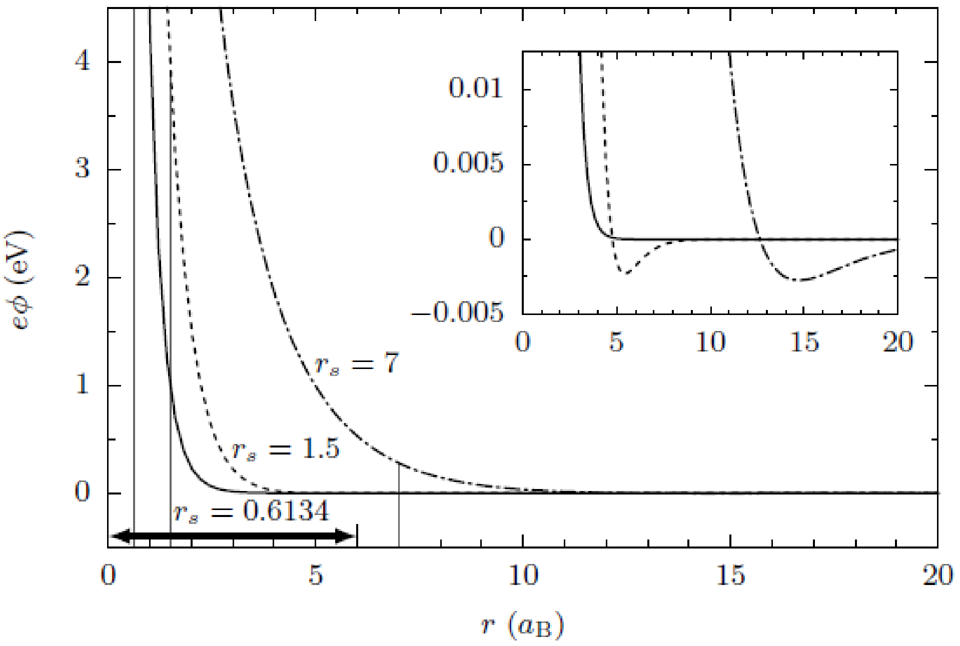
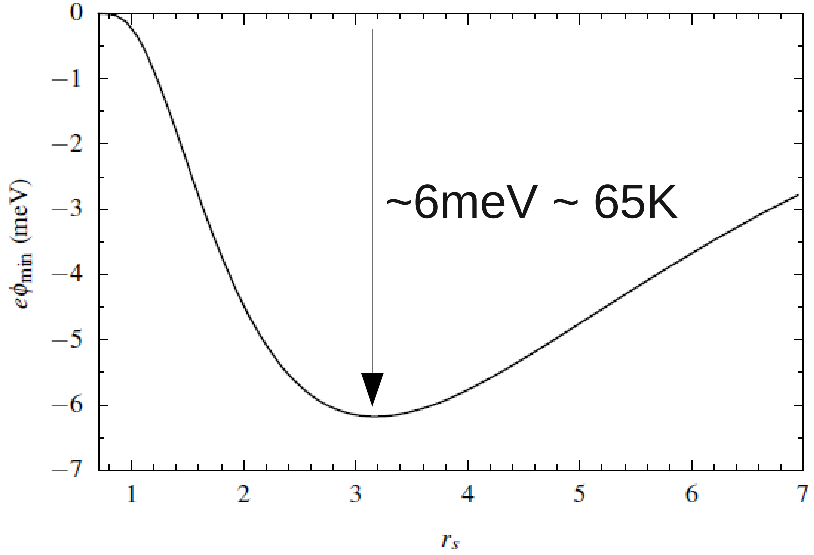
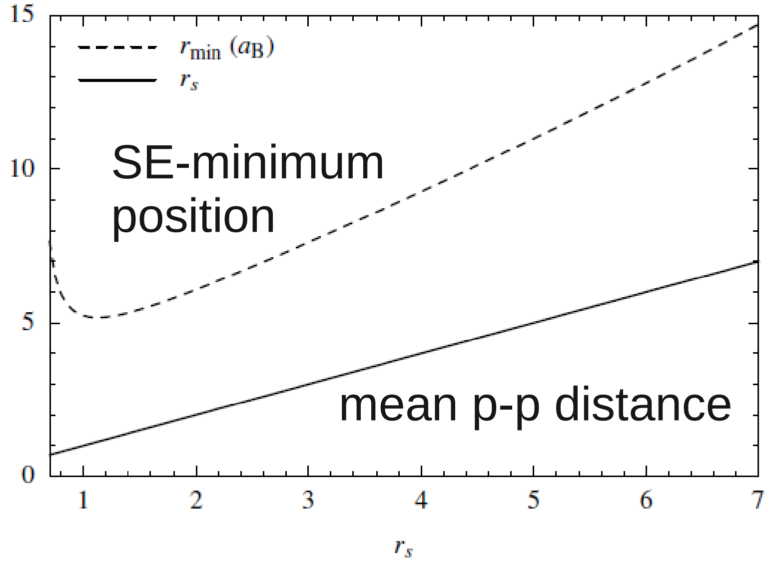


FIG. 2. Screened proton potential of SE for three densities. A single negative minimum is observed, shown more clearly in the inset. The location of the minimum and its depth are shown in Figs. 3 and 4, respectively. Thin vertical lines indicate the equilibrium nearest neighbor distance of two protons, cf. Fig. 3. The black arrow marks the range of values of r shown in Fig. 5.

Depth of SE-minimum



~6meV ~ 65K



SE-minimum position

mean p-p distance

→ even if the SE-attraction would exist
it could not lead to proton crystals

Ab initio H_2 molecules in dense hydrogen

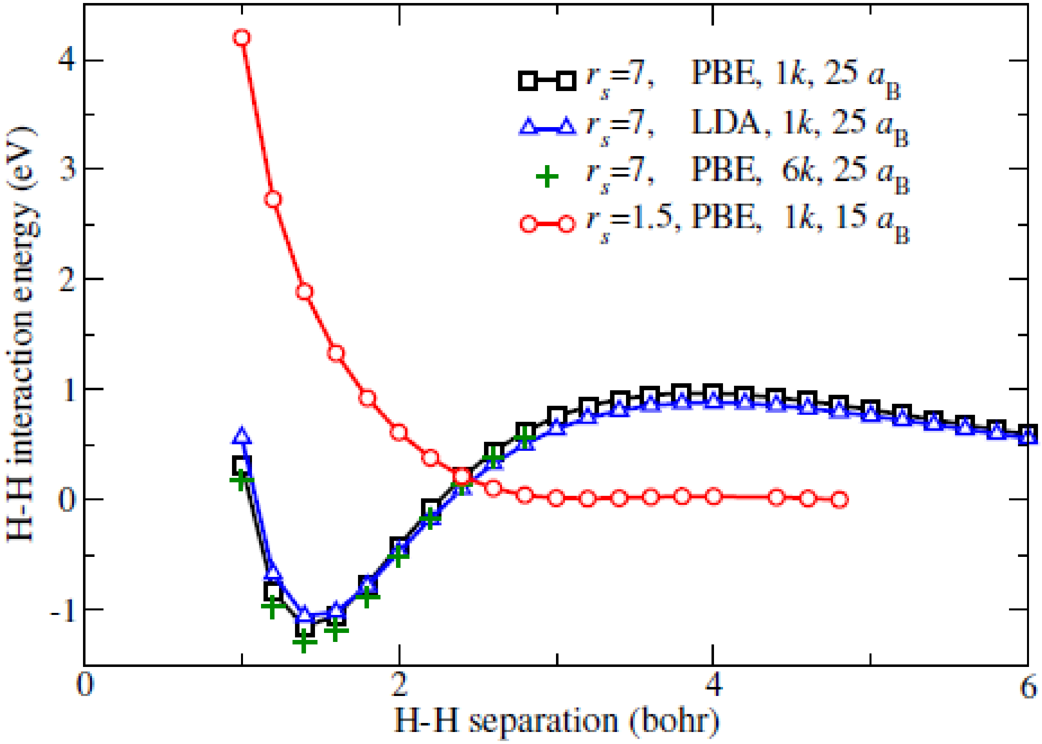


FIG. 6. (color online) Interaction energy of two H-atoms immersed in jellium for two densities. While for $r_s = 7$ a minimum around the hydrogen molecule bond length in vacuo (1.4 bohr) is observed, for $r_s = 1.5$, the molecular bound state is unstable. The DFT data have been calculated in a cubic box (with a size as noted in the inset) using PBE-GGA or LDA for the exchange-correlation energy-functional, a single or 6 k-points in the irreducible part of the Brillouin zone, and a plane-wave cutoff-energy of 100 Ry.

DFT results

r_s>1.5: H_2 molecules
r_s<1.5: proton repulsion

Friedel oscillations present (very shallow)

No additional minima

Bonitz, Pehlke, Schoof,
PRE **87**, 033105 (2013)

Ab initio proton potential in dense hydrogen

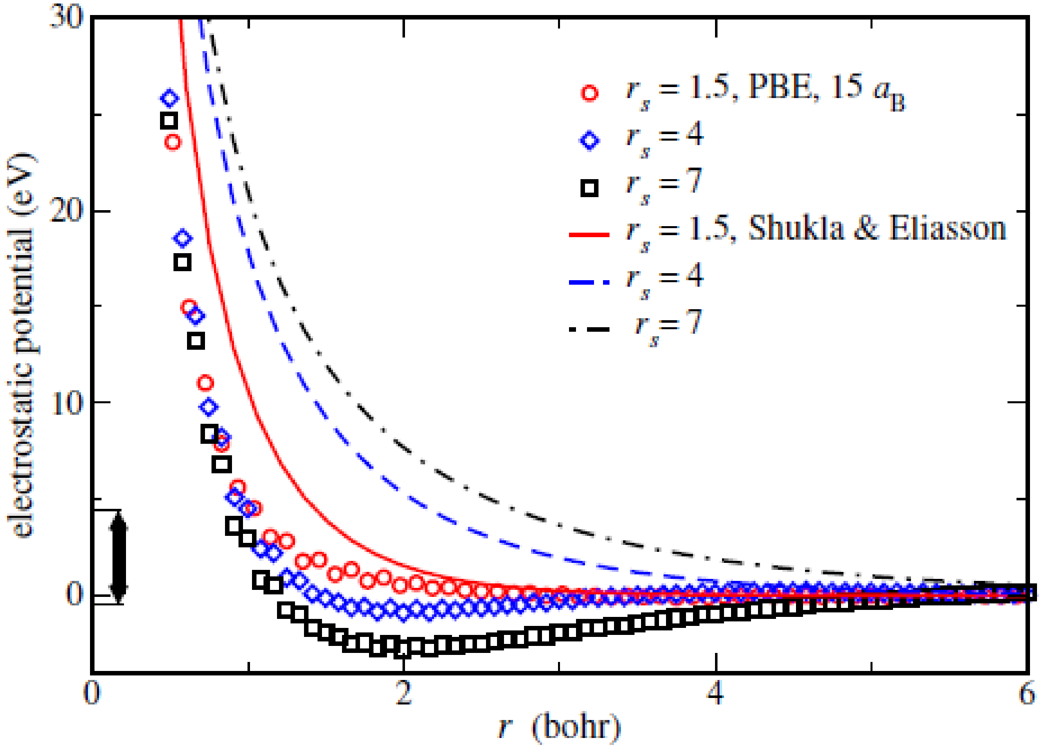


FIG. 5. (color online) Electrostatic potential around an H-atom immersed in jellium. r is the distance from the proton. DFT data have been calculated in a cubic box (size $15a_0$) using the PBE-GGA for the exchange-correlation energy-functional, a single k-point, and a plane-wave cutoff-energy of 200 Ry ($r_s = 1.5$) or 300 Ry ($r_s = 4$ and $r_s = 7$). The DFT data (symbols) are compared to the electrostatic potential from LQHD of Shukla and Eliasson, Ref. [1] (lines). The black arrow marks the voltage range shown in Fig. 2.

DFT results (symbols)

- the SE-potential (lines) is qualitatively wrong.
- wrong density dependence
- the SE minimum (few meV around 10 a_B) is irrelevant

Bonitz, Pehlke, Schoof,
PRE **87**, 033105 (2013)

Phys. Scripta **88**, 057001 (2013)

Quantum hydrodynamics (QHD)

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0$$

$$m_*\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = e\nabla\phi - n^{-1}\nabla P + \nabla V_{xc} + \nabla V_B$$

$$\nabla^2\phi = \frac{4\pi e}{\epsilon}(n - n_0) - 4\pi Q\,\delta(\mathbf{r}),$$

- 1-particle problem (exact): Madelung, Bohm

- Extension to N fermions assuming independent particles Manfredi/Haas (2001)

Approximations:

- ideal Fermi pressure, T=0
- no Fermi statistics
- phenomenological Xc-corrections (from DFT)
- average over small volume
- linear response

V_B= $(\hbar^2/2m_*)(1/\sqrt{n})\nabla^2\sqrt{n}.$ „Bohm potential“

V_XC= $-0.985(e^2/\epsilon)n^{1/3}[1+(0.034/a_B n^{1/3})\ln(1+18.37 a_B n^{1/3})]$

Linearization (LQHD) yields dielectric function D and screened potential:

$$\phi(\mathbf{r}) = \frac{Q}{2\pi^2}\int\frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{k^2 D}d^3k$$

$$D = 1 + \frac{\omega_{pe}^2}{k^2(v_*^2 + v_{\mathrm{ex}}^2) + \hbar^2 k^4/4m_*^2}$$

Summary: failure of LQHD for dense hydrogen

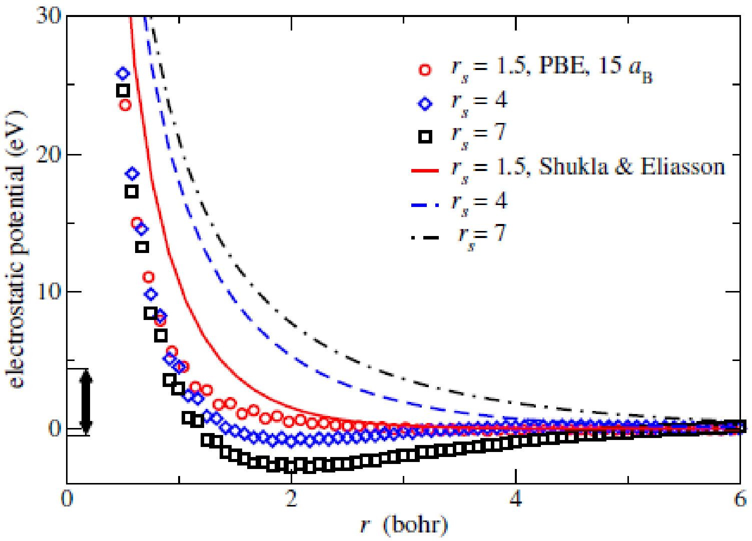
Approximations used in LQHD

- TD equilibrium, T=0, Fermi EOS
- no Pauli principle
- phenomenological xc-corrections
- average over small volume
- linear response

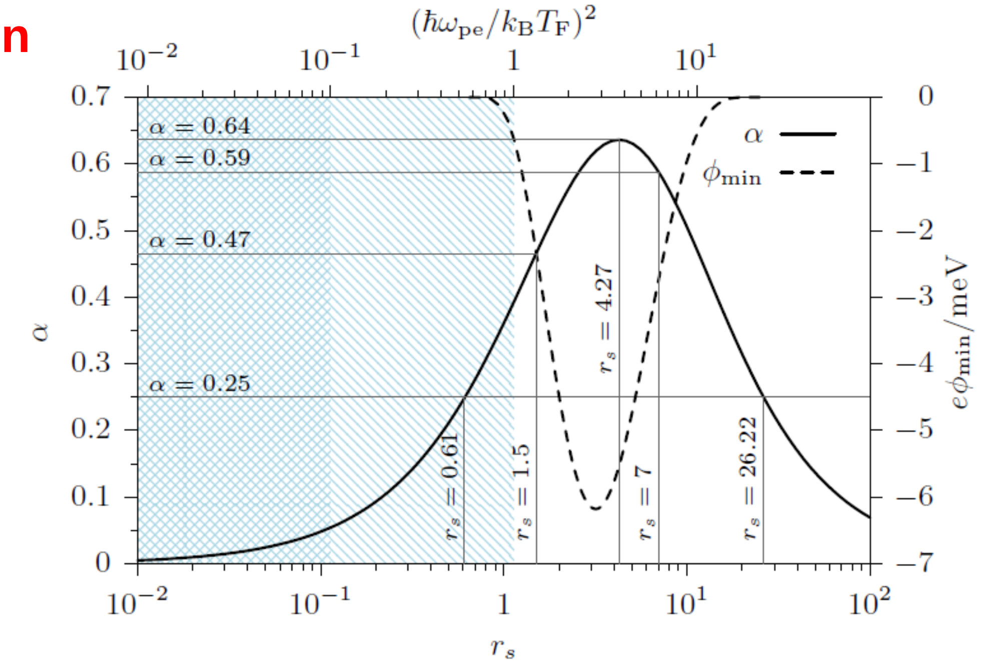
Hydrogen: LQHD restricted to r_s <<1,
distances >> a_B.

- ignored by Shukla/Eliasson
- **SE blame DFT for discrepancy**
(„misses Bohm potential“)

DFT more accurate than QHD by construction



SE-potential is qualitatively wrong.
SE minimum is an artefact of LQHD



no atomic-scale resolution
no novel bound states or proton crystal

Summary 2: implications for physics

Errors are unavoidable and have to be excused. However:

Bold claims without scientific justification
No comparison with earlier results, key references ignored
No discussion of applicability limits of SE-potential
No critical test of the made predictions, parameters

cannot be tolerated by the scientific community

- This style has become common in quantum hydrodynamics
- damages reputation of plasma physics in the borader community
- Journals and referees should restore good scientific practice

Similar critical analysis:

J. Vranjes, B. P. Pandey and S. Poedts, EPL **99**, 55001 (2012),
„On quantum plasma: A plea for a common sense“

G.S. Krishnaswami, R. Nityananda, A. Sen, A. Tyagaraja, „A critique of recent theories of spin half quantum plasmas“, arXiv:1306.1774 (2013)

Review: S. Khan, M. Bonitz, chapter in „Complex Plasmas“, Springer 2013, arxiv: 1310.0283
http://www.theo-physik.uni-kiel.de/~bonitz

APS Guidelines for professional conduct

Each physicist is a citizen of the community of science.
Each shares responsibility for the welfare of this community.

Science is best advanced when there is mutual trust, based upon honest behavior, throughout the community. Acts of deception, or any other acts that deliberately compromise the advancement of science, are unacceptable.

Honesty must be regarded as the cornerstone of ethics in science. Professional integrity in the formulation, conduct, and reporting of physics activities reflects not only on the reputations of individual physicists and their organizations, but also on the image and credibility of the physics profession as perceived by scientific colleagues, government and the public.

It is important that the tradition of ethical behavior be carefully maintained and transmitted with enthusiasm to future generations.