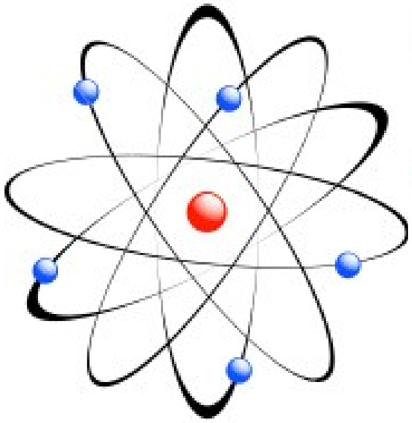
# How well do we understand the properties and characteristics of ions in plasma ?

S. Fritzsche
Oulu University and GSI Darmstadt
2th May 2011



## Questions of this talk:

i) How much help and information can atomic physics provide for modeling plasmas ?

ii) How does the electronic structure of ions (may) affect the diagnostics of plasma ?

iii) How well do we actually understand the behavior of – free as well as embedded -- atoms ?

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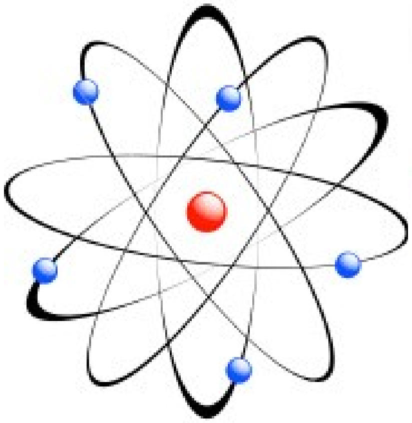

## Outline of this talk:

i) Atomic properties in plasma: A theoretician's viewpoint

ii) Extreme conditions: High-Z limit & “hollow” ions

iii) (Some) microscopic models for describing the electronic-structure response to plasma

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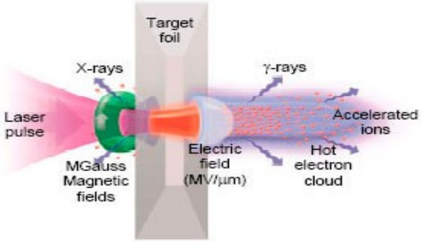
# Atomic and ionic “signatures” in plasma

## -- useful properties for the diagnostics and modeling

### Plasma diagnostics:

- Level shifts; magnetic-field shifts
- Oscillator strength and lifetimes; radiative cascades
- Line shapes & Stark broadening
- Nuclear-spin quenching



### Laser-induced plasmas:

- Index of refraction: dispersion and absorption
- Electric conductivity of plasma
- X-ray interferograms
- Charge-state distributions, optical depths
- (Super-) configuration averaging

### Plasma-wall interactions:

- Electron-impact rates; reaction rates
- Radiative and dielectronic recombination; collisional cascades
- Electron and radiation transport
- Auger channels & high-Rydberg states

# Atomic and ionic “signatures” in plasma

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### Plasma diagnostics:

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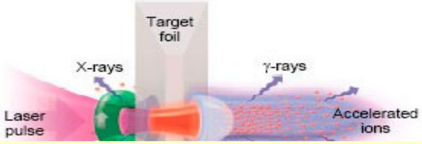


### Laser-induced plasmas:

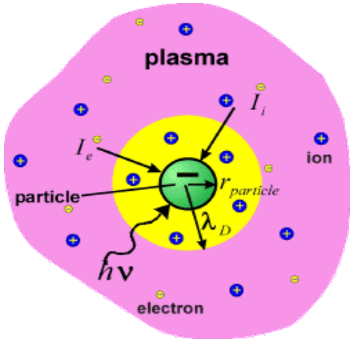
- Index of refraction: dispersion and absorption
- Electric conductivity of plasma

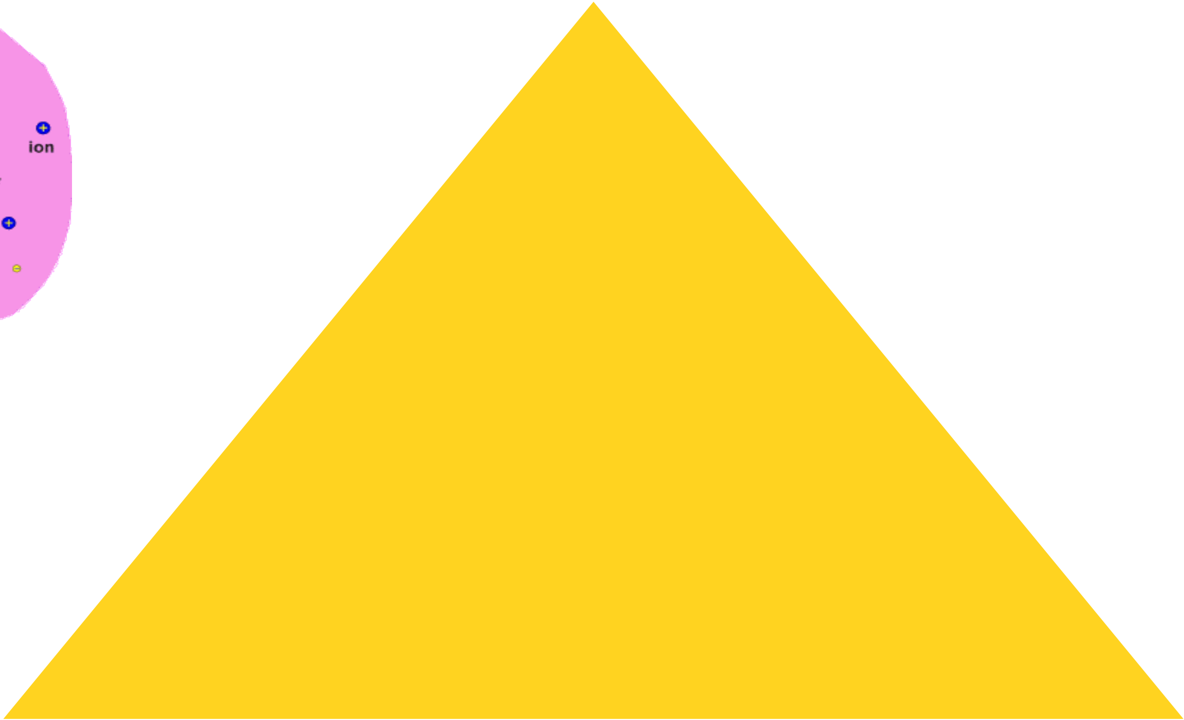
### Current questions and interests:

- Predicting understanding and control of plasma transport

  (w.r.t. thermal, electric, particle, momentum, ...)
- How are (turbulent) plasmas structured and to be confined ?
- How can the details from experiment and simulations be developed into understanding ?
- Inner- and subvalence shell ionization of high-Z materials

# Atomic properties in plasma: A theoretician's viewpoint





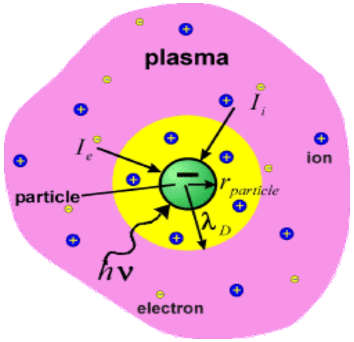
(strongly-) correlated motion of particles

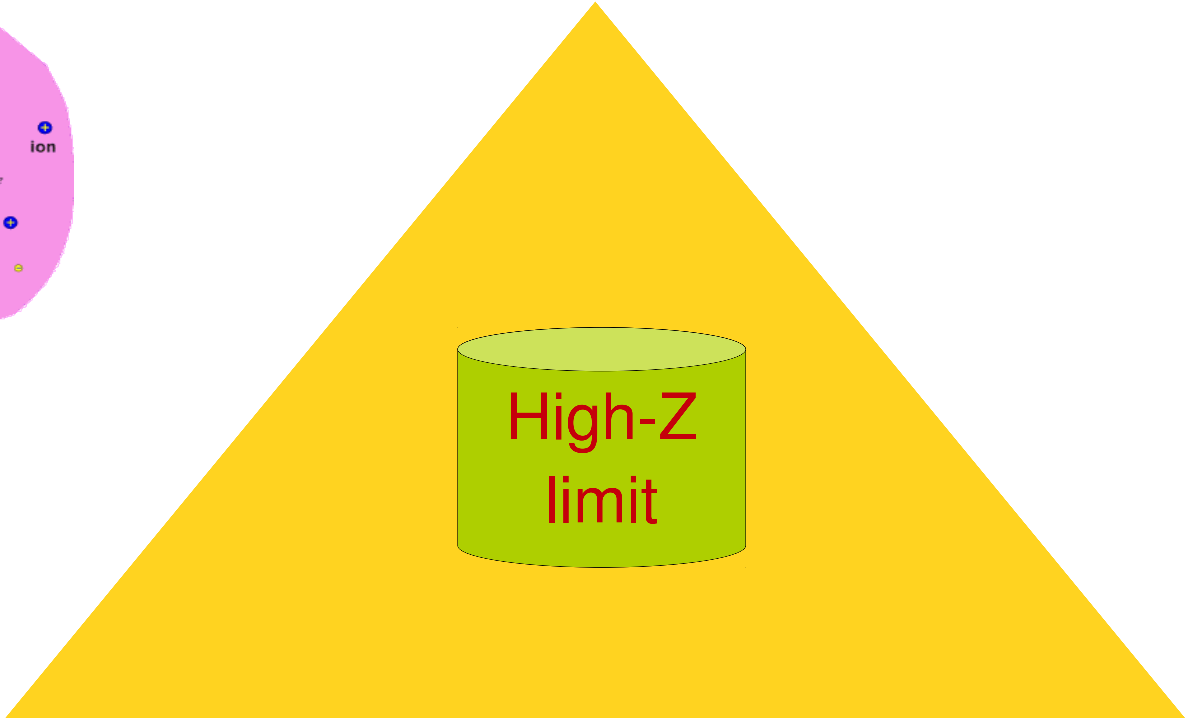
plasma
coupling &
environments

relativity

# Atomic properties in plasma: A theoretician's viewpoint

– via highly-charged ions and their exact quantum states





(strongly-) correlated motion of particles

High-Z limit

plasma coupling & environments

relativity

G. Friesecke and B.D. Goddard, PRA 81 (2010) 032516

# Level-structure of highly-charged, few-electron ions

## -- in the limit of large Z

For Z → ∞, a closed form can be found for the low-lying quantum states

(with convergence in a least-square sense along each iso-electronic sequence):

→ useful for predicting electronic configuration and term values

For example, the $^1S_0$ ground state of beryllium-like ions:

$$\frac{1}{\sqrt{1+c^2}}\left(|1s^2 2s^2\rangle + c\,\frac{1}{\sqrt{3}}\left(|1s^2 2p_1^2\rangle + |1s^2 2p_2^2\rangle + |1s^2 2p_3^2\rangle\right)\right)$$

$$c = -\frac{\sqrt{3}}{59049}\left(2\sqrt{1509308377} - 69821\right) = -0.2310995\ldots$$

Remarkable $p^2$ admixture along the whole beryllium iso-electronic sequence.

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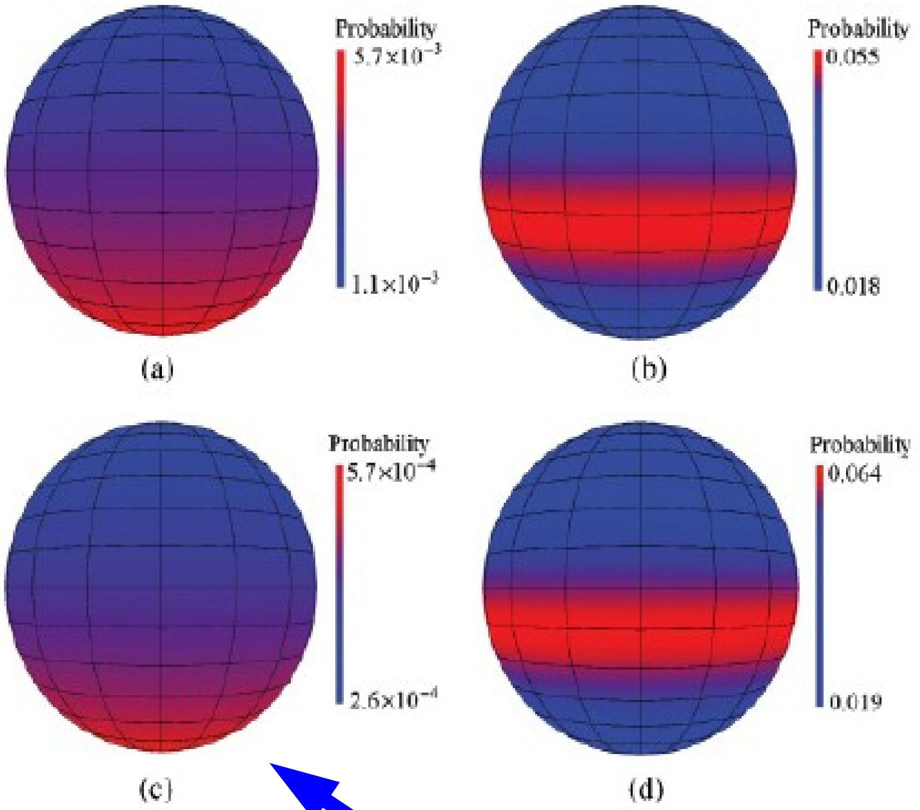
# Level-structure of highly-charged, few-electron ions

## -- in the limit of large Z

For Z $\to \infty$, a closed form can be found for the low-lying quantum states (with convergence in a least-square sense along each isoelectronic sequence):

Be-like
$Z \to \infty$

neutral



N-like
$Z \to \infty$

Quantum probability of finding a second electron anywhere on the sphere of radius N/Z a.u. when the first electron is at the north pole for the ground states.

Explains molecular geometries:

- $BeH_2$ is linear, while
- $NH_2$ is a bent molecule

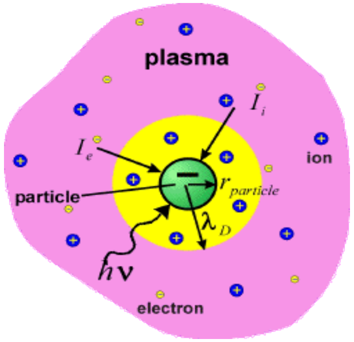
(due to dominant correlation anlge)

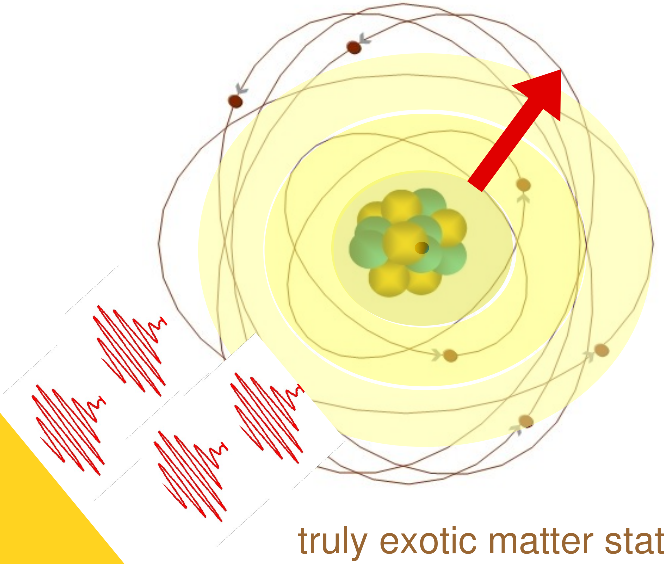
Remarkable $p^2$ admixture along the whole beryllium iso-electronic sequence.

# Atomic properties in plasma: A theoretician's viewpoint

– ionic processes in intense FEL radiation

(strongly-) correlated motion of particles





truly exotic matter states

plasma
coupling &
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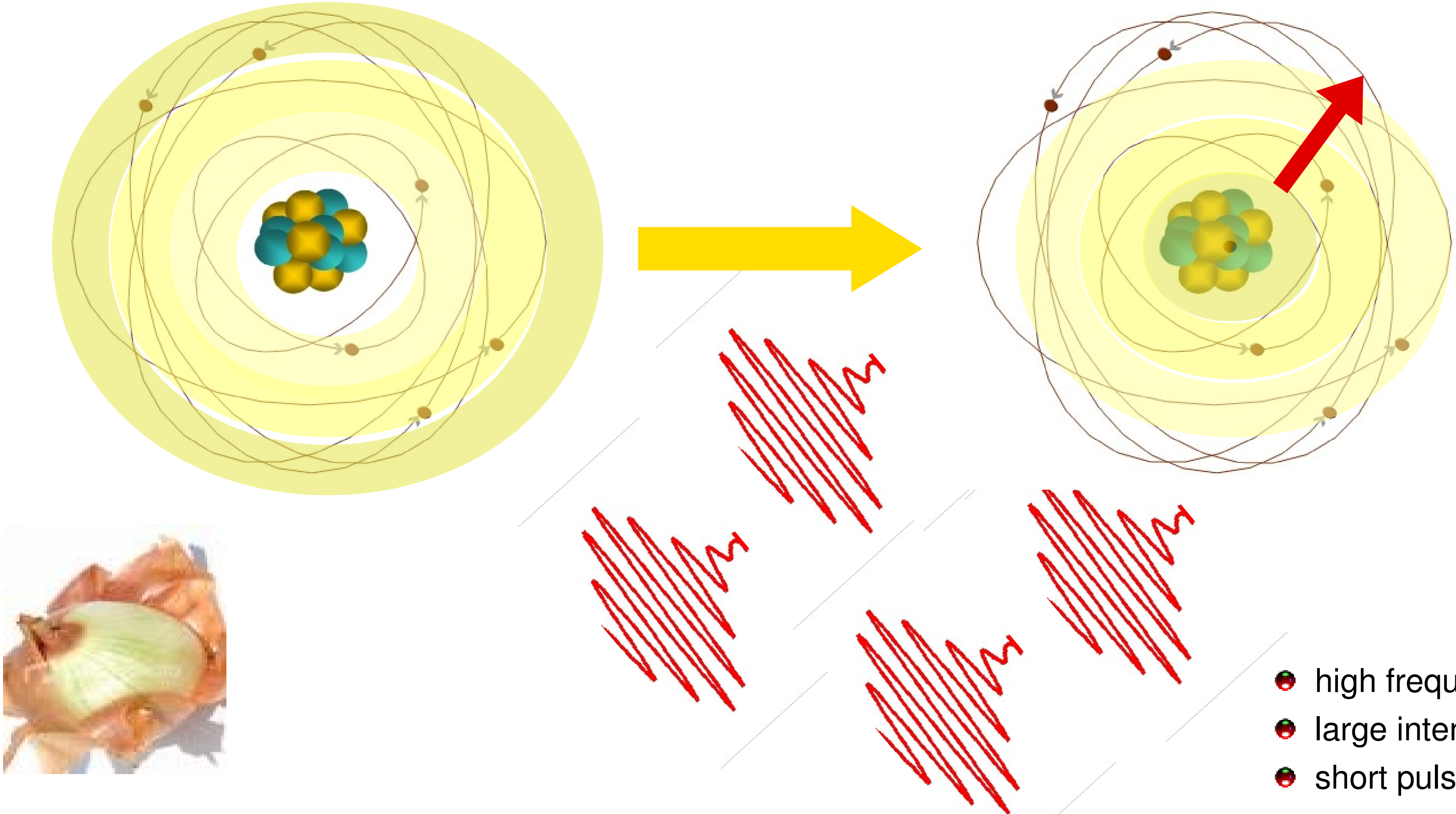
relativity

# Peeling the onion from inside

-- creation of truly exotic matter states

Intense optical and VUV laser

Intense x-rays



- high frequencies
- large intensities
- short pulses

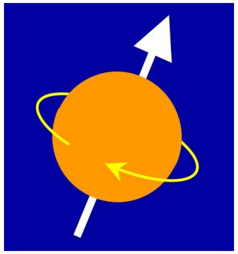
# Generation of „hollow atoms“

## -- strong coupling of the ionization and decay dynamics

### Generalized Bloch-type equations:

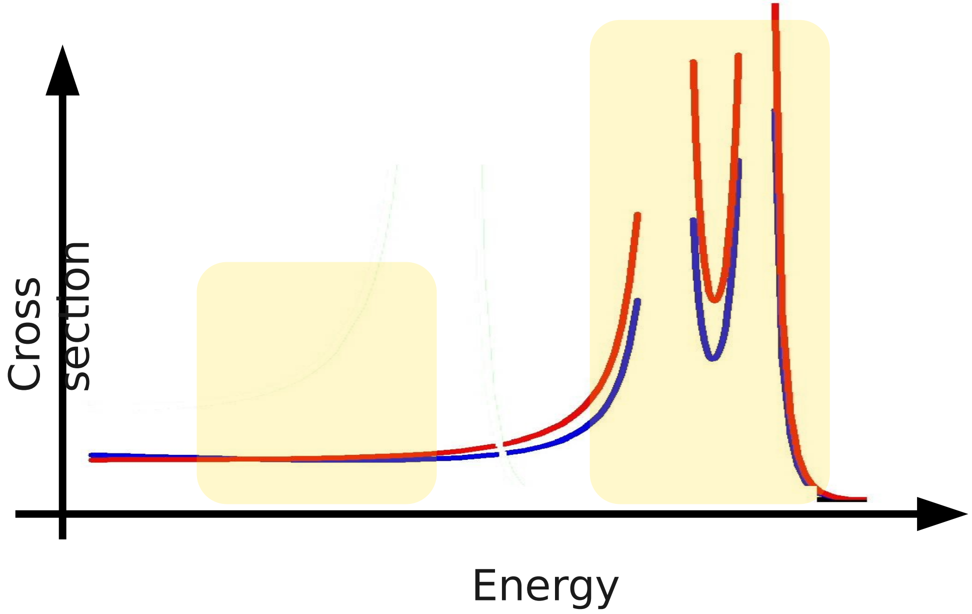
- time-dependent density matrix (theory)
- keeping the physical insight alive
- competition of ionization and decay
- interplay of different time and complexity scales
- entanglement evolution

$$\begin{aligned} \frac{\partial \rho_{21}}{\partial t} + (\gamma_2 + i\omega_{21})\rho_{21} &= i\frac{pE}{\hbar}n \\ \frac{\partial n}{\partial t} + \gamma_1(n - n_0) &= 2i\frac{pE}{\hbar}(\rho_{21} - \rho_{21}^{*}), \end{aligned}$$



### Creation of inner-shell holes:

- nonresonant vs. resonant regions
- isolated & non-isolated resonances
- inherent coupling with valence shells
- different interaction regimes
    - multi-photon ionization
    - fast Auger processes



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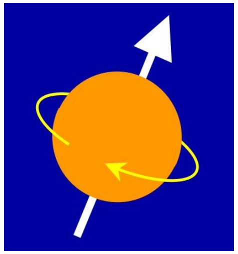


## Creation of inner-s

- nonresonant vs. reso
- isolated & non-isolat
- inherent coupling wit
- different interaction r
  - multi-photon ior
  - fast Auger proce

## Current interests and challenges

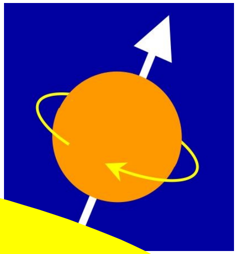
- two-photon double ionization: direct vs. sequential
- ionization of dressed ionic states: sidebands, Raman, ...
- multiple ionization in short pulses ($Xe^{21+}$, ...)
- multi-photon excitation of inner-shell hole: fast Auger, ...
- depolarization and quantum beats

# Generation of „hollow atoms“

-- strong coupling of the ionization and decay dynamics

## Generalized Bloch-type ns:

$$\frac{\partial\rho_{21}}{\partial t} + (\gamma_2 + i\omega_{21})\rho_{21} = i\frac{pE}{\hbar}n$$



- time-dependent density
- keeping th
- c

Interesting dynamics and a hot topic today

... but NOT well understood so far

and very complex

## Creation of inner-s

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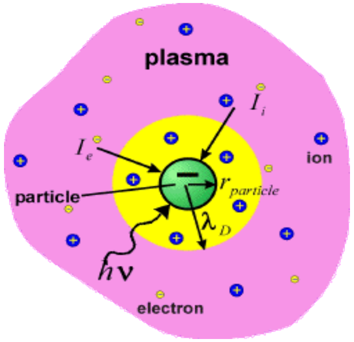
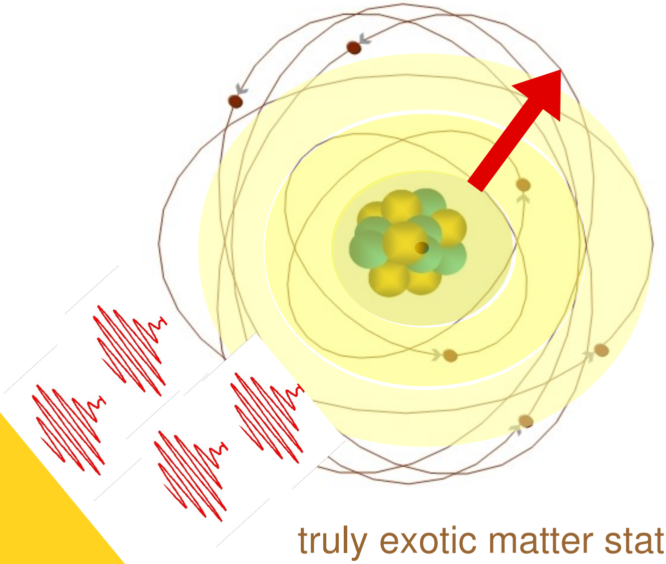
# Atomic properties in plasma: A theoretician's viewpoint

– ionic processes in intense FEL radiation

(strongly-) correlated motion of particles





truly exotic matter states

plasma coupling & environments

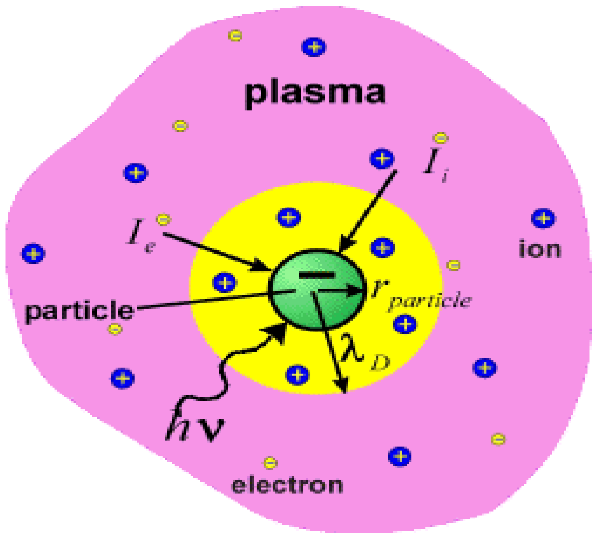
relativity

Plasma models based on ion-electron coupling

- Debye & ion-sphere
- Free & averaged-atom model
- Collisional-radiative model
- Particle-in-cell model, ...

# Hierarchy of inner-atomic interactions

## -- with the plasma environment treated by effective potentials



*Effective plasma potential due to dominant processes and coupling strength*

- Nuclear potential
- Instantaneous Coulomb repulsion between all pairs of electrons
- Spin-orbit interaction
- Relativistic electron velocities; magnetic contributions and retardation

- QED: radiative corrections
- Hyperfine structure
- Electric and magnetic nuclear moments (isotopes)

# Coulomb coupling parameter of plasma

## -- also known as plasma or `correlation' parameter

### Ratio of potential and kinetic energy

- Typical strength $0 < \Gamma \lesssim 100$
- Help to classify plasma regimes and phase transitions

### Weakly-coupled plasma ($\Gamma << 1$)

- Gaseous discharge plasma: $T \sim 10^4$ K, $n \sim 10^{11}$ cm$^{-3}$
-

### Calculations under external confinement:

- Interpretation of spectral line shifts in artificial atoms and laser produced plasma.
- Level populations, intensities, etc. obtained from such (for instance, collisional-radiative) models cannot be more accurate than underlying data.
- For laser-induced plasmas ($T \sim 1$ keV, $n \sim 10^{24}$/cm$^{-3}$), computations are suitable for deriving population kinetics, radiation flow as well as the line formation.
- Of course, use of plasma parameter is not comprehensive to characterize the dynamics of plasma
- Related also to quantum-dot studies and ultra-cold gases.

# Effective microscopic models

-- use of different potentials to deal with e-n and e-e interactions

Schrödinger equation for electronic motion in an effective (plasma) potential:

$$\left[\frac{p^2}{2m} - \frac{Z}{r} + V\right] u_a(\boldsymbol{r}) = \epsilon u_a(\boldsymbol{r})$$

Free-electron model: V(r) … derived from the free-electron gas

Averaged-atom model: $V(r) = V_{dir} + V_{exc}^{(LDA)}$ ; $\nabla^2 V_{dir} = -4\pi\rho$

Fermi distribution and chemical potential μ to ensure neutrality of the Wigner-Seitz cell of the ion with radius R.

Debye model:

$$-\frac{Z}{r} + V \longrightarrow -\frac{Ze^{-r_i/r_D}}{r_i} + \sum_{j \neq i} \frac{e^{-r_{ij}/r_D}}{r_{ij}}$$

Ion-sphere model:

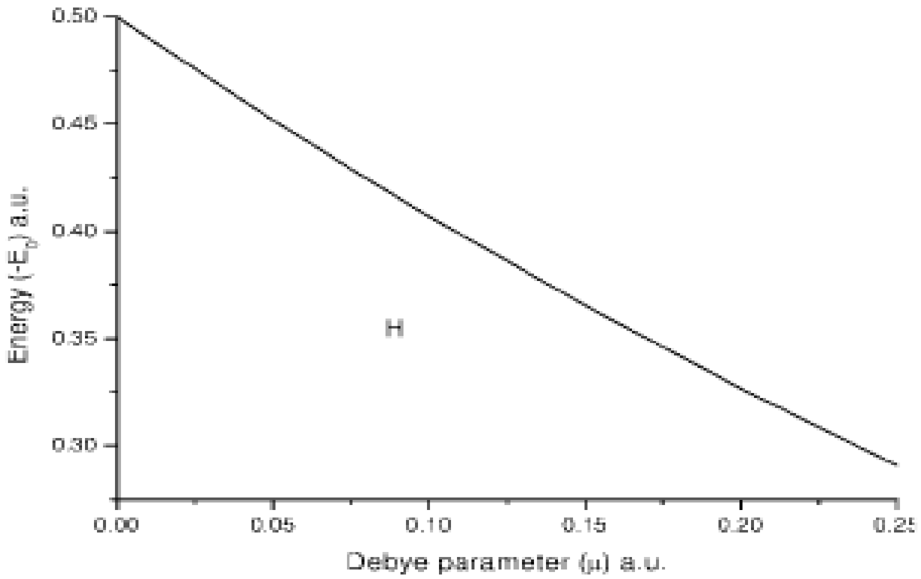
$$V \longrightarrow \frac{Z-N}{2R}\left[3 - \left(\frac{r_i}{R}\right)^2\right] + \sum_{j \neq i} \frac{1}{r_{ij}}$$

In plasma, the effective potential depends apparently on the plasma parameters.

# Debye plasma: Energy shifts and radiative rates

## – studied so far mainly for light few-electron ions

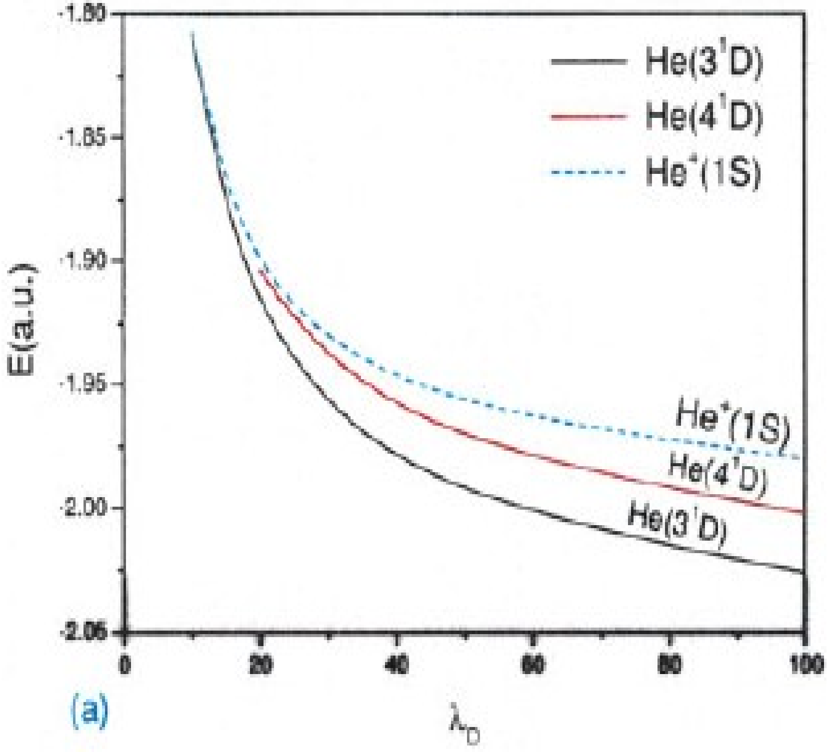
In experiments, exotic atoms are created inside of a neutral plasma environment when particles are slowed down in matter.



Ground-state energy of H a function of Debye parameter.

A. N. SIL et al, Int. J. Quant. Chem. 107 (2007) 2708.

$$r_{\mathrm{D}} = \left( \frac{4\pi(1+Z)n_e}{kT} \right)^{-1/2}$$



Bound 1s3d $^1$D and 1s4d $^1$D-state energies of helium in plasmas for various Debye lengths.

S. Kar and Y. K. Ho., Int. J. Quant. Chem. 107 (2007) 353.

B. Saha and S. Fritzsche, PRE 73 (2006) 036405.

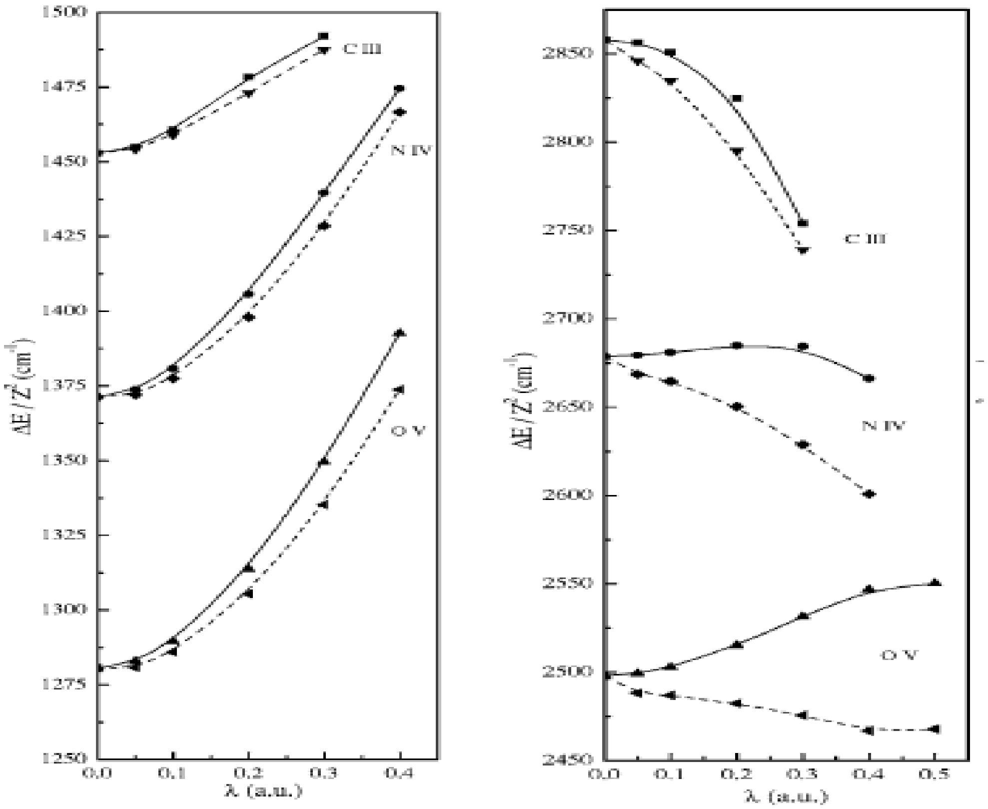
# Debye plasma: Energy shifts and radiative rates

## – along the beryllium isoelectronic sequence

Plasma screening on the 2s$^2$ $^1S_0 \to$ 2s2p $^3P_1$ intercombination and 2s$^2$ $^1S_0 \to$ 2s2p $^1P_1$ resonance transitions:

Relativistic theory; screening with regard to e-n (solid lines) and e-e (dashed lines) interaction.

Increasing blueshift of the intercombination line as Z is increased, while the resonance line is either red- or blueshifted, in dependence on Z and the coupling strength.

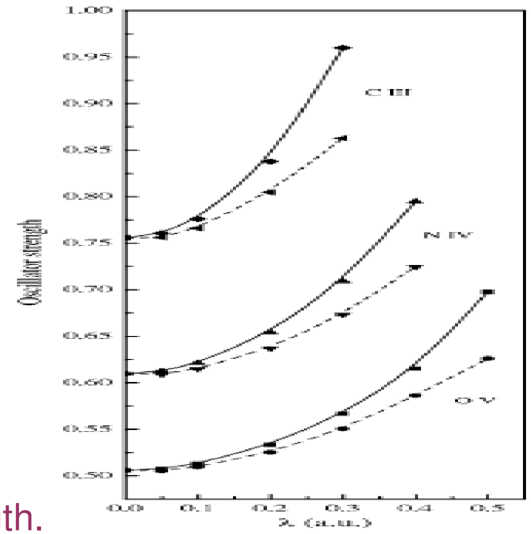


intercombination

resonance

Excitation energies, scaled by $1/Z^2$, as function of the plasma screening.

resonance



Oscillator strength.

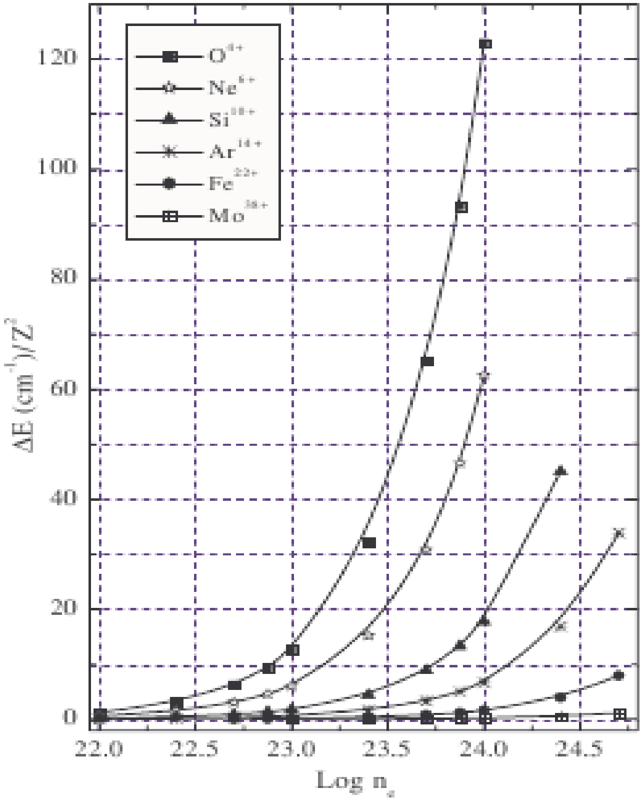
B. Saha and S. Fritzsche, JPB 40 (2007) 259.

# Ion-sphere model: Energy shifts and radiative rates

## – along the beryllium isoelectronic sequence

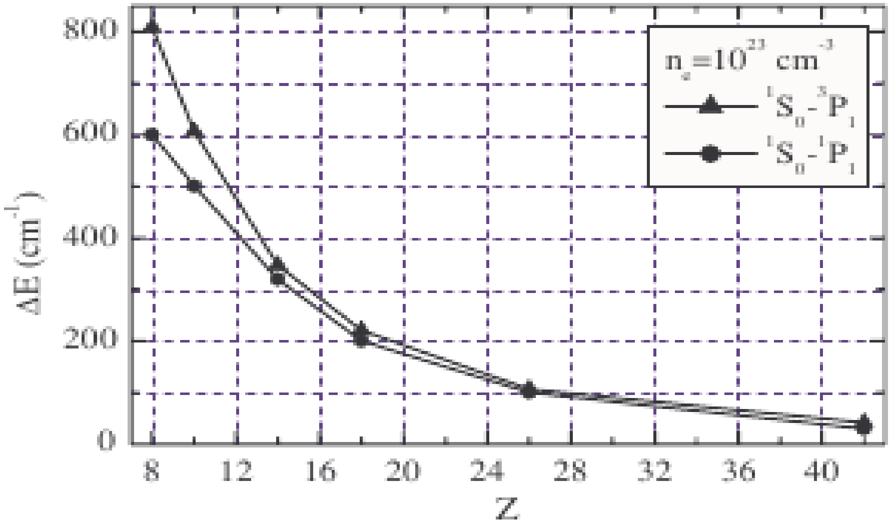
**Again,** ion-sphere plasma screening on the $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^3P_1$ intercombination and $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^1P_1$ resonance transitions:

The plasma screening is found to increase the excitation energy along the whole isoelectronic sequence, leading to a quite sizeable blueshift for both, the intercombination and resonance lines.



Intercombination line

Excitation energies, scaled by $1/Z^2$, as function of electron density (in $cm^{-3}$).



Plasma shifts ΔE as function of Z ($n=10^{23}\ cm^{-3}$).

B. Saha and S. Fritzsche, JPB 40 (2007) 259.

# Ion-sphere model: Energy shifts and radiative rates

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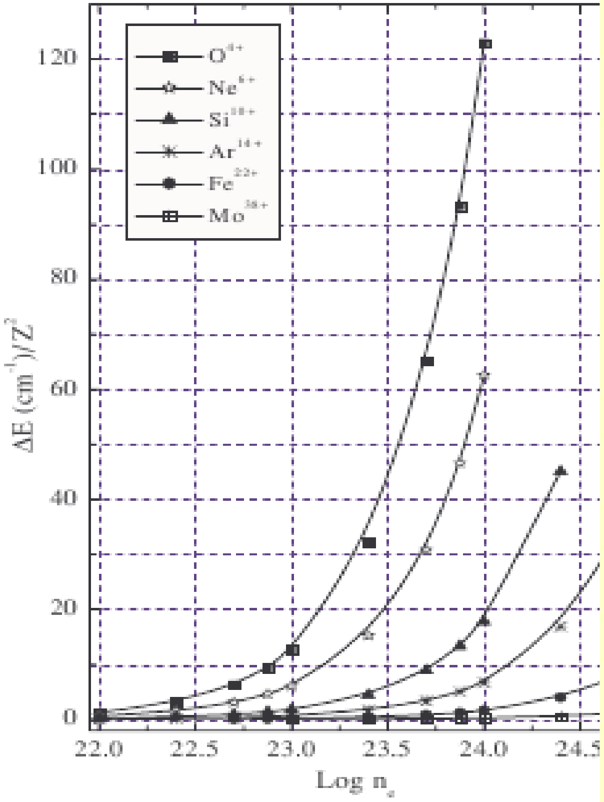

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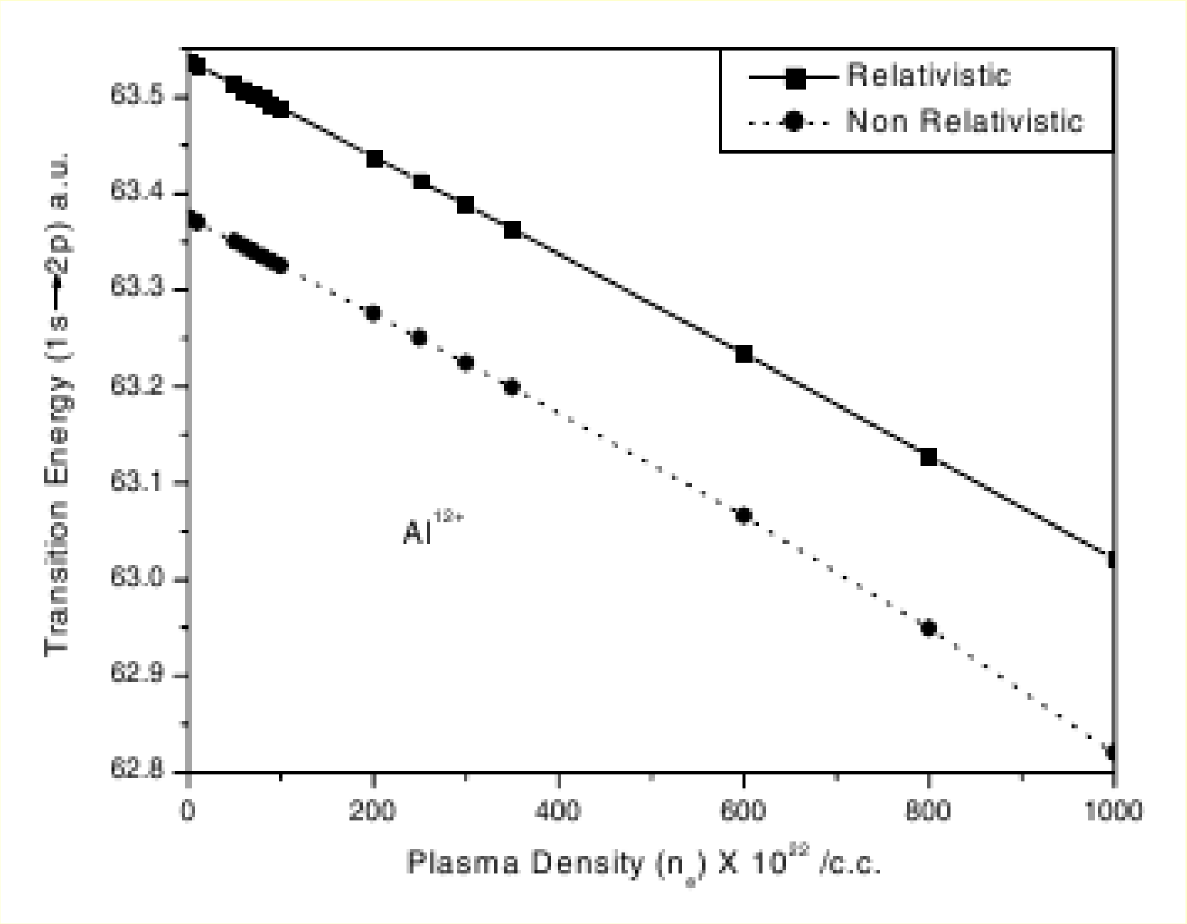

Plot of relativistic and nonrelativistic 1s → 2p transition energies (a.u.) as function of electron density in the IS model.

S. Bhattacharyya et al, EPJ D46 (2008) 1.

W.R. Johnson et al, JQRST 99 (2006) 327.

# Average-atom model

## – for studying optical properties of laser-irradiated plasmas

Fermi distribution and chemical potential μ to ensure neutrality of the Wigner-Seitz cell of the ion with radius R:

$$Z = \int_{r<R} d^3r\,\rho(r) = 4\pi \int_{r<R} dr\, r^2\, (\rho_b(r) + \rho_c(r))$$

$$4\pi r^2\, \rho_b(r) \sim \sum_{nl} f_{nl}\, P^2_{nl}(r) = \sum_{nl} \frac{P^2_{nl}(r)}{1 + \exp\left[(\epsilon - \mu)/kT\right]}$$

Averaged-atom form of Kubo-Greenwood formula:

(for the conductivity of the plasma)

$$\sigma(\omega) = \frac{2\pi e^2}{\omega\, V_{\text{atom}}} \sum_{ij} (f_i - f_j)\, |\langle j\,|v_z|\,i\rangle|^2\, \delta(\epsilon_j - \epsilon_i - \omega)$$

Contains contributions from:

- Free-free transitions (inverse bremsstrahlung)
- Bound-bound transitions (photoexcitation)
- Bound-free transitions (photoionization)

W.R. Johnson et al, JQRST 99 (2006) 327.

# Average-atom model

## – contribution to conductivity for Al plasma

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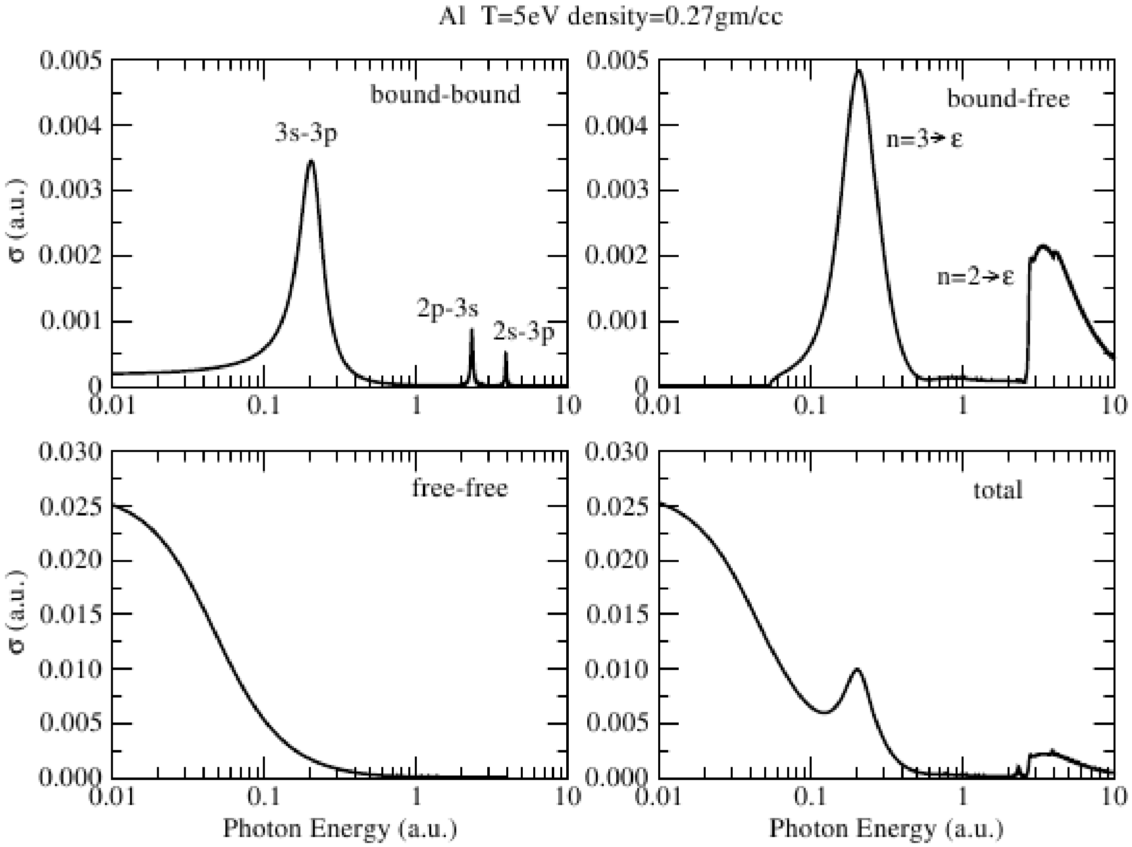


Contains contributions from:

- Free-free transitions (inverse bremsstrahlung)
- Bound-bound transitions (photoexcitation)
- Bound-free transitions (photoionization)

Contributions to the conductivity for an average atom of Al (5eV and 1/10 metallic density) as functions of the photon energy.

W.R. Johnson et al, JQRST 99 (2006) 327.

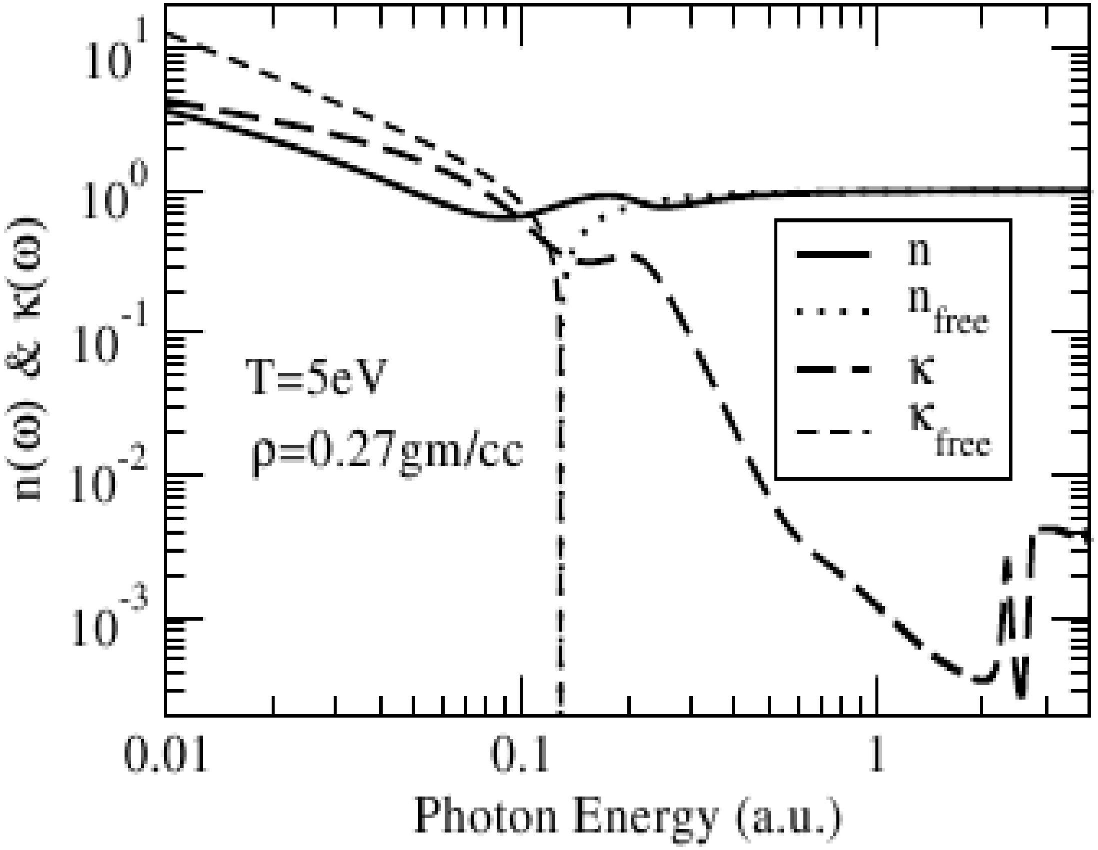
# Average-atom model

## – contribution to conductivity for Al plasma

Conductivity
$\sigma(\omega)$

Kramers-Kronig
dispersion relations

dielectric function
$\varepsilon_r(\omega)$



$$n(\omega) + i\kappa(\omega) = \sqrt{\epsilon_r(\omega)}$$

Refraction index

- Dispersion
- Photoabsorption coefficient of plasma
- Information about electron density

Real $n(\omega)$ and imaginary $\kappa(\omega)$ parts of the index of refraction for an average atom of Al (5eV and 1/10 metallic density) given as functions of the photon Energy ω. The lightly dashed and dotted lines show n and κ in the free-electron approximation. The singularity in the free-electron case occurs at the plasma frequency.

W.R. Johnson et al, JQRST 99 (2006) 327.

# Average-atom model

– contribution to conductivity for Al plasma

Conductivity
$\sigma(\omega)$

Kramers-Kronig
dispersion relations

dielectric function
$\varepsilon_r(\omega)$

## In the end

- A great deal of atomic data is needed to model the dynamics and radiation emitted from plasmas.
- Simple scaling rules on level energies and oscillator strength may reveal certain inconsistencies … but need to be considered with care.
- Atomic calculation help determine electron temperatures and densities within different plasma environments --- if inner-shell processes are suppressed.
- Creation of multiple holes (in the ionic core) usually results in truly exotic states of matter and are far away from being understood.