Atomic Physics and High Energy Density Plasmas

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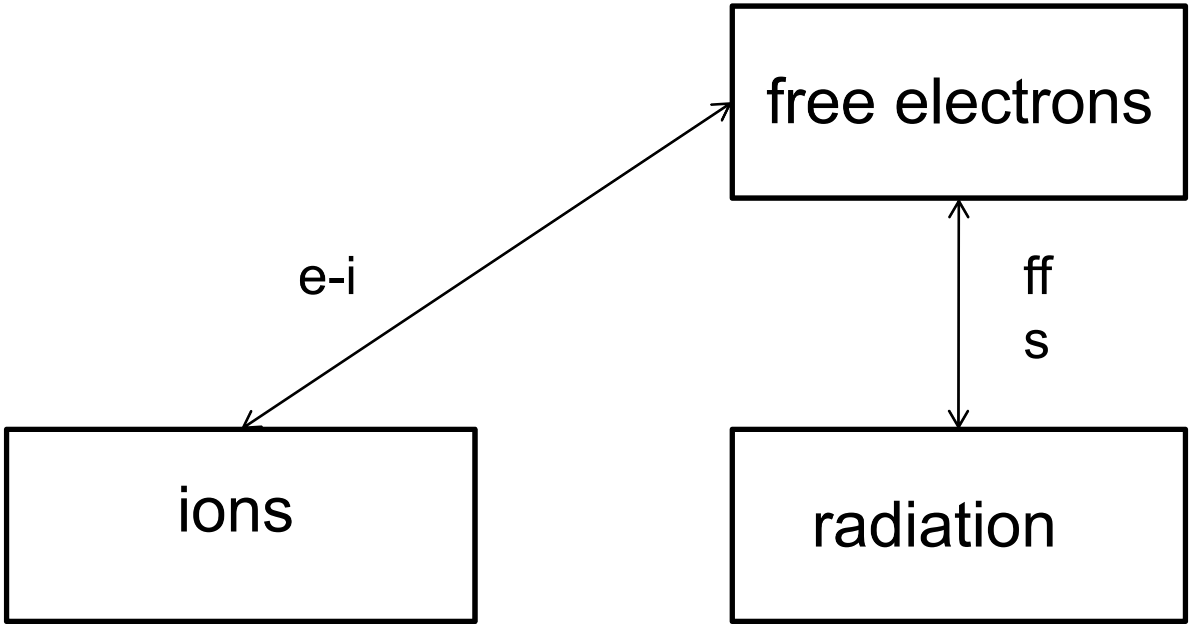
Fully- ionised plasma



free electrons

ions

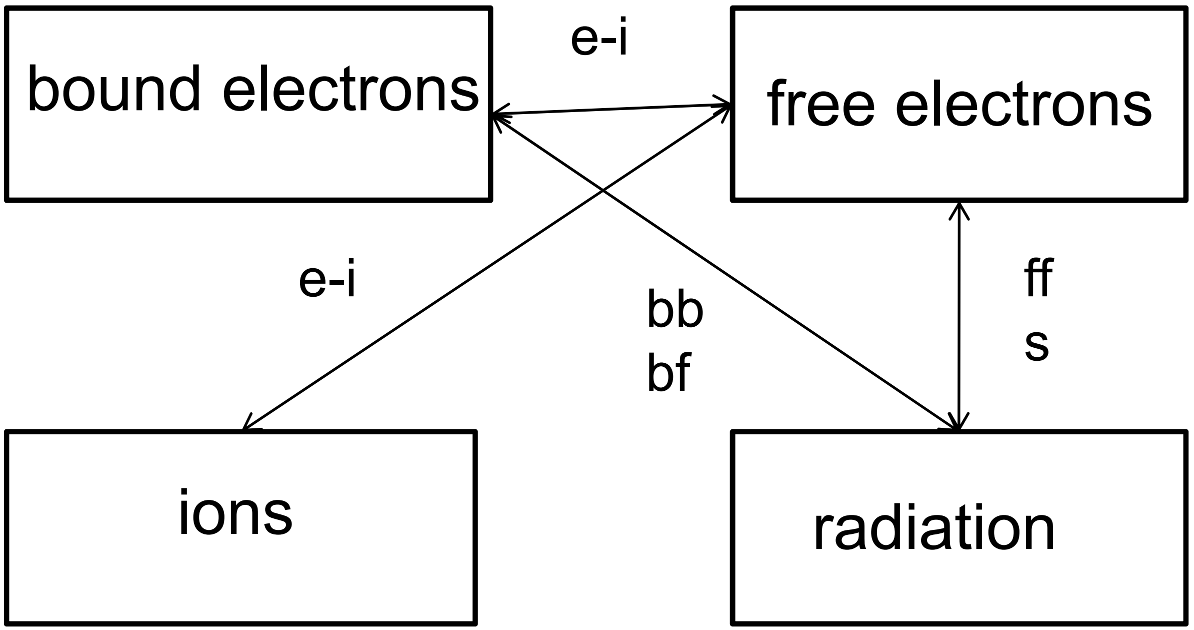
radiation

e-i

ff

s

Partially- ionised plasma



Low and high density plasma pictures

Low-density picture

- Debye-Huckel theory holds (weak coupling)
- Maxwellian free electron velocity distribution
- Bound electronic structure same as in the free ion

High-density picture

- Debye-Huckel theory does not hold (strong coupling)
- Fermi degeneracy of free electron distribution
- Bound electronic structure altered from that of free ion
  - Continuum lowering / pressure ionisation
  - Bound electronic wavefunction overlap

Strong-coupling

$$\Gamma_{ii} = \frac{Z^{*2}e^2}{\underbrace{4\pi\varepsilon_0 R}_{\text{potential energy}}kT_i}$$

kinetic energy

$\Gamma_{ii} < 1$ weak coupling – Debye-Huckel theory holds

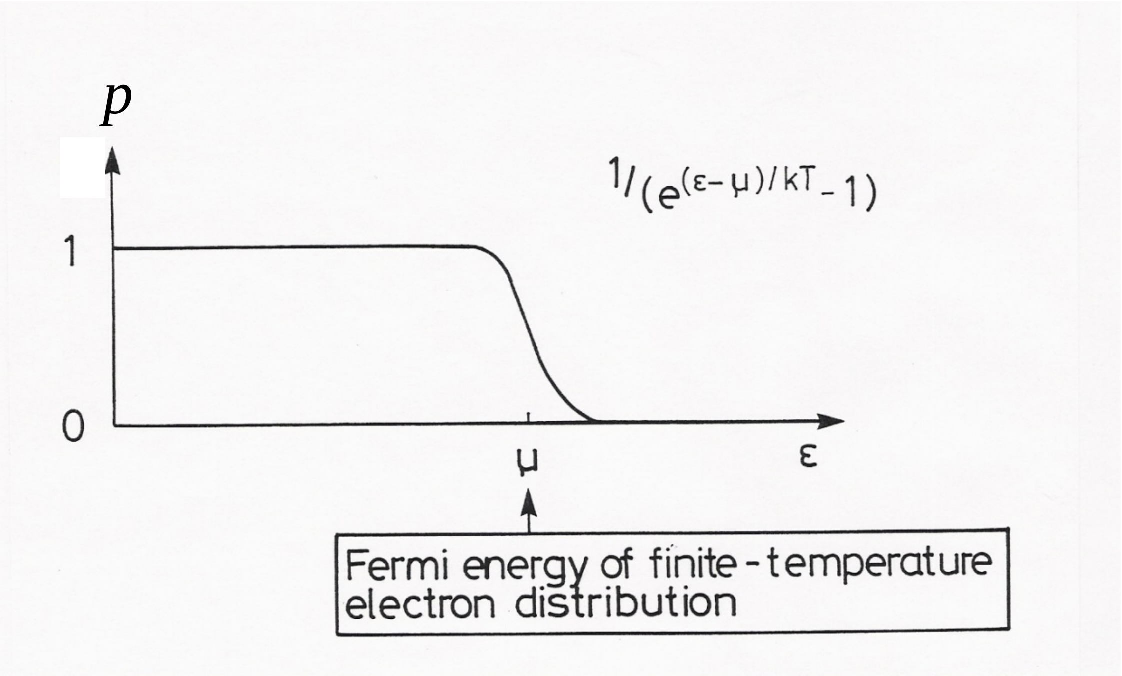
$\Gamma_{ii} > 1$ strong coupling – Debye-Huckel theory does not holds

Free electron degeneracy

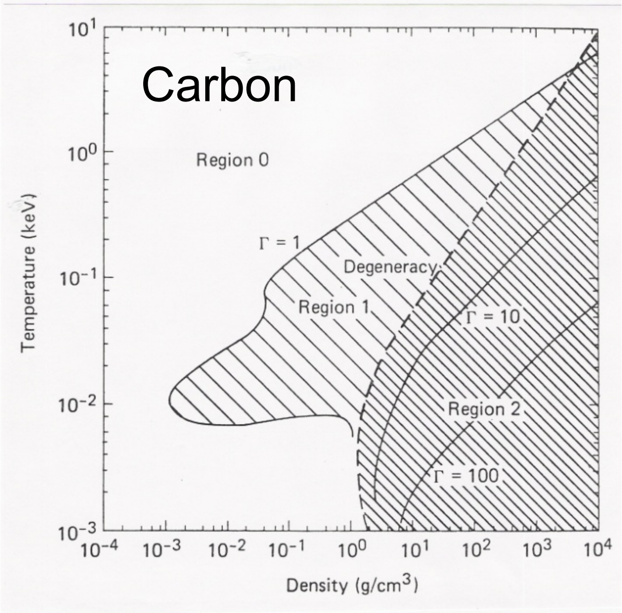
The probability of occupancy of a free electron state is

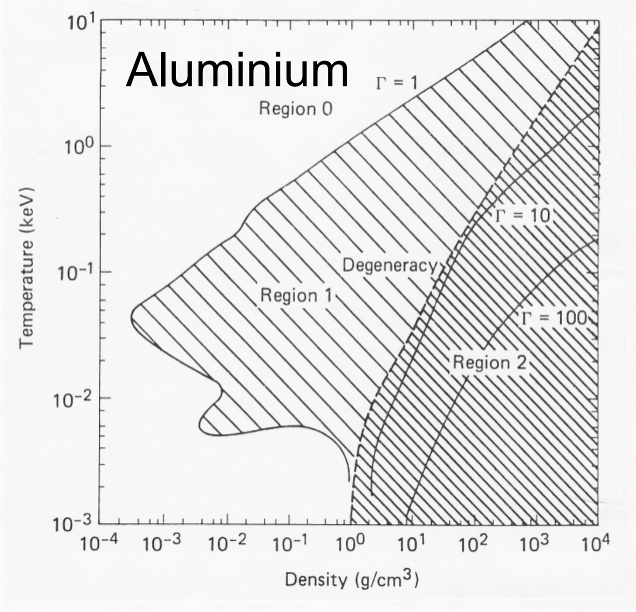
$$p = \frac{1}{\left[\exp(\varepsilon - \mu)/kT\right] - 1} \qquad \mu / kT = \eta$$

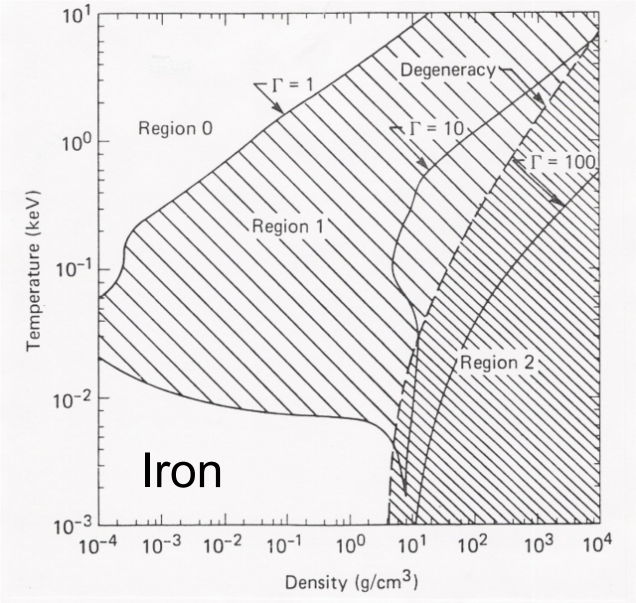
$\lambda << r_{ee}$	$\eta << 0$	non-degenerate
$\lambda >> r_{ee}$	$\eta >> 0$	degenerate

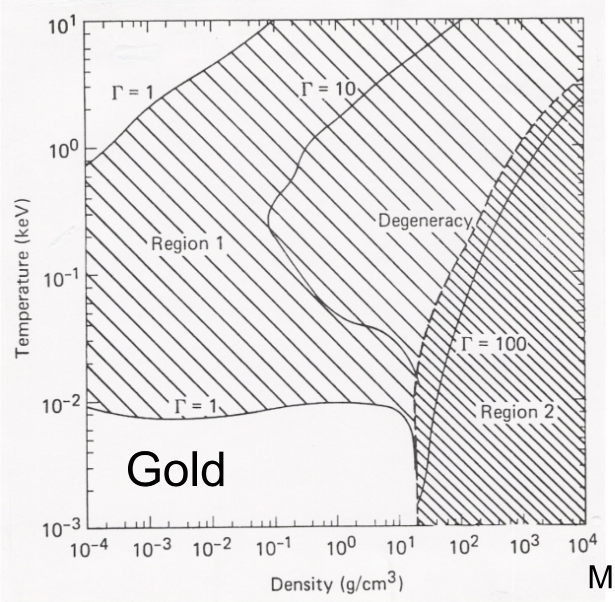


Strong-coupling and degenerate regions in plasmas





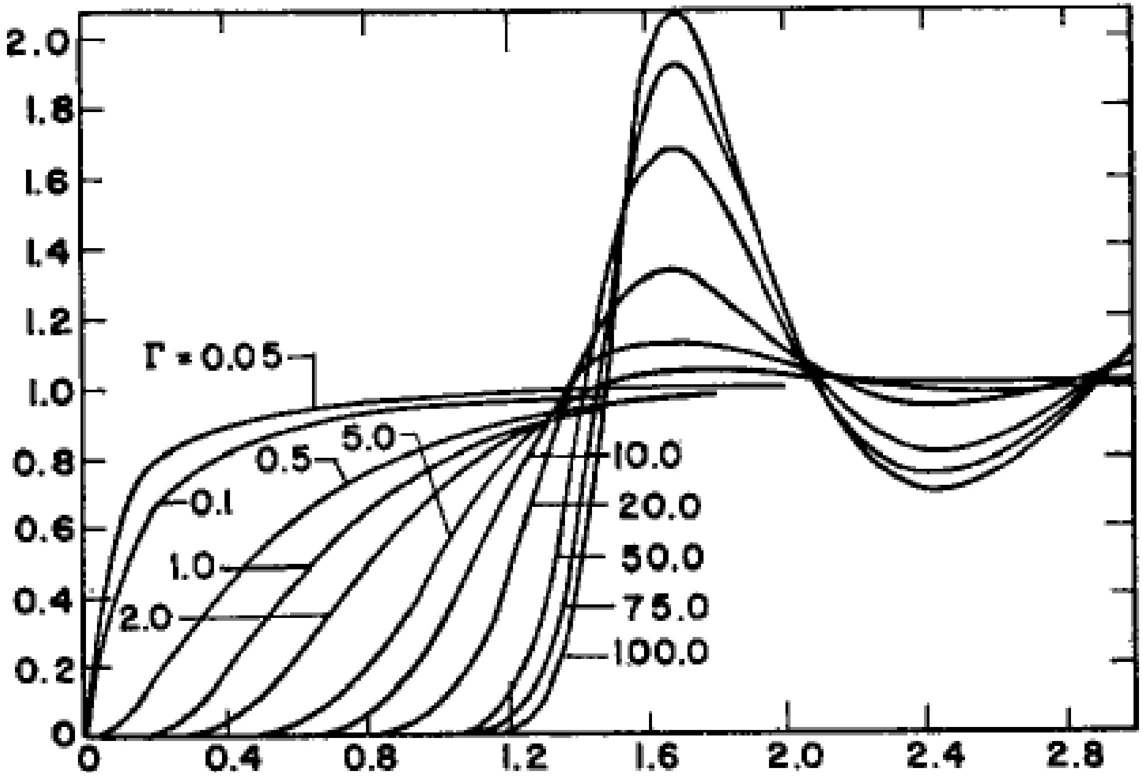




More, UCRL-84991, 1982

Effect of strong-coupling on ion distribution

$n_i(r)/n$

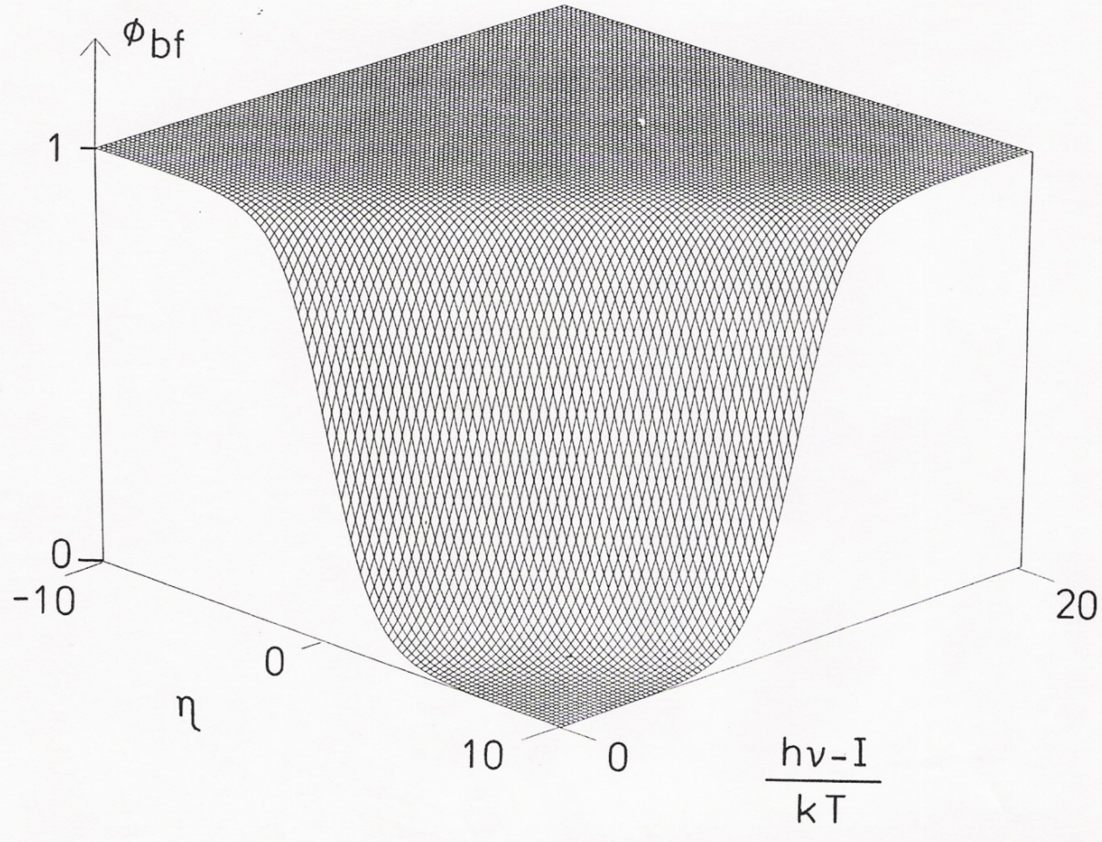


r/R

Brush, Salin and Teller, JChemPhys (1966)

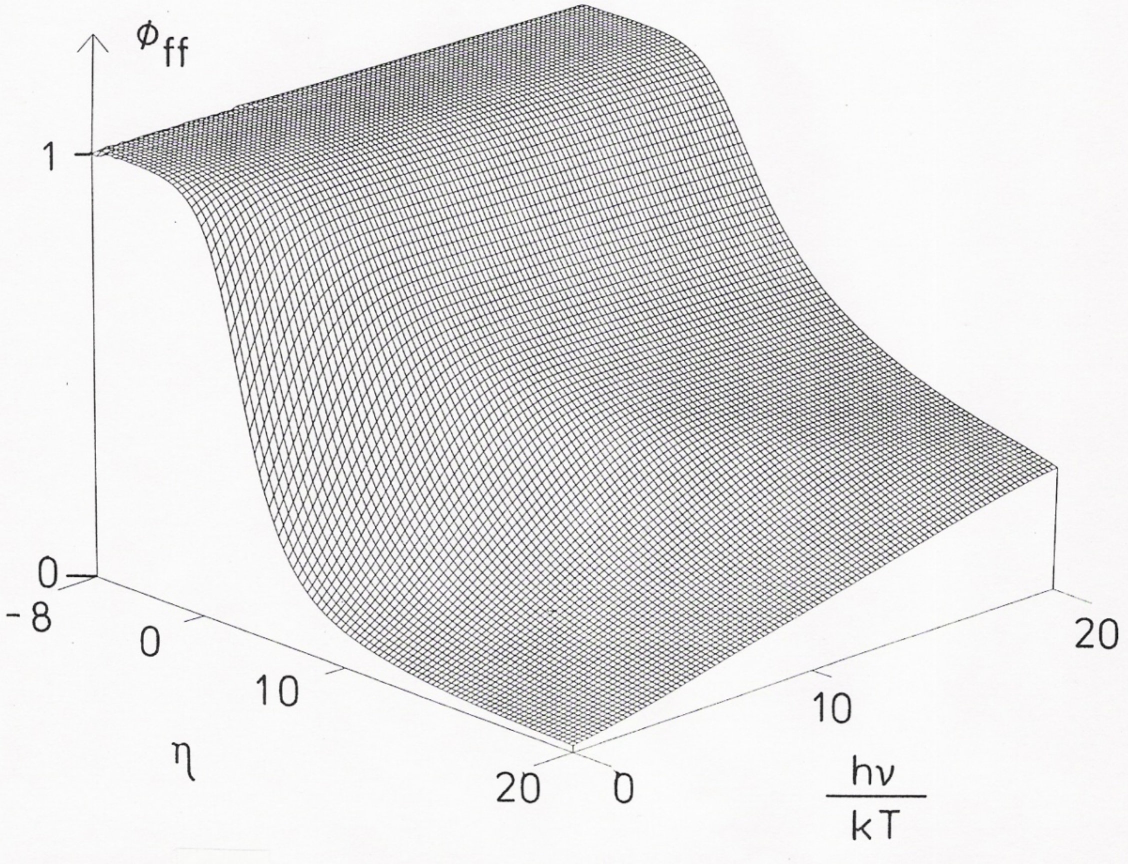
Correction factor for degeneracy in bound-free transitions

$$\phi_{bf} = \frac{1}{1+\exp\left\{-\left[\frac{h\nu - I}{kT}\right]+\eta\right\}}$$

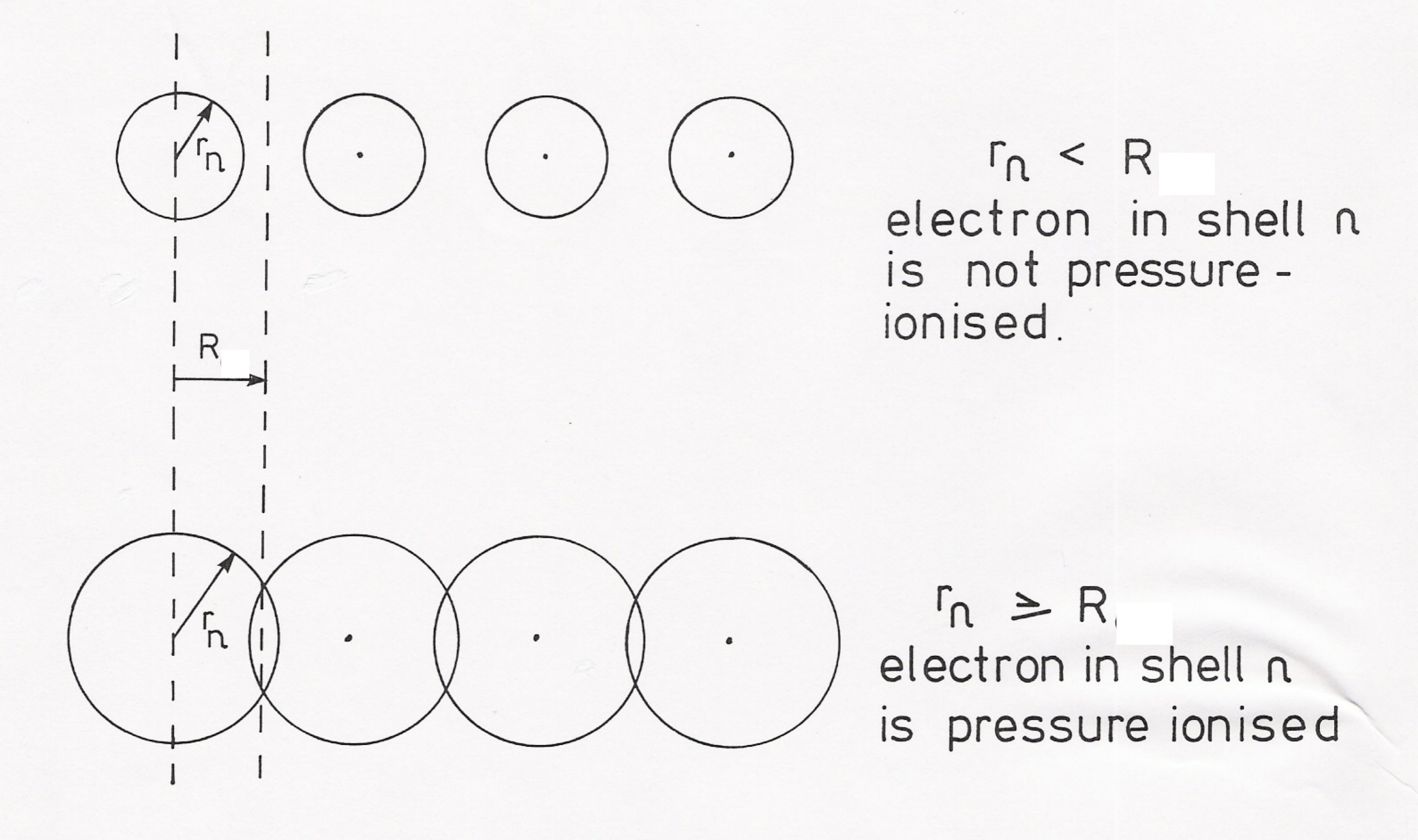


Correction factor for degeneracy in free-free transitions

$$\phi_{ff} = \frac{\sqrt{\pi}}{2I_{1/2}(\eta)(1-e^{-u})} \ln\left[\frac{1+e^{\eta}}{1+e^{\eta-u}}\right]$$



Continuum lowering / pressure ionisation



$r_n < R$
electron in shell n
is not pressure-
ionised.

$r_n \geq R$
electron in shell n
is pressure ionised

Saha equation and continuum lowering

$$\frac{n_{i+1}n_e}{n_i} = \frac{2Q_{i+1}(T)}{Q_i(T)} \frac{\left(2\pi m_e kT\right)^{3/2}}{h^3} e^{-I/kT}$$

$$Q_i(T) = \sum_r g_{r,i} \exp\left(-(\varepsilon_{r,i} - \varepsilon_{1,i})/kT\right)$$

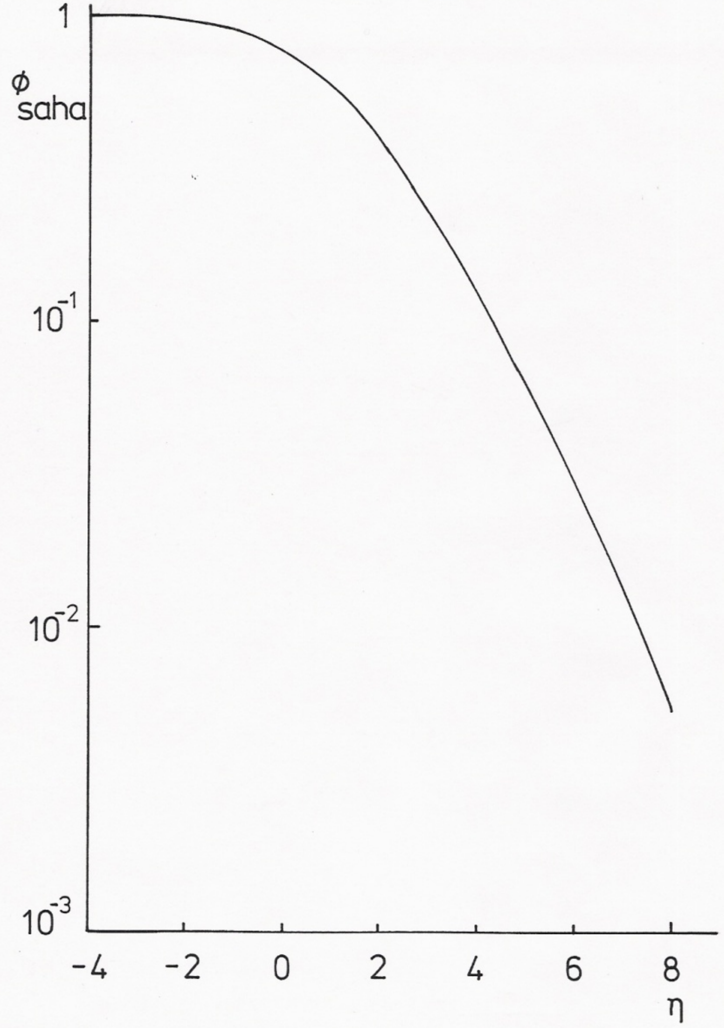
For a H-like ion the sum diverges

$$Q(T) = \sum_{n=1}^{N} 2n^2 \exp\left(-\frac{Z^2 I_H}{kT}\left[1 - \frac{1}{n^2}\right]\right)$$

Sum diverges as N→∞

Degeneracy correction to ionisation equilibrium

$$\phi_{Saha} = \frac{2}{\sqrt{\pi}} I_{1/2}(\eta) e^{-\eta}$$



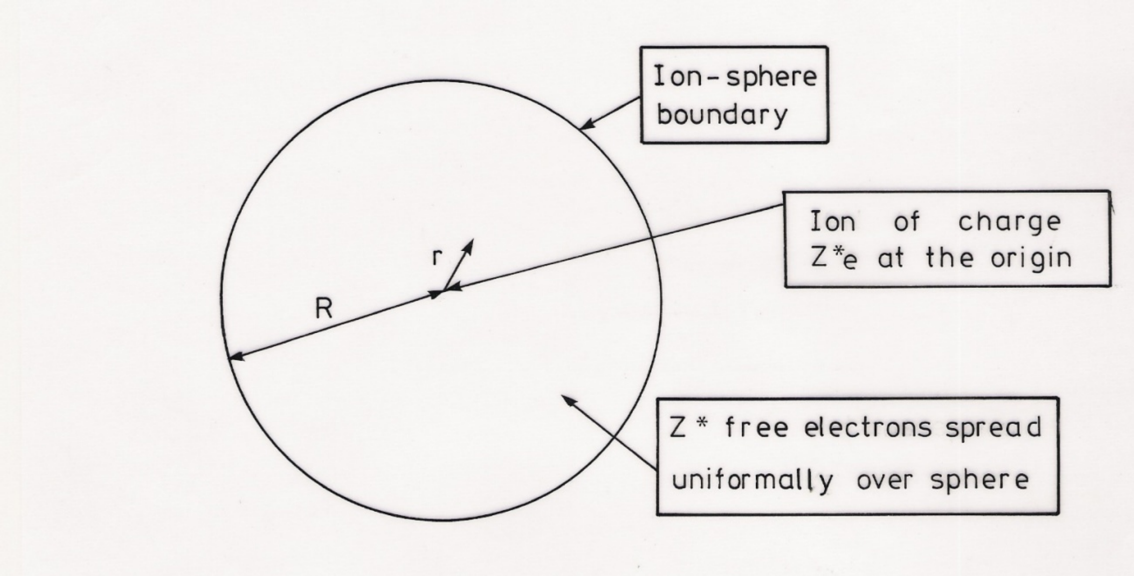
Usual calculation of the electronic structure of a partially-ionised plasma

- Calculate the isolated ion structure. The effect of the plasma is included by perturbation theory.

- Calculate the (spherically-symmetric) potential including the effect of the plasma neighbours. Calculate the electronic structure using this potential.

- Each treatment uses single-centre wavefunctions.

Continuum lowering in the ion-sphere model



potential at radius r $$V(r) = \frac{Z^* e}{8\pi\varepsilon_0 R}\left[\frac{r^2}{R^2} - 3\right]$$

perturbation from field-free case $$\Delta\varepsilon = \int d\tau(-e\psi^2)V$$

Continuum lowering in the ion-sphere model II

K-shell ionisation

$$\Psi_i \longrightarrow \Psi_f$$

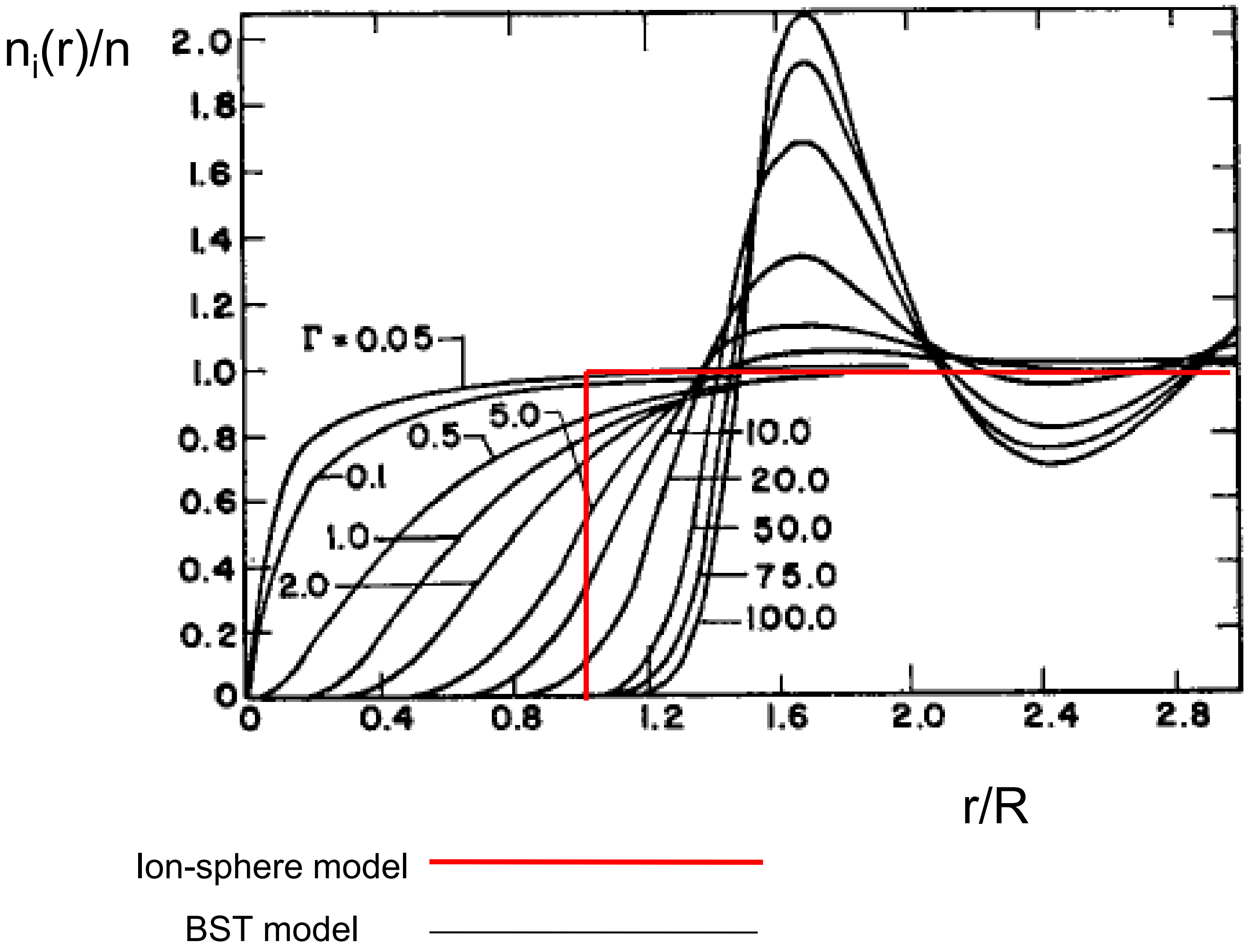
$$\Delta E = \int(-e\psi_f^2)\frac{Z^*e}{8\pi\varepsilon_0 R}\left[\frac{r^2}{R^2}-3\right]d\tau - \int(-e\psi_i^2)\frac{Z^*e}{8\pi\varepsilon_0 R}\left[\frac{r^2}{R^2}-3\right]d\tau$$

shift in transition energy

$$\Delta E = \frac{Z^*e^2}{8\pi\varepsilon_0 R}\left[\frac{\sum_k n_k^f\langle r_k^2\rangle^f - \sum_k n_k^i\langle r_k^2\rangle^i}{R^2}-3\right]$$

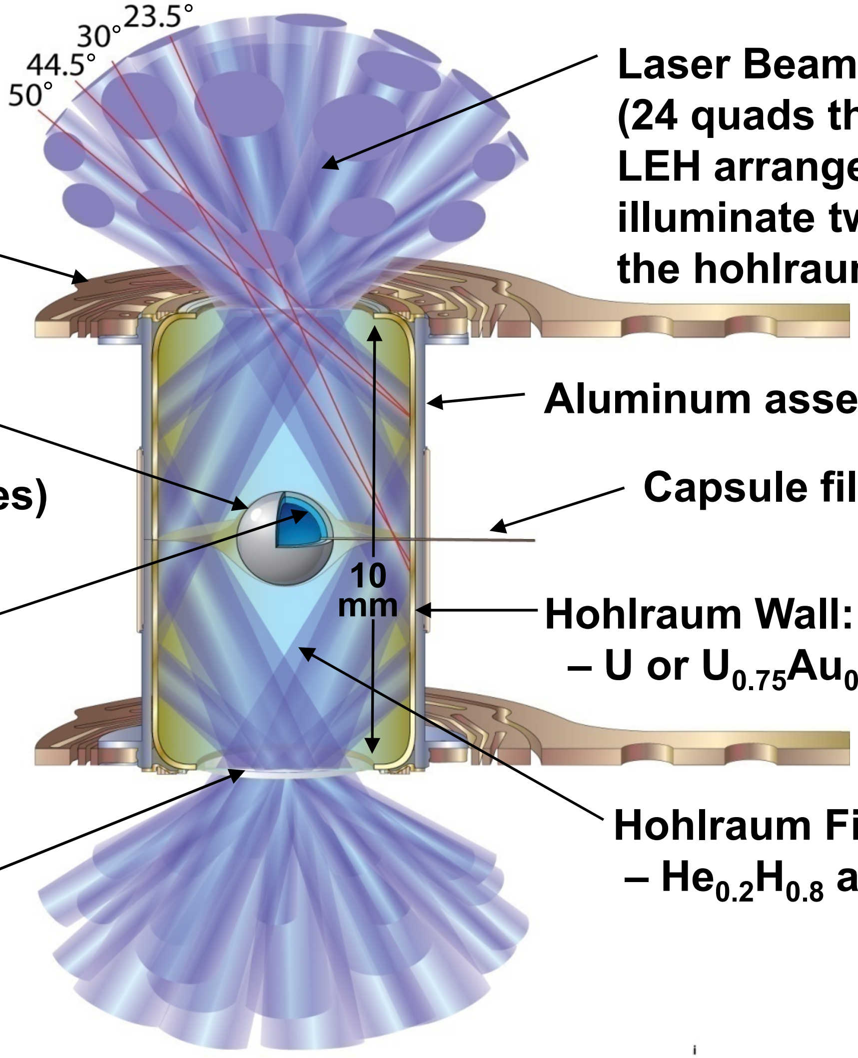
$$\Delta E = -\frac{3Z^*e^2}{8\pi\varepsilon_0 R} + \frac{Z^*e^2\Delta\langle r^2\rangle}{8\pi\varepsilon_0 R^3}$$

Effect of strong-coupling on ion distribution



Brush, Salin and Teller, JChemPhys (1966)

The NIF ignition target



Laser Beams
(24 quads through each LEH arranged to illuminate two rings on the hohlraum wall)

Cryo-cooling Ring

Graded-doped Be Capsule (CH and Diamond are alternates)

Aluminum assembly sleeve

Capsule fill tube

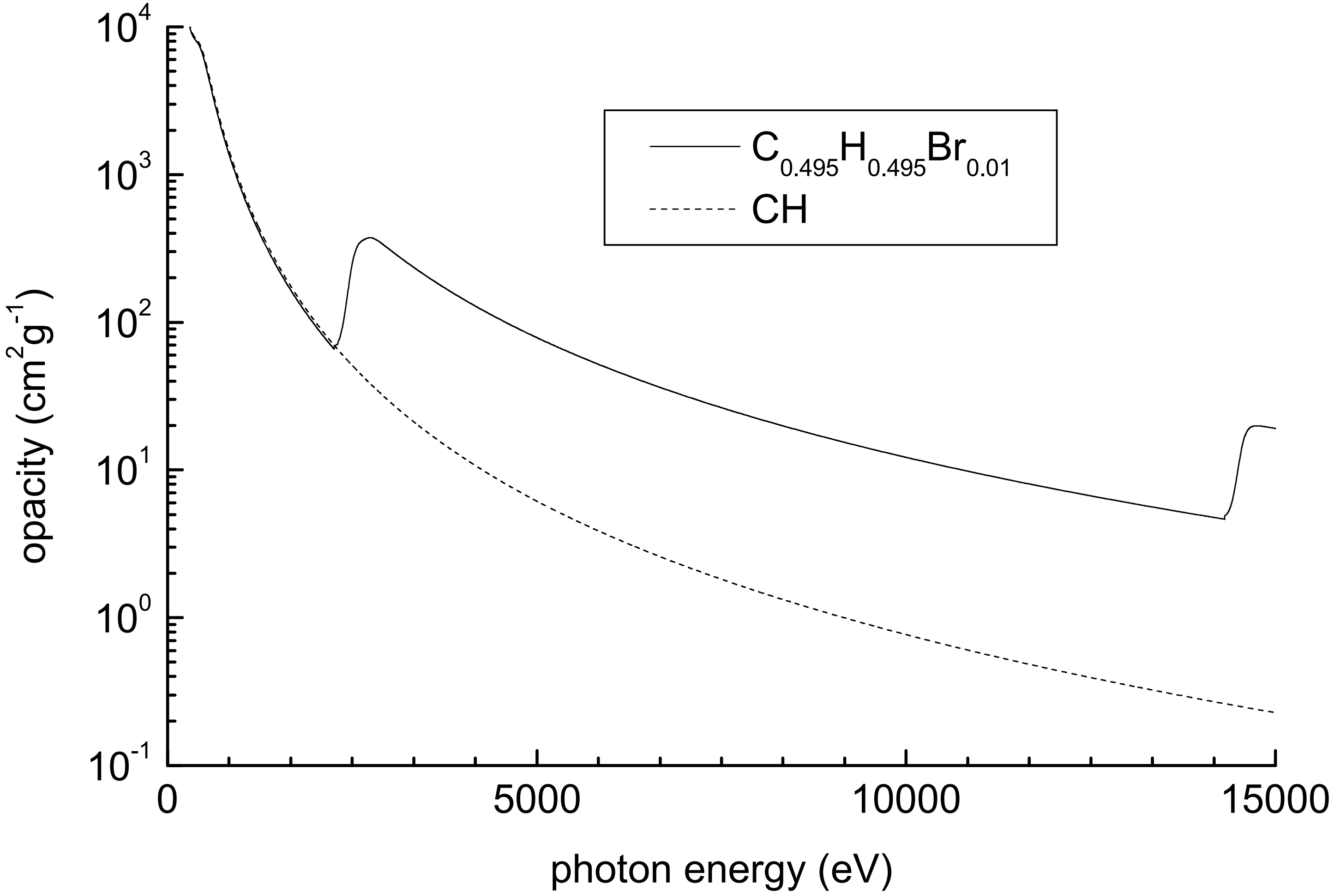
Solid DT fuel layer

Hohlraum Wall:
- **U or $U_{0.75}Au_{0.25}$**

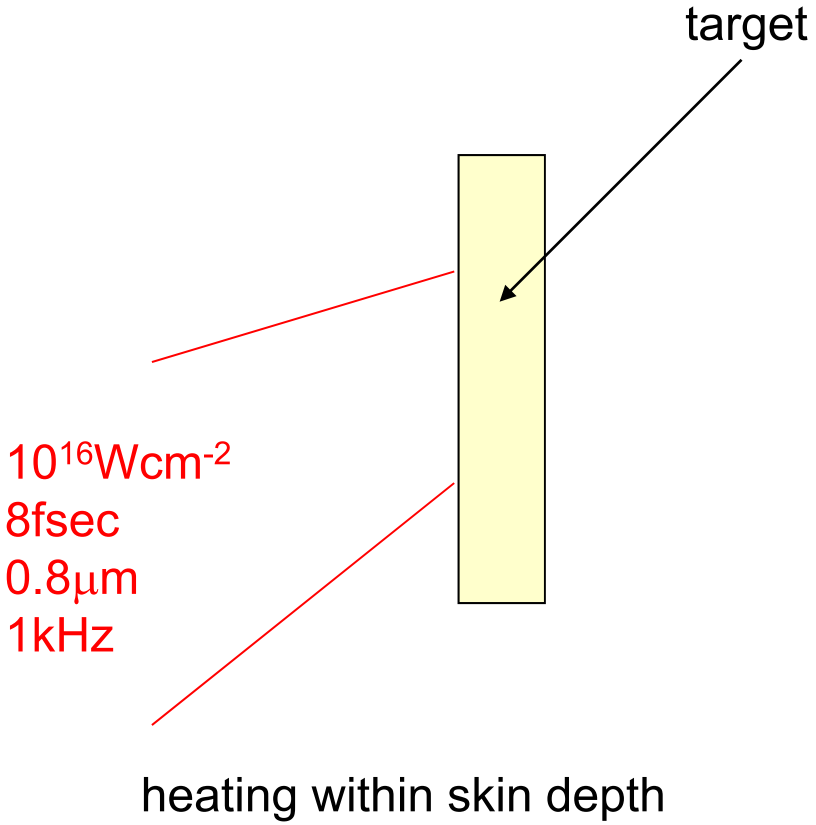
Hohlraum Fill
- **$He_{0.2}H_{0.8}$ at 0.7 mg/cm^3**

Laser Entrance Hole (LEH) with window

Bromine doped plastic opacity
(50eV and 70gcm^{-3})



Ultra-short-pulse (sub 10fsec) beam can produce moderate temperature, solid density plasma

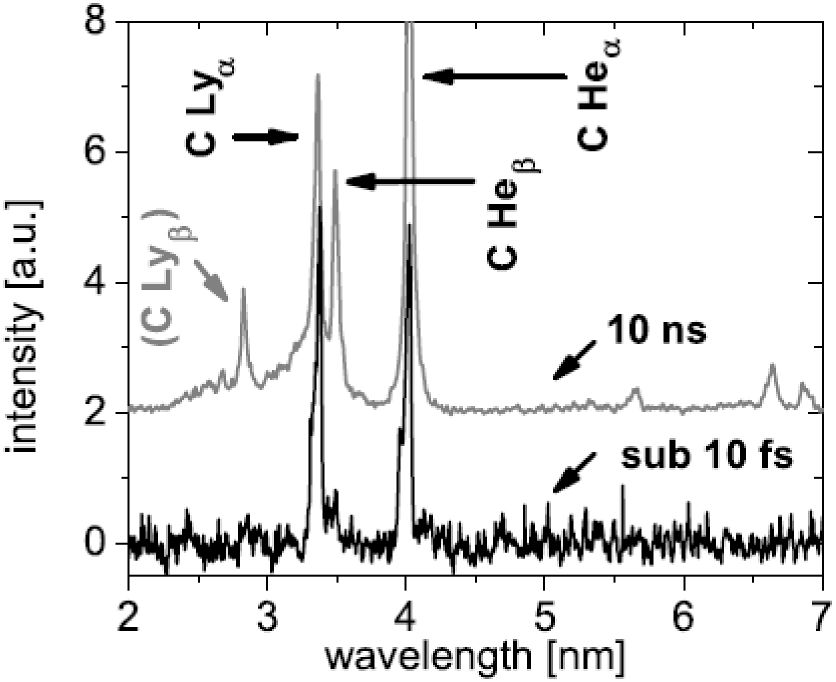


target

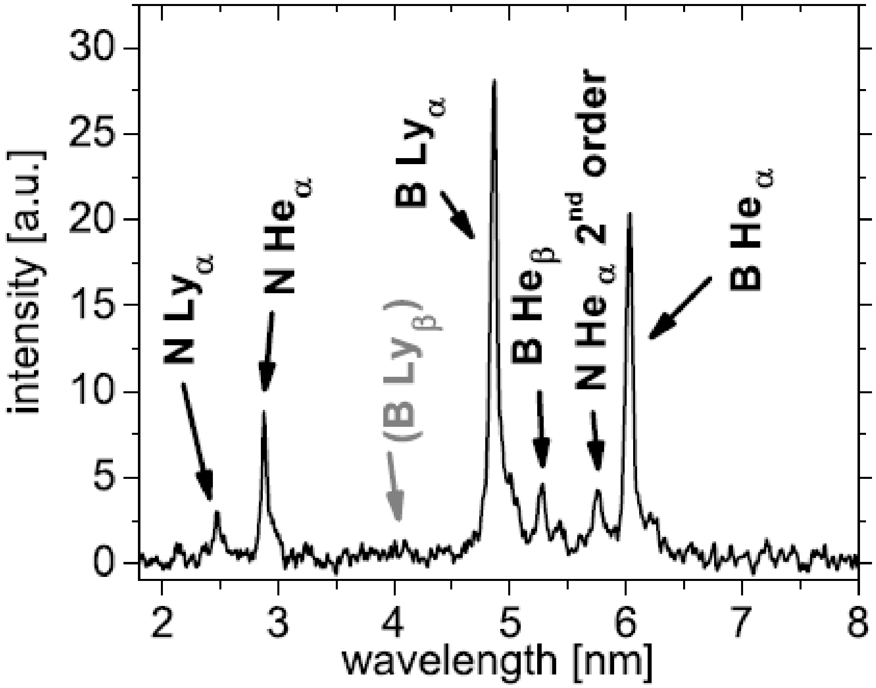
10^{16}Wcm^{-2}
8fsec
0.8μm
1kHz

heating within skin depth

XUV spectroscopy of sub 10fsec laser-solid interaction



Carbon target

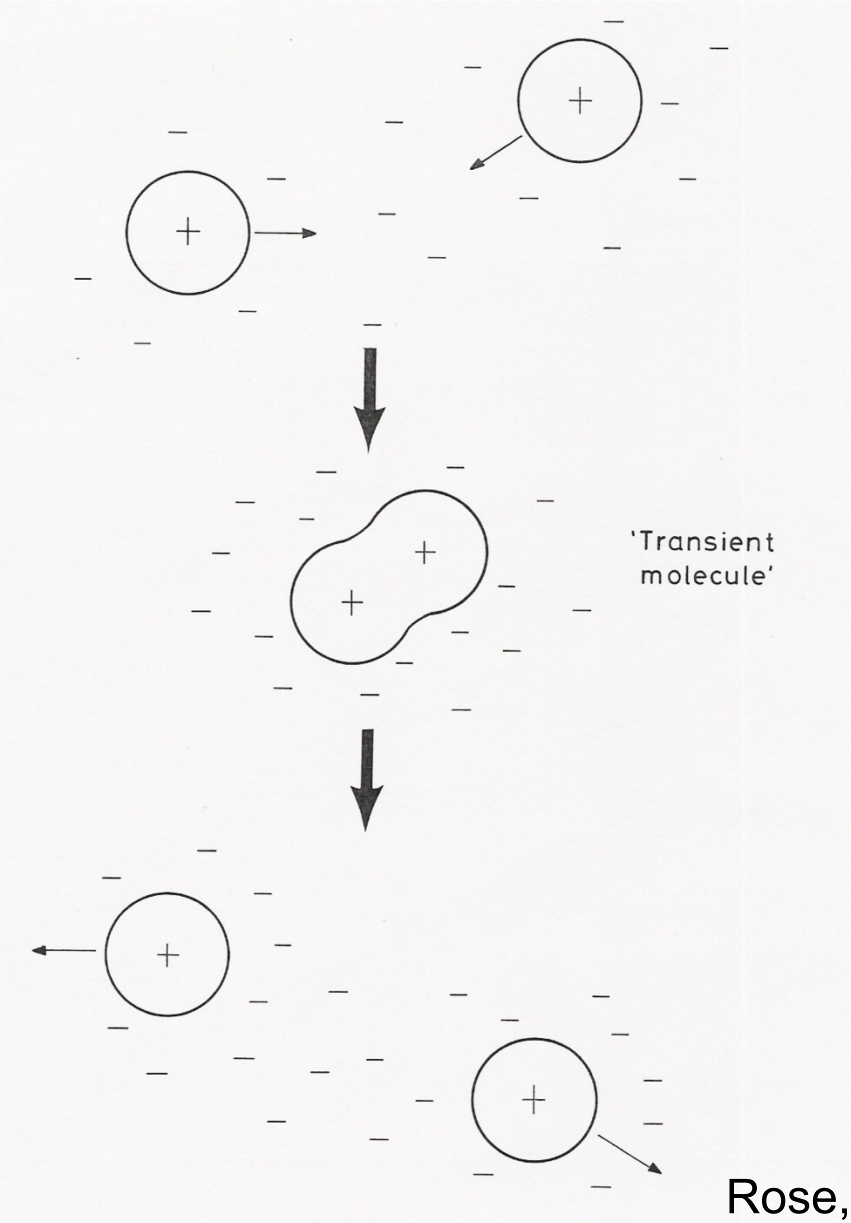


Boron Nitride target

- Ly-α and He-α lines indicate hot (approximately 100eV) plasma
- Lack of Ly-β or He-β lines indicates near solid density (approximately 1gcm^{-3}) plasma

Osterholz et al, Physical Review Letters (2005), Physics of Plasmas (2006)

Transient molecules in a plasma



Rose, J. de Physique (1983)

Transient chemistry revealed by molecular wavefunctions

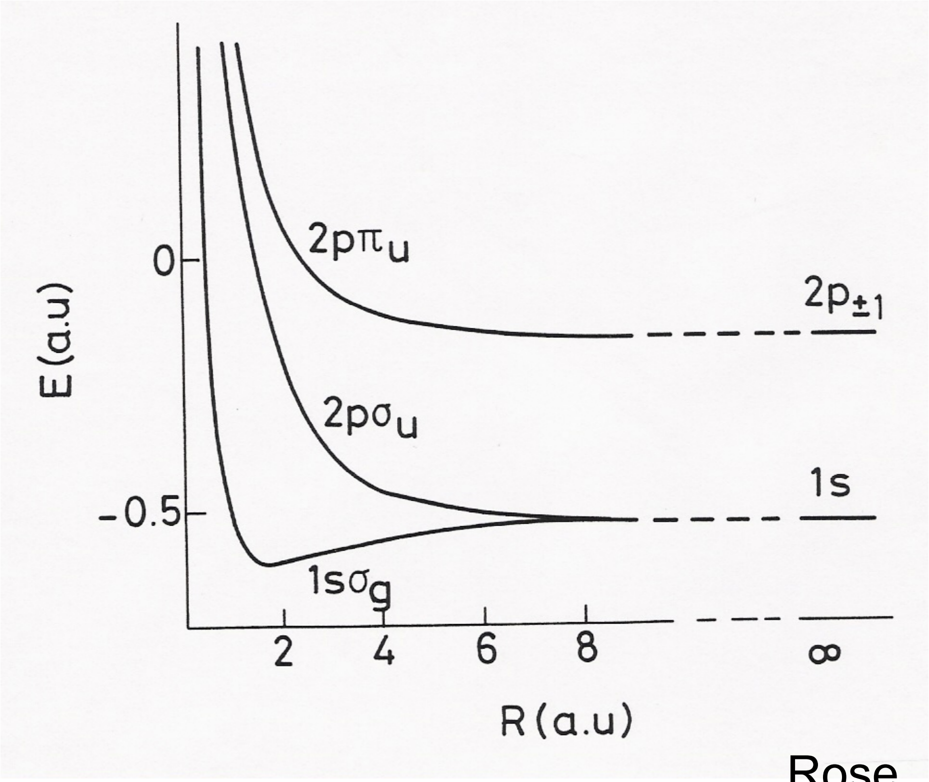
- A consideration of transient molecules predicts contributions to plasma properties not arising in single-centre treatments.

- Transient chemistry is only revealed by use of two-centre (or in general multi-centre) electronic wavefunctions.

Rose, J. de Physique (1983)

H_2^+ transient molecules in a low-temperature, partially-ionised plasma

- Accurate wavefunctions known for H_2^+
- Two transitions studied

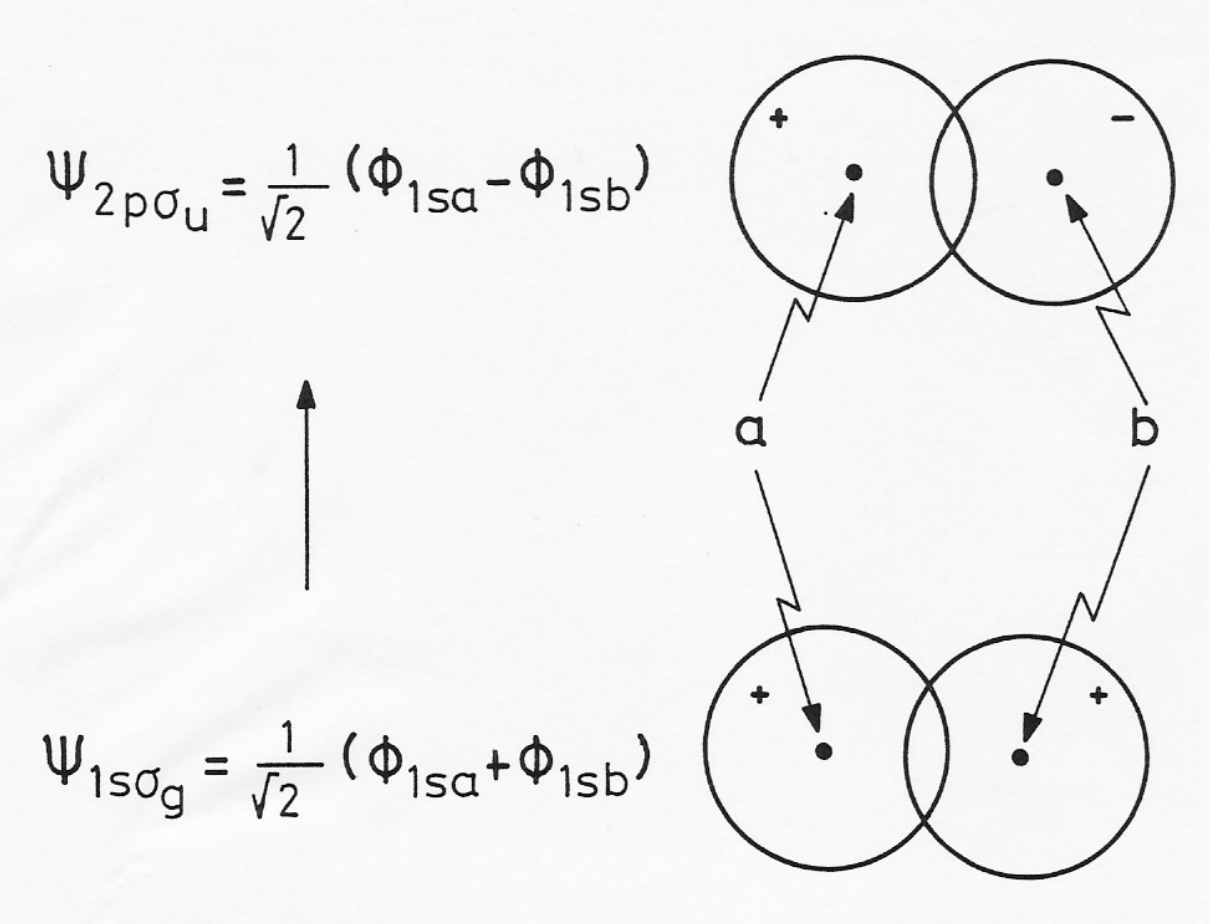


Rose, J. de Physique (1983)

H_2^+ $1s\sigma_g \rightarrow 2p\sigma_u$ transition

- Bonding – antibonding transition

- Photon absorption moves electron density from between the nuclei to either side of the nuclei

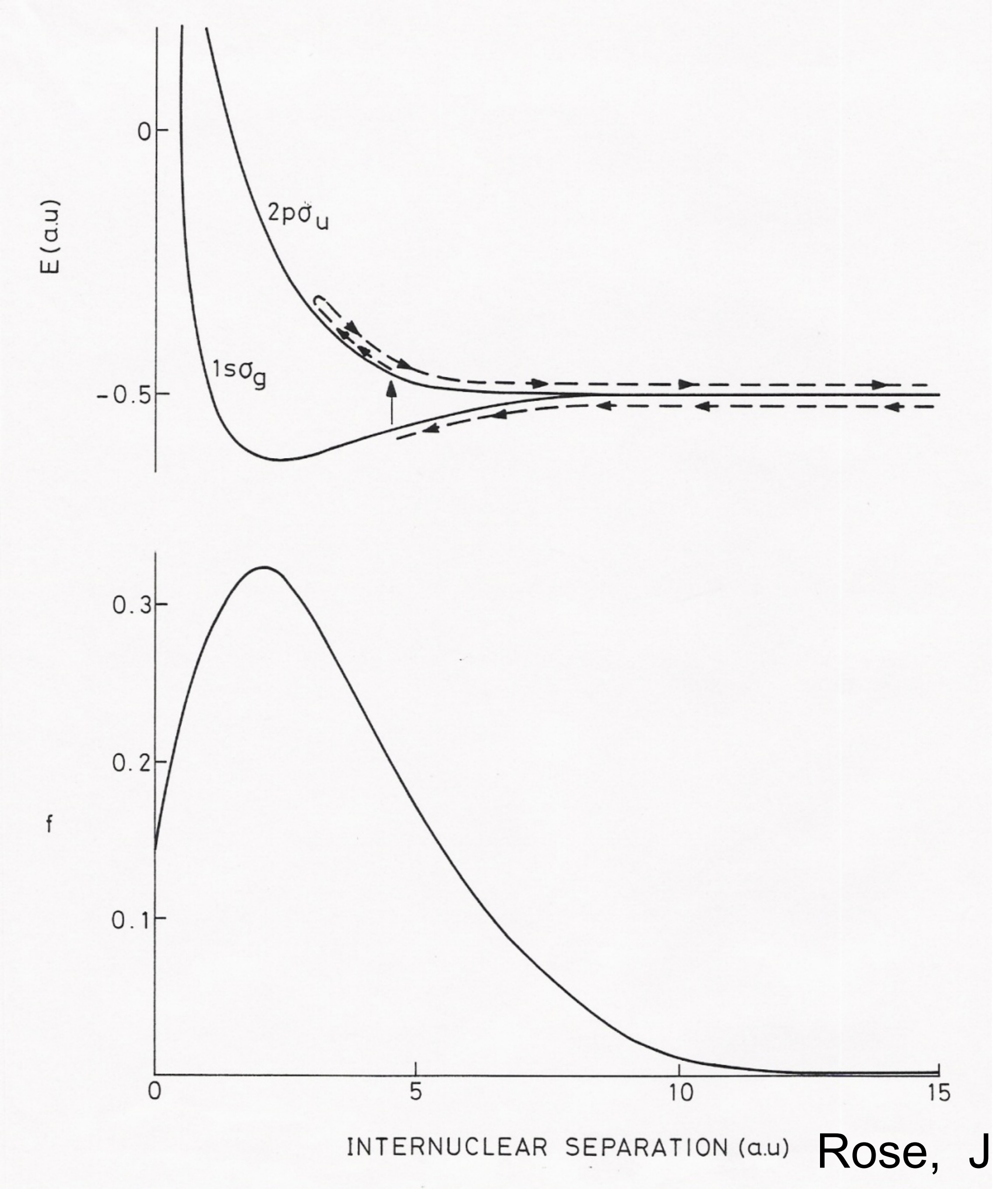


$$\Psi_{2p\sigma_u} = \frac{1}{\sqrt{2}}(\Phi_{1sa} - \Phi_{1sb})$$

$$\Psi_{1s\sigma_g} = \frac{1}{\sqrt{2}}(\Phi_{1sa} + \Phi_{1sb})$$

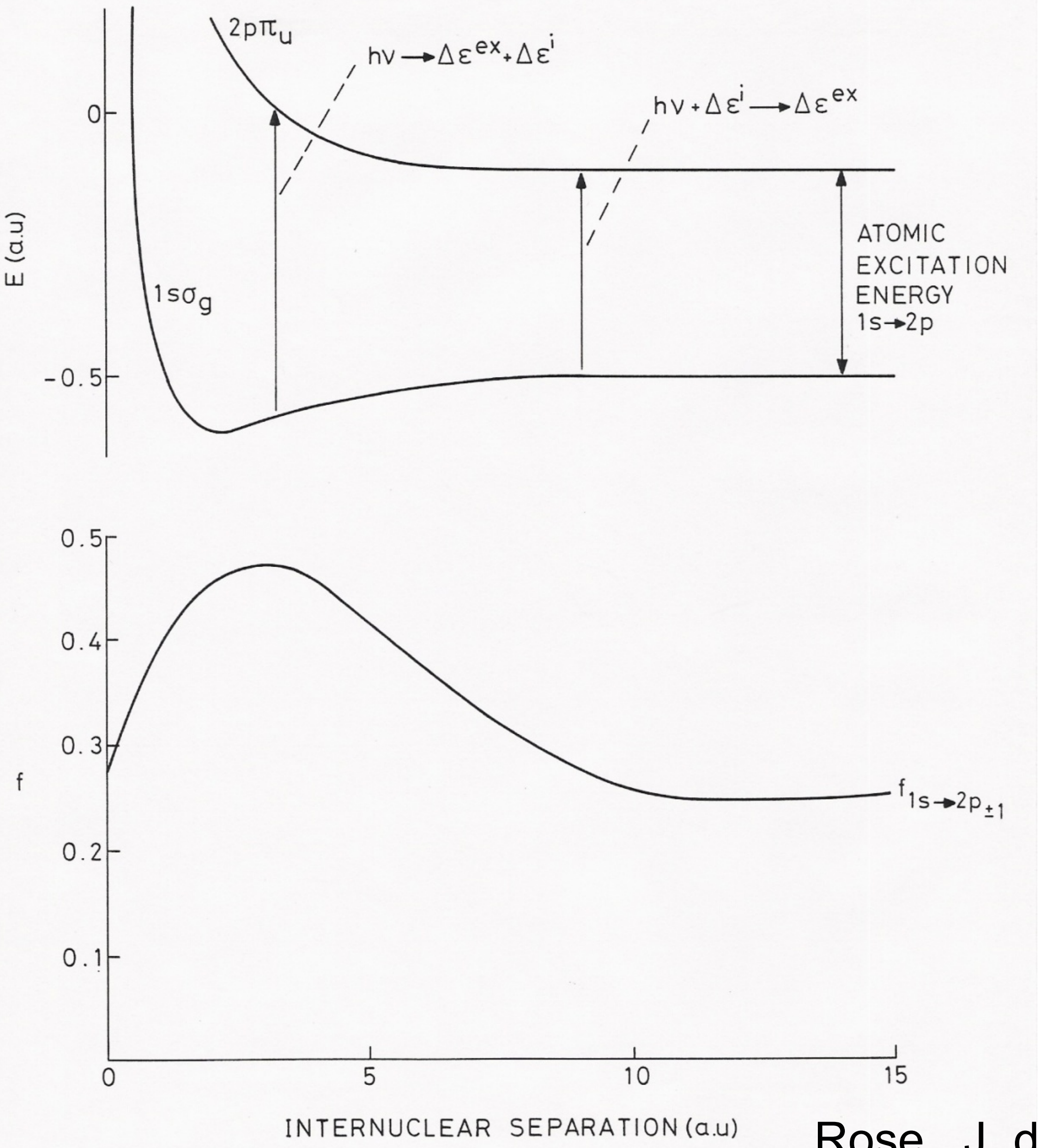
Rose, J. de Physique (1983)

Bonding – antibonding transition transfers photon energy to kinetic energy of ions



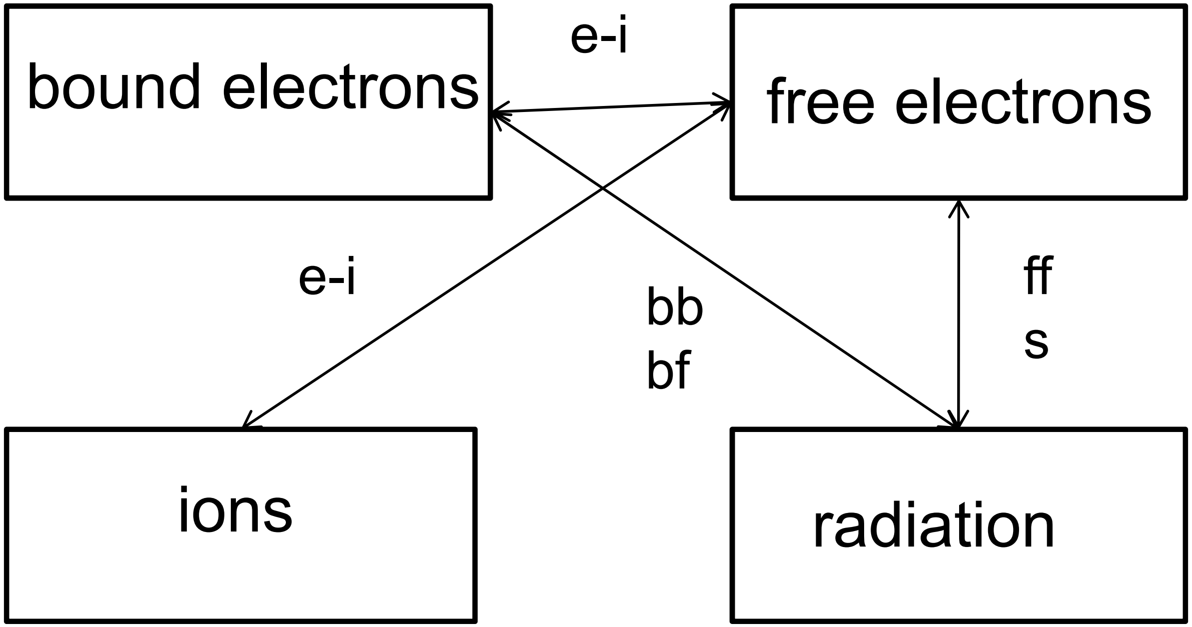
Rose, J. de Physique (1983)

H_2^+ $1s\sigma_g \rightarrow 2p\pi_u$ transition



Rose, J. de Physique (1983)

Partially- ionised plasma



bound electrons

free electrons

ions

radiation

e-i

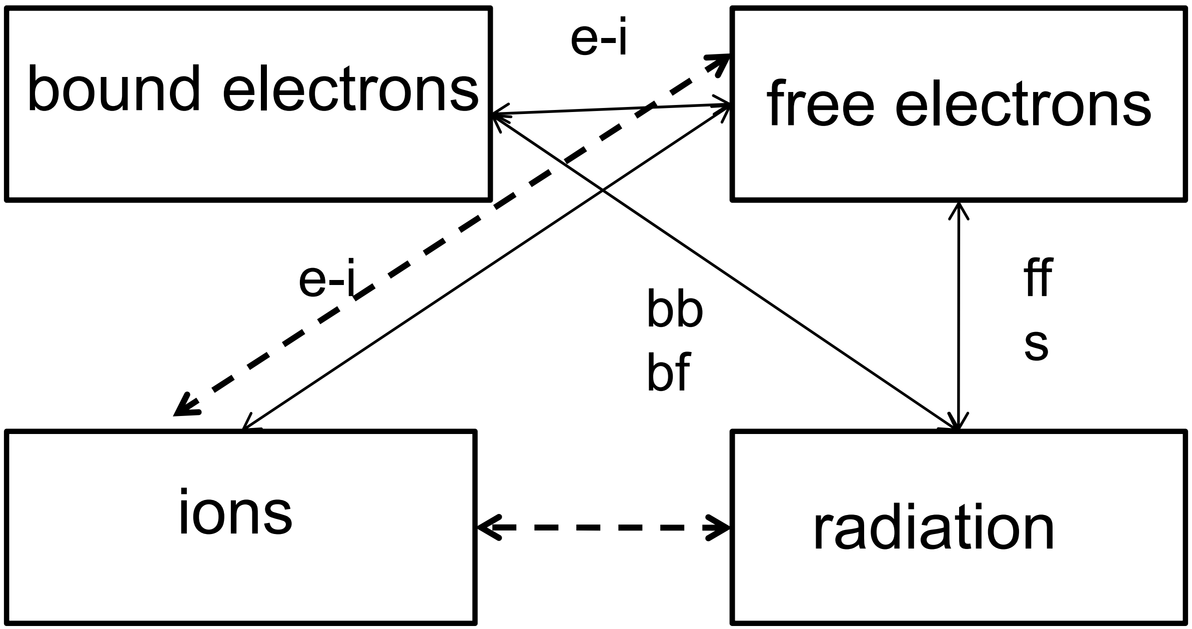
e-i

bb
bf

ff
s

Rose, J. de Physique (1983)

Transient molecules predicts new energy couplings



bound electrons

e-i

free electrons

e-i

bb

bf

ff

s

ions

radiation

Rose, J. de Physique (1983)

General expression for the partition of energy

Assume low-density limit (potential energy curves horizontal at average internuclear separation).

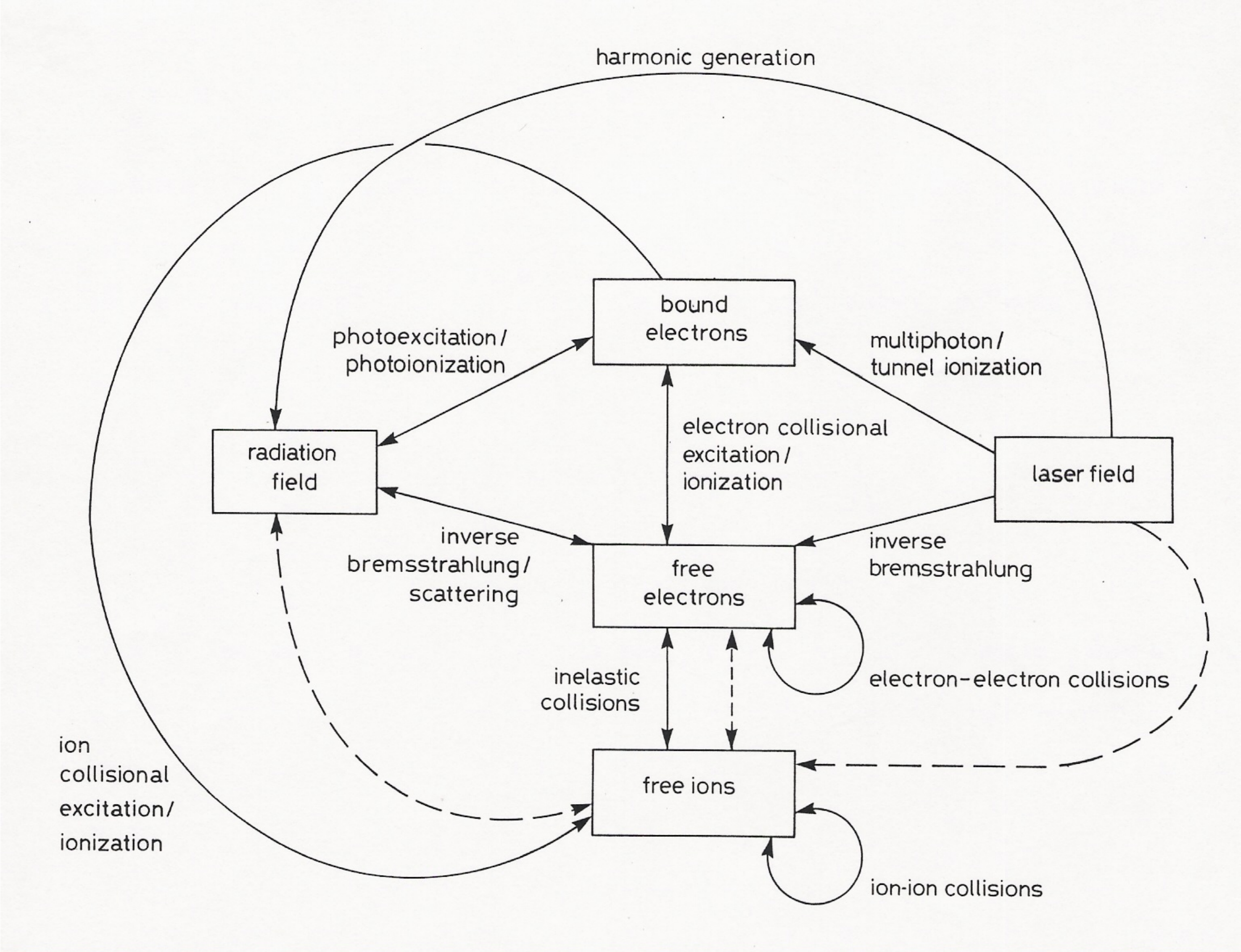
$$\underbrace{\Delta\varepsilon^{i}}_{\text{change in ionic kinetic energy}} = \underbrace{h\nu}_{\text{photon energy absorbed}} - \underbrace{\Delta\varepsilon^{ex}}_{\text{excitation energy in the limit of large internuclear separation}}$$

$1s\sigma_g \rightarrow 2p\sigma_u \qquad \Delta\varepsilon^{ex} = 0 \qquad \Delta\varepsilon^{i} = h\nu$

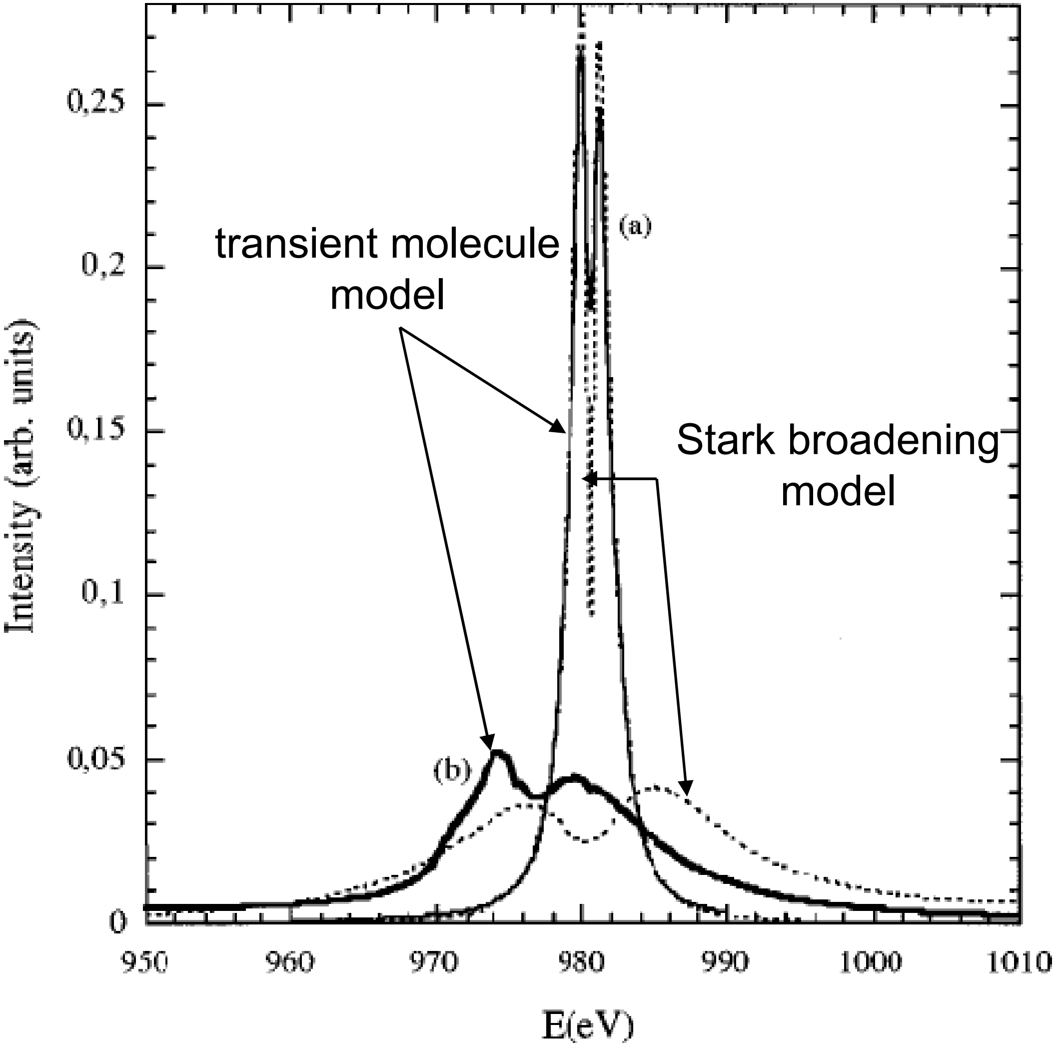
$$1s\sigma_g \rightarrow 2p\pi_u \begin{cases} h\nu > \Delta\varepsilon^{ex} & \Delta\varepsilon^{i} > 0 \\ h\nu < \Delta\varepsilon^{ex} & \Delta\varepsilon^{i} < 0 \end{cases}$$

Rose, J. de Physique (1983)

Energy pathways in HEDP plasma



Transient molecular method provides a new line shape model



transient molecule model

Stark broadening model

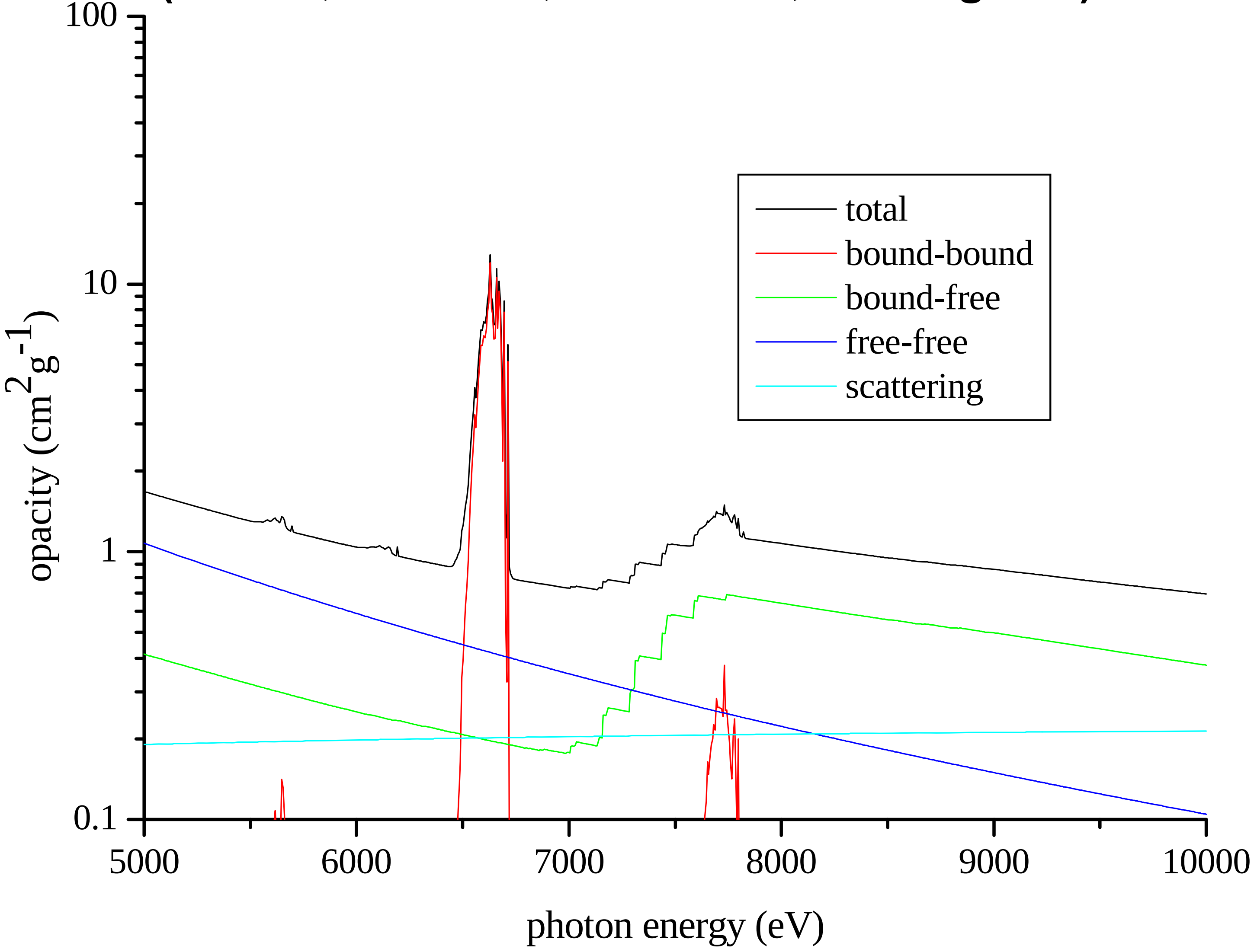
F IX Lyβ

(a) $n_e=10^{22}cm^{-3}$

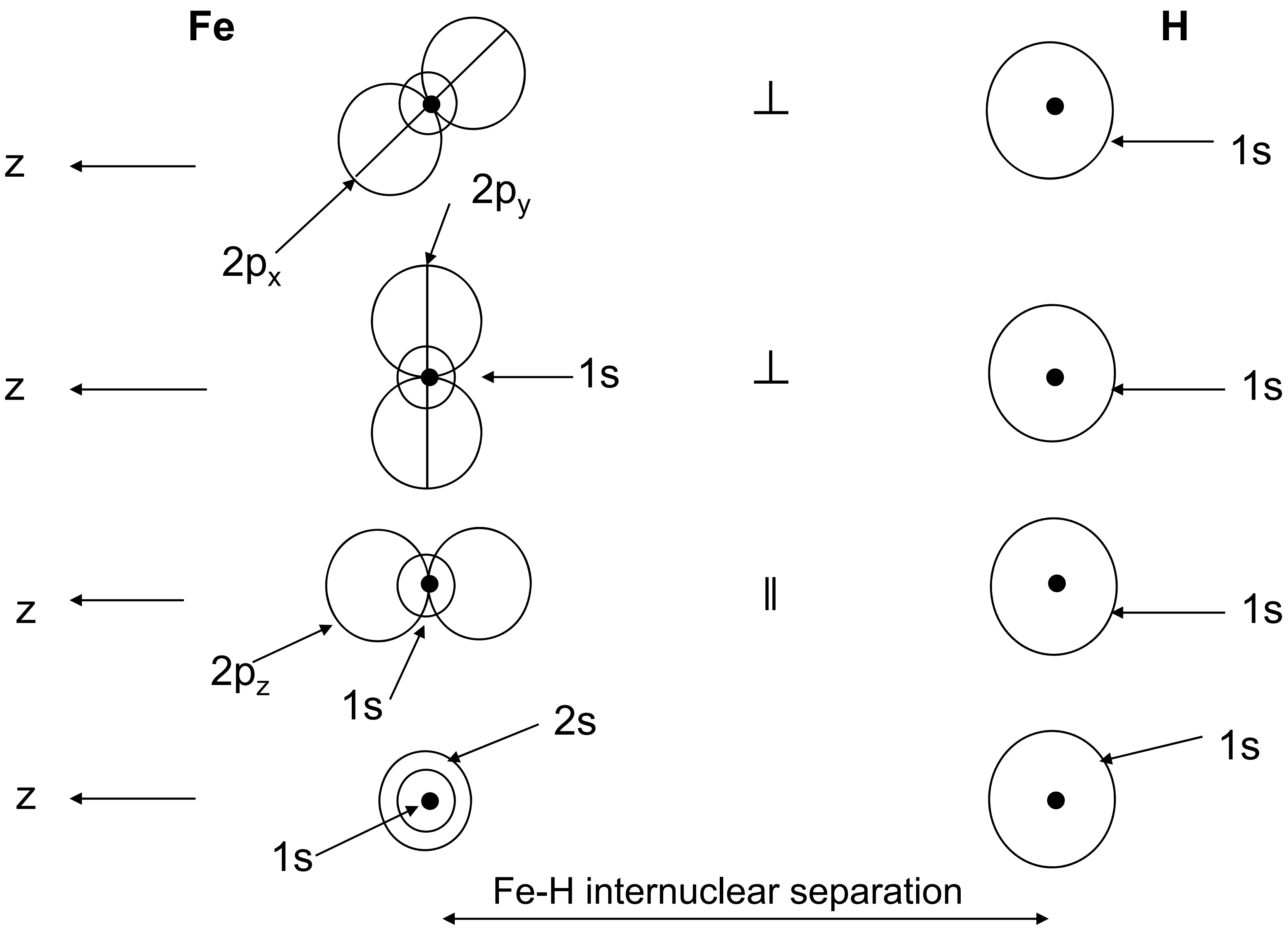
(b) $n_e=2x10^{23}cm^{-3}$

Gauthier, Rose et al, PRE, (1998)

Grevesse 20 element stellar opacity at Sun centre (X=0.35, Z=0.0195, 1.3621keV, 157.02gcm^{-3})

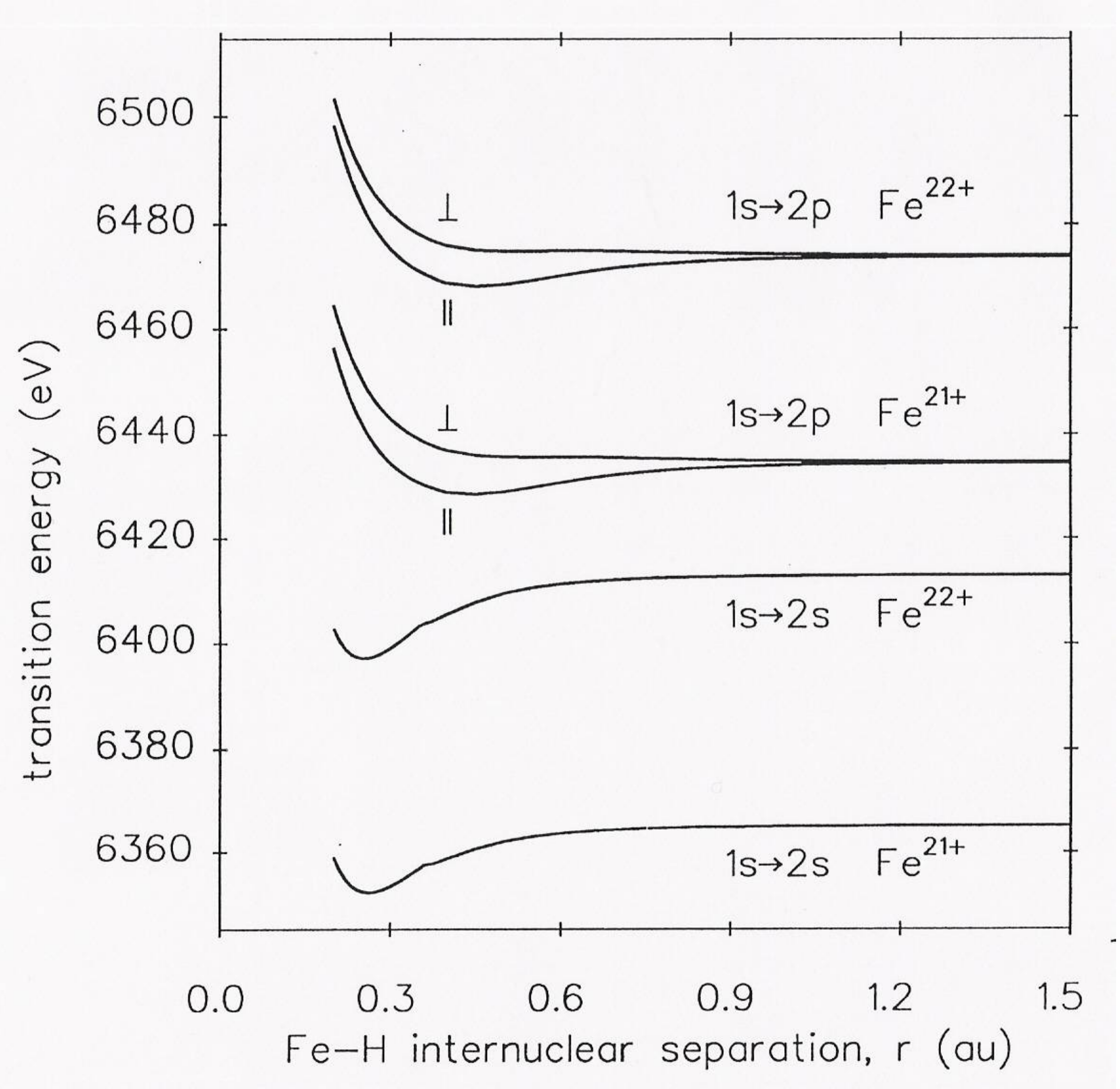


Transient molecules at the Sun centre



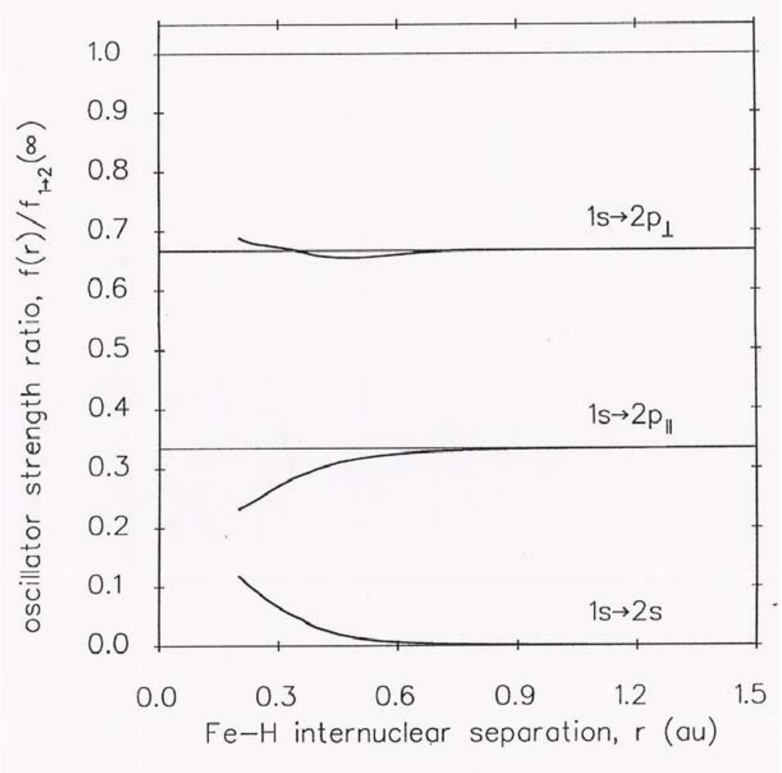
Rose, Foulis and Beynon, J Phys B, (1998)

One-electron transition energies for 1s→2s and 1s→2p in Fe^{21+} and Fe^{22+}



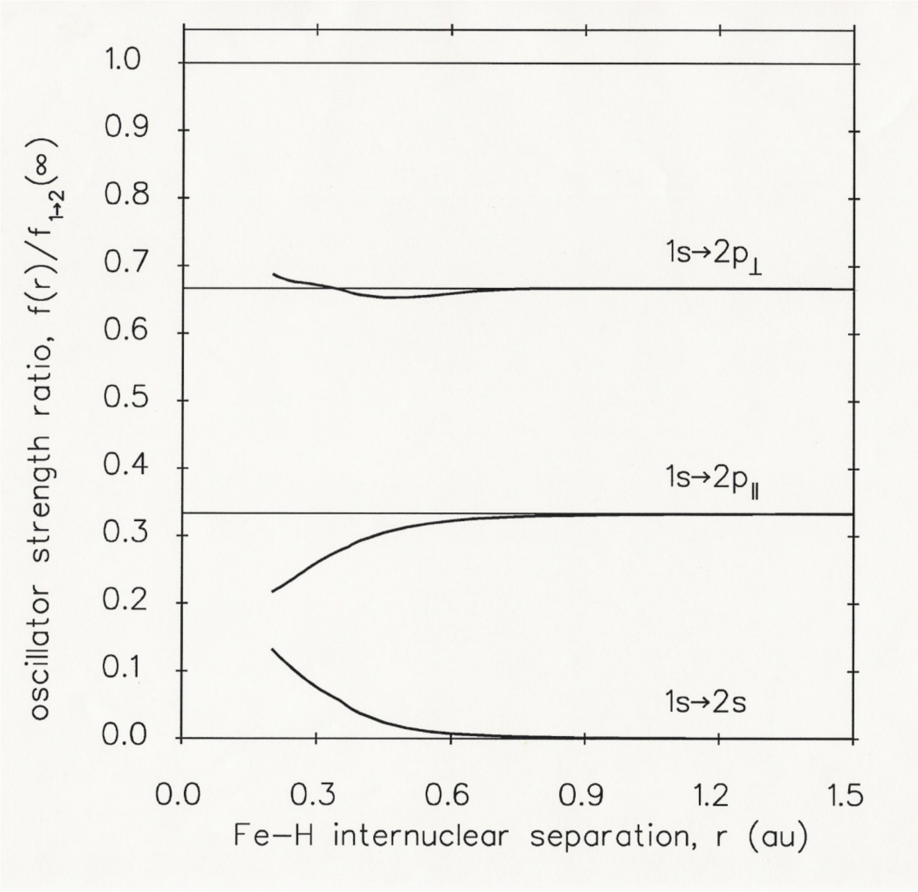
Rose, Foulis and Beynon, J Phys B, (1998)

Ratio of oscillator strength $f(r)/f_{1\rightarrow 2}(\infty)$ for 1s→2s and 1s→2p



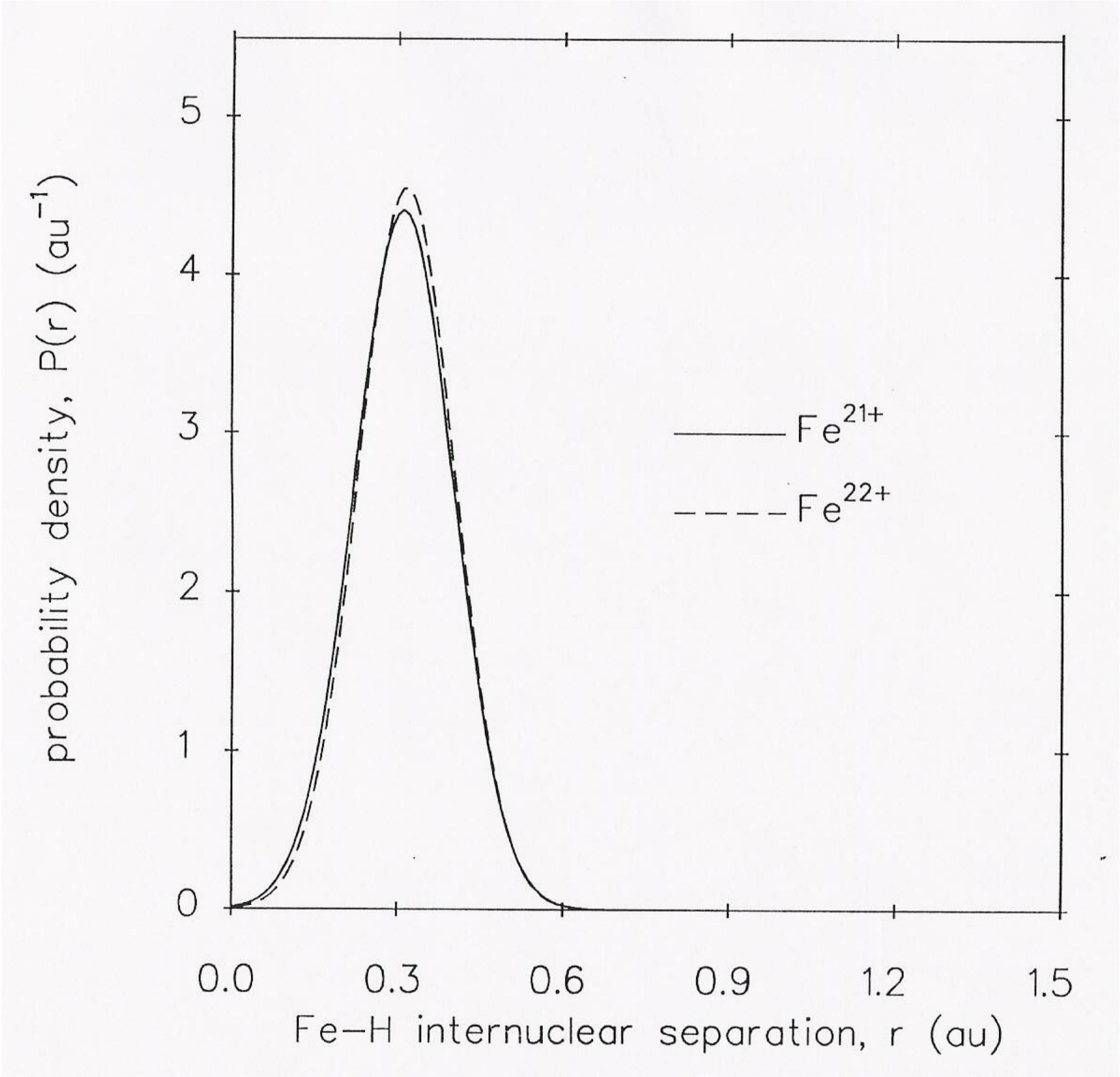
Fe^{21+}

Fe^{22+}



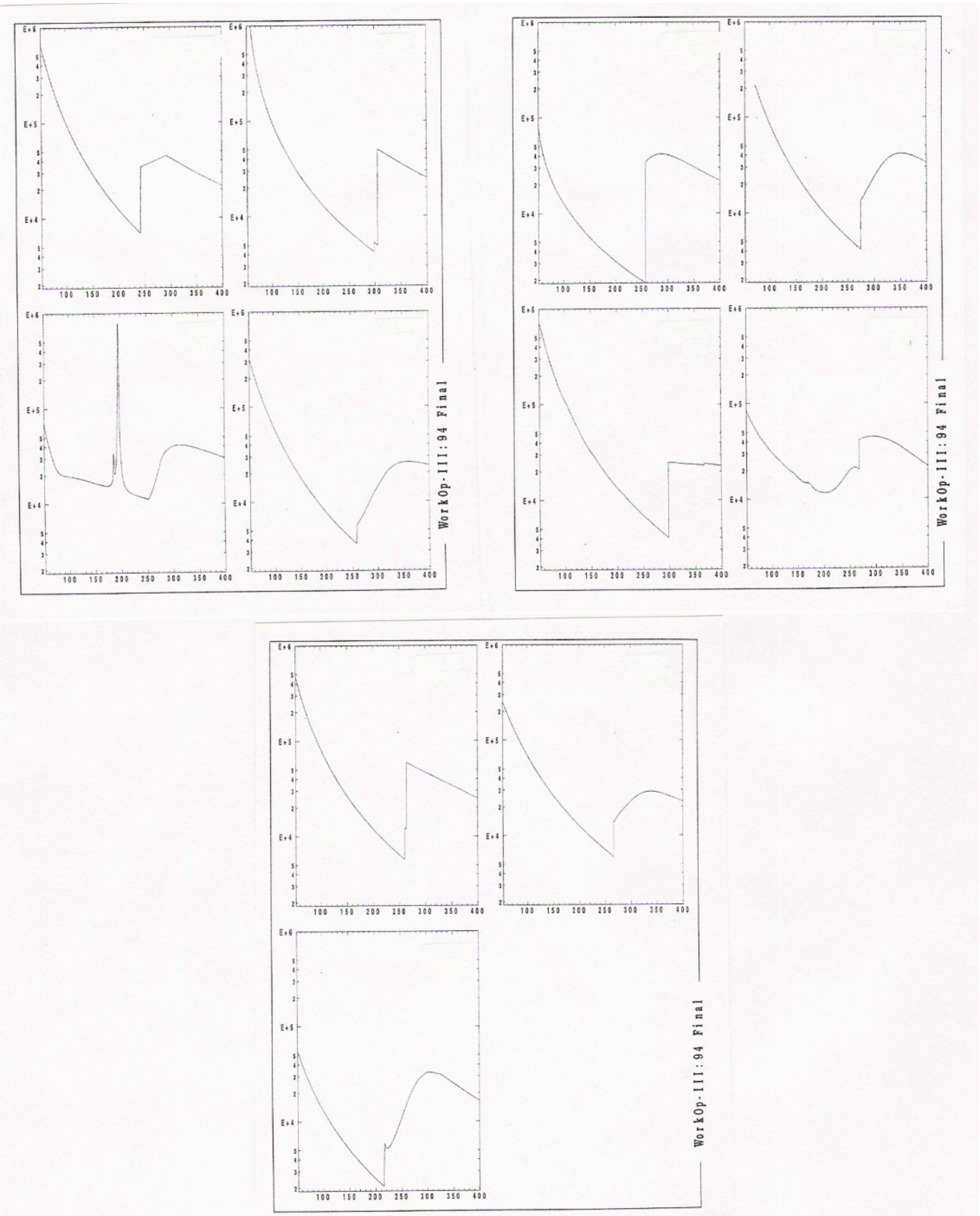
Rose, Foulis and Beynon, J Phys B, (1998)

Nearest neighbour distribution of protons around iron ions at Sun’s centre



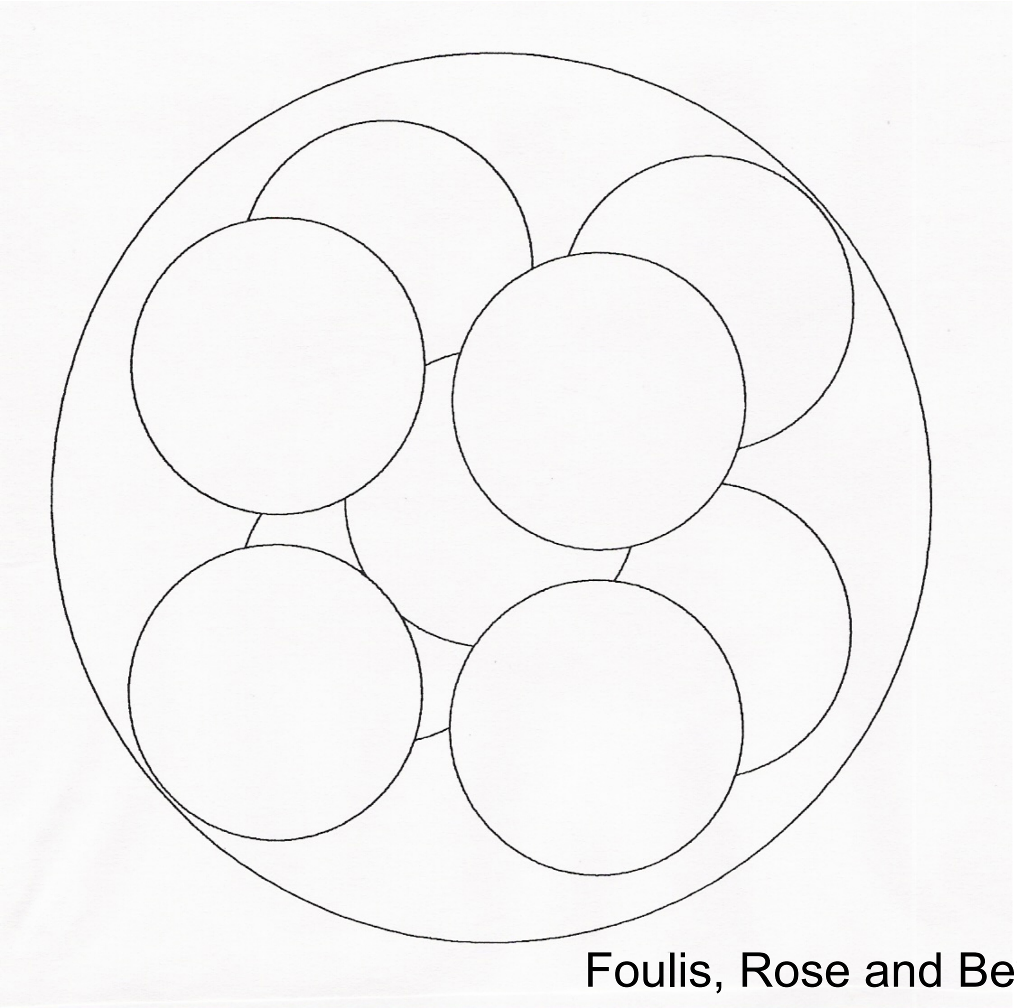
Rose, Foulis and Beynon, J Phys B, (1998)

Workshop shows large disagreement between codes
Carbon (20eV, 10gcm^{-3})



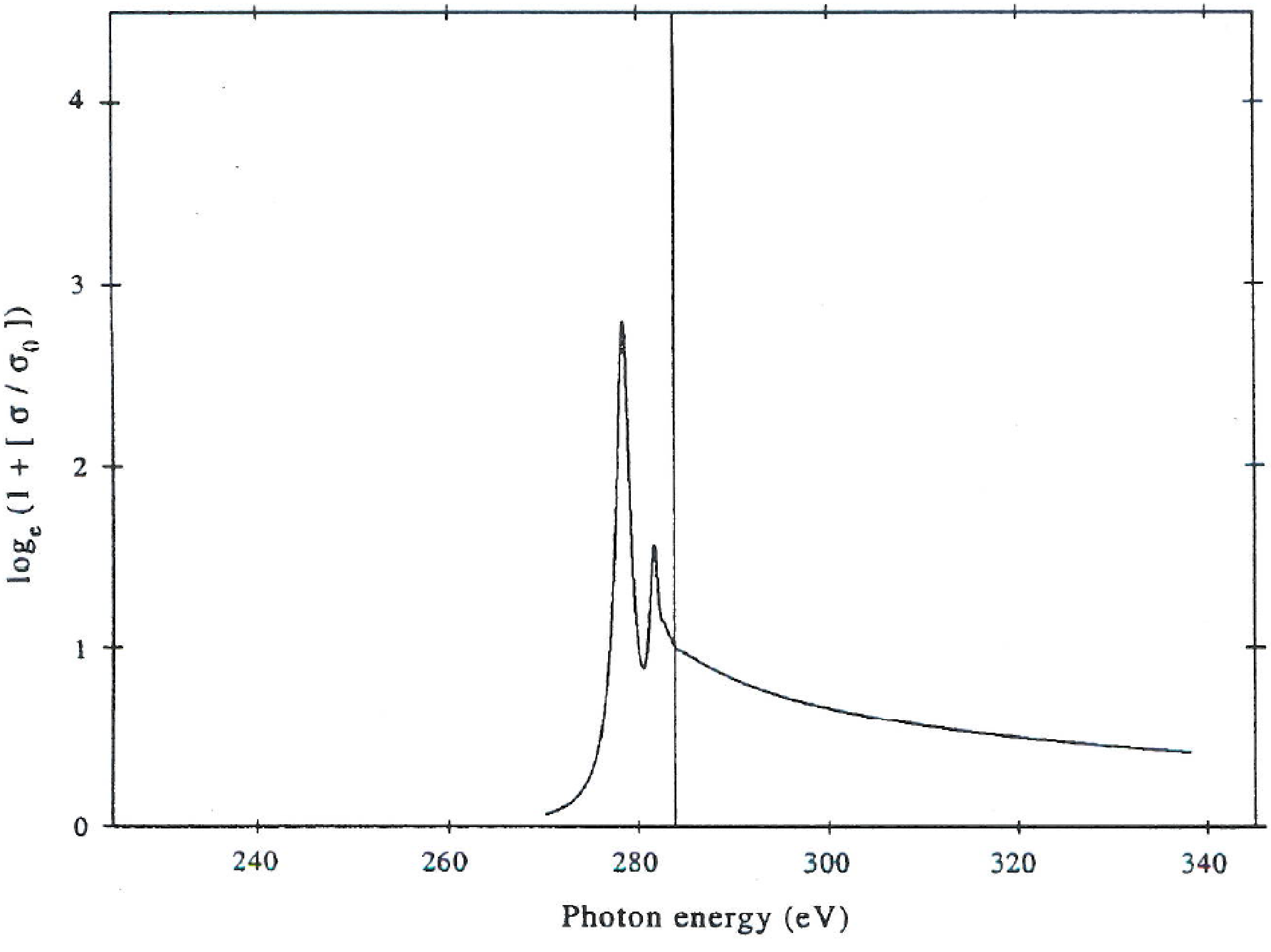
Calculation of K-shell photoabsorption in carbon (20eV, $10gcm^{-3}$) using multicentre wavefunctions

CC_8 cluster in a super cell



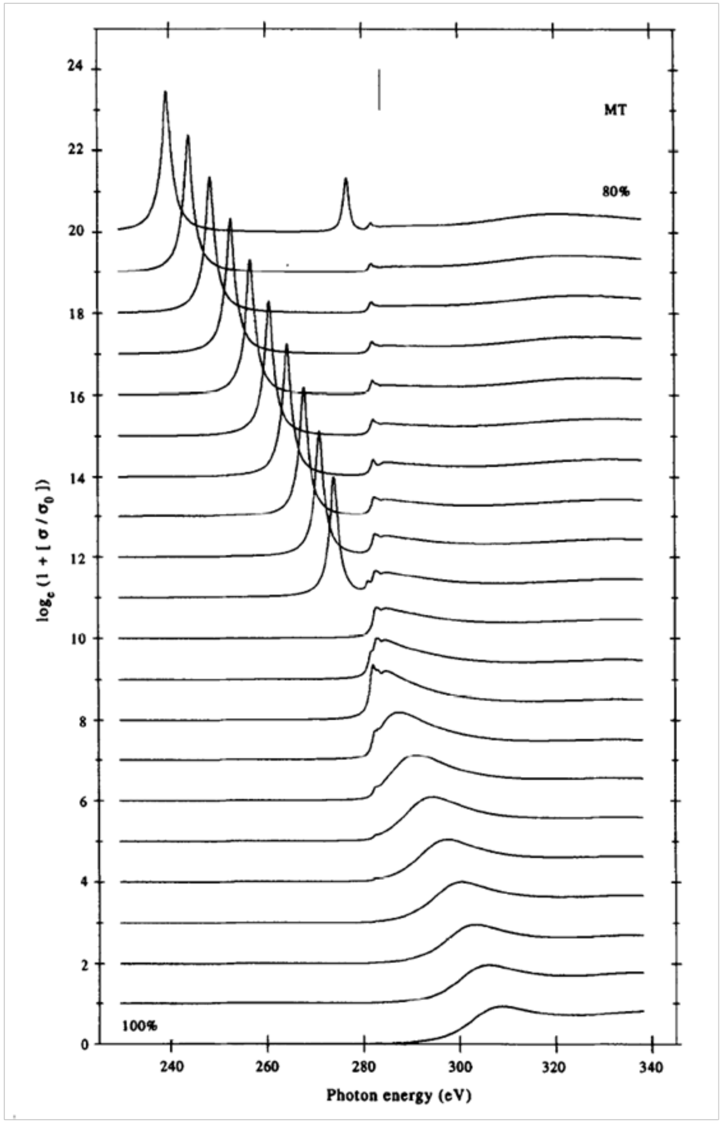
Foulis, Rose and Beynon, JQSRT, (1997)

Calculation of C^{4+} K-shell photoabsorption in carbon (20eV, 10gcm^{-3}) using single-centre wavefunctions



Foulis, Rose and Beynon, JQSRT, (1997)

Variation in C^{4+} photoabsorption cross-section in carbon (20eV, $10gcm^{-3}$) using multi-cetre wavefunctions with contraction in the $A1_g$ (breathing mode) of CC_8 cluster



Foulis, Rose and Beynon, JQSRT, (1997)

Transient molecules predict new effects

- Single-centre wavefunctions cannot account completely for the change in wavefunction due to neighbouring ions in a plasma.

- Two-centre (in general multicentre) wavefunctions are needed.

- Calculations that involve the wavefunctions (rather than using density functional theory which have been undertaken for equation of state calculations) are very complex – even for today's computers

- Atomically allowed absorption altered.

- Extra absorption mechanisms introduced.

- Stark line shapes are altered.

- Energy coupling altered - ω_{ri} and ω_{ei} introduced.

- Validity of Born-Oppenheimer approximation – need to break the approximation to allow electron-ion energy exchange.