# Configurations and superconfigurations models in Atomic Physics

## X-ray radiation in hot plasmas

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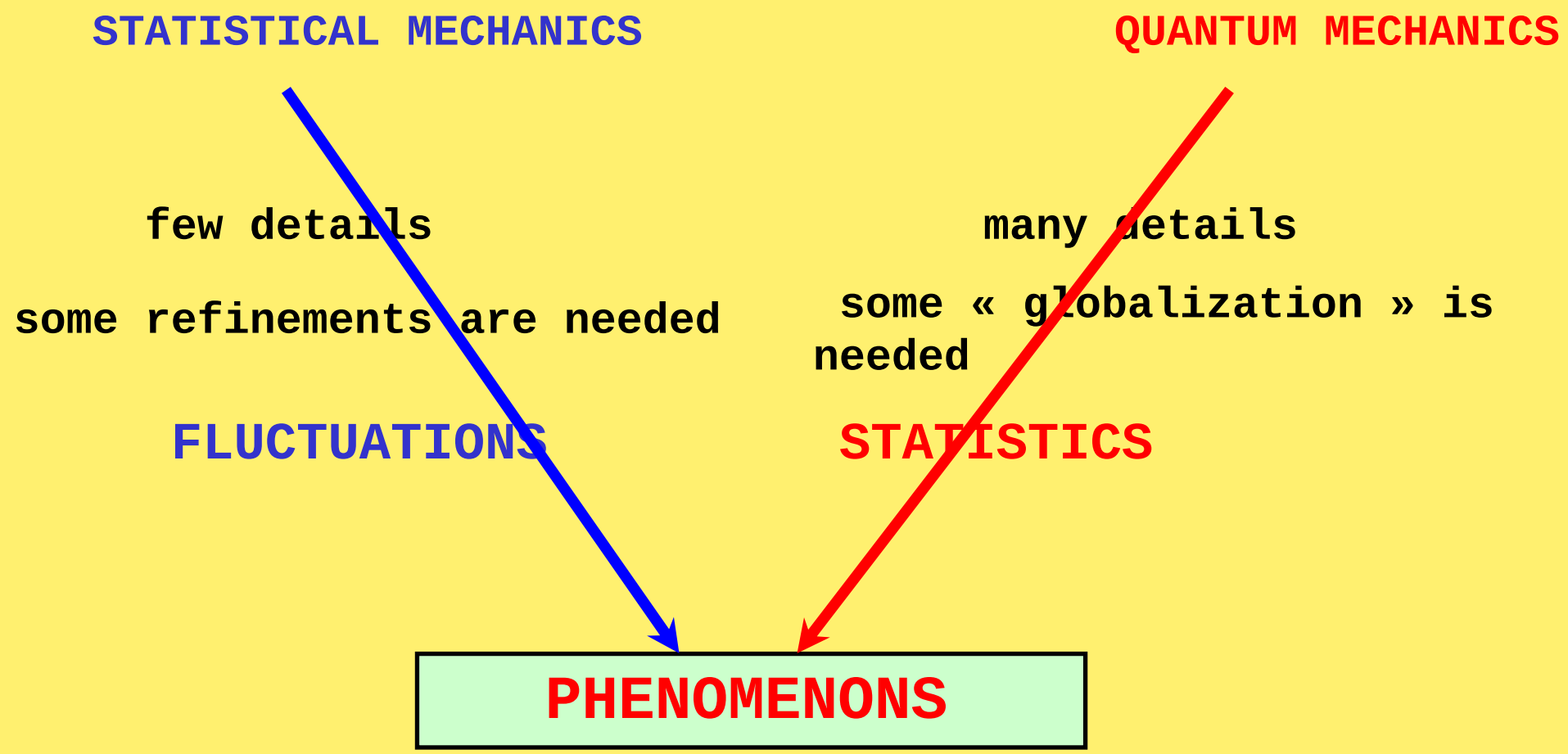
# TWO DIFFERENT APPROACHES



# Outline

**I. Introduction**

**II. Statics** (structures)

**III. Dynamical equilibrium** ($dN_i/dt = 0$)

**IV. Dynamics** ($dN_i/dt \neq 0$)

**V. Conclusion**

# I. INTRODUCTION

## Basic theoretical *ab-initio* methods

Central field (radial potential)

Hartree-Fock method

Average Atom

Tensor Operators

Second Quantization

Statistical distributions

# Central field

In Slater's approach, an atom is a sphere, centered at which is the center of symmetry of the system.

The simplest form of the Hamiltonian

$$H = -\sum_{i=1,N} \frac{\vec{p}^2}{2m} - \sum_{i=1,N} \frac{Ze^2}{r_i} + \sum_{i<j=1,N} \frac{e^2}{r_{ij}} + \sum_{i=1,N} \xi(r_i)(\vec{s}_i.\vec{\ell}_i)$$

has also spherical symmetry.

$$H_0 = -\sum_{i=1,N} \frac{\vec{p}^2}{2m} + \sum_{i=1,N} V(r_i)$$ is the zeroth-order Hamiltonian

$$H_r = -\sum_{i=1,N} V(r_i) - \sum_{i=1,N} \frac{Ze^2}{r_i} + \sum_{i<j=1,N} \frac{e^2}{r_{ij}} + \sum_{i=1,N} \xi(r_i)(\vec{s}_i.\vec{\ell}_i)$$ is the residual Hamiltonian.

# Central field (cont'd)

**Zeroth-order solutions :**

the configurational *states*, which gather into degenerate electronic *configurations*. These states are made of *angular* and *spin* functions, and of *radial* functions.

**Higher-order solutions :**

the states obtained by diagonalizing the H matrix
- for one configuration (this is a calculation of *intermediate coupling*)
- for several configurations (this is a calculation of *configuration interaction*).

An approximate *ab-initio* V(r) radial potential is generally obtained through the variational optimization of an expansion in terms of Slater basis functions $r^n e^{-\alpha r}$.

The central-field model can be chosen to be relativistic c

# Tensor operators, and graphical methods

The tensor-operator methods have been invented by Gi
and fully explained, and extended by Brian R. Judd. They
the angular and spin parts of the configurational states,
computation of the corresponding matrix elements of the o

For very complicated cases, it is convenient to use the graphical
methods developed by A. P. Jucys et al.

# Second-Quantization formalism

The Second-Quantization formalism has been adapted
Physics by Brian R. Judd. In his version, the well-known
annihilation operators do not relate to photons, or to nu
electrons.

This formalism is extremely efficient for the calcu
quantities, e.g., moments of statistical distributions, su
subspaces, or averages, or correlation factors.

# II. STATICS

## Statistics of configuration states and leve

An electronic configuration is denoted $(nl)^N (n'l')^{N'} (n''l'')^{N''} \ldots$, i.e., a suite of open subshells $(nl)^N$. Each of its quantum states corresponds to a pair of quantum numbers $(J, M_J)$ which are, in $h$ units, the values of the total angular momentum $J$ and of its projection on the $z$ axis, respectively. The degeneracy of each $J$ *level* is equal to $(2J+1)$.

It is remarkable that the number of $(J,M_J)$ states of the configuration, for example, is the well-known combinatorial factor, $\binom{4\ell+2}{N}$, whereas no simple formula has yet been found for the number of J levels. However, the statistical distribution of the J values is related to the derivative vs $M_J$ of that of the $M_J$ values, which can be expressed as a Gram-Charlier distribution, whose moments are computed *exactly*.

# tistics of configuration states and levels (con

The Gram-Charlier distribution function of $M_J$ (denoted M) in the $(l)^N$ configuration reads

$$D(M) = g\,(2\pi v)^{-1/2} \exp\left(-M^2/2v\right)\left[1 + (\alpha_4 - 3)\,(3 - 6M^2/v + M^4/v^2)/24 + \ldots\right]$$

with the *distribution moments* $\mu_n(M) = \Sigma_i M_i^n / g$

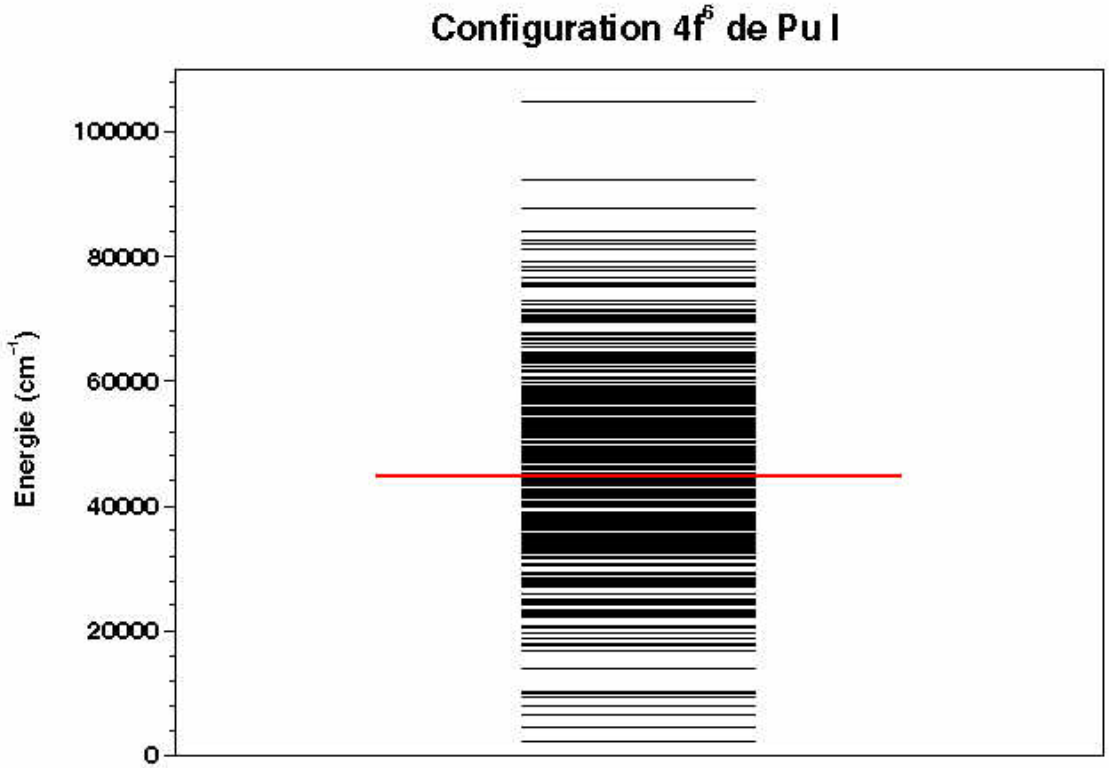
$\mu_2$ (the *variance* v) $= N(4l - N + 2)\,(4l^2 + 4l + 3) / (4l + 1)$

$\mu_4 = N(4l - N + 2)\,[N(4l - N + 2)\,x(l) + y(l)]$

(where $x(l)$ and $y(l)$ are polynomials in $l$)

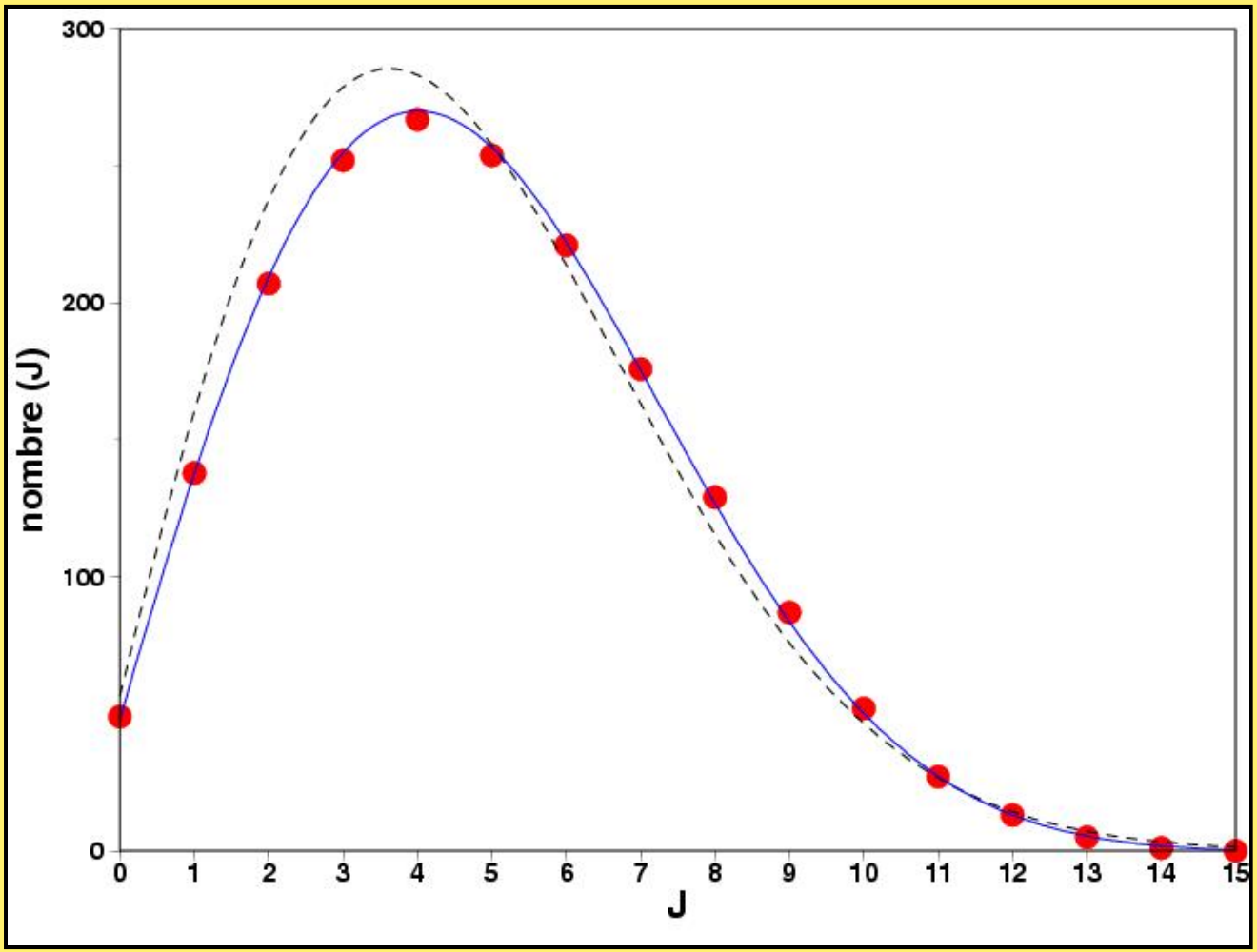
and the *kurtosis* coefficient $\alpha_4 = \mu_4 / (\mu_2)^2$.

# Configuration levels



# J distribution of the levels of configurations

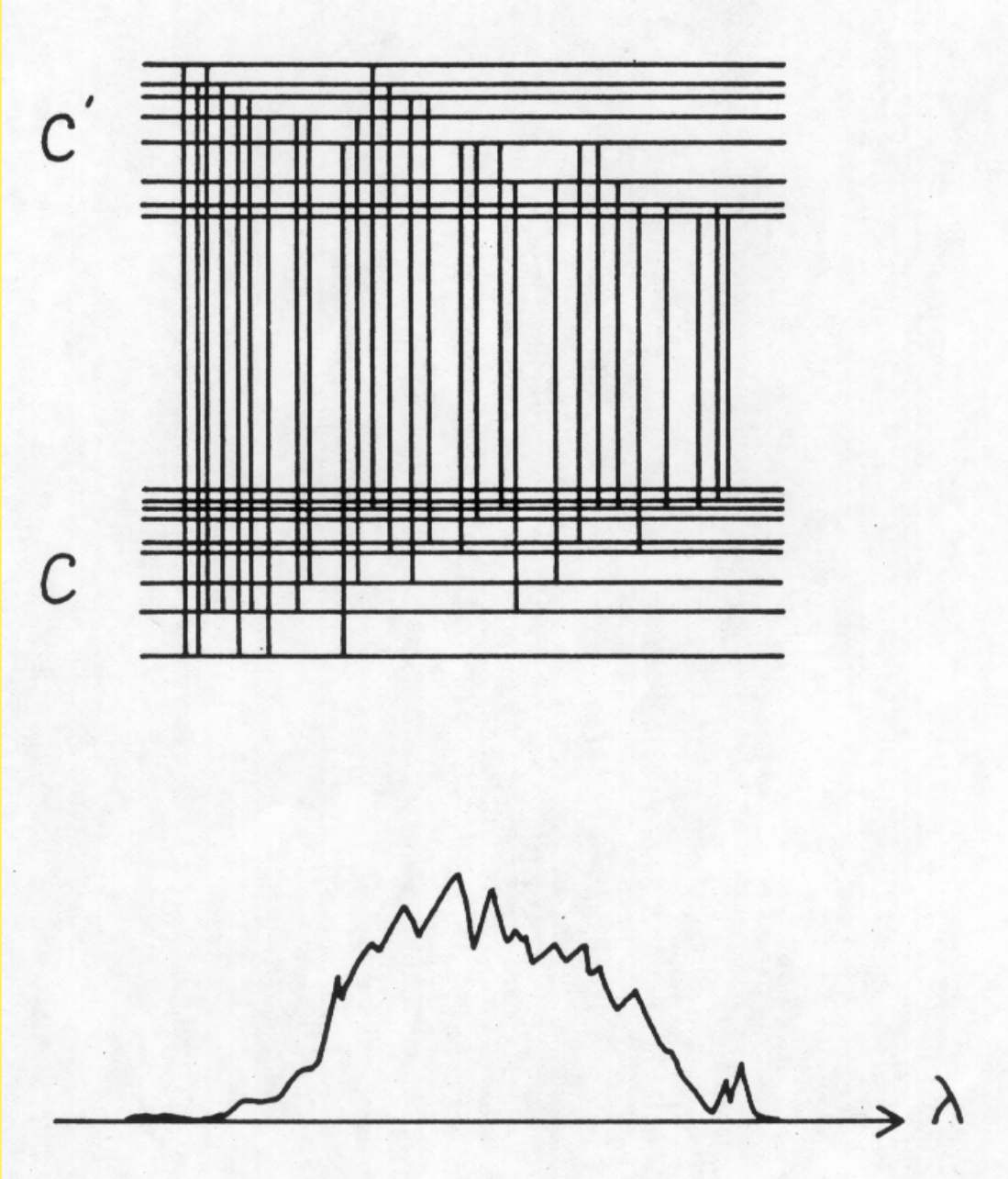
## Example: $4f\ ^5 5d$



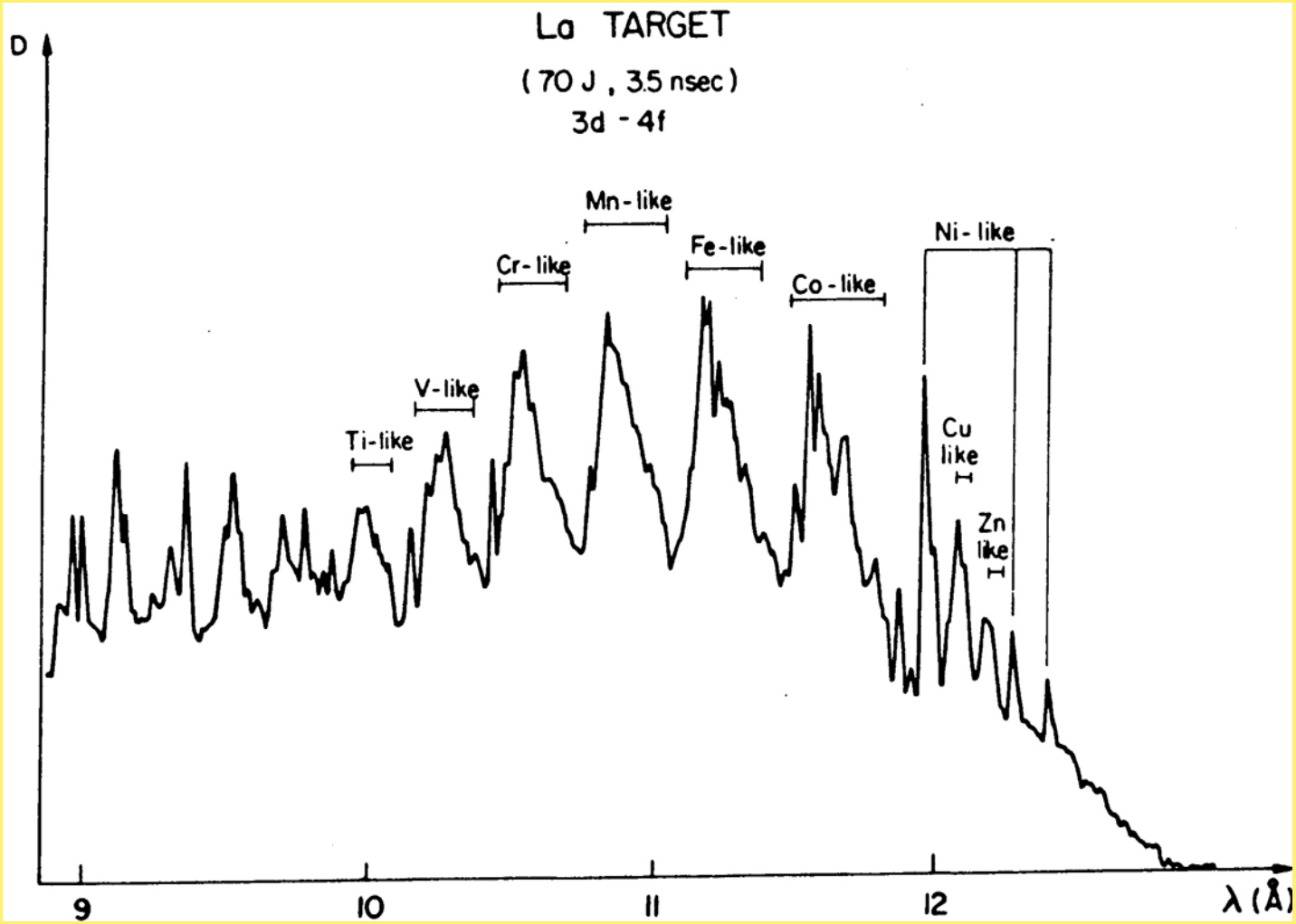
# Transition arrays

A transition array is the ensemble of the radiativ
which link two configurations.

# Transition array

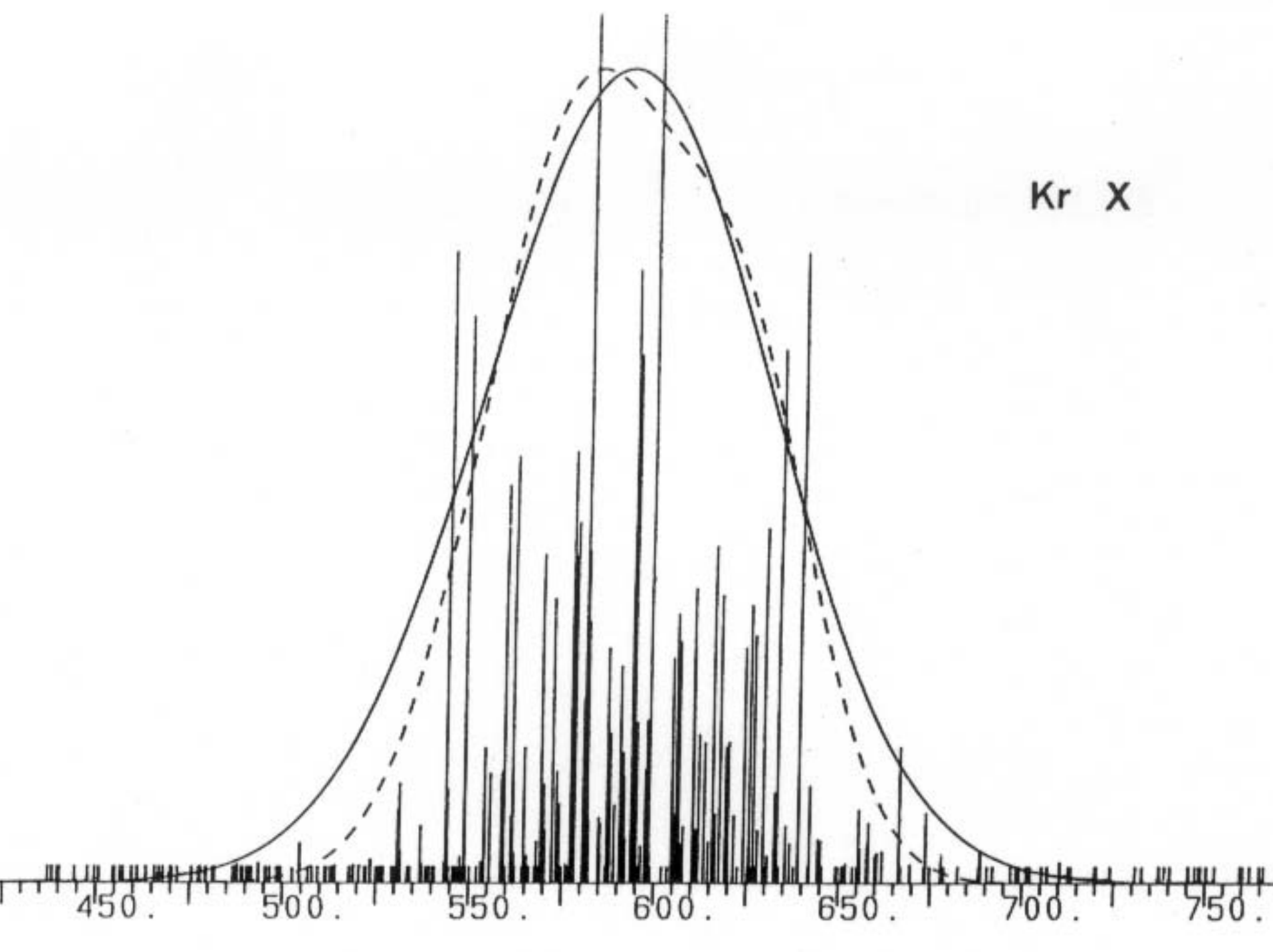


# Lanthanum spectrum



# The Unresolved Transition Array (UTA) model

In most arrays, the linewidths and the spectral de
lines are large enough for the line profiles to *coalesce*
continuous band. That band can be simulated as a Gaussian
(or skewed-Gaussian) feature, using the analytical expans
the strength-weighted two (or three) lowest-order moments
line wavenumbers.


Kr X
450.
500.
550.
600.
650.
700.
750.

# NUMBERS OF LINES IN TRANSITION ARRAYS

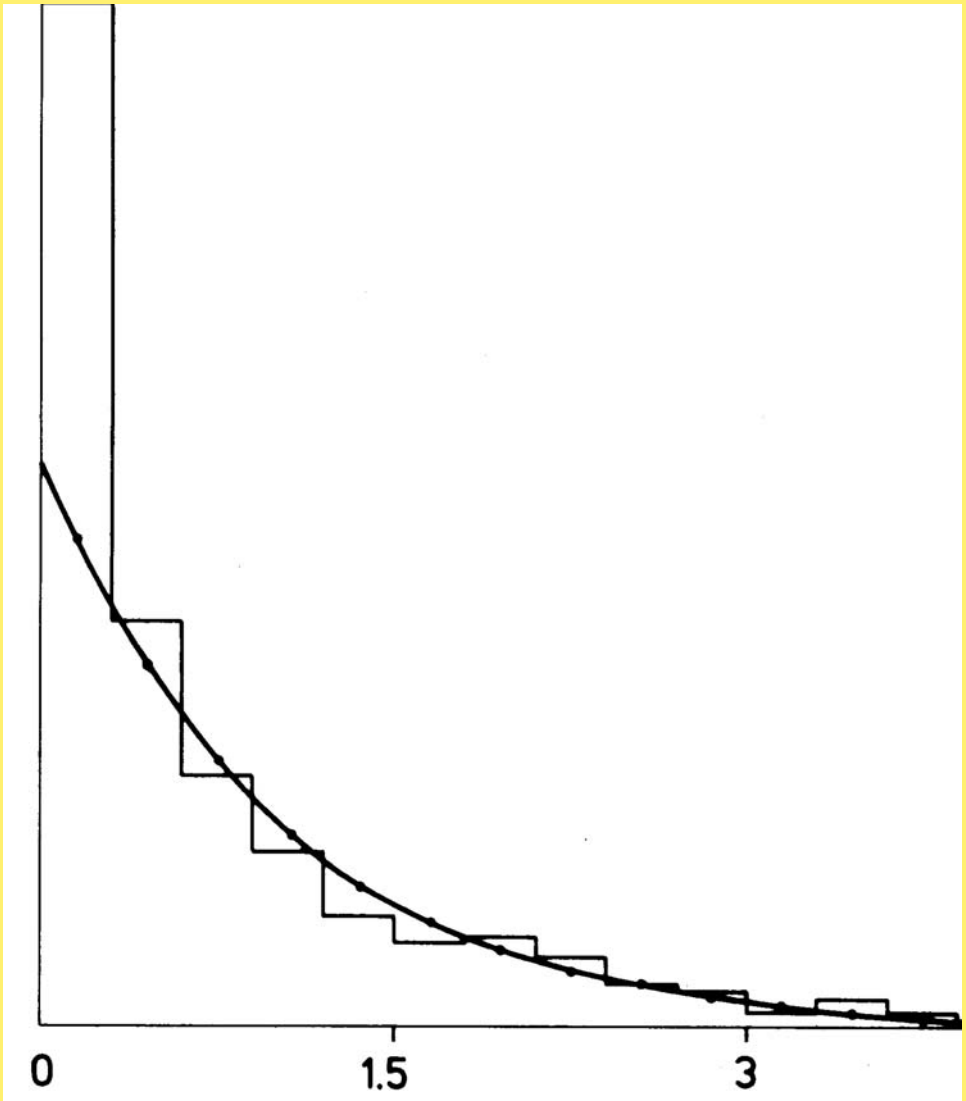
| Transition array | Number of lines | | Relative error (%) |
|---|---|---|---|
| | | *Exact* | |
| $p^3 - p^2s$ | 37 | 35 | +5.5 |
| $d^9 - d^8p$ | 59 | 60 | -1.7 |
| $d^8 - d^7f$ | 728 | 721 | +1.0 |
| $d^8p - d^8d'$ | 1 574 | 1 554 | +1.3 |
| $d^4 - d^3p$ | 1 741 | 1 718 | +1.3 |
| $f\ ^3s^2 - f\ ^3sp$ | 7 429 | 7 402 | +0.4 |
| $f\ ^{13}d^2s - f\ ^{13}dsp$ | 16 027 | 15 821 | +1.3 |
| $d^7f - d^6fp$ | 162 289 | 160 887 | +0.9 |
| $f\ ^8 - f\ ^7d$ | 279 112 | 277 827 | +0.5 |
| $d^6f - d^5f\ ^2$ | 293 376 | 291 521 | +0.6 |

# Statistics of strengths in a transition array

Porter and Thomas have proved that the radiative a
of the lines nearly obey a Poisson distribution (the stre
to $a^2$).

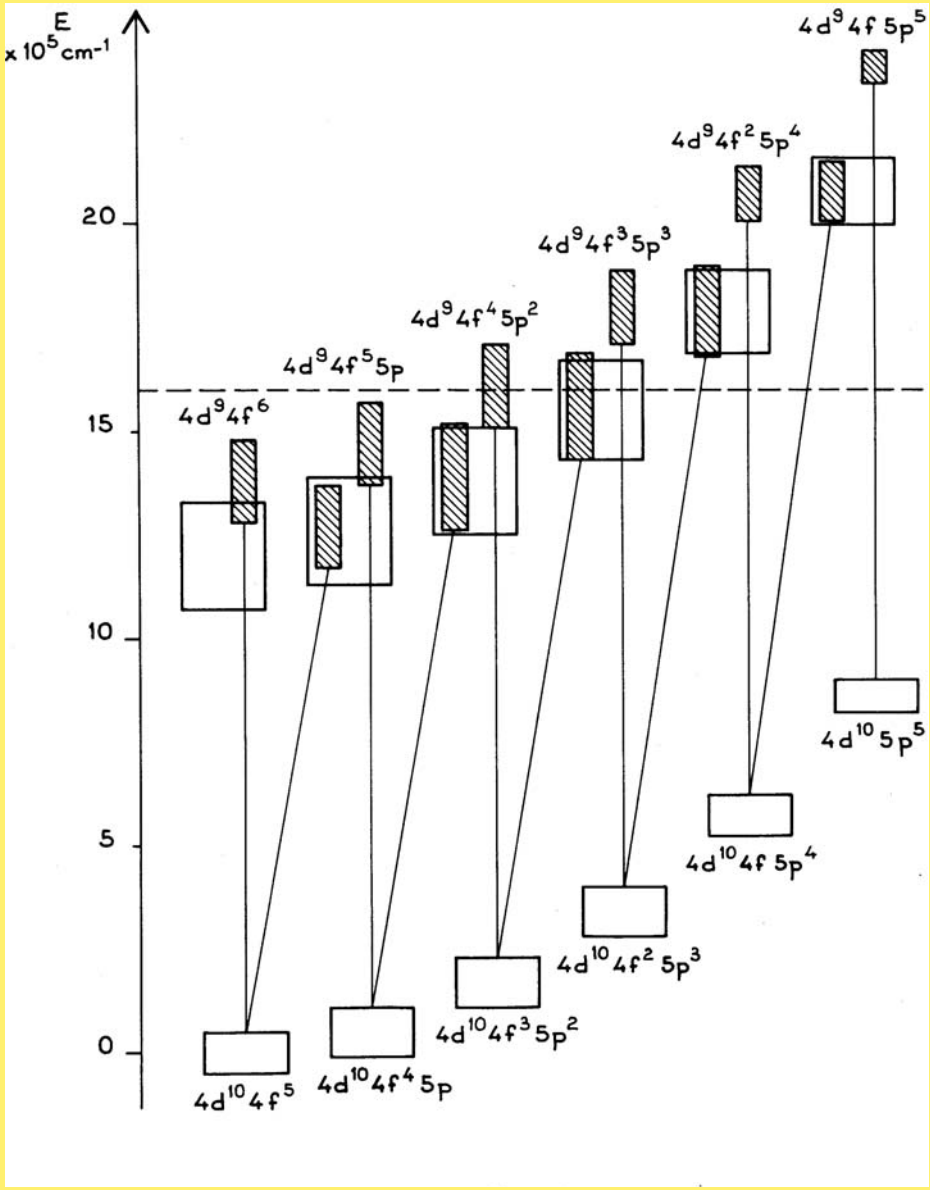
This agrees with the fact that most (allowed) line
array are very weak.

# Amplitude distribution in $Fe^{4+}$ $3d^4$ - $3d^3 4p$




|a|

# Emissive zones

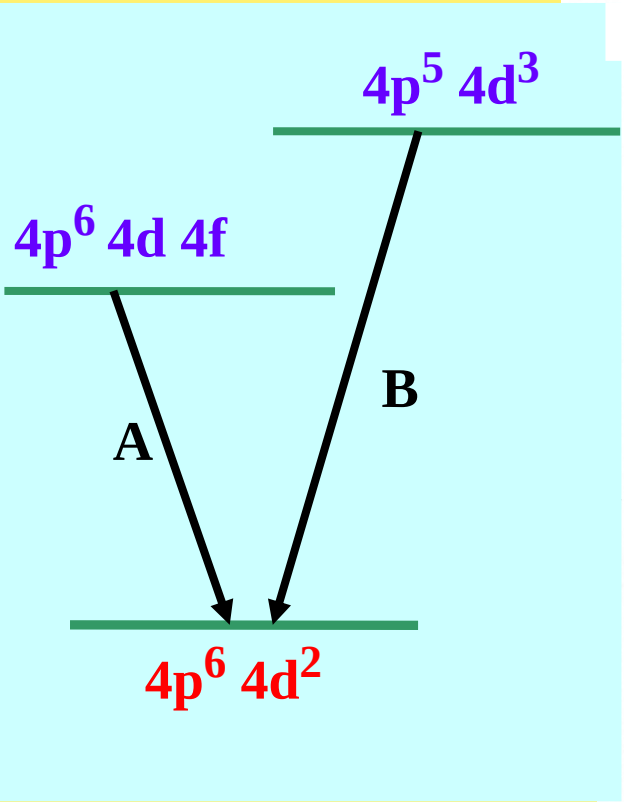


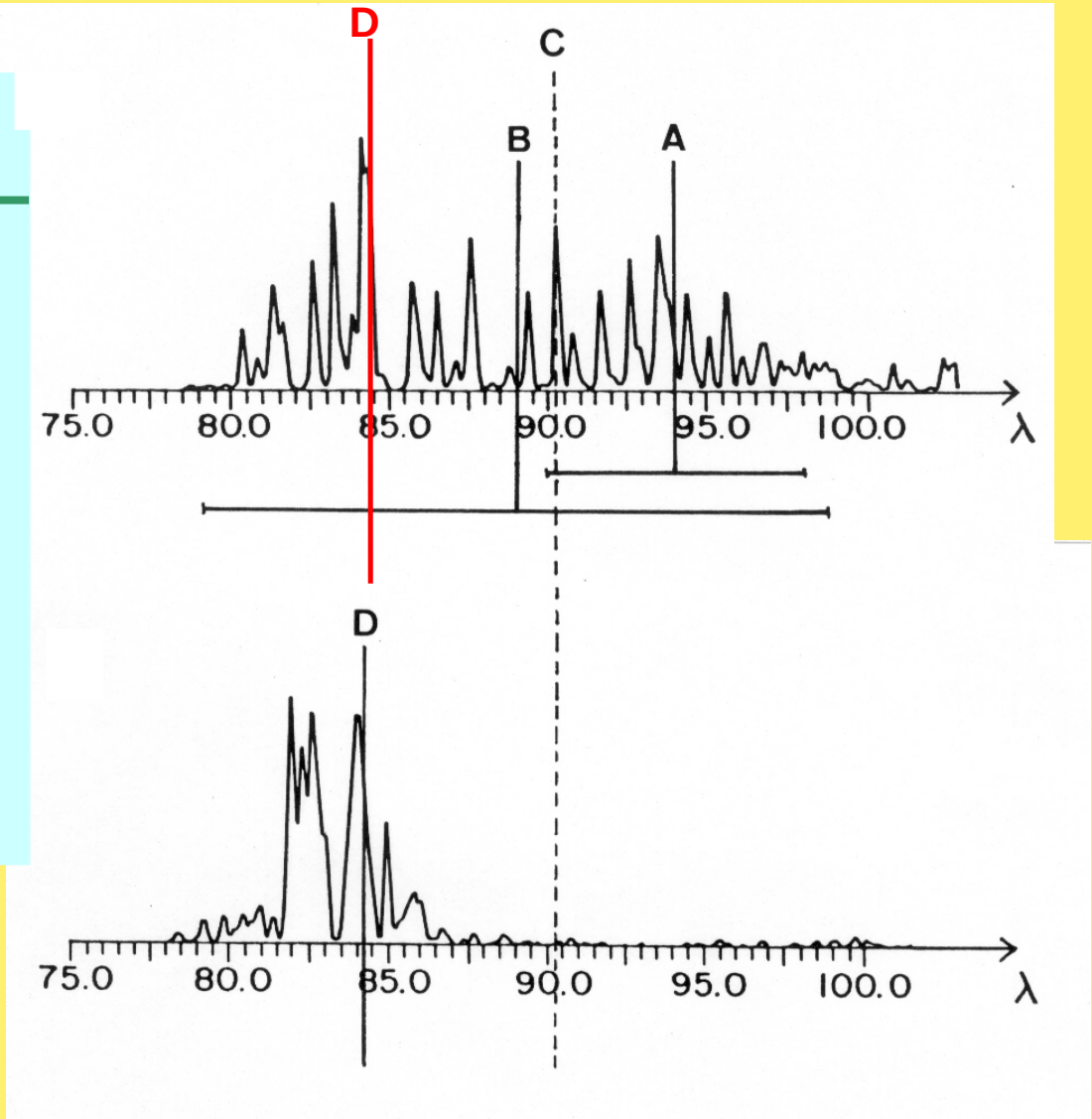
# Configuration interaction effects between UTAs

It may happen that a configuration is linked radia
other ones, which are mixed by the residual Hamiltonian $H$
energies are perturbed very little (to the second order o
but the strengths are perturbed to the first-order. There
possible to predict the qualitative (and quantitative) ch
UTAs without diagonalizing $H_r$ .

# Configuration-interaction effects

**Pr XXII $4p^6\,4d^2 - (\,4p^5\,4d^3 + 4p^6\,4d\,4f\,)$**

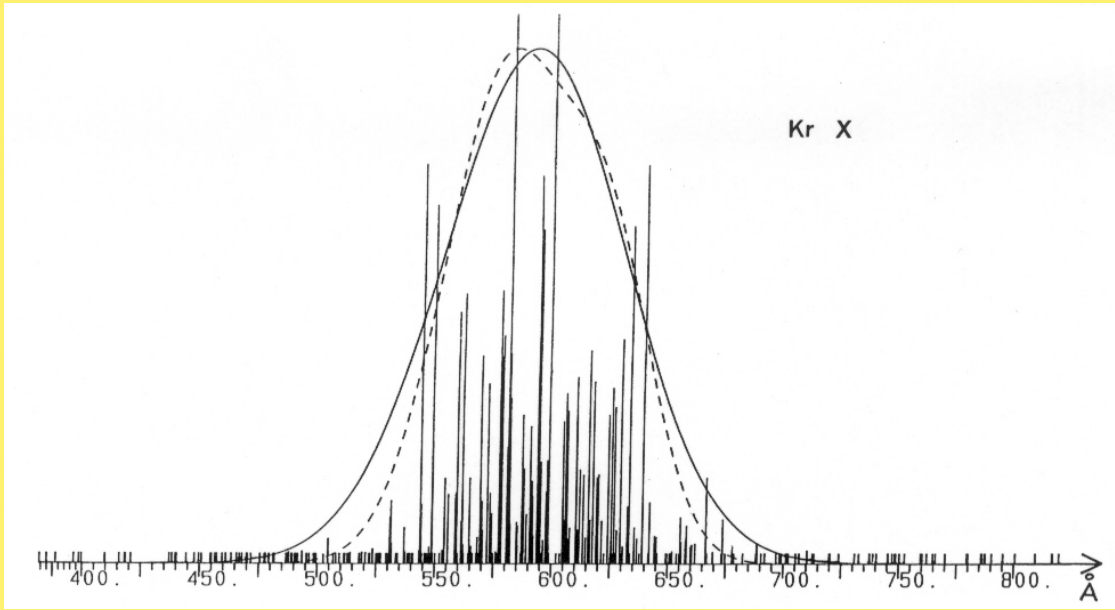


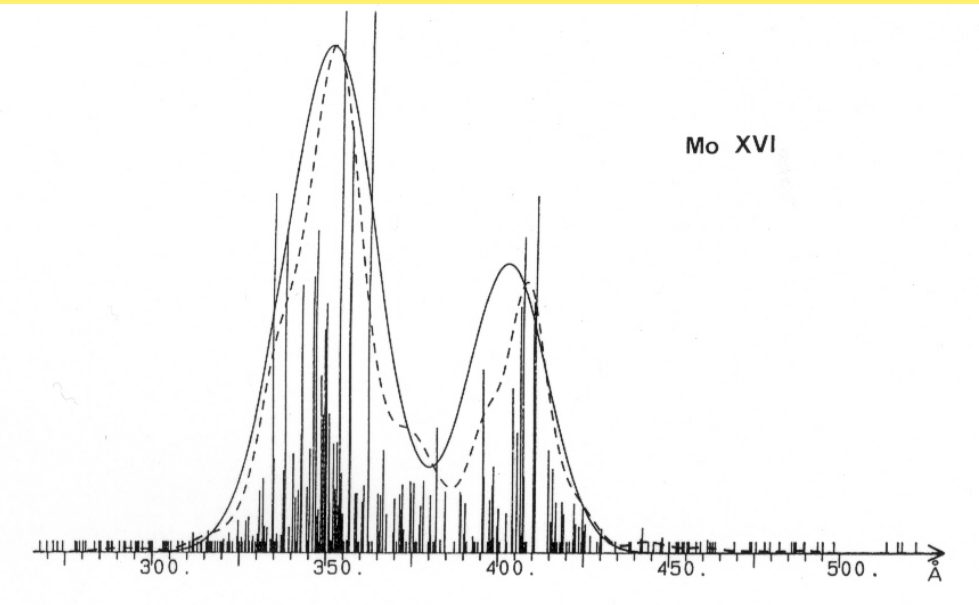



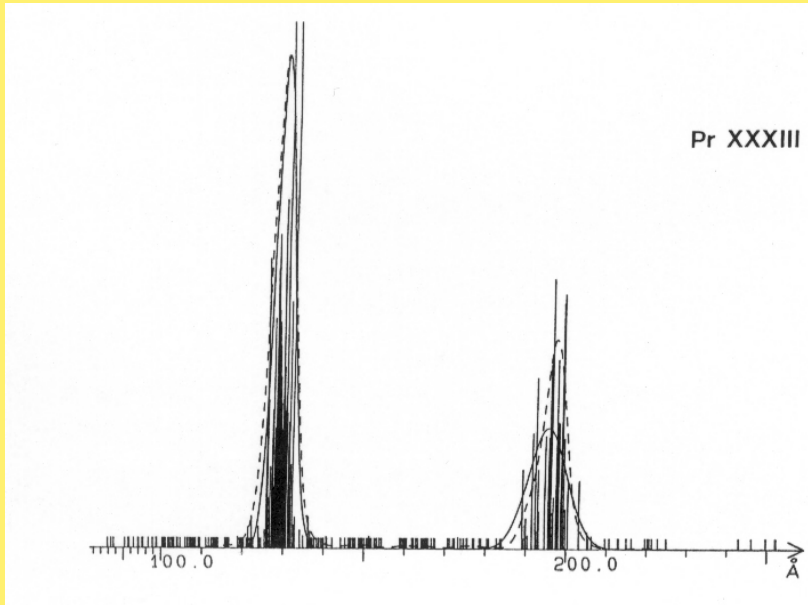
# The Spin-Orbit-Split-Array (SOSA) model

It may happen that the spin-orbit interactions are so large that the UTA Gaussian feature is split into two or three smaller ones, called *sub-arrays*. Other specific global formulas can be used, in pure j-j coupling.

# The $3d^8 4s - 3d^8 4p$ array



# The Resolved Transition Array (RTA) model

For computing the monochromatic absorption, a smooth curve like the Gaussian functions of the UTA model ought to be replaced by a line-by-line model, because the gaps between the lines are essential data. For achieving an RTA model, one uses the same energy variance and total strength as for the relevant UTA. The individual-line characteristics are picked at random in the following joint triple distribution of the upper and lower level energies E and E', and of the line amplitudes a:

$$D(E, E', a) = N \exp\left(-\frac{E^2/2v + E'^2/2v' - \lambda a^2}{}\right)$$

where v and v' are the energy variances of the configurations,
and $\lambda$ is a correlation factor.

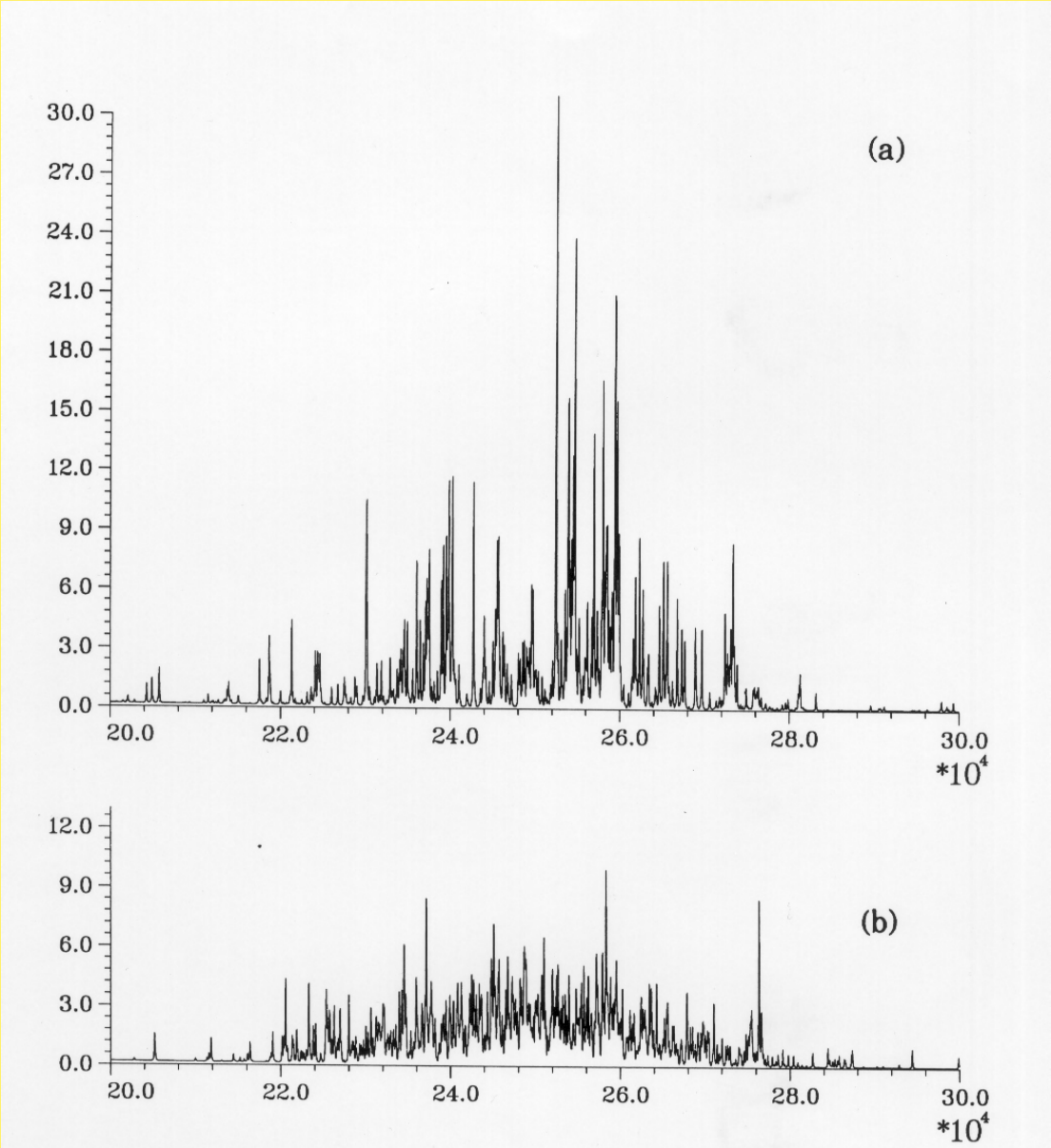
# Correlation between energies and strengths
# The propensity law

In most $C_1 - C_2$ transition arrays, the higher (lower) levels of $C_1$ are more strongly linked to the higher (lower) levels of $C_2$.

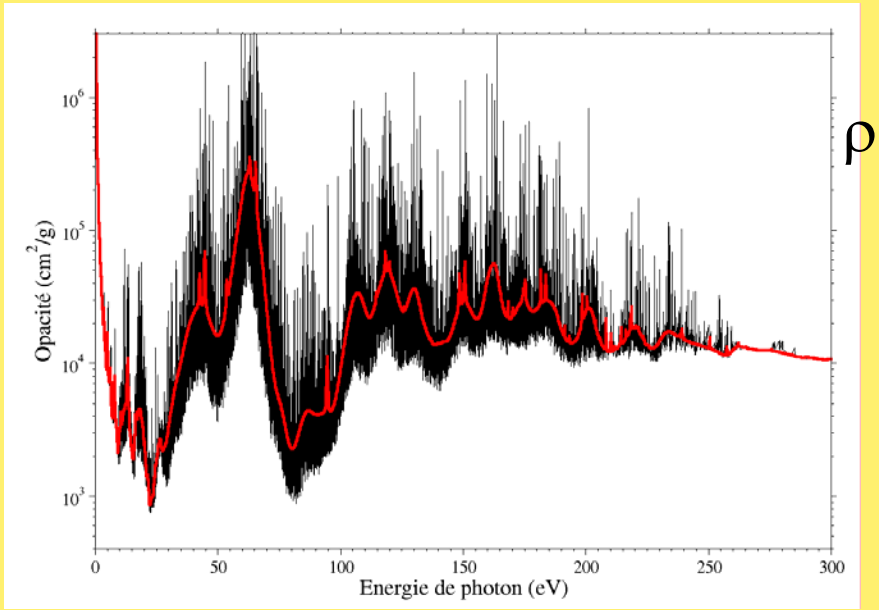
# The more intense lines are closer to the center of the array

**Exact line-by-line calculation**

**statistical calculation, without correlation**

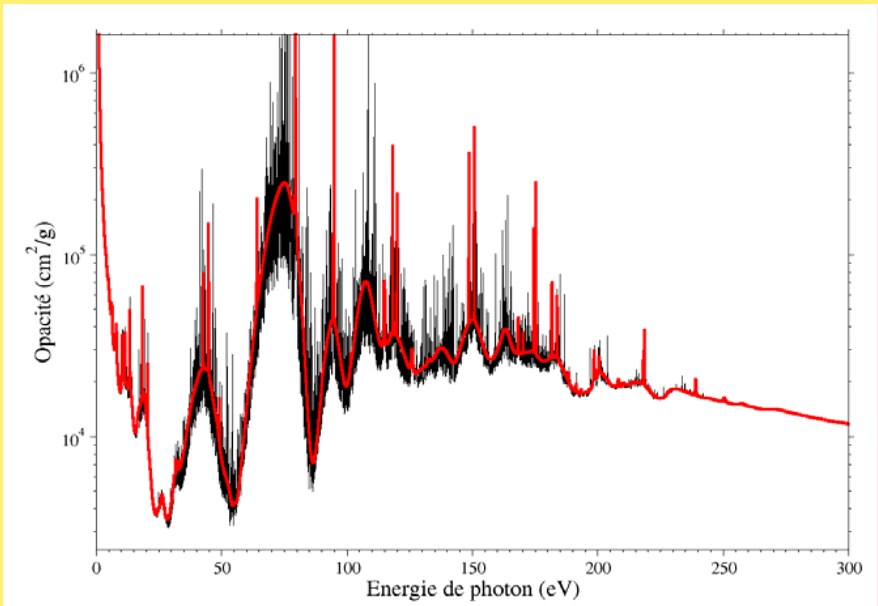


# RTA model: the Iron absorption spectrum (T=20 eV)

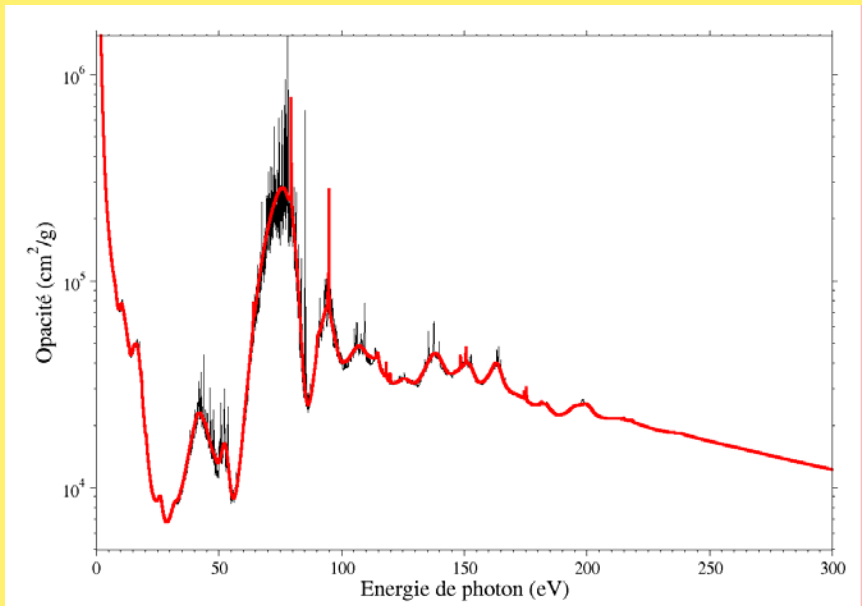



$\rho = 10^{-4}$ g/cc

$\rho = 10^{-3}$ g/cc




$\rho = 10^{-2}$ g/cc



# III. DYNAMICAL EQUILIBRIUM

## The Local Thermodynamical Equilibrium (LTE)

Four simple laws, from **Statistical Mechanics**, are enough for calculating the populations of all the levels of all the ions .

1) Planck's law (the radiation spectral distribution)

2) Maxwell's law (the free-particle kinetic-energy distribution)

3) Boltzmann's law (the populations of the J levels)

4) Saha's law (the populations of the ions)

# The Local Thermodynamical Equilibrium (LTE) (cont'd)

n the LTE plasma conditions, the population of each aJ level

$$N(\alpha J) = (2J + 1)\,\mathbf{N}\ \exp\left[ - \Delta E(\alpha J) / kT_e \right]$$

where **N** is a calibration factor and $\Delta E(\alpha J)$ is the energy of level referred to the ground level of the relevant ion. A properties can be deduced.

However, when too many levels are involved, it is mor to achieve the calculations by using configurations, or e superconfigurations. Codes like STA and SCO have been wri that purpose.

# Definition of superconfigurations

A superconfiguration is the totality of all the co
electrons possess the same ensemble of principal quantum nu
For example,

$(3)^2$ represents all the two-electron configurations wi

$3s^2$
3s3p
3s3d
$3p^2$
3p3d
$3d^2$

# Superconfigurations in Xe (Fe-like)

| | | | |
|---|---|---|---|
| $(3)^{16}$ | 6 configurations | | |
| $(3)^{15}\ (4)^{1}$ | 36 configurations | $(3)^{14}\ (4)^{2}$ | 120 configurations |
| $(3)^{15}\ (5)^{1}$ | 45 configurations | $(3)^{14}\ (4)^{1}\ (5)^{1}$ | 240 configurations |
| $(3)^{15}\ (6)^{1}$ | 54 configurations | $(3)^{14}\ (4)^{1}\ (6)^{1}$ | 288 configurations |
| $(3)^{15}\ (7)^{1}$ | 63 configurations | $(3)^{14}\ (4)^{1}\ (7)^{1}$ | 336 configurations |
| $(3)^{15}\ (8)^{1}$ | 72 configurations | $(3)^{14}\ (4)^{1}\ (8)^{1}$ | 384 configurations |
| $(3)^{14}\ (5)^{2}$ | 180 configurations | | |
| $(3)^{14}\ (5)^{1}\ (6)^{1}$ | 360 configurations | | |
| $(3)^{14}\ (6)^{2}$ | 252 configurations | | |

**2436 configurations**

**5 700 000 levels**

*$(n)^{N}$ : N electrons in the n shell .*

*e.g. $(3)^{15}\ (4)^{1}$ : $(3s\ 3p\ 3d)^{15}\ (4s\ 4p\ 4d\ 4f)^{1}$*

# Non-LTE cases

Practically, LTE situations are very rarely fou
Planck’s law is rarely obeyed, due to the escape of photo
medium. In those NLTE cases, one has to study the compet
between the atomic processes.

The balance equation is used. A Collisional-Radi
of homogeneous linear equations is obtained.

# NLTE: balance equation

$$\frac{dN_i}{dt} = \sum_{j \neq i\, P} N_j R^P_{ji} - N_i \sum_{j \neq i\, P} R^P_{ij} = 0$$

# NLTE codes for levels, configurations, and/or superconfigurations

**Pairs of atomic processes:**

| | |
|---|---|
| **spontaneous emission** | **radiative absorption** |
| **photoionization** | **radiative recombination** |
| **collisional excitation** | **collisional de-excitation** |
| **collisional ionization** | **3-body recombination** |
| **autoionization** | **resonant electron capture** |

**NLTE codes**

**for levels**

HULLAC, FAC are very accurate NLTE codes.

**for configurations**

In ATOMIC, the CR system is solved for configura
adapted rates

**for superconfigurations**

In AVERROES, the CR system is solved for SCs, as
in each SC, the reduced configuration populatio
decreasing-exponential law vs energy, for tempera

# NLTE codes (cont'd)

**For superconfigurations** (cont'd)

In MOST/AVERROES, the CR system is solved for SC
assuming that, in each SC, the reduced configuration popu
follow a decreasing-exponential law vs energy, for temper
specific to the different SCs. The CR system can be split
systems of the same size, one for the reduced populations
one for the 1/T(SC) values.

**For levels, configurations, and/or superconfigurations**

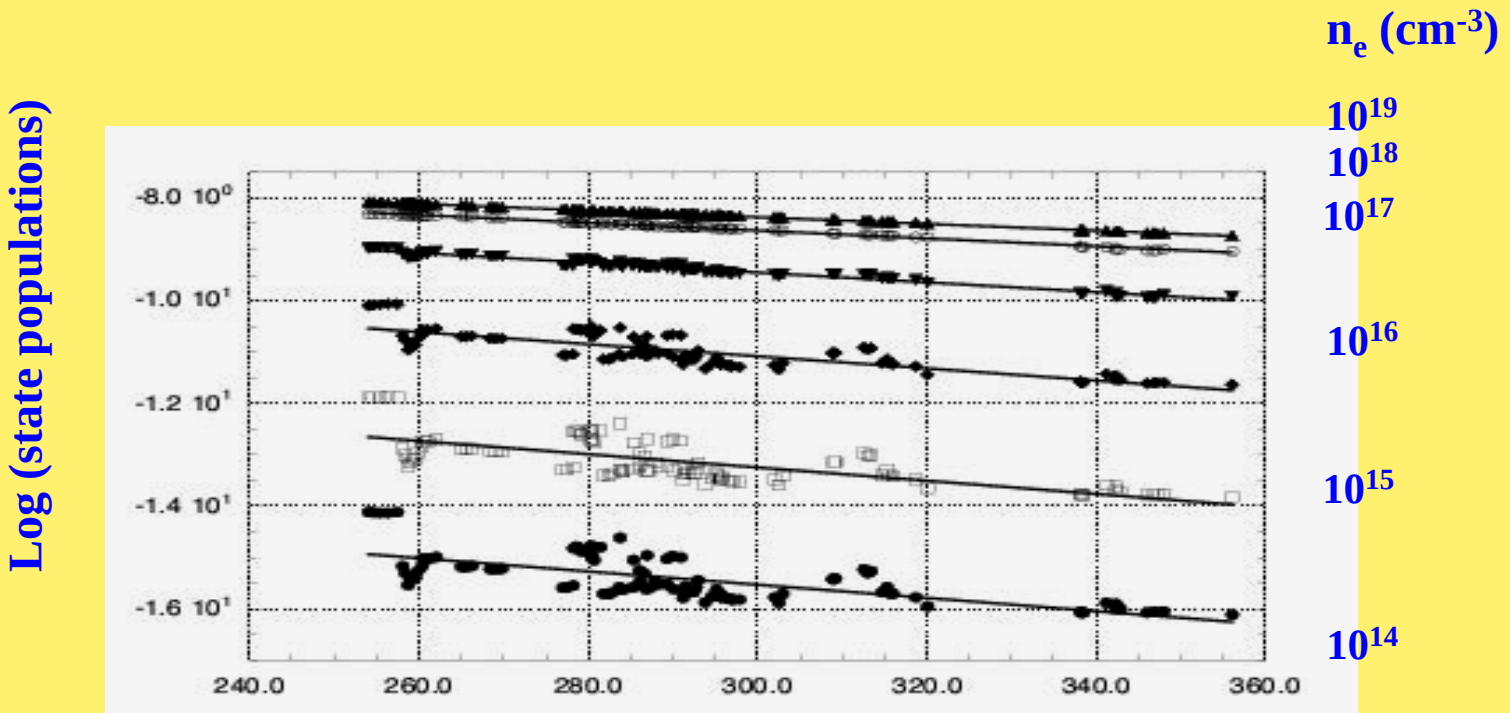
In SCRAM/HYBRID, the CR system is solved for lo
lowly-excited configurations, and highly-excited SCs, wi

In SCROLL, an iteration/convergence procedure i
At the beginning, the CR system contains many SCs. Furthe
depending on the results of the comparisons between succe
some SCs may be discarded, and others may be split into c
and/or superconfigurations, with adapted rates, at each

# Configuration temperatures

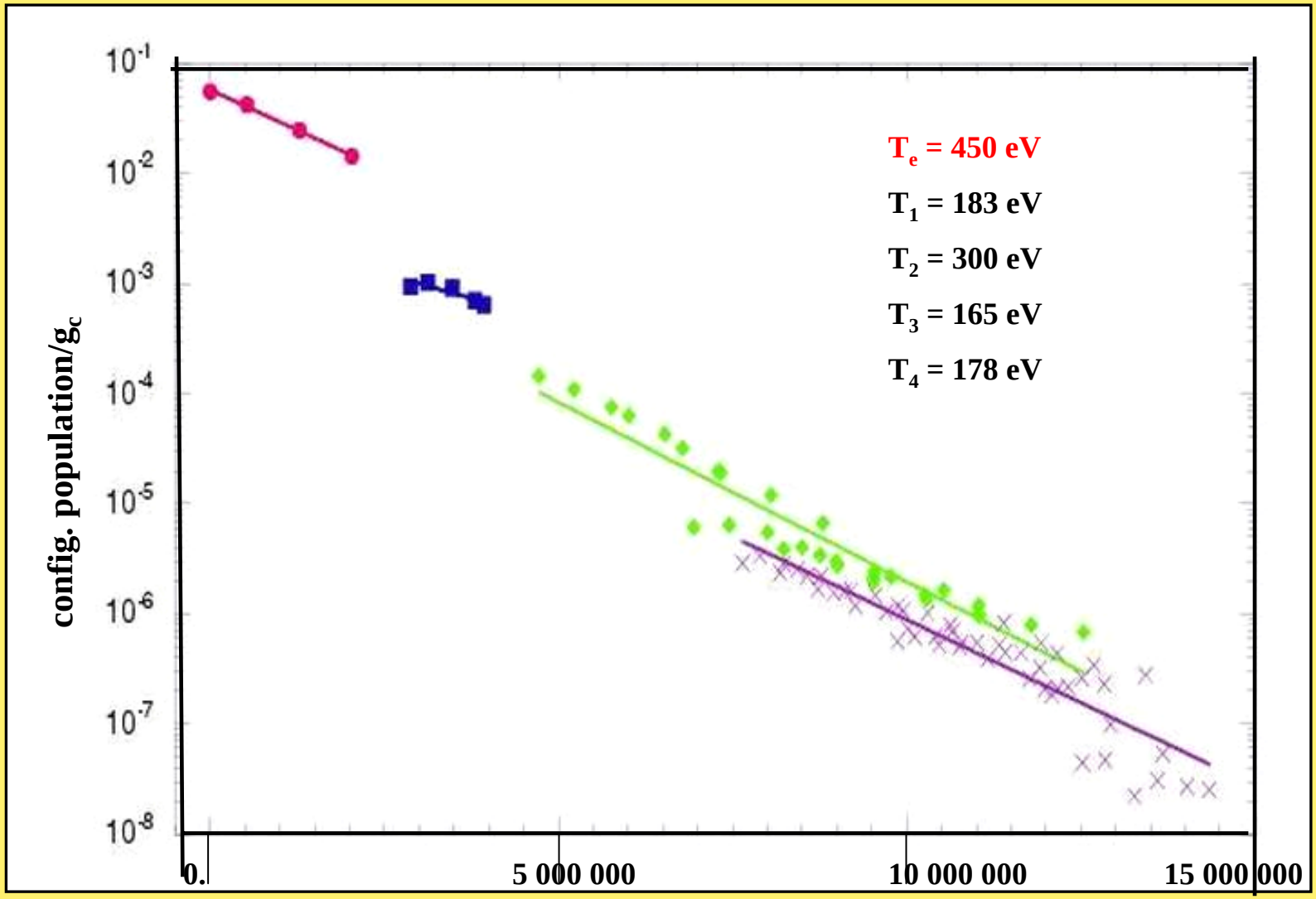
## $T_e$ = 20 eV

**Collisional-radiative calculations in Fe IV, V, VI (4668 levels)**

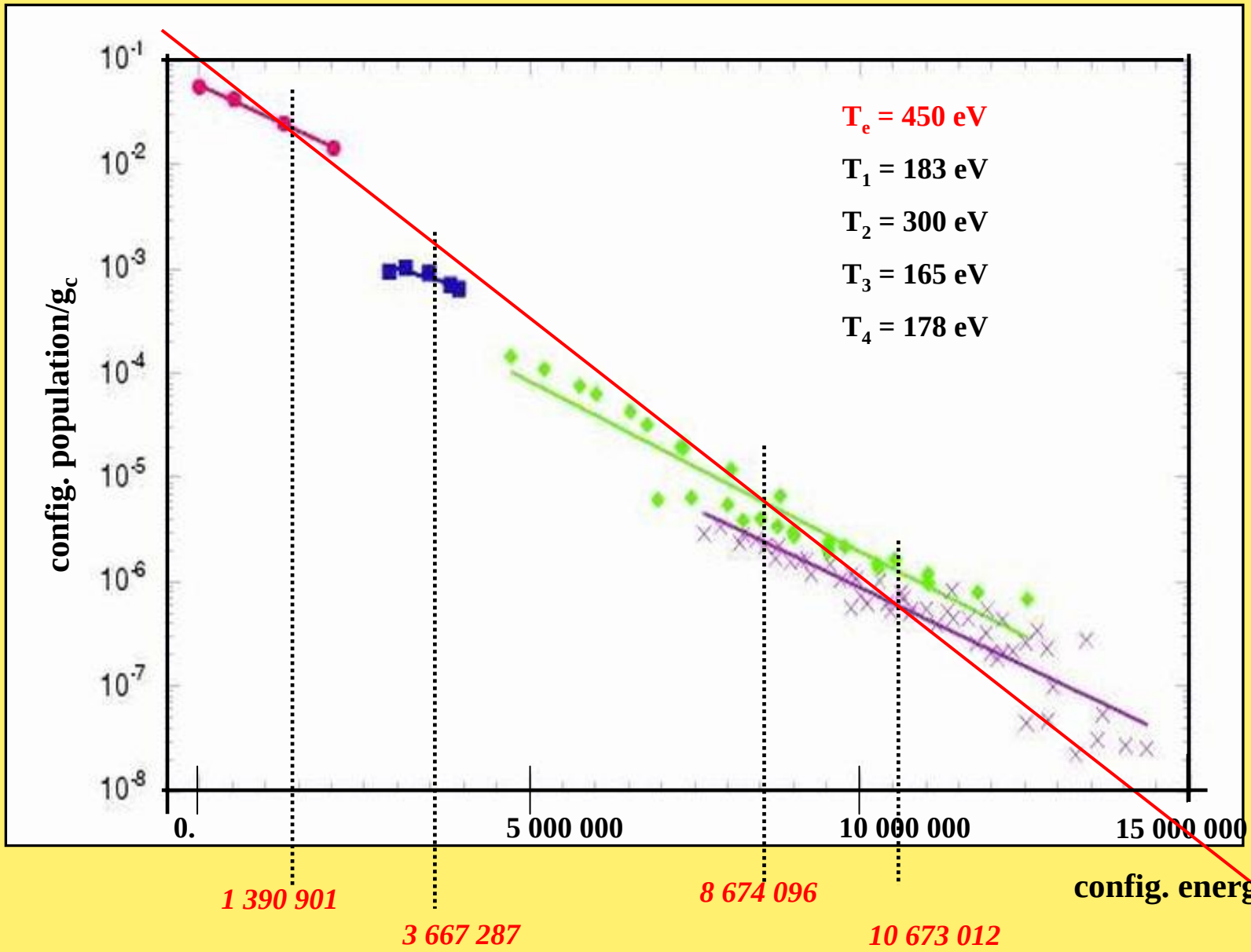



**Energies of $3d^3 4p$ states**

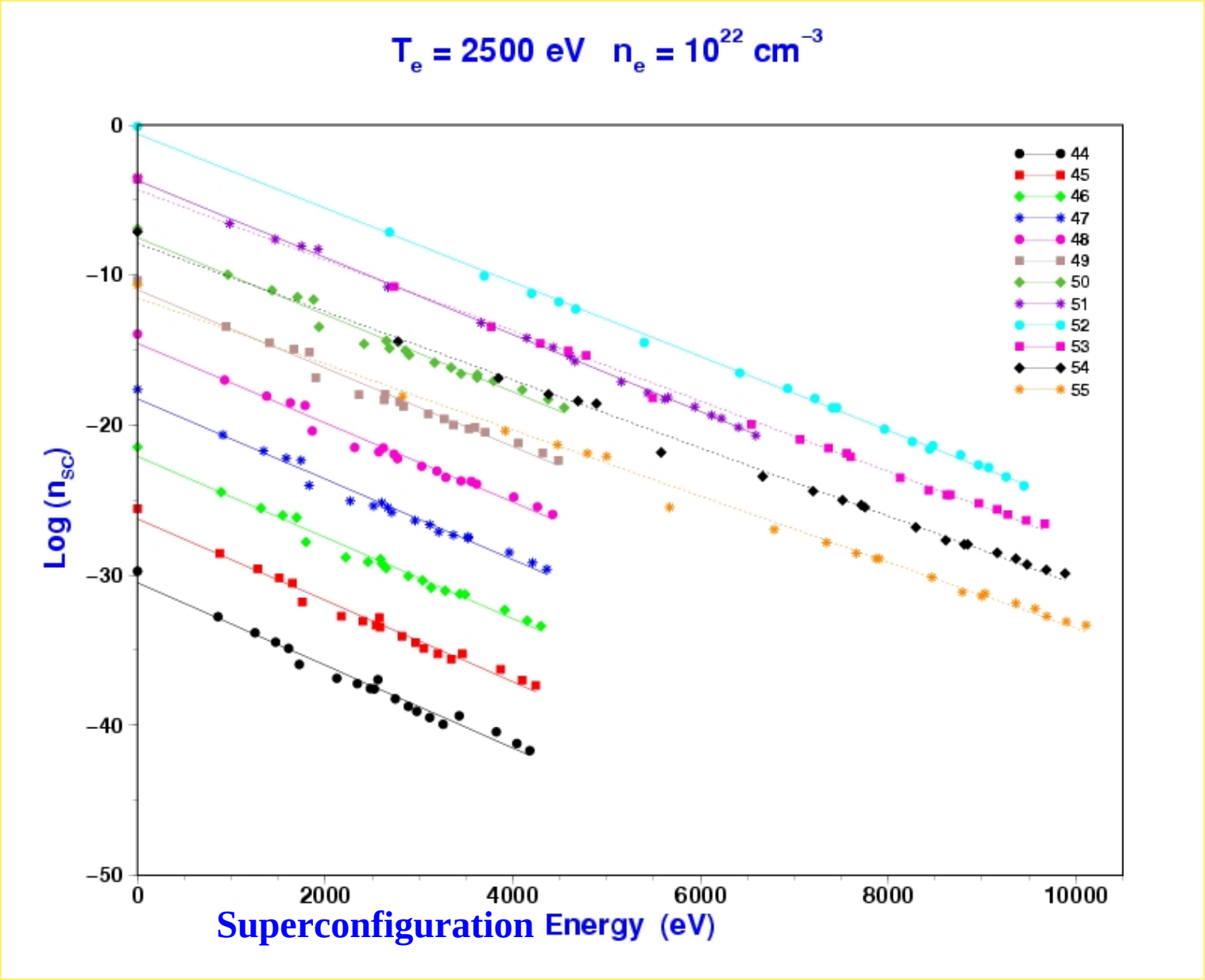
# uperconfiguration temperatures in Xe (Cu-like)



# Ionic excitation temperature in Xe (Cu-L

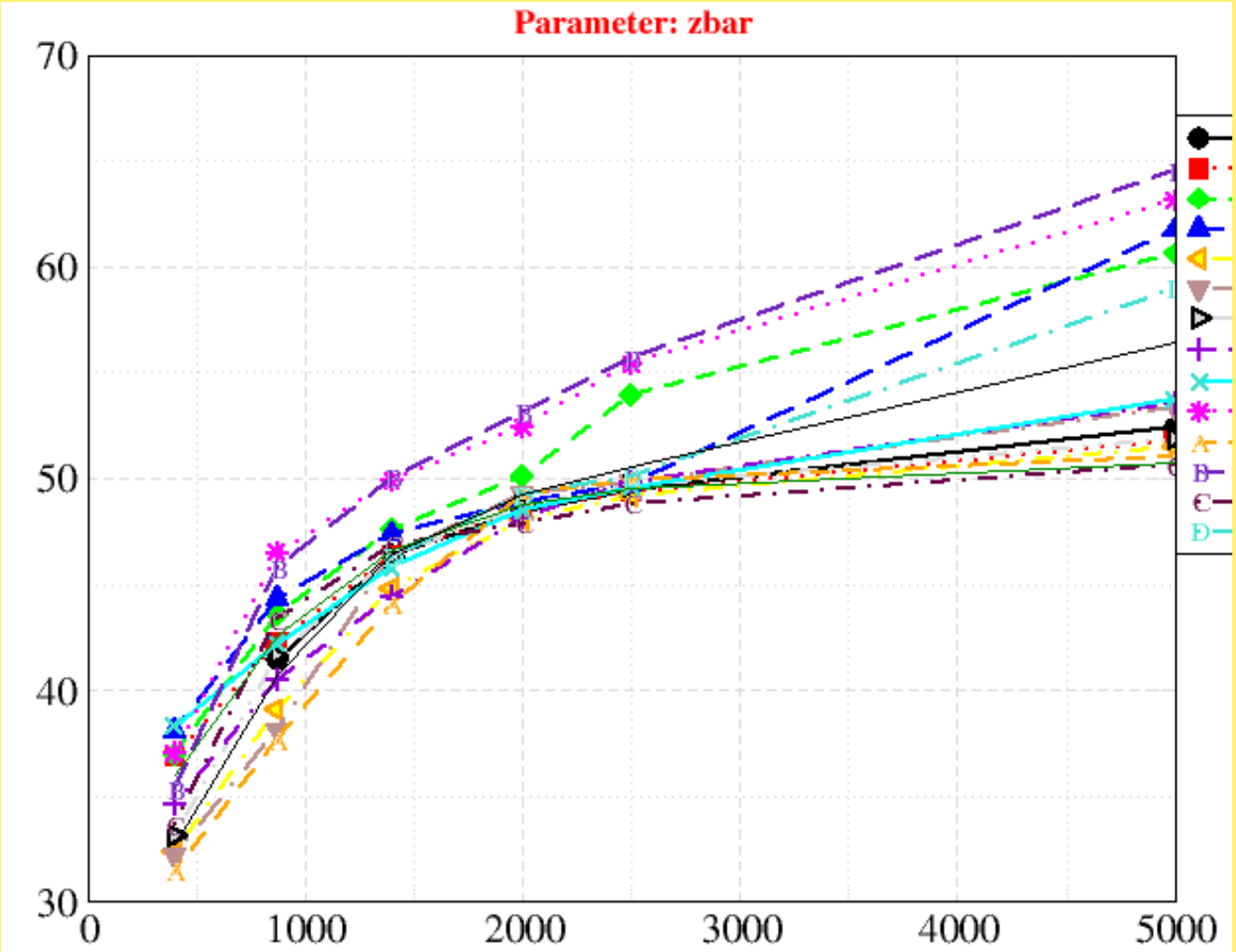


# Ionic excitation temperatures in Gold



# <Z> values for Gold ($N_e$=1.$10^{21}$ $cm^{-3}$)

## (NLTE-4 Workshop data base)



# IV. DYNAMICS

The balance equation written above only holds for the stationary cases, i.e., in the assumption that no ions escape from the plasma. It is much more complicated, but necessary, to study the dynamic cases. In the genuine physical situations, the plasma exchanges ions with its environment (this is *hydrodynamics*), and photons (this is *radiative transfer* and *radiative power loss*).

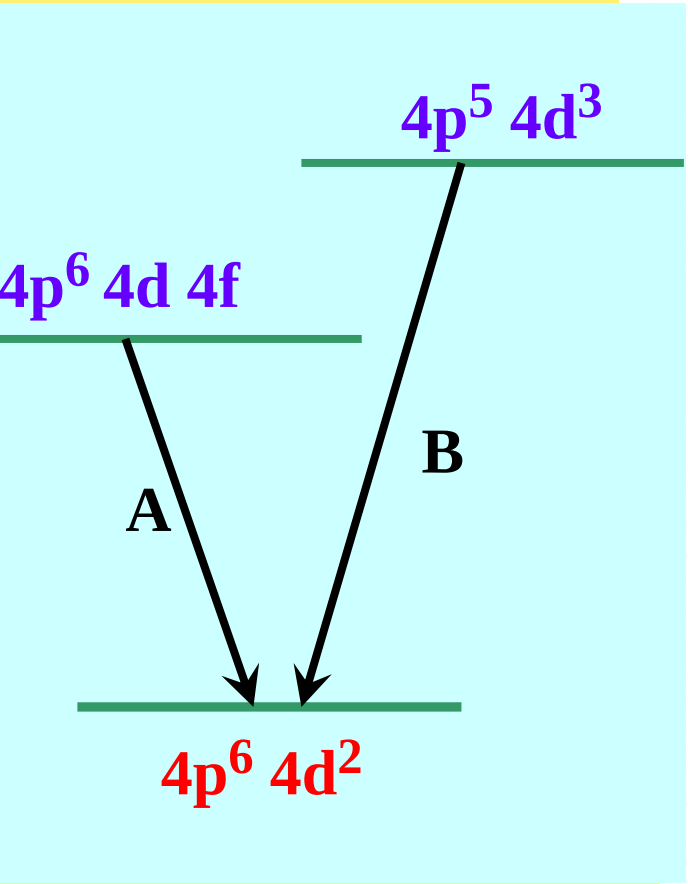
# V. CONCLUSION

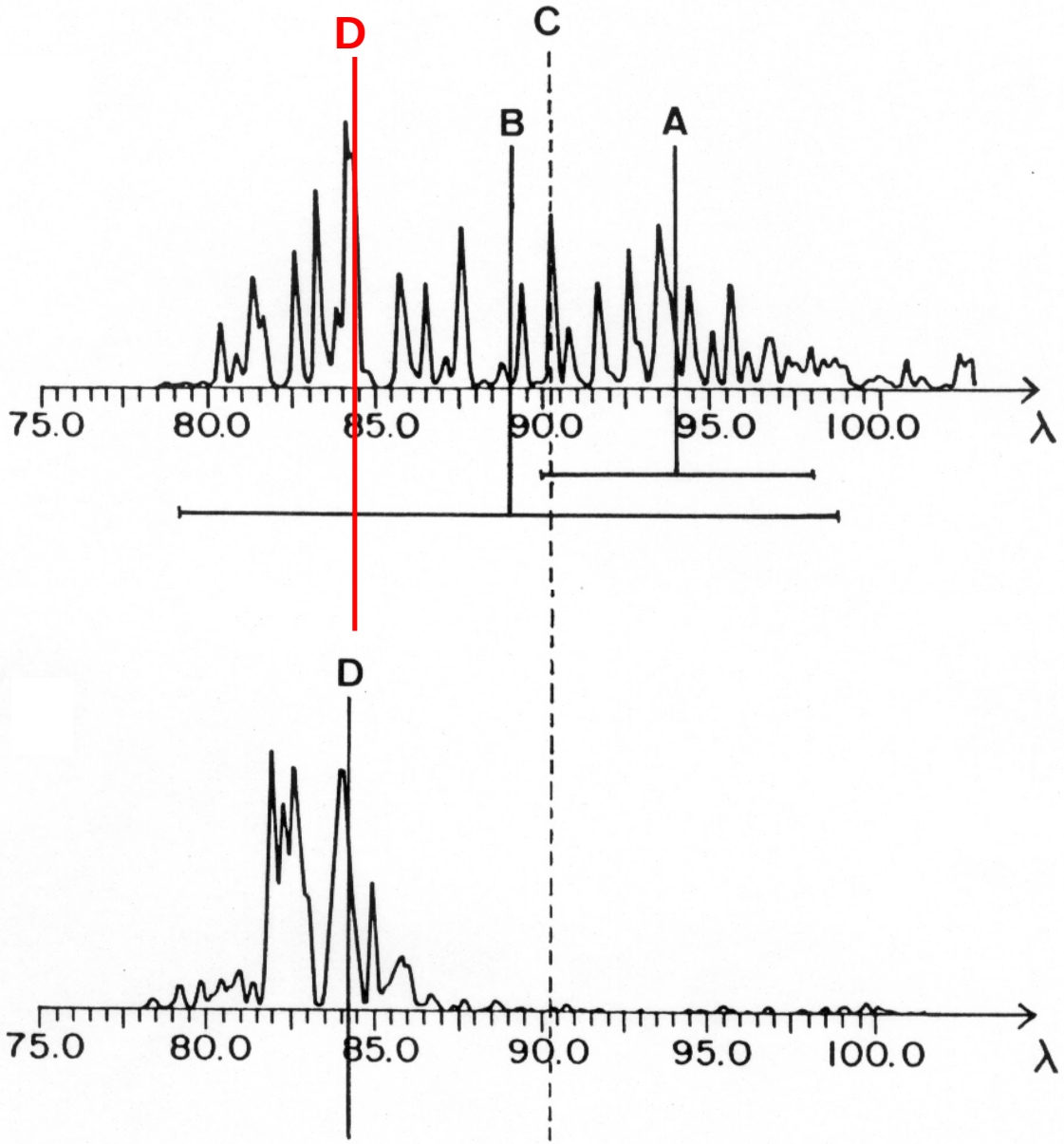
Work is in progress in many laboratories. A new scientific journal, entitled *High Energy Density Physics*, has been created recently by Dick Lee (Livermore) and Steve Rose (Oxford). This proves that many new methods and results are still expected.

Finding the best compromise between accuracy (of th completeness (of the plasma description), and time reductio computing times) is a challenge.

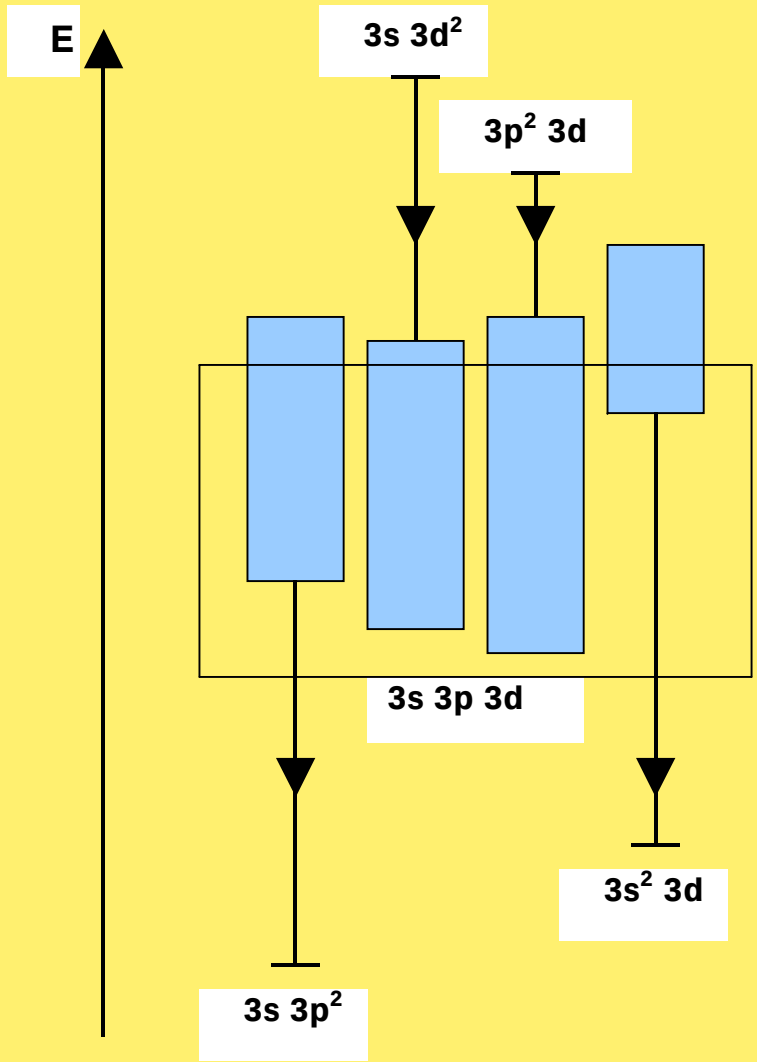
For that purpose, global methods are recommended. T the advantage of putting some phenomenons into evidence. In when one only produces millions of numerical results, « *One cannot see the wood for the trees!* ».

# Pr XXII $4p^6\ 4d^2 - (\ 4p^5\ 4d^3 + 4p^6\ 4d\ 4f\ )$



# Emissive zones



# THE TRANSFER EQUATION

$$\frac{dN(C_i)}{dt} = \sum_j R(C'_j \rightarrow C_i) \quad g(C'_j) \quad n_{SC'} \exp\left[-\frac{\Delta E(C'_j)}{kT(SC')}\right]$$

2nd correlation

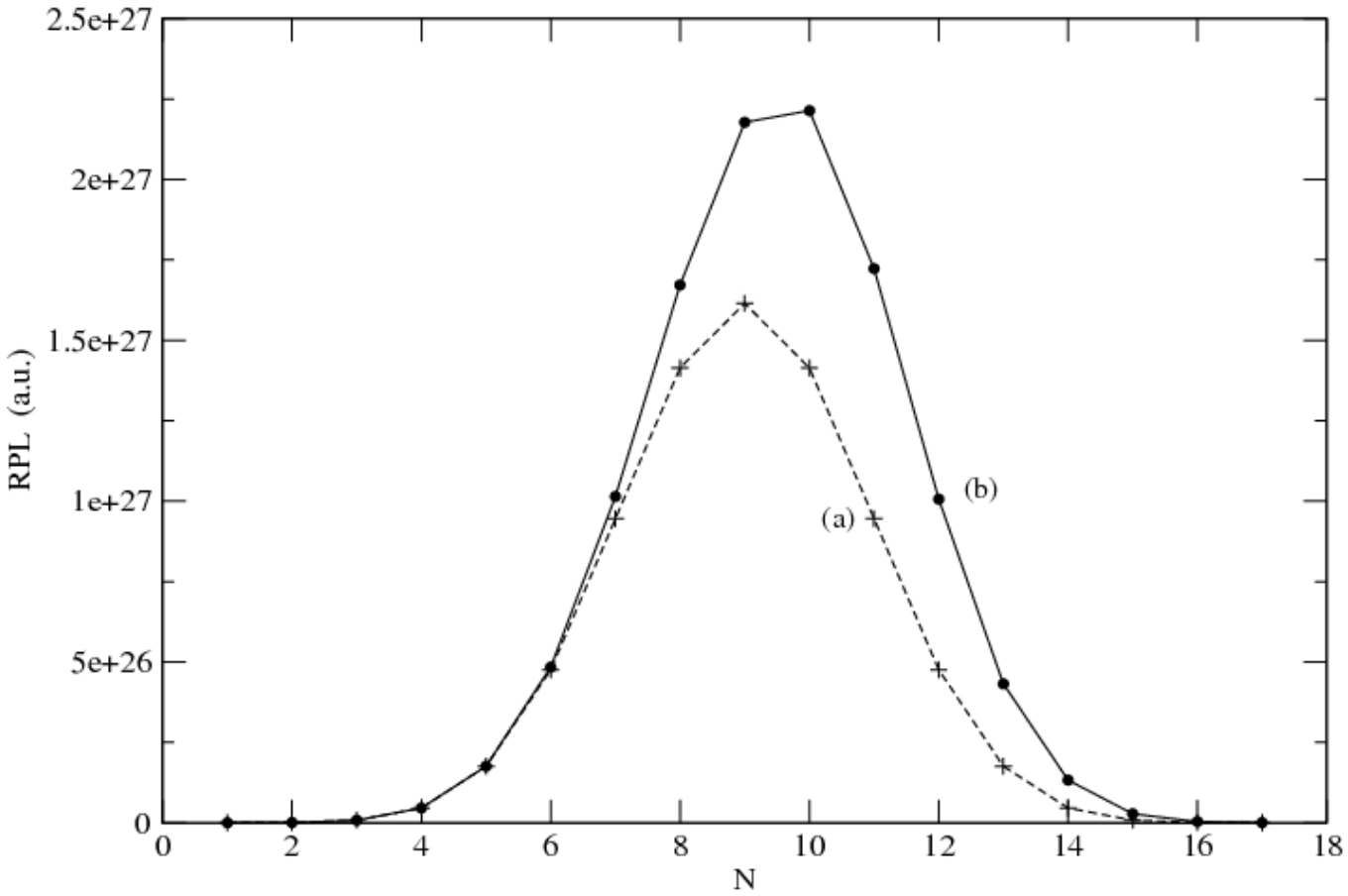
1st correlation

$$= g(C_i)\,[\alpha + \beta \Delta E(C_i)] \quad n_{SC'} \exp\left[-\rho \frac{\Delta E(C_i)}{kT(SC')}\right]$$

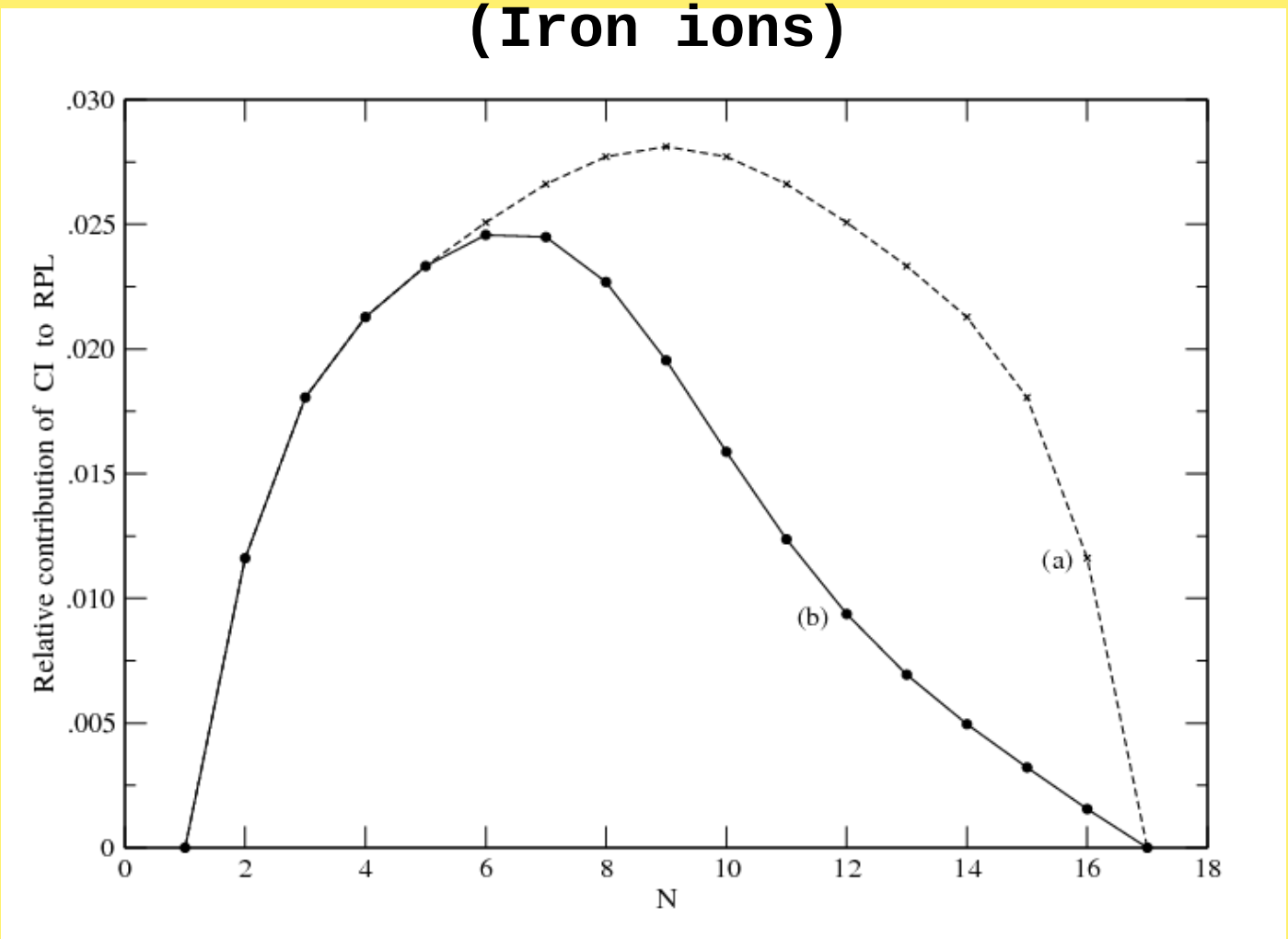
where $\Delta E(C_i) = E(C_i) - E_{av}(SC)$.

$n_{SC'}$ is the population of the "average state" of $SC'$.

# Total radiative power loss of the $(3)^N$ superconfigurations (Iron ions)



# Relative configuration-interaction contribution to the total RPL of the $(3)^N$ superconfigurations (Iron ions)



# Hartree-Fock methods

Essentially, a Hartree-Fock calculation consists in minimizing the total energy of a configurational state of given angular and spin parts, through a variational optimization of the electronic radial functions.

In general, for the computed state, the results are better than those of any central field. But, in principle, the obtained radial quantities are not valid for the other levels of the same configuration, in contrast with the one-electron central field approach.

Configuration interaction can be accounted for by assuming th to be optimized is a linear combination of the states of configurations. The corresponding code is a MultiConfigur Hartree-Fock (MCHF) code, or Dirac-Fock (MCDF) code.

# Ionic excitation temperatures in $Au^{52+}$ (Co-like)

$T_e = 2500$ eV  $n_e = 10^{22}$ cm$^{-3}$