Modelling of emission line shapes in high parameter aluminium plasma

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Outline

Motivation

Line shapes

Theoretical basis of the present work

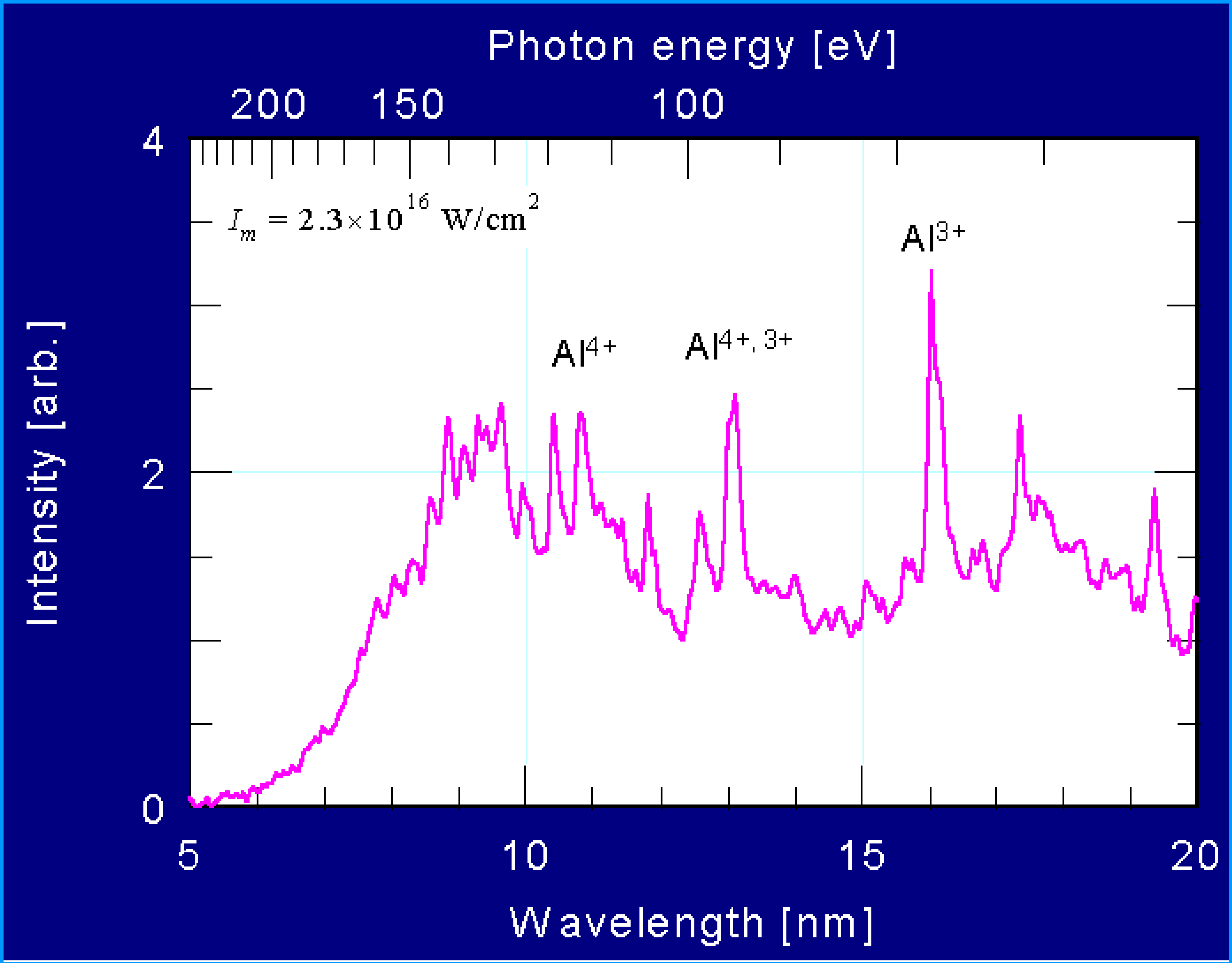
The database

Parametrizing the database

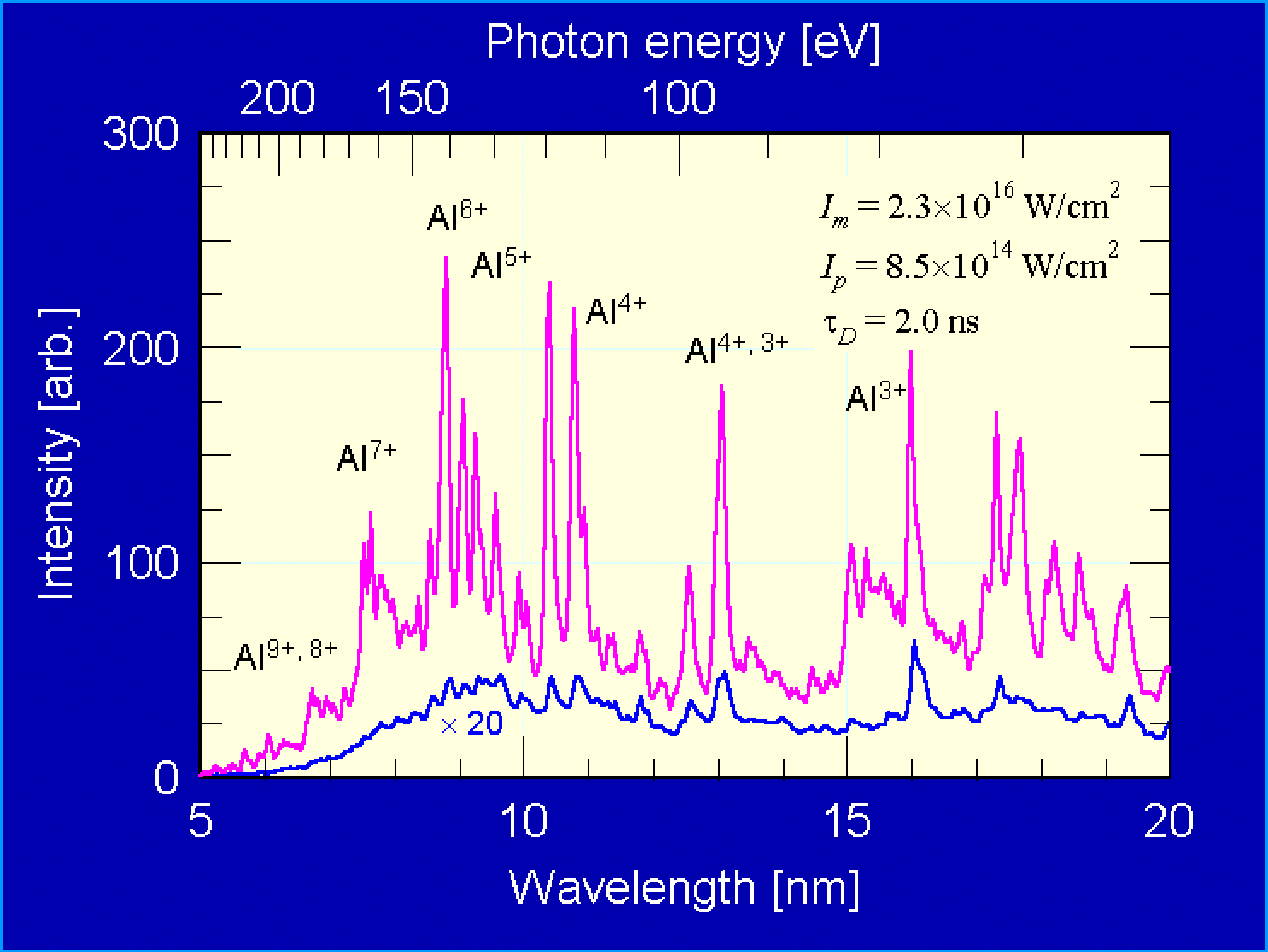
Conclusion

Motivation

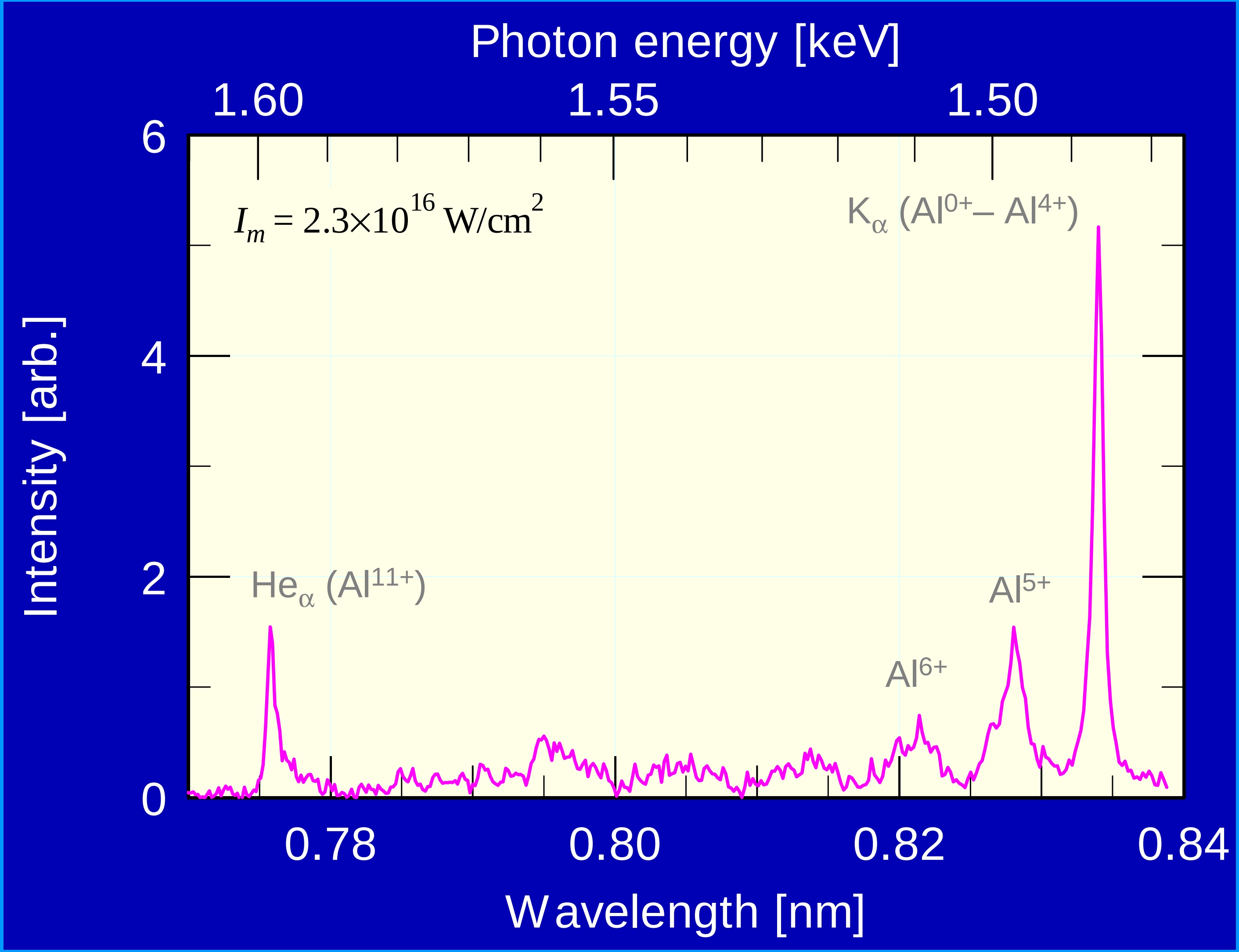
Spectrum of soft X-rays from Al-plasma



Soft X-ray emission enhanced by a prepulse



Spectrum of x-ray in keV-range from Al-plasma



Line shapes

Line shapes, broadening

Line Broadening: Lorentz, Doppler, Voigt profiles

Stark broadening

electron broadening

Lorentzian Lineshape

Pressure broadening results from collisions between molecules in a gas. It is the most important source of broadening when pressures are high. The simplest treatment of pressure broadening produces a Lorentzian lineshape centered at the transition frequency ν_0 and given by the functional form

$$\phi(\nu) = \frac{1}{\pi} \frac{\alpha_L}{(\nu - \nu_0)^2 + \alpha_L{}^2}$$

where α_L is the Lorentzian half-width.

$$\begin{aligned} F(\omega) &\approx \tfrac{1}{2} f_0 [\tfrac{1}{2}\gamma - i(\omega - \omega_0)]^{-1} \\ |F(\omega)|^2 &= \frac{f_0{}^2}{\gamma^2} \frac{\tfrac{1}{4}\gamma^2}{(\omega - \omega_0)^2 + \tfrac{1}{4}\gamma^2} \\ &= \frac{f_0{}^2}{\gamma^2} \frac{\gamma^2}{4(\omega - \omega_0)^2 + \gamma^2}. \end{aligned}$$

If $f(t)$ is the radiated field, the curve $|F(\omega)|^2$ is known as the Lorentzian lineshape. Collision shortens the duration of emission, widening the peak.

Doppler Lineshape

The broadening of a spectral line as a result of the thermal motion of a gas. Doppler line-broadening results from the random motion of radiating molecules, and is therefore dependent on temperature. The Doppler lineshape takes the form of a Gaussian,

$$\phi(\nu) = \frac{1}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}\, e^{-(\ln 2)(\nu-\nu_0)^2/\alpha_D{}^2},$$

where the Doppler half-width is given by

$$\alpha_D \equiv \frac{\nu_0}{c}\sqrt{\frac{2\ln 2RT}{M}} = 1.131 \times 10^{-8}\sqrt{\frac{T}{M}}\,\nu_0$$

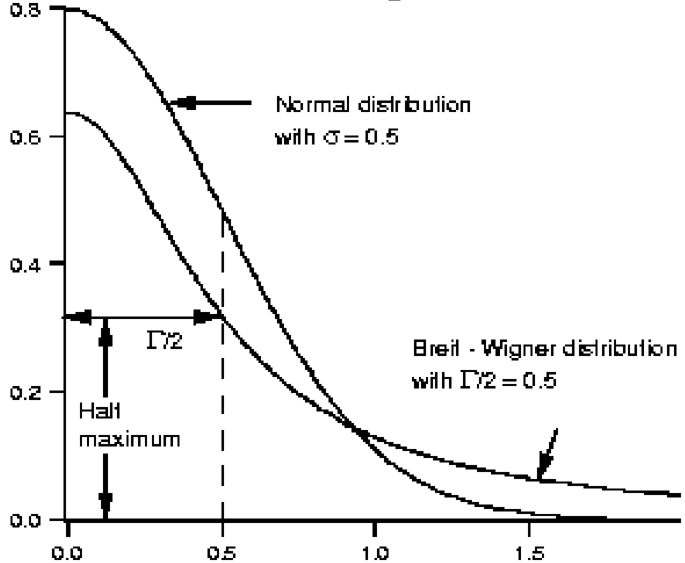
(Townes and Schawlow 1975, pp. 337-338). In (0), R is the universal gas constant, T is the thermal temperature, M is the mean molar mass (in kg), and c is the speed of light.

Breit-Wigner Distribution (also known as Lorentz Distribution)

The Breit-Wigner (also known as Lorentz) distribution is a generalized form originally introduced ([Breit36], [Breit59]) to describe the cross-section of resonant nuclear scattering in the form

$$\sigma(E) = \frac{\Gamma}{(2\pi)[(E - E_0)^2 + (\Gamma/2)^2]} ,$$

The equation follows from that of a harmonic oscillator with damping, and a periodic force. A normal (Gaussian) distribution decreases much faster in the tails than the Breit-Wigner curve.

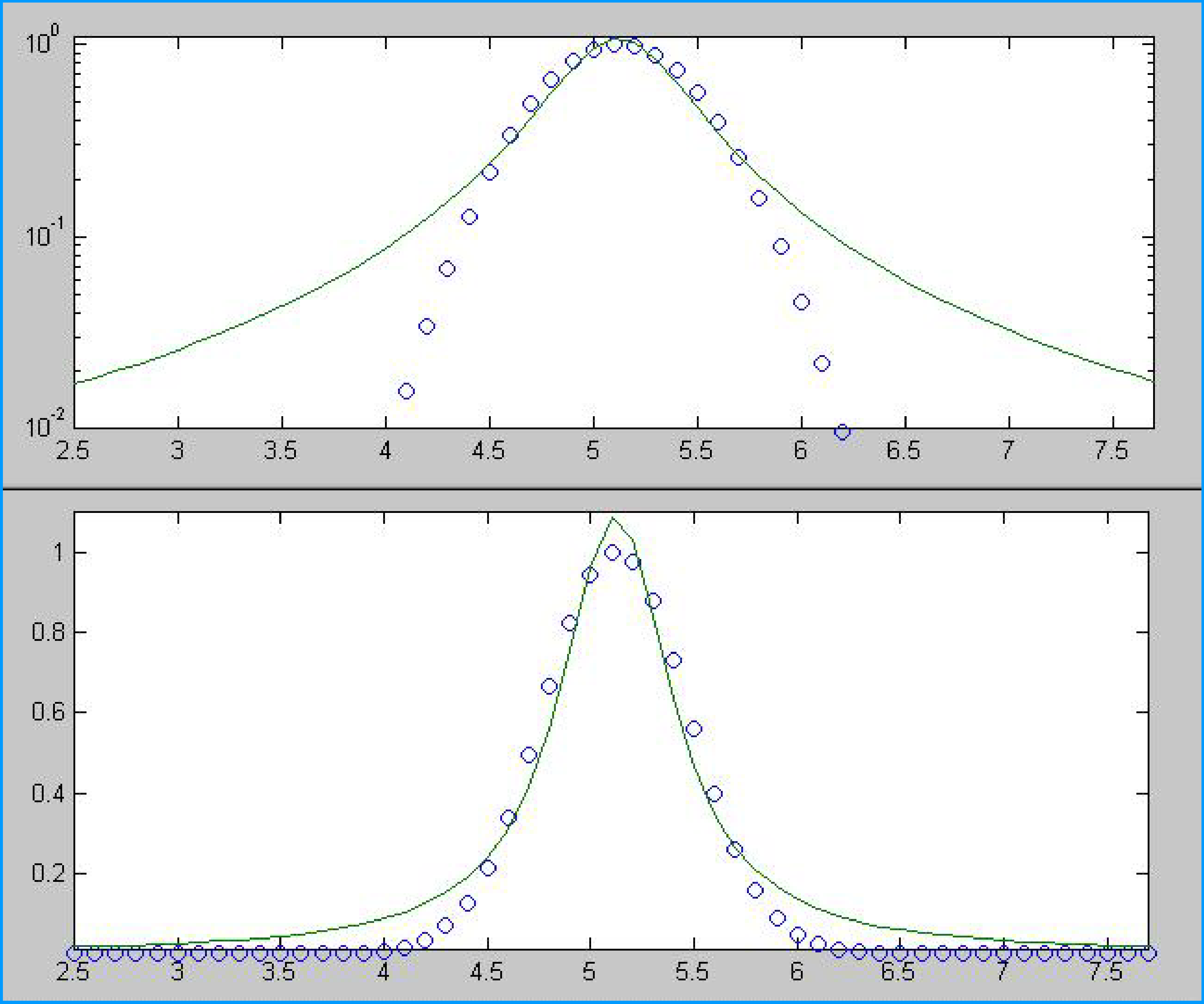


The distribution is fully defined by E_0, the position of its maximum (about which the distribution is symmetric), and by Γ , the full width at half maximum (FWHM), as obviously

$$\sigma(E_0) = 2\sigma(E_0 \pm \Gamma/2) .$$

Γ and the lifetime τ of a resonant state are related to each other by Heisenberg's uncertainty principle ($\Gamma\tau = h/2\pi$).

After Rudolf K. Bock, 7 April 1998 http://rkb.home.cern.ch/rkb/AN16pp/AN16pp.html



10^0
10^-1
10^-2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5
1
0.8
0.6
0.4
0.2
2.5
3
3.5
4
4.5
5
5.5
6
6.5
7
7.5

Voigt Lineshape

The Voigt profile is the spectral line shape which results from a superposition of independent Lorentzian and Doppler line broadening mechanisms (e.g., Armstrong 1967). It is given by the expression

$$\phi(\nu) = \frac{1}{\alpha_D}\sqrt{\frac{\ln 2}{\pi}}K(x, y),$$

where $K(x, y)$ is the "Voigt function"

$$K(x, y) \equiv \frac{y}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{y^2 + (x - t)^2}\,dt.$$

In (2),

$$y \equiv \frac{\alpha_L}{\alpha_D}\sqrt{\ln 2}$$

is the ratio of Lorentz to Doppler widths and

$$x \equiv \frac{\nu - \nu_0}{\alpha_D}\sqrt{\ln 2}$$

is the frequency scale in units of Doppler lineshape half-width α_D .

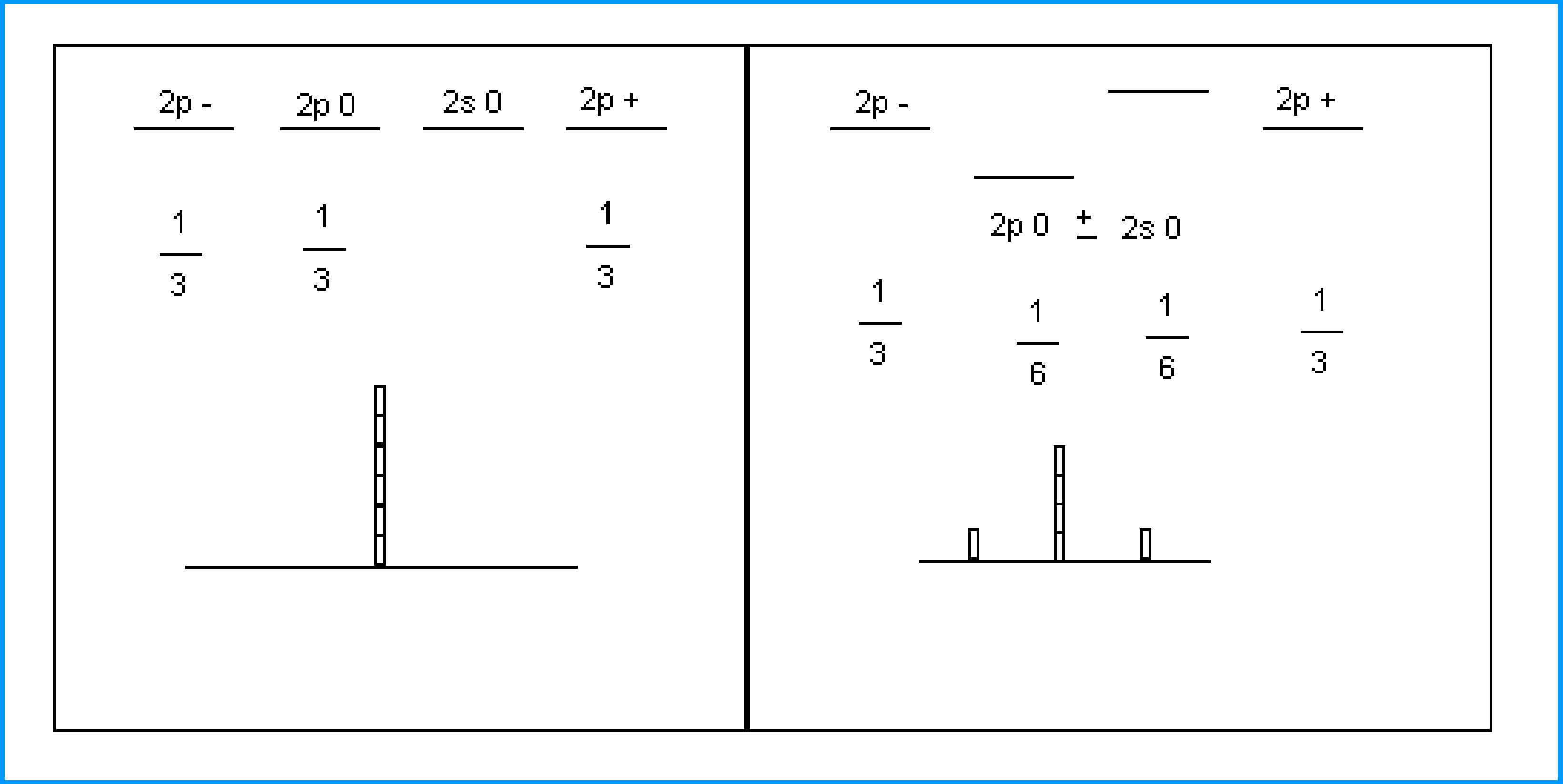
Stark broadening

due to the fields of neighbouring ions

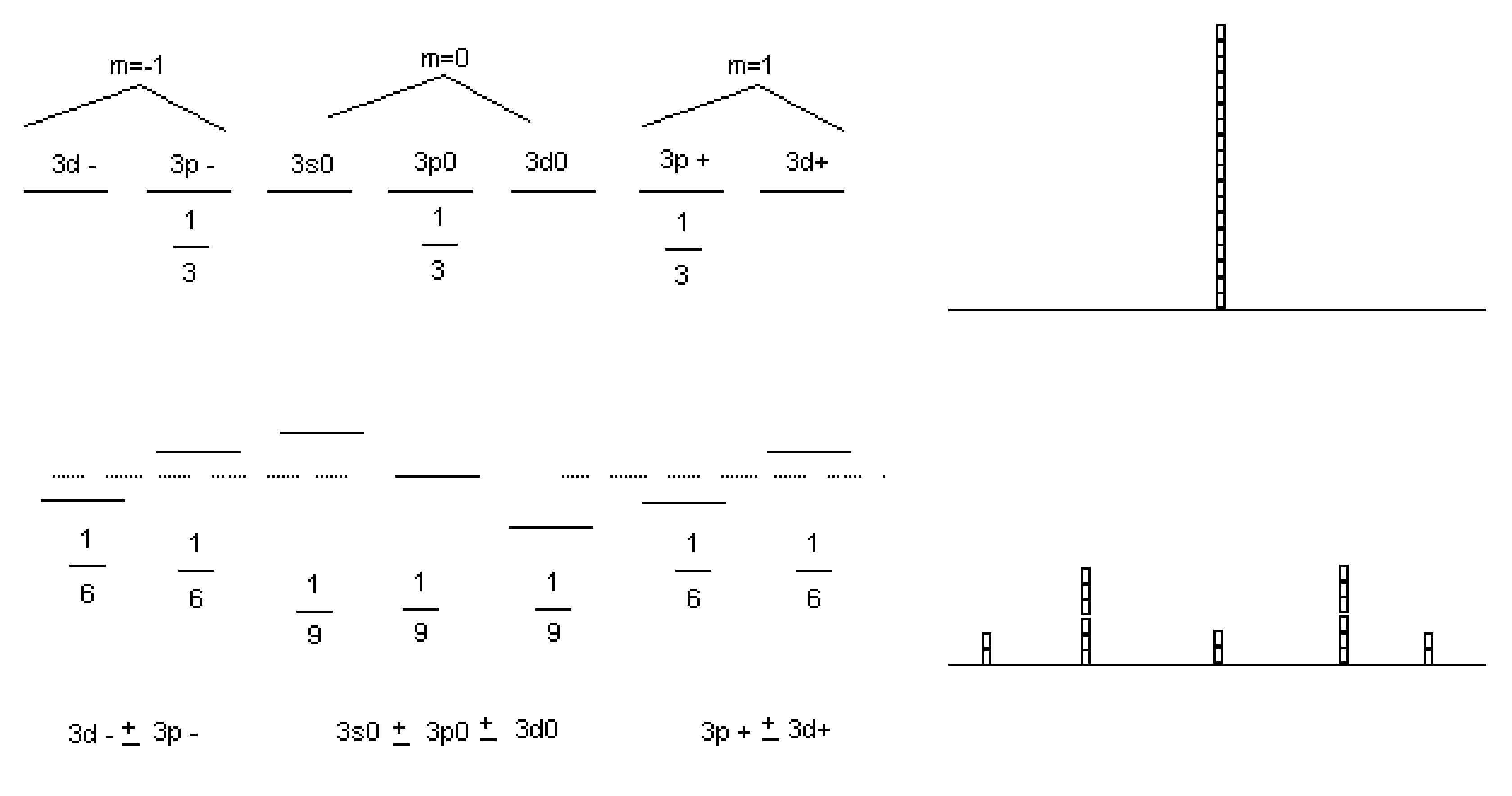
Ion microfields

Distribution of microfields (static)
Holtsmark 1919

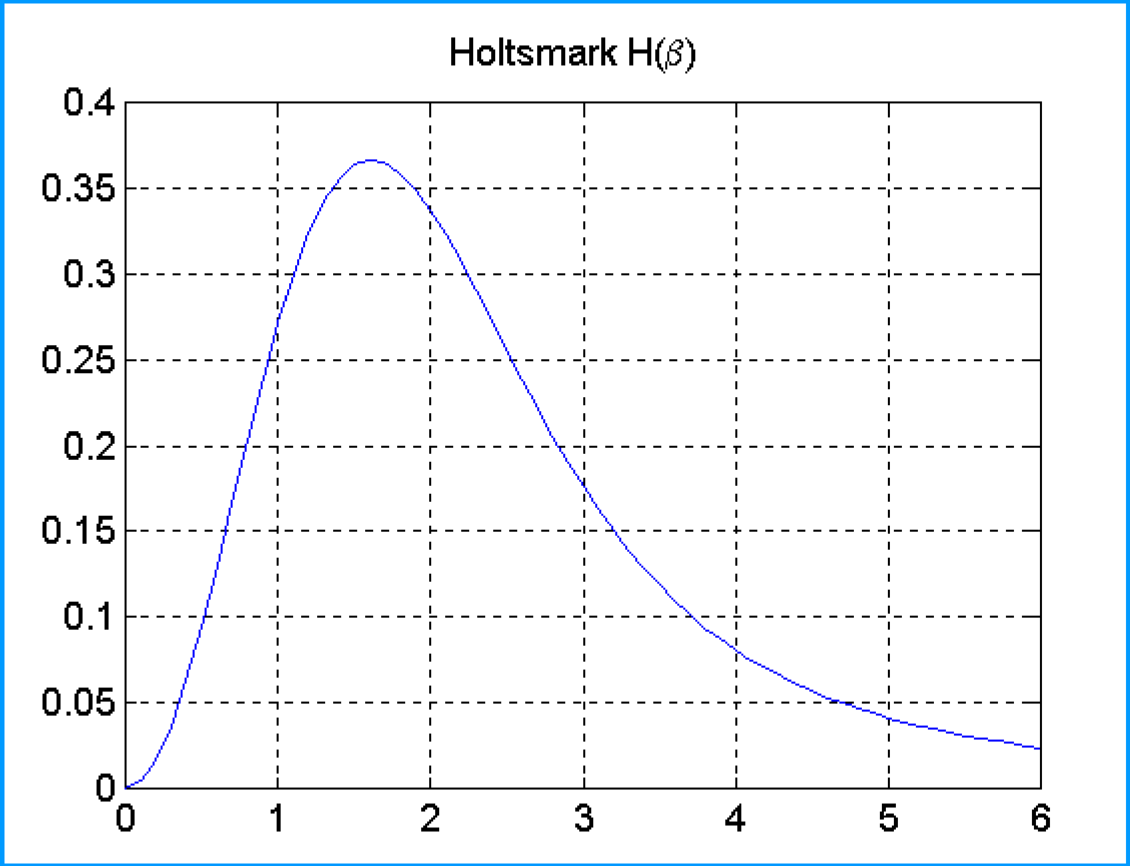
Microfields determine states of the emiter



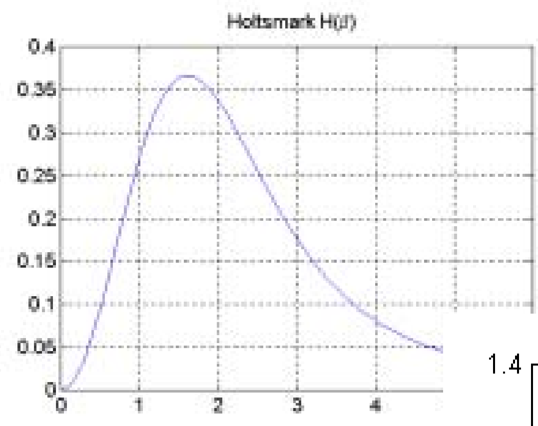
n=2 in hydrogen-like ion (atom)

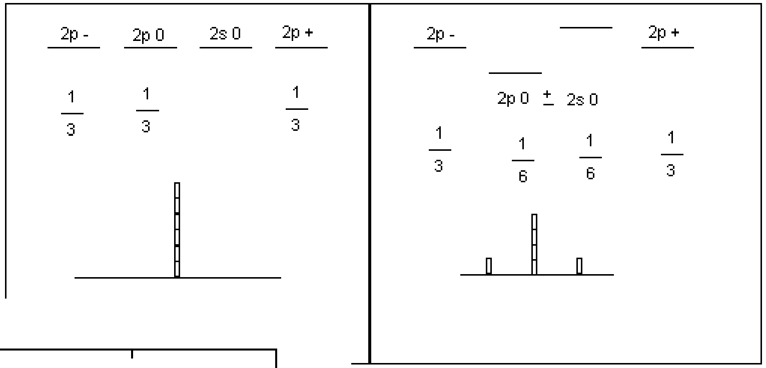


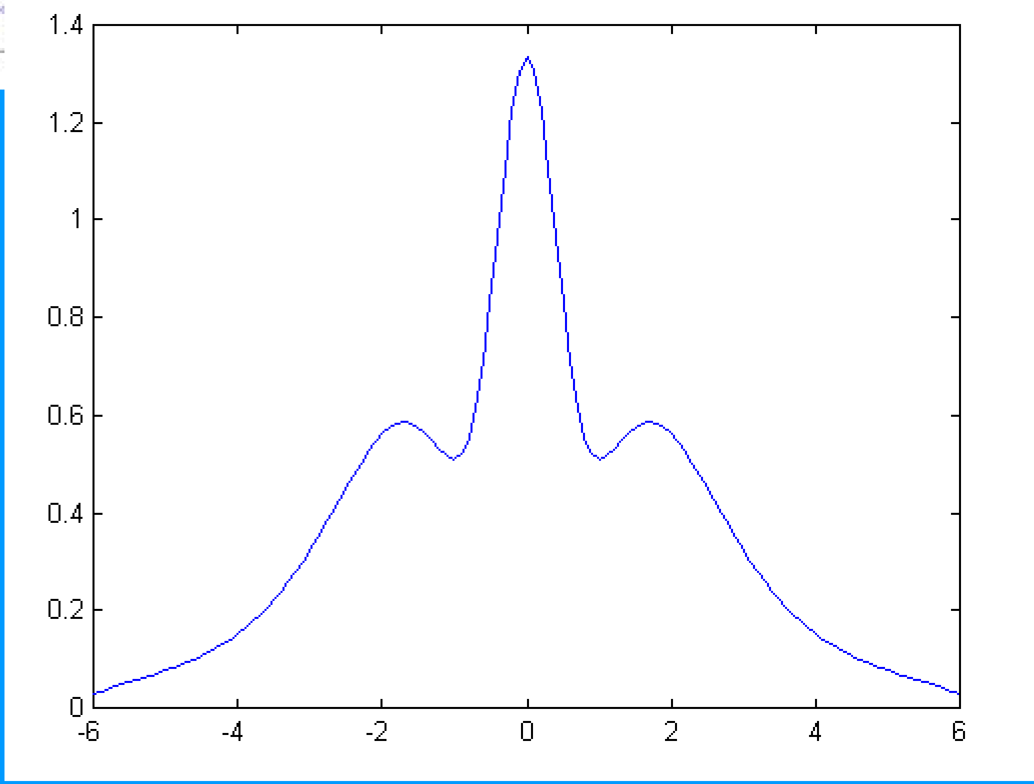
n=3 in hydrogen-like ion (atom)



Holtsmark function used to evaluate the distribution of electric field strength due to ions. β is scaled electric field strength.

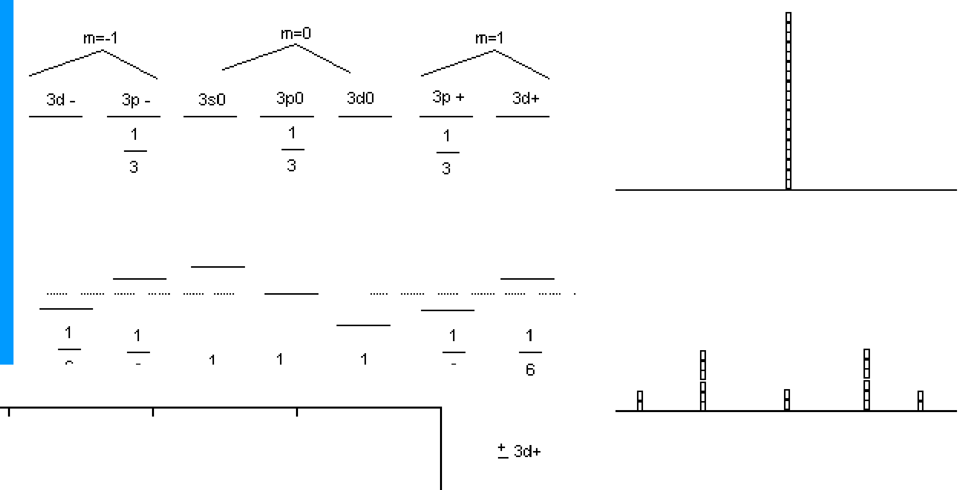


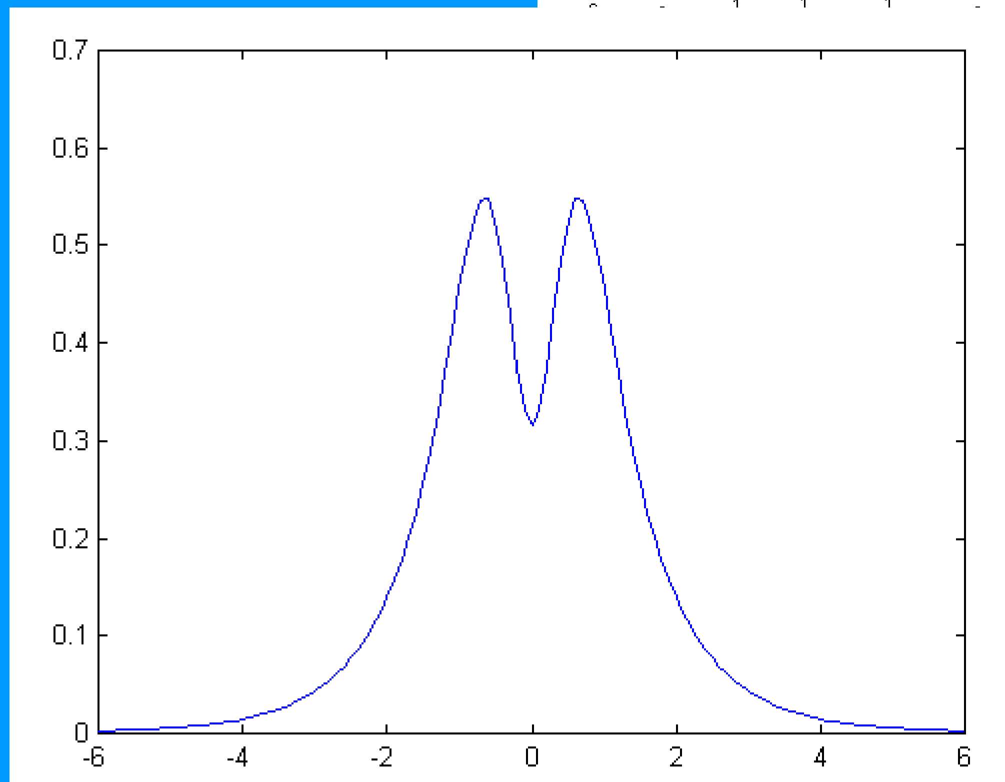




Stark brodened n=2 to n=1 in hydrogenic ion

(model, from Holtsmarks distribution) Ly_{α}





Stark brodened n=3 to n=1 in hydrogenic ion

(model, from Holtsmarks distribution) Ly_β

Broadening due to electron impact

Which means also
due to the presence of unbound electrons

Classical motion (semiclassical model)
Quantal: Baranger's formulation

(coherent broadening - single emitor)

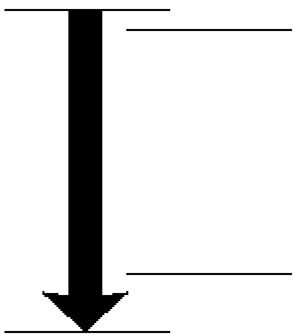
Baranger's formula for electronic broadening

For an isolated line corresponding to a transition $u \rightarrow l$ the full collisional width (frequency width)at half-maximum (FWHM) is given by:

$$w = N_e \int_0^\infty v F(v) \left\{ \sum_{u' \neq u} \sigma_{uu'}(v) + \sum_{l' \neq l} \sigma_{ll'}(v) + \int \left| f_u(\theta, v) - f_l(\theta, v) \right|^2 d\Omega \right\} dv$$

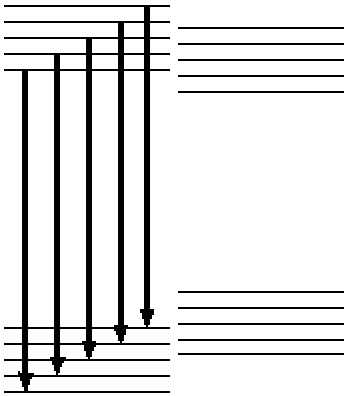
where Ne is the electron density, v is the velocity of the scattering electron, and F (v) is the Maxwellian electron velocity distribution. The electron impact cross sections $\sigma_{uu'}$ (represent contributions from transitions connecting the upper (lower) level with other perturbing levels (indicated by primes).

the $f_u(\Omega; v)$ and $f_l(\Omega; v)$ are elastic scattering amplitudes for the target ion in the upper and lower states, respectively, and the integral is performed over the scattering angle Ω, with $d\Omega$ being the element of solid angle.

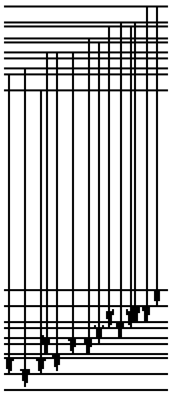


Isolated system

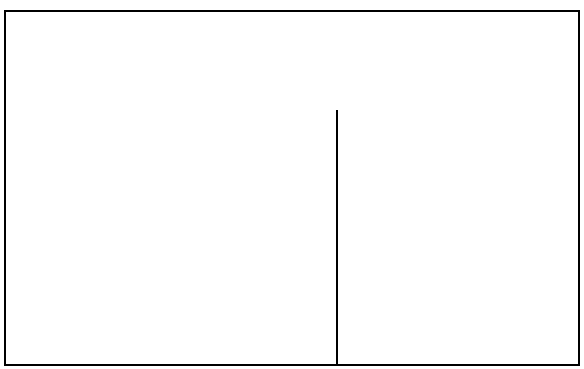
Perturbing system



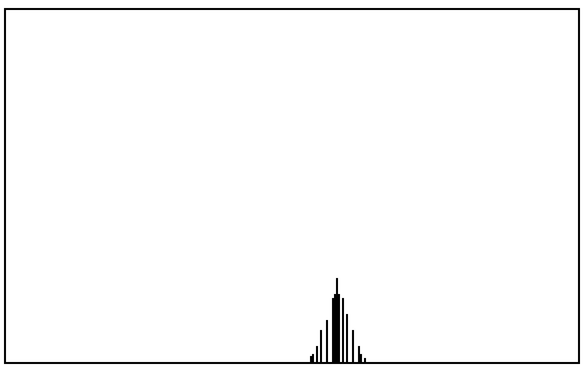
Combined levels without interaction



Combined levels with interaction



Combined levels without interaction



Combined levels with interaction

The perturbing system:

Continuum electrons present in the neighboourhood

Their density of states

Their distribution over these states

This makes the multiparticle manifold of perturbing states

Generalized formulations

several approaches exist

(fully quantal, semiclassical)

Density matrix formulation

(can incorporate both coherent and incoherent broadening)

Theoretical basis of the present work

Line shape modeling of multielectron ions in plasmas

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G.V. BAYDIN, V.V. POPOVA,
and S.V. KOLTCHUGIN

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All Russian Institute of Technical Physics
Snezhinsk, Chelyabinsk region, Russia

Laser and Particle Beams **18** (2000), 275–289.

$$\rho = \rho^0 + \rho^\mu,$$

$$[\partial/\partial t + \boldsymbol{v}_i \nabla]\rho^0 = -\frac{i}{\hbar}[H + V_F, \rho^0] + R\rho^0 + Q,$$

$$[\partial/\partial t + \boldsymbol{v}_i \nabla]\rho^\mu = -\frac{i}{\hbar}[H + V_F, \rho^\mu] + R\rho^\mu - \frac{i}{\hbar}[V_\mu, \rho^0].$$

Here, $\boldsymbol{v}_i$ is a velocity of the emitter, ρ^μ is a small value induced by the quasi-resonant interaction V_μ of the emitter with the electromagnetic field mode μ, and H is the diagonal Hamiltonian matrix of the isolated emitter.

The perturbation V_F induced by an ion microfield $\boldsymbol{F}$ is described by the nondiagonal operator $V_F = -\boldsymbol{dF}$, where $\boldsymbol{d}$ is the emitter dipole operator.

The operator $R = R_c + R_r + R_a$ responsible for ion-state relaxation due to electron collisional (R_c), radiative (R_r) and autoionizing (R_a) transitions is a tetradic, or four-index operator in the Liouville space, with the elements

$$(R\rho)_{ab} = \sum_{a'b'} R_{ab}^{a'b'} \rho_{a'b'},$$

$$\begin{aligned}
\rho^{\mu}_{\alpha\beta}(\omega)\big[i(\omega - \omega_{\alpha\beta} - \boldsymbol{k}\boldsymbol{v}_i) - \Gamma_{\alpha\beta}\big] \\
+ \sum_{\alpha'\beta'}{}' R^{\alpha'\beta'}_{\alpha\beta}\, \rho^{\mu}_{\alpha'\beta'}(\omega) \\
- \frac{i}{\hbar} \sum_{\alpha'\beta'} \big[(V_F)_{\alpha\alpha'}\, \rho^{q}_{\alpha'\beta}(\omega) - \rho^{q}_{\alpha\beta'}(\omega)(V_F)_{\beta'\beta}\big] \\
= \frac{i}{\hbar} \sum_{\alpha'\beta'} \big[\rho^{0}_{\alpha\alpha'}(d_q)_{\alpha'\beta} - (d_q)_{\alpha\beta'}\, \rho^{0}_{\beta'\beta}\big],
\end{aligned}$$

spectral function $S(\omega)$

$$S(\omega) = \frac{I(\omega)}{I_\infty}, \quad I_\infty = \int_0^\infty I(\omega) d\omega,$$

specifying the line profile of spontaneous emission, where

$$I(\omega) = -\frac{4\omega^4}{3\pi c^3} \cdot \mathrm{Re} \left\langle \sum_{\alpha\beta, q} (d_q)^*_{\alpha\beta} \rho^q_{\alpha\beta}(\omega) \right\rangle_{v_i, F}$$

is the spectral power of spontaneous emission

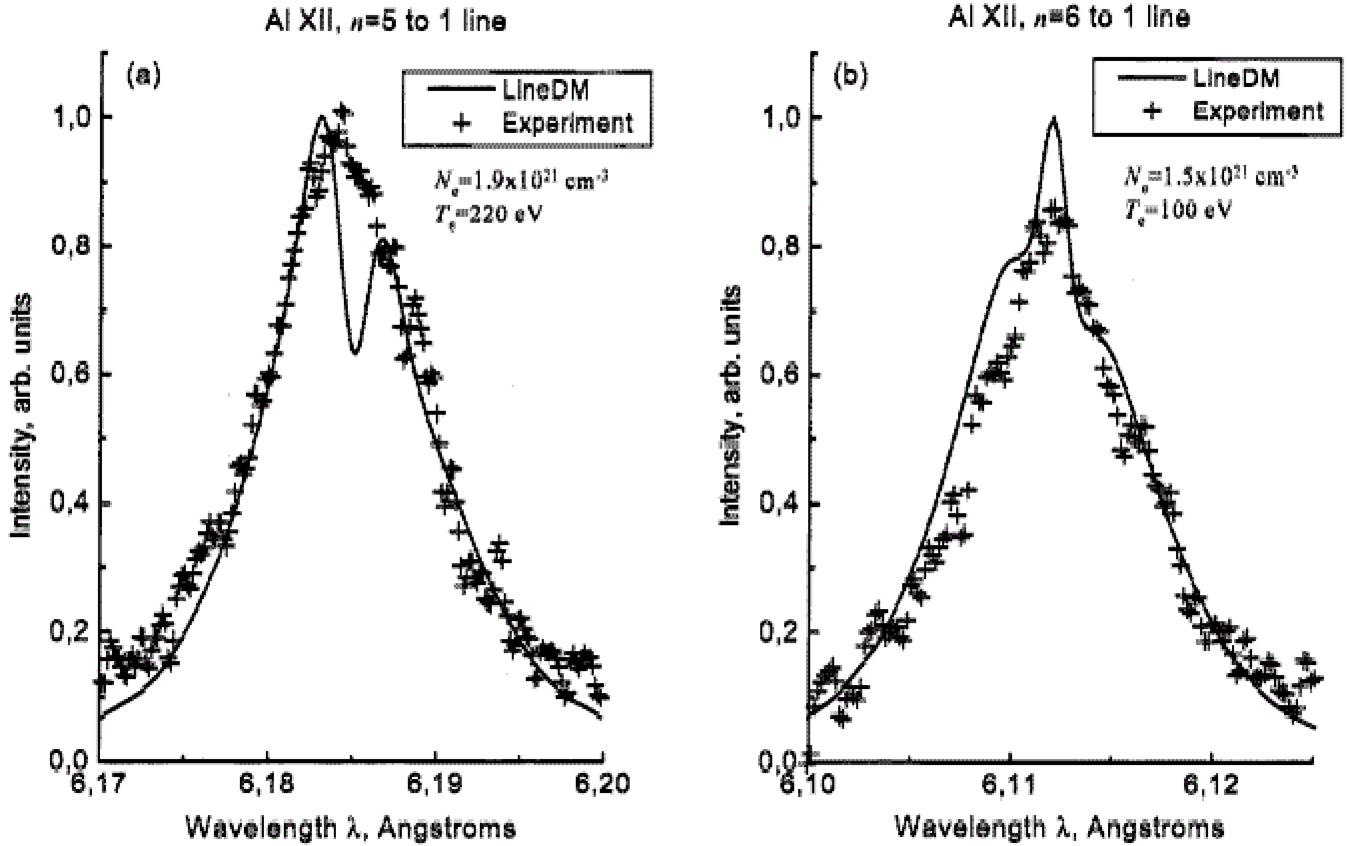


Fig. 3. Profiles of the $n = 5$ to 1(a) and $n = 6$ to 1(b) resonance lines of Al XII at a close distance $x \approx 30\ \mu m < d_f$ (d_f is the focal spot diameter) from the target surface. Solid curves represent LineDM-calculated profiles, while the pluses correspond to the experimental data of Stepanov *et al.* (1998) and Faenov (1998). The values of electron density N_e and temperature $T_e = T_i$ providing the best agreement of calculated and experimental data are given in the plots.

Hydrodynamics codes

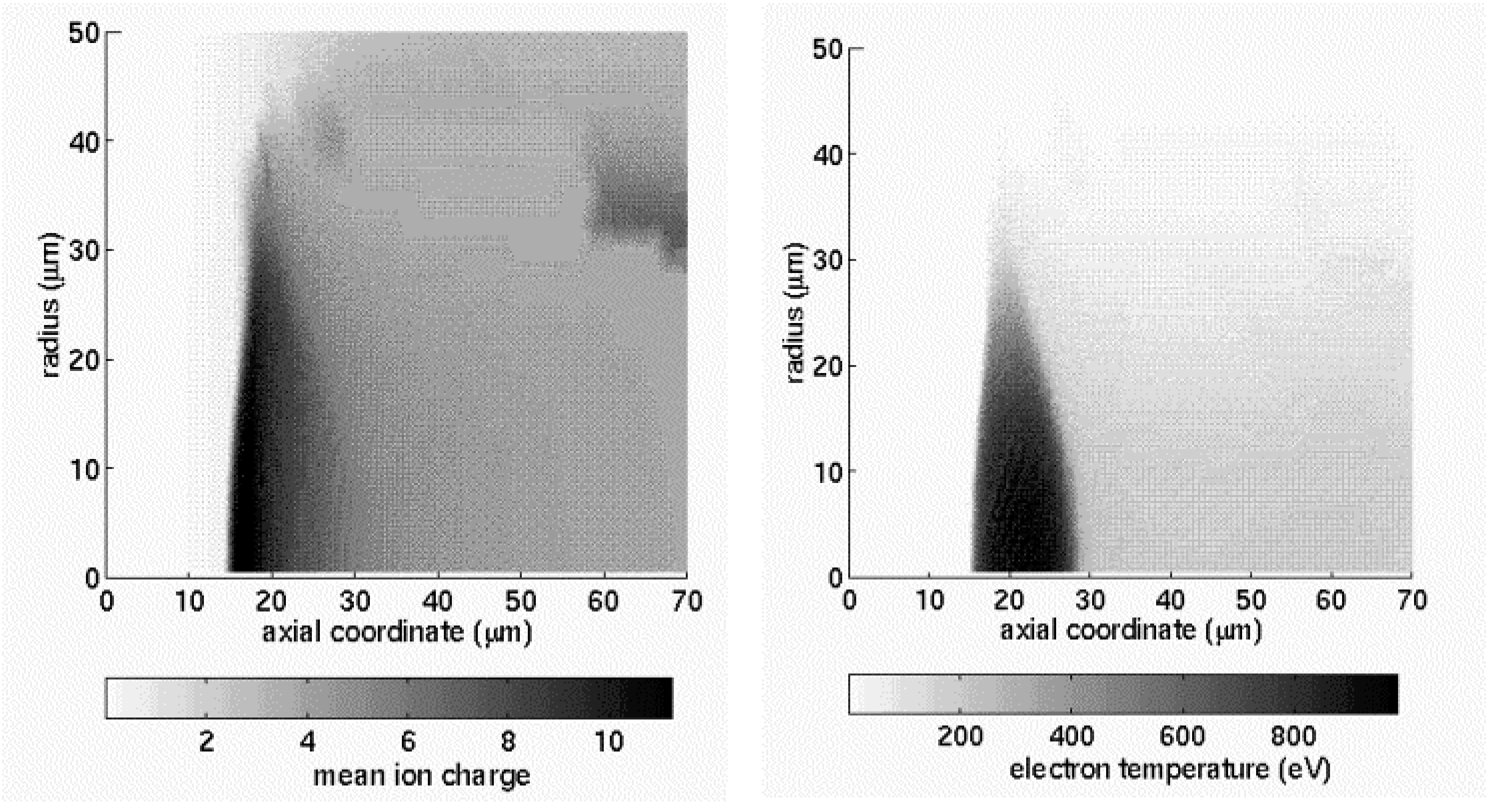
N_e, T_e, Z_{av}, T_i, $N_i (Z)$

As function of position

Postprocessing:
Needs spectra as function of

N_e, T_e, Z_{av}, T_i, $N_i (Z)$

Gives spectra integrated over space region or/and time



Ion mean charge and electron temperature spatial distributions
2 ps after main pulse maximum (laser incident from the right)
for main pulse delay 2 ns.

The database

The data has been produced by the Snezhinsk code in the framework of a project of

Bergen Computational Physics Laboratory

April 2001

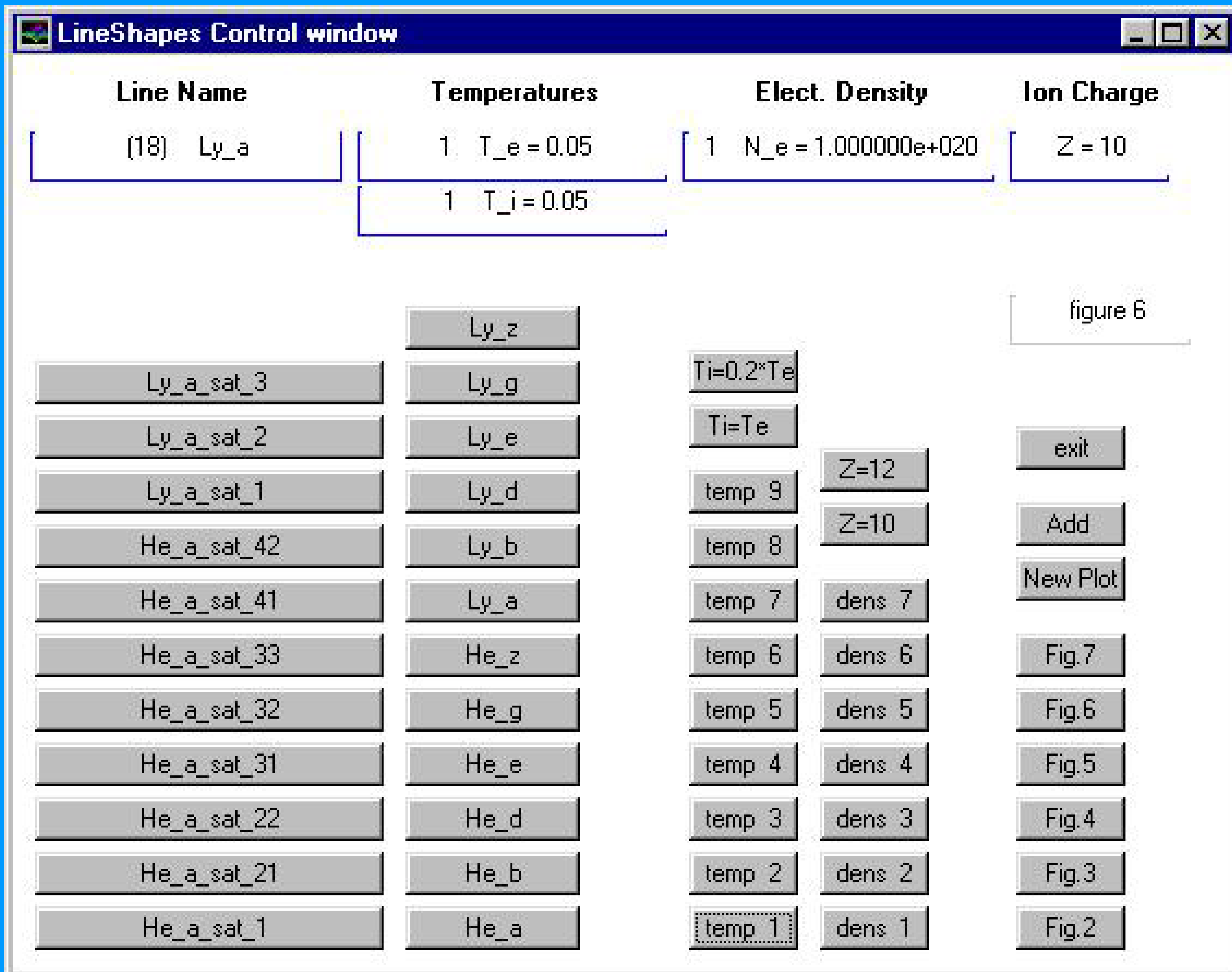
The ranges of the aluminium line database

Ly_{α} , Ly_{β} …… Ly_{ζ}

He_{α} , He_{β} …… He_{ζ} Satellites

N_e	T_e
$1.000\ 10^{20}\ cm^{-3}$	0.050 keV
$3.162\ 10^{20}\ cm^{-3}$	0.100 keV
$1.000\ 10^{21}\ cm^{-3}$	0.200 keV
$3.162\ 10^{21}\ cm^{-3}$	0.400 keV
$1.000\ 10^{22}\ cm^{-3}$	0.600 keV
$3.162\ 10^{22}\ cm^{-3}$	0.900 keV
$1.000\ 10^{23}\ cm^{-3}$	1.200 keV
	1.600 keV
	2.000 keV

$Z_{av}=\{\ 10,12\ \}$ $T_i = \{\ 0.2\ T_e\ , T_e\ \}$



LineShapes Control window
Line Name
Temperatures
Elect. Density
Ion Charge
(18) Ly_a
1 T_e = 0.05
1 N_e = 1.000000e+020
Z = 10
1 T_i = 0.05
figure 6
Ly_z
Ly_a_sat_3
Ly_g
Ti=0.2*Te
Ly_a_sat_2
Ly_e
Ti=Te
exit
Z=12
Ly_a_sat_1
Ly_d
temp 9
Z=10
Add
He_a_sat_42
Ly_b
temp 8
New Plot
He_a_sat_41
Ly_a
temp 7
dens 7
He_a_sat_33
He_z
temp 6
dens 6
Fig.7
He_a_sat_32
He_g
temp 5
dens 5
Fig.6
He_a_sat_31
He_e
temp 4
dens 4
Fig.5
He_a_sat_22
He_d
temp 3
dens 3
Fig.4
He_a_sat_21
He_b
temp 2
dens 2
Fig.3
He_a_sat_1
He_a
temp 1
dens 1
Fig.2

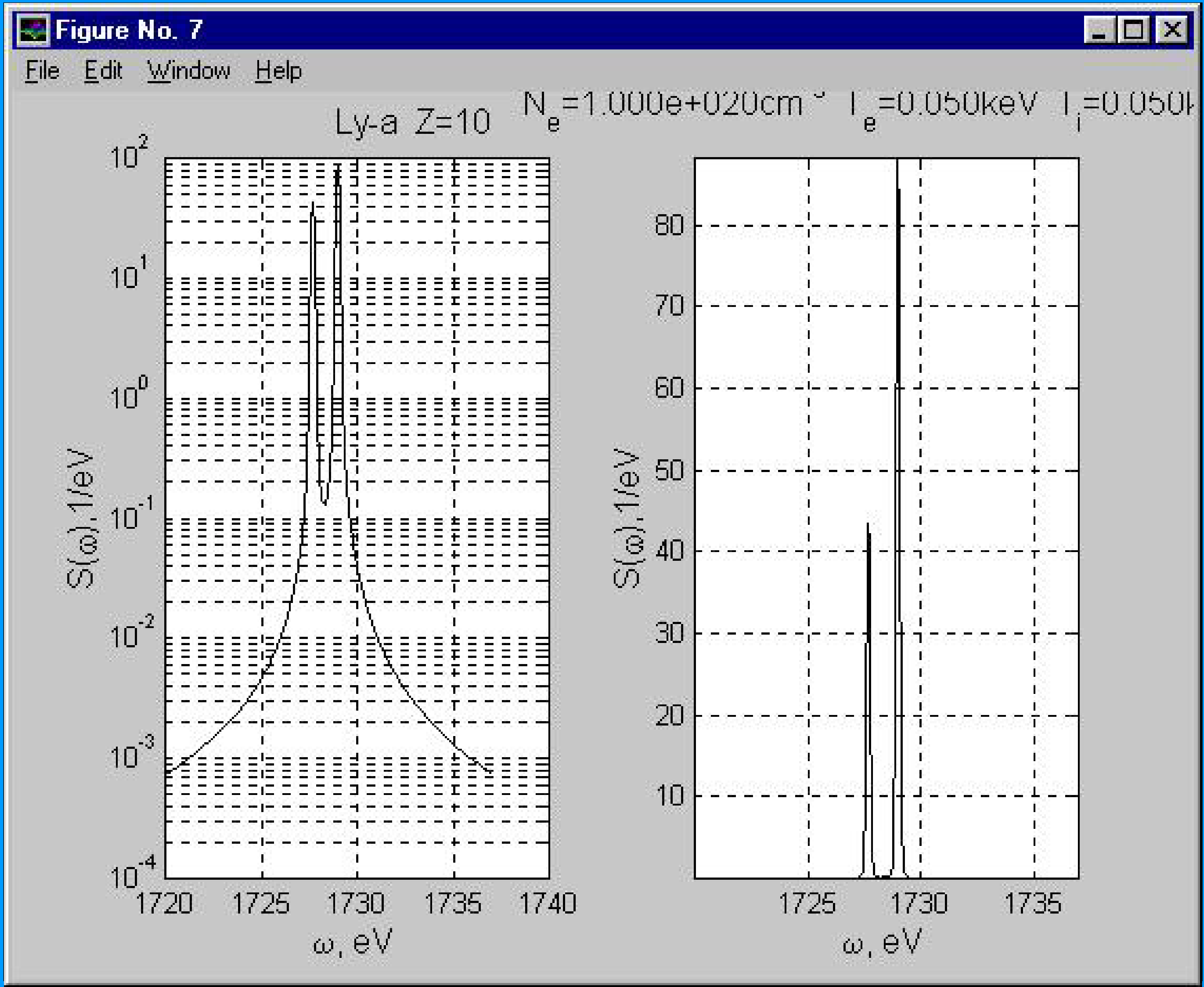
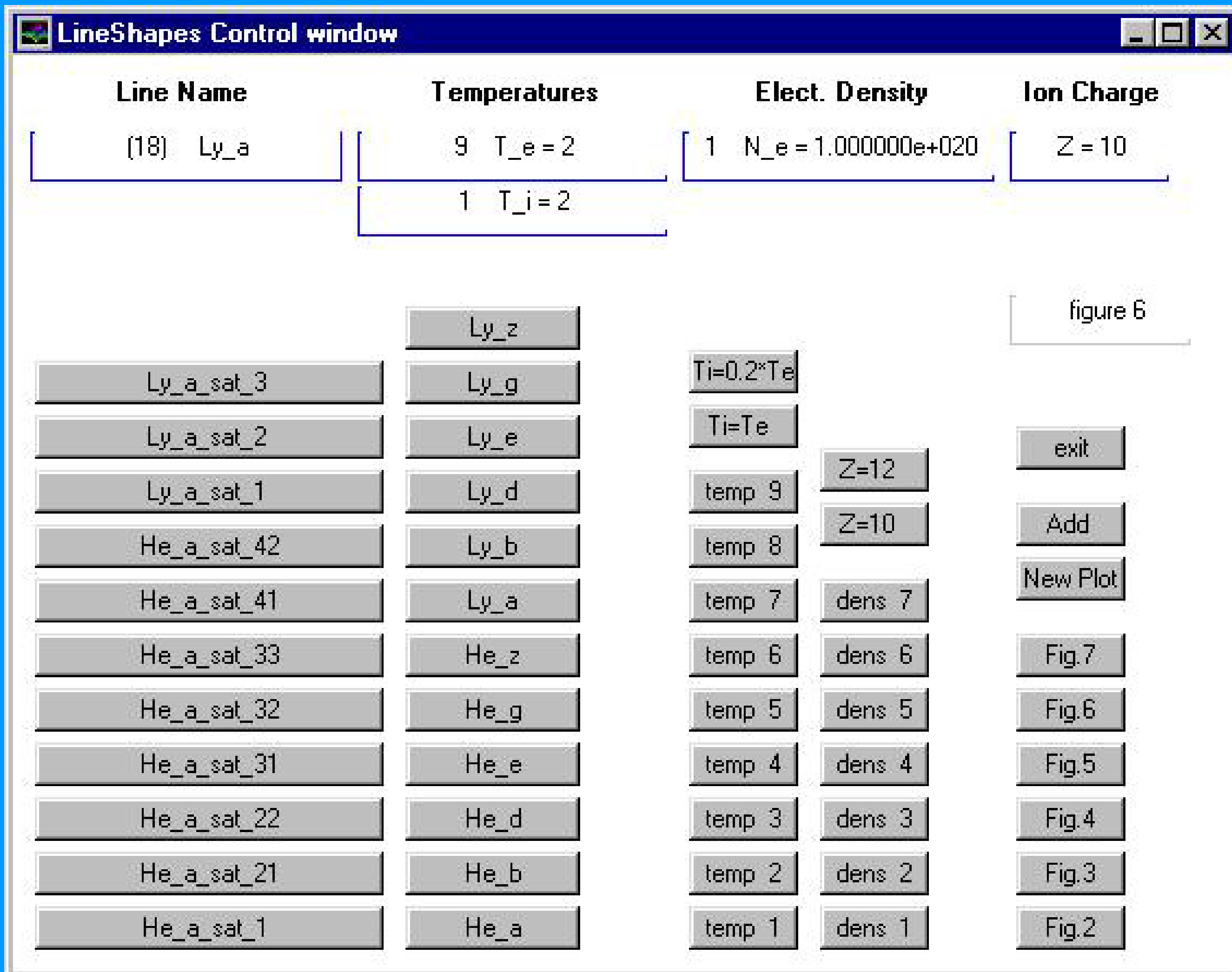


Figure No. 7
File Edit Window Help
Ly-a Z=10
N_e=1.000e+020cm
T_e=0.050keV
T_i=0.050
S(ω), 1/eV
ω, eV
1720
1725
1730
1735
1740
10
20
30
40
50
60
70
80


LineShapes Control window
Line Name
Temperatures
Elect. Density
Ion Charge
(18) Ly_a
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1 T_i = 2
1 N_e = 1.000000e+020
Z = 10
figure 6
Ly_z
Ly_a_sat_3
Ly_g
Ti=0.2*Te
Ly_a_sat_2
Ly_e
Ti=Te
exit
Ly_a_sat_1
Ly_d
temp 9
Z=12
He_a_sat_42
Ly_b
temp 8
Z=10
Add
New Plot
He_a_sat_41
Ly_a
temp 7
dens 7
He_a_sat_33
He_z
temp 6
dens 6
Fig.7
He_a_sat_32
He_g
temp 5
dens 5
Fig.6
He_a_sat_31
He_e
temp 4
dens 4
Fig.5
He_a_sat_22
He_d
temp 3
dens 3
Fig.4
He_a_sat_21
He_b
temp 2
dens 2
Fig.3
He_a_sat_1
He_a
temp 1
dens 1
Fig.2

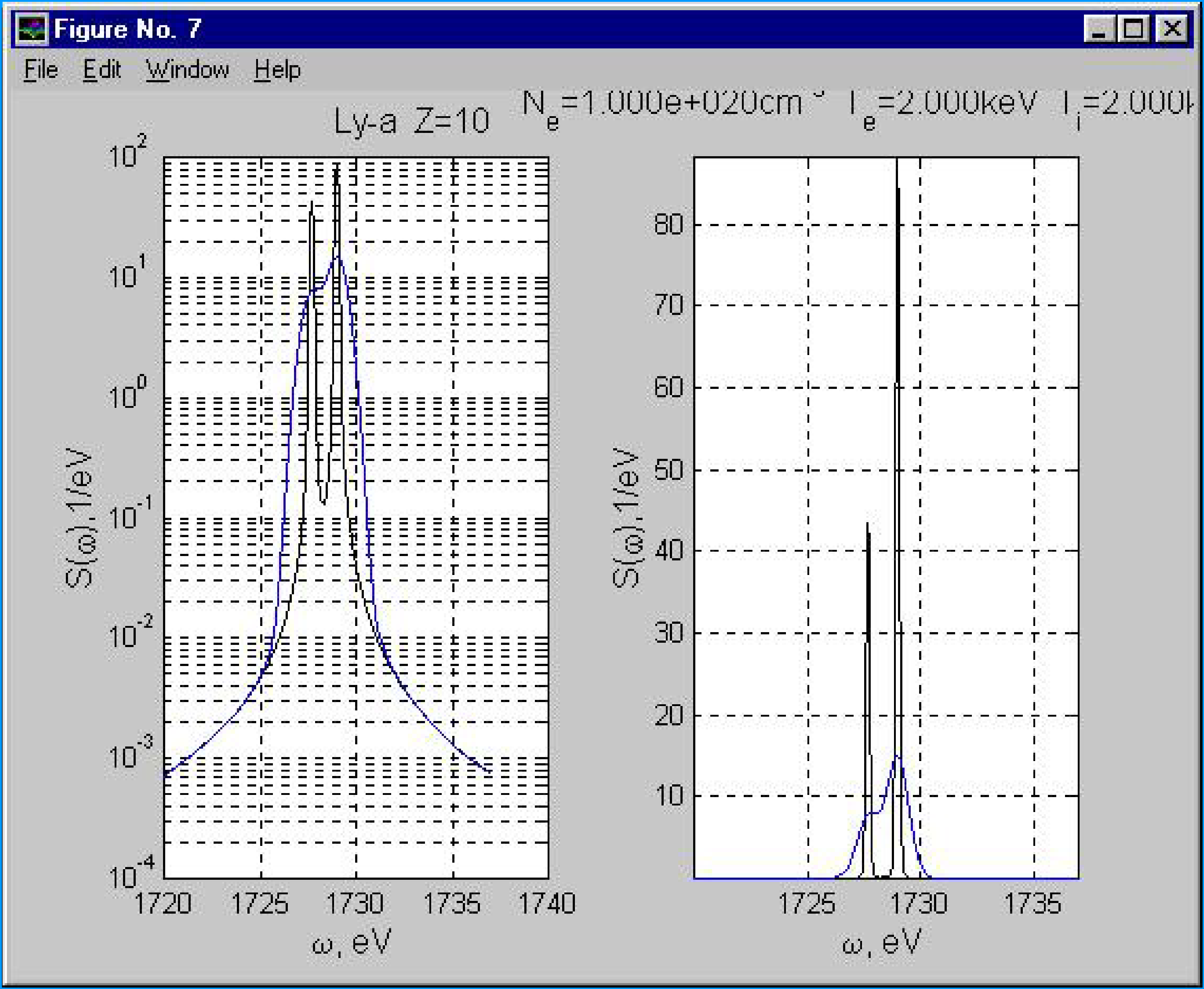
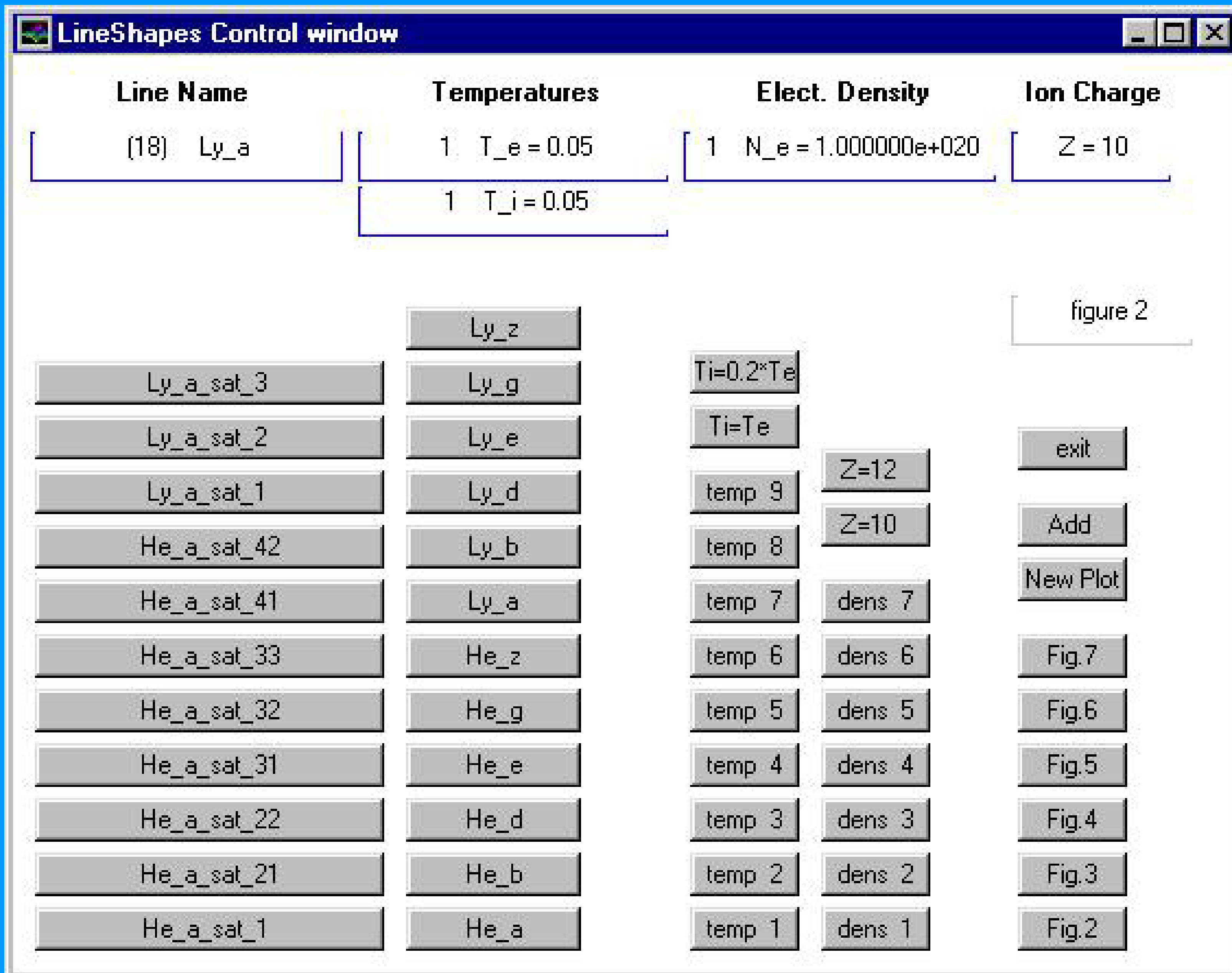


Figure No. 7
File Edit Window Help
Ly-a Z=10
N_e=1.000e+020cm^-3 T_e=2.000keV T_i=2.000k
S(ω), 1/eV
ω, eV
1720 1725 1730 1735 1740
10^2 10^1 10^0 10^-1 10^-2 10^-3 10^-4
80 70 60 50 40 30 20 10



LineShapes Control window
Line Name
Temperatures
Elect. Density
Ion Charge
(18) Ly_a
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1 N_e = 1.000000e+020
Z = 10
1 T_i = 0.05
figure 2
Ly_z
Ly_a_sat_3
Ly_g
Ti=0.2*Te
Ly_a_sat_2
Ly_e
Ti=Te
exit
Ly_a_sat_1
Ly_d
temp 9
Z=12
He_a_sat_42
Ly_b
temp 8
Z=10
Add
He_a_sat_41
Ly_a
temp 7
dens 7
New Plot
He_a_sat_33
He_z
temp 6
dens 6
Fig.7
He_a_sat_32
He_g
temp 5
dens 5
Fig.6
He_a_sat_31
He_e
temp 4
dens 4
Fig.5
He_a_sat_22
He_d
temp 3
dens 3
Fig.4
He_a_sat_21
He_b
temp 2
dens 2
Fig.3
He_a_sat_1
He_a
temp 1
dens 1
Fig.2

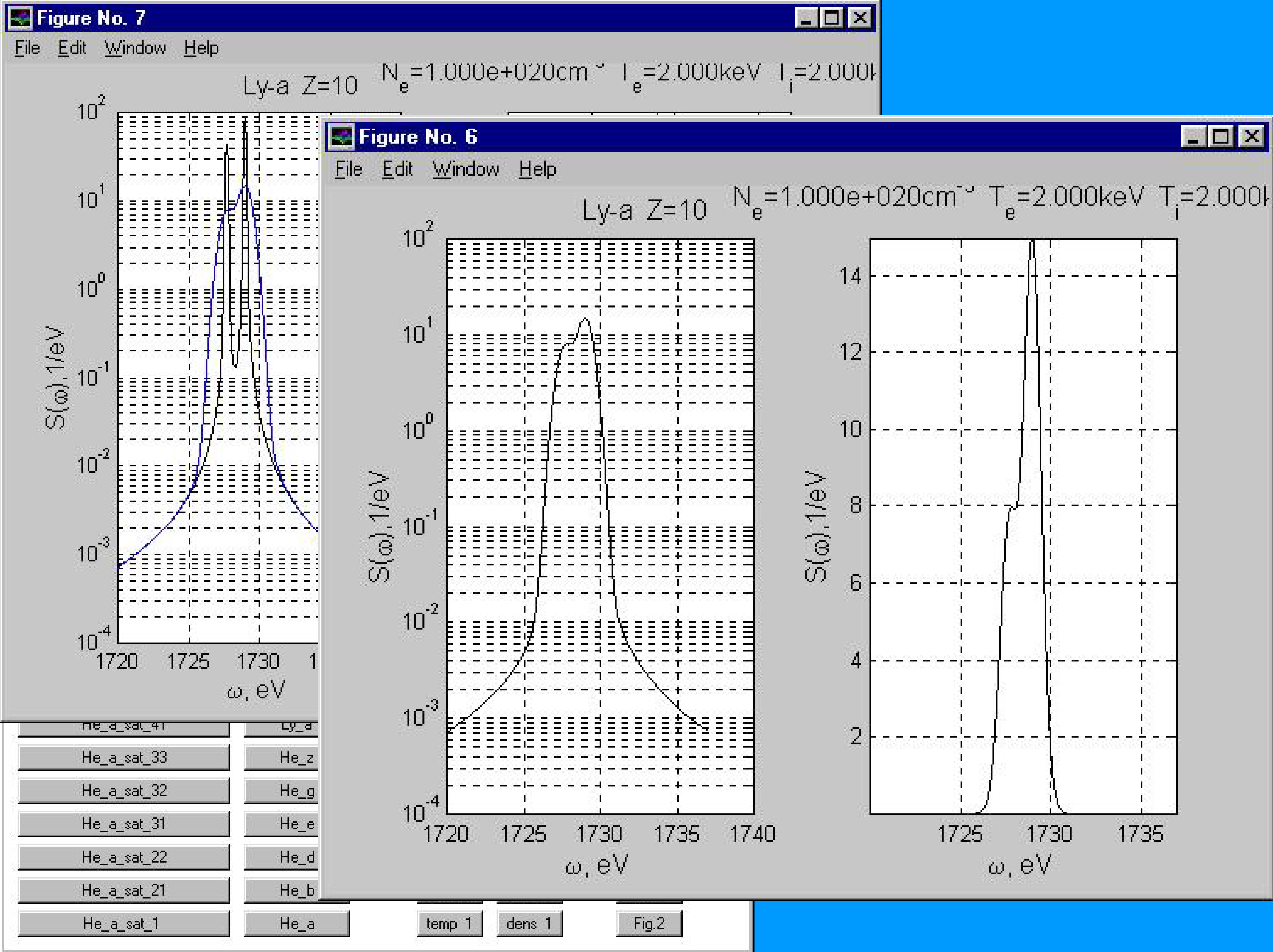
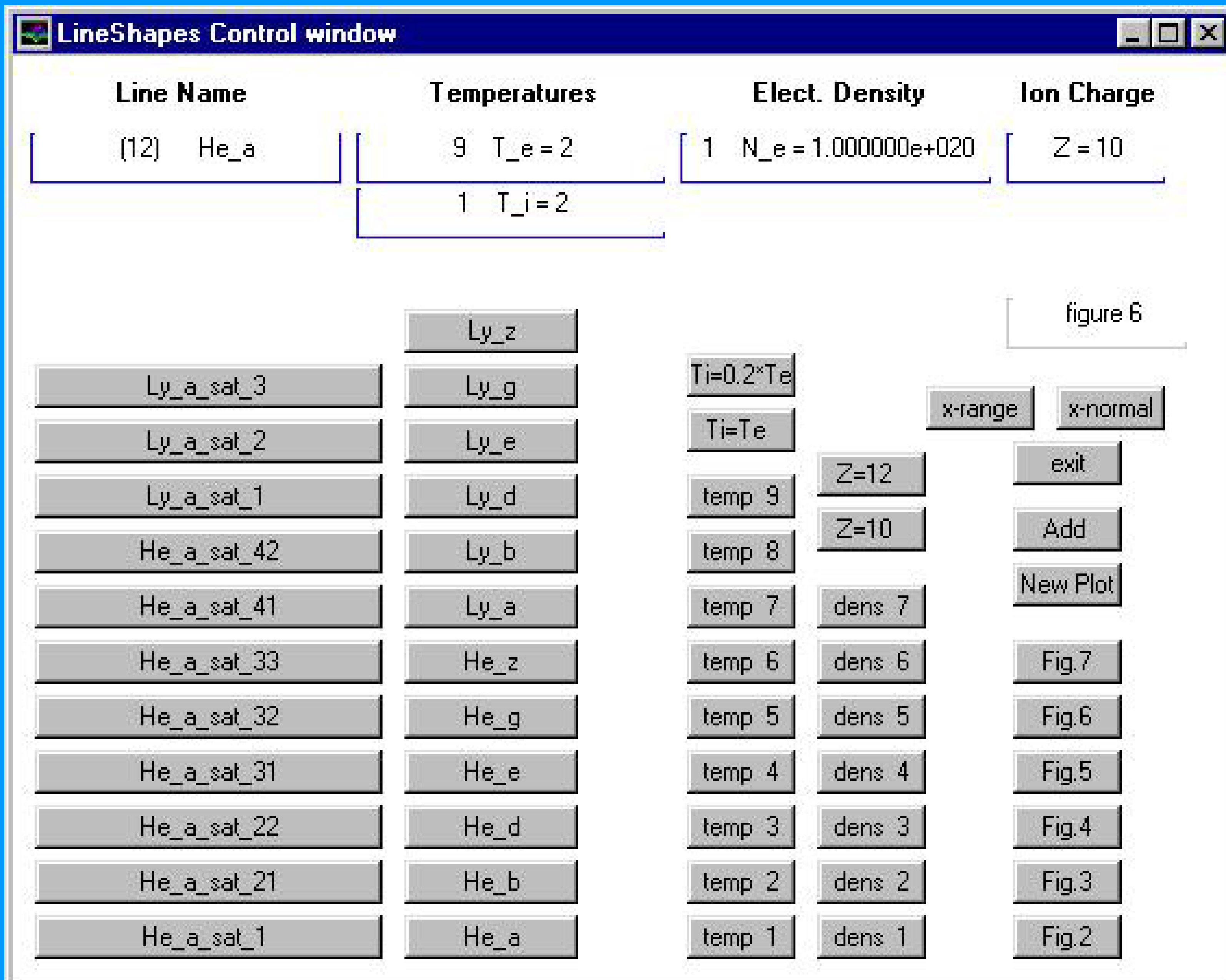


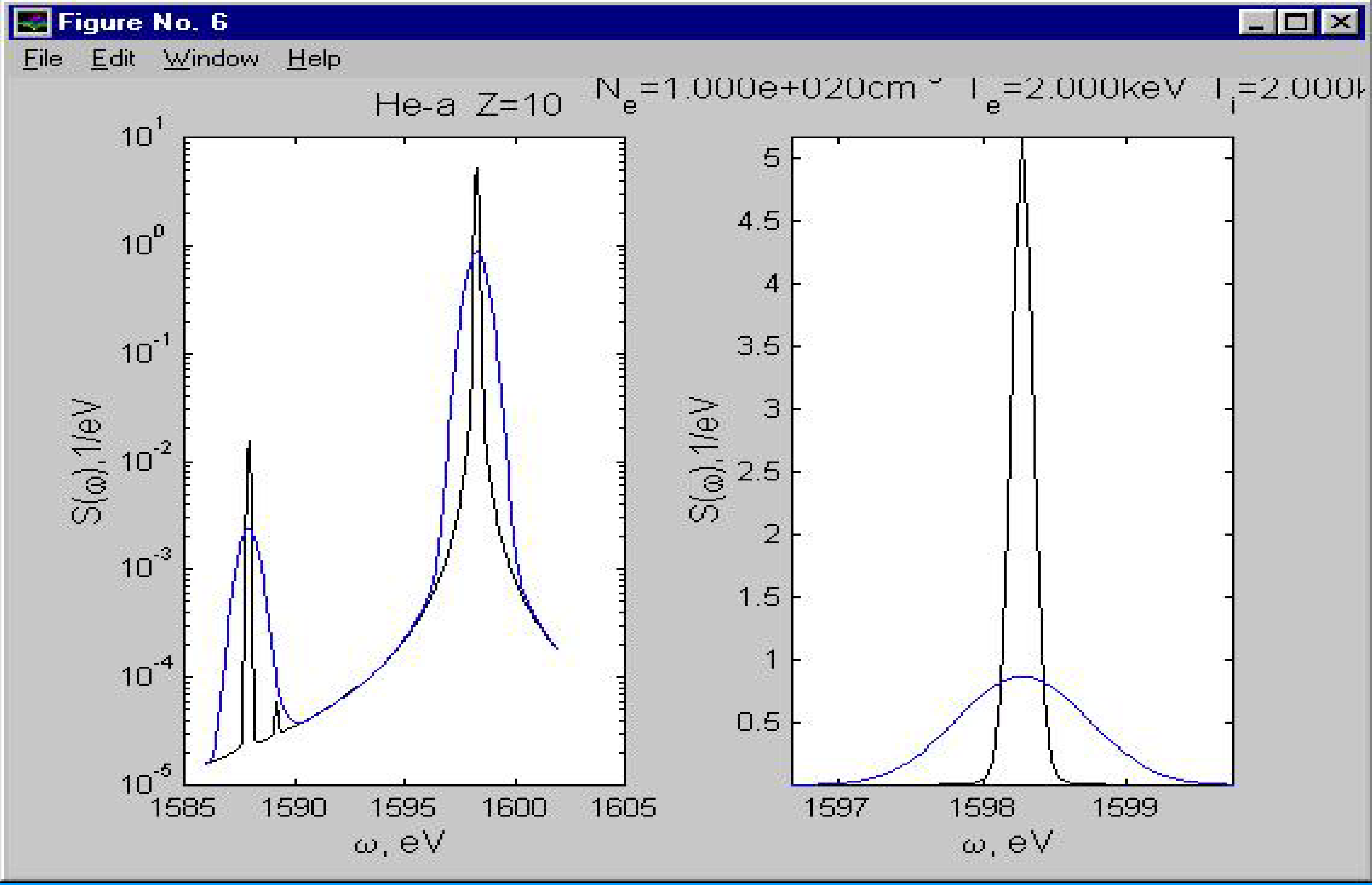
Figure No. 7
File Edit Window Help
Ly-a Z=10
N_e=1.000e+020cm^{-3} T_e=2.000keV T_i=2.000k
S(ω), 1/eV
ω, eV
Figure No. 6
File Edit Window Help
Ly-a Z=10
N_e=1.000e+020cm^{-3} T_e=2.000keV T_i=2.000k
S(ω), 1/eV
ω, eV
1720 1725 1730 1735 1740
S(ω), 1/eV
ω, eV
1725 1730 1735
He_a_sat_33
He_a_sat_32
He_a_sat_31
He_a_sat_22
He_a_sat_21
He_a_sat_1
He_z
He_g
He_e
He_d
He_b
He_a
temp 1
dens 1
Fig.2

MATLAB Command Window

File Edit Window Help

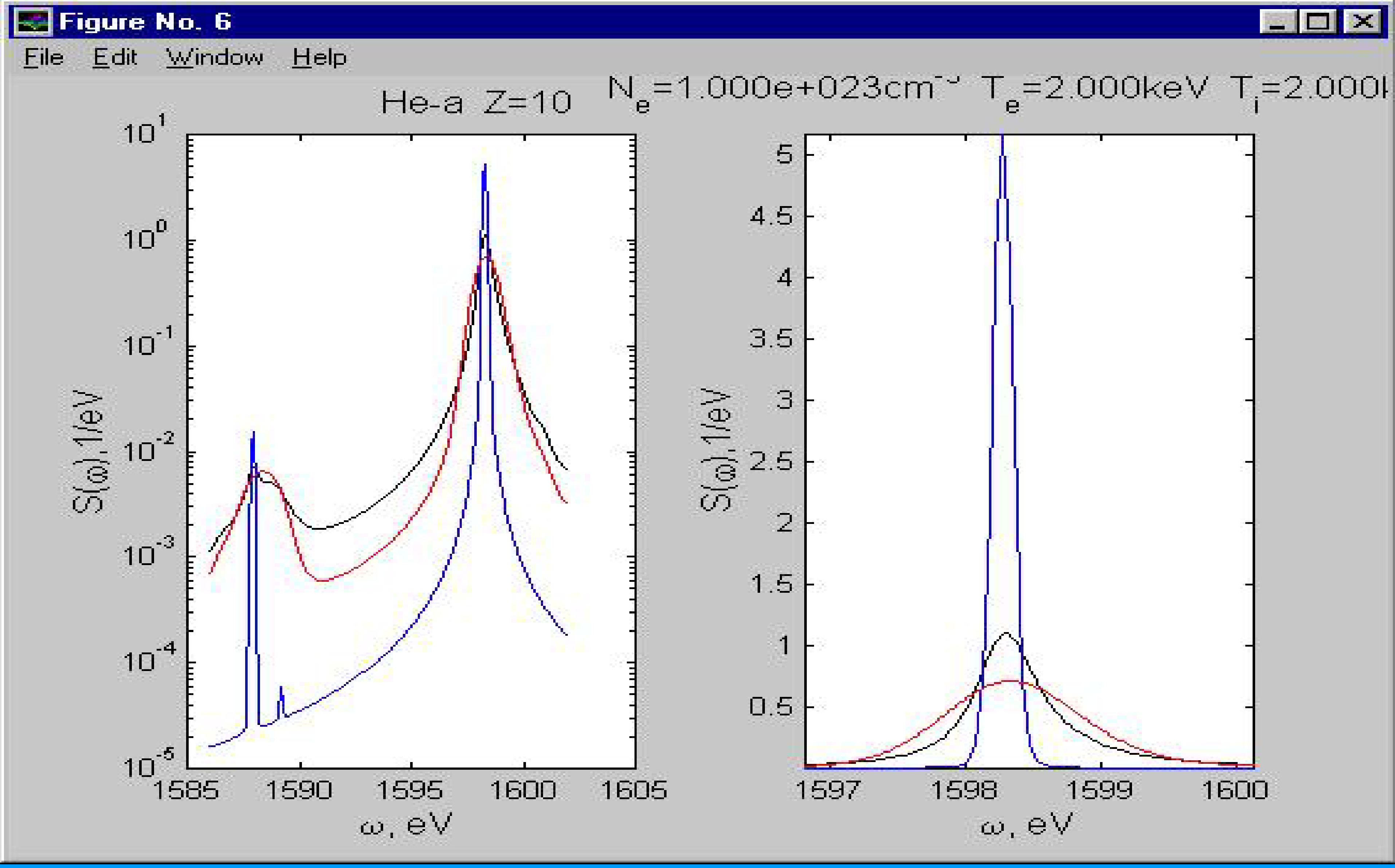
```
>>
>>
>>
>> gview
>>
>>
figure 7  plots
          Ly-a  Z=10 N_e=1.000e+020cm^{-3}  T_e=0.050keV  T_i=0.050keV
          Ly-a  Z=10 N_e=1.000e+020cm^{-3}  T_e=2.000keV  T_i=2.000keV

figure 6  plots
          Ly-a  Z=10 N_e=1.000e+020cm^{-3}  T_e=2.000keV  T_i=2.000keV
>>
>>
```


LineShapes Control window
Line Name
Temperatures
Elect. Density
Ion Charge
(12) He_a
9 T_e = 2
1 T_i = 2
1 N_e = 1.000000e+020
Z = 10
figure 6
Ly_z
Ly_a_sat_3
Ly_g
Ti=0.2*Te
x-range
x-normal
Ly_a_sat_2
Ly_e
Ti=Te
exit
Ly_a_sat_1
Ly_d
temp 9
Z=12
Add
He_a_sat_42
Ly_b
temp 8
Z=10
New Plot
He_a_sat_41
Ly_a
temp 7
dens 7
He_a_sat_33
He_z
temp 6
dens 6
Fig.7
He_a_sat_32
He_g
temp 5
dens 5
Fig.6
He_a_sat_31
He_e
temp 4
dens 4
Fig.5
He_a_sat_22
He_d
temp 3
dens 3
Fig.4
He_a_sat_21
He_b
temp 2
dens 2
Fig.3
He_a_sat_1
He_a
temp 1
dens 1
Fig.2



He-a Z=10 N_e=1.000e+020cm^{-3} T_e=0.050keV T_i=0.050keV

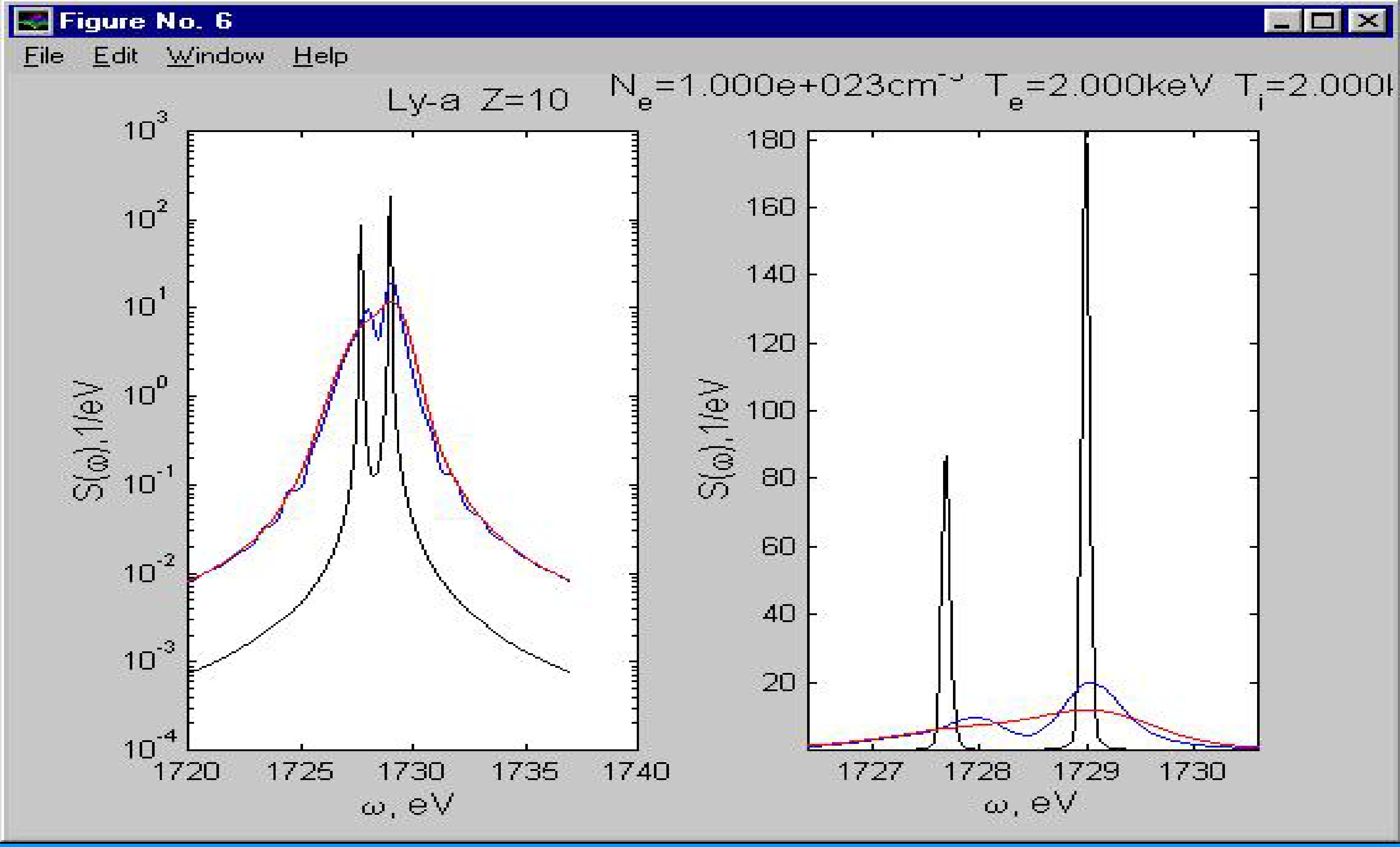
He-a Z=10 N_e=1.000e+020cm^{-3} T_e=2.000keV T_i=2.000keV



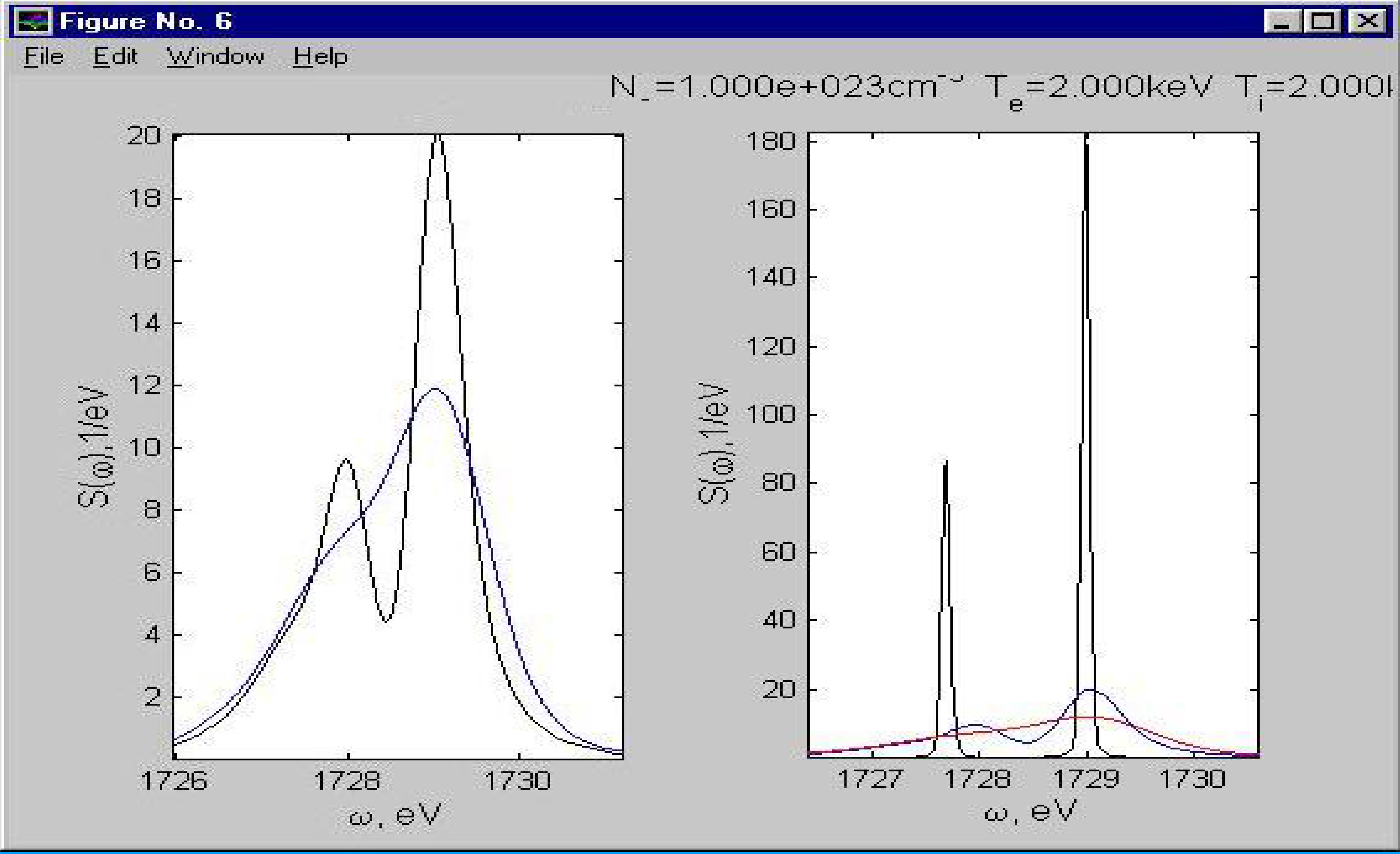
He-a Z=10 N_e=1.000e+023cm^{-3} T_e=0.050keV T_i=0.050keV

He-a Z=10 N_e=1.000e+020cm^{-3} T_e=0.050keV T_i=0.050keV

He-a Z=10 N_e=1.000e+023cm^{-3} T_e=2.000keV T_i=2.000keV

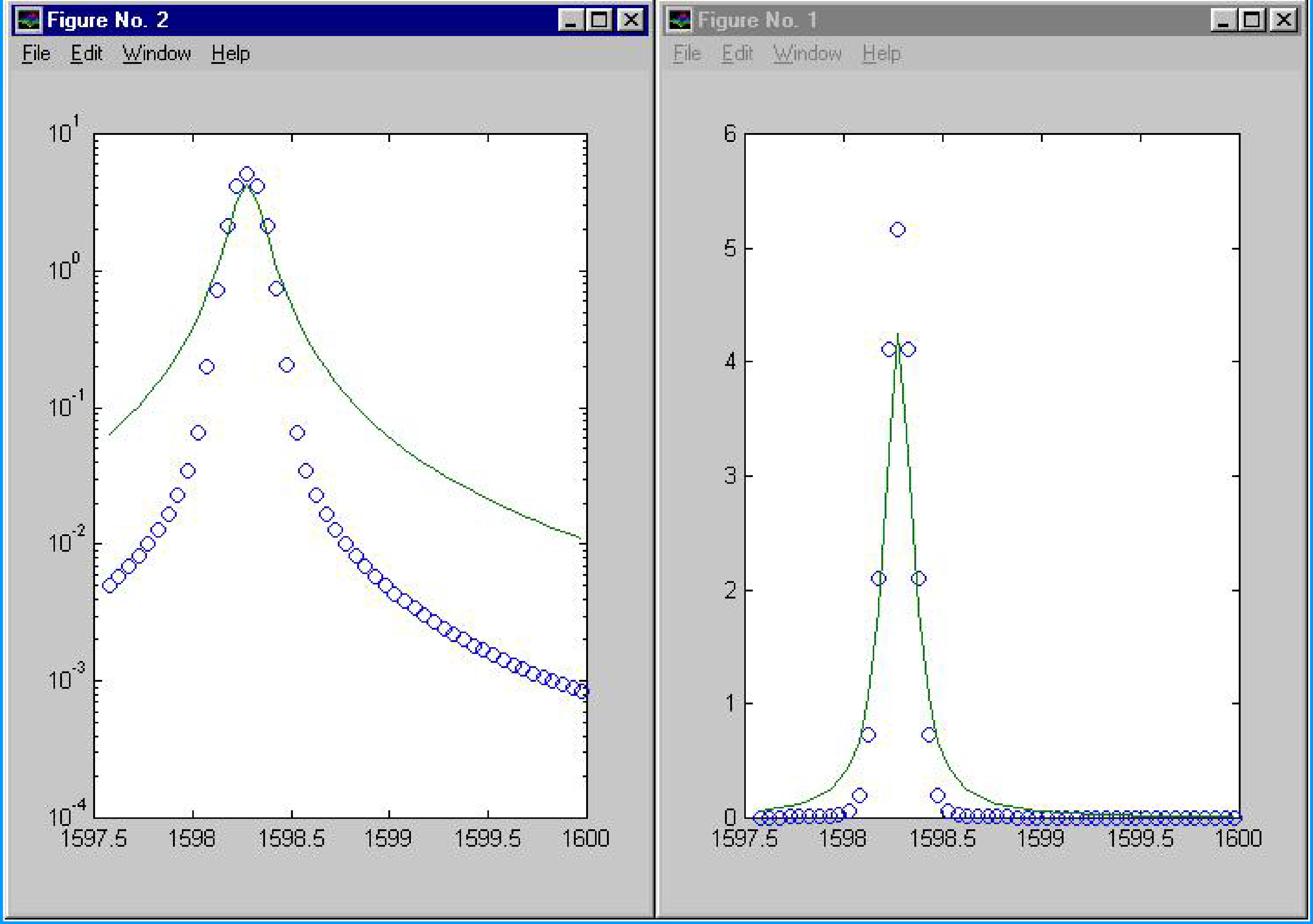


Ly-a Z=10 N_e=1.000e+020cm^{-3} T_e=0.050keV T_i=0.010keV
Ly-a Z=10 N_e=1.000e+023cm^{-3} T_e=2.000keV T_i=0.400keV
Ly-a Z=10 N_e=1.000e+023cm^{-3} T_e=2.000keV T_i=2.000keV

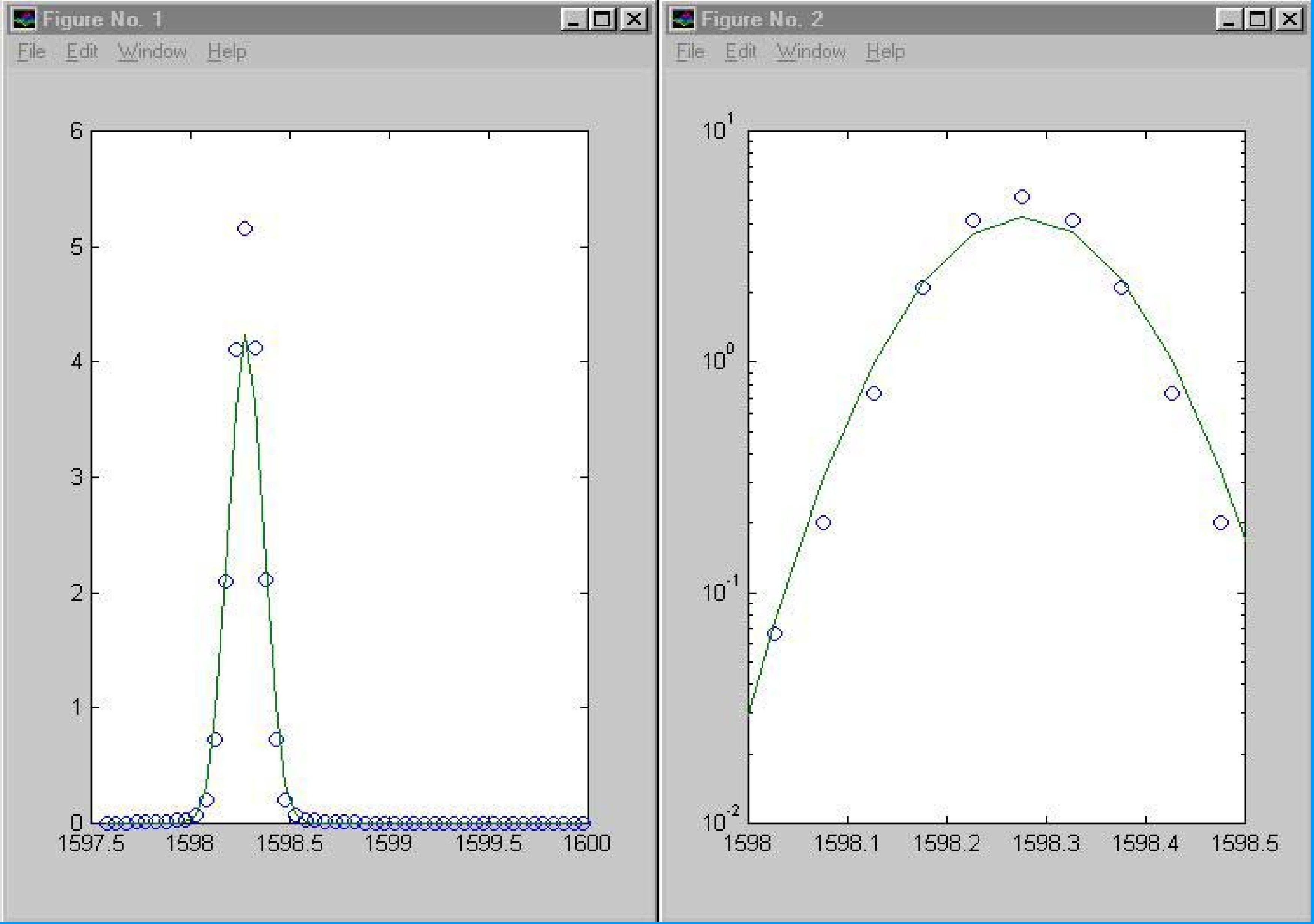


Ly-a Z=10 N_e=1.000e+020cm^{-3} T_e=0.050keV T_i=0.010keV
Ly-a Z=10 N_e=1.000e+023cm^{-3} T_e=2.000keV T_i=0.400keV
Ly-a Z=10 N_e=1.000e+023cm^{-3} T_e=2.000keV T_i=2.000keV

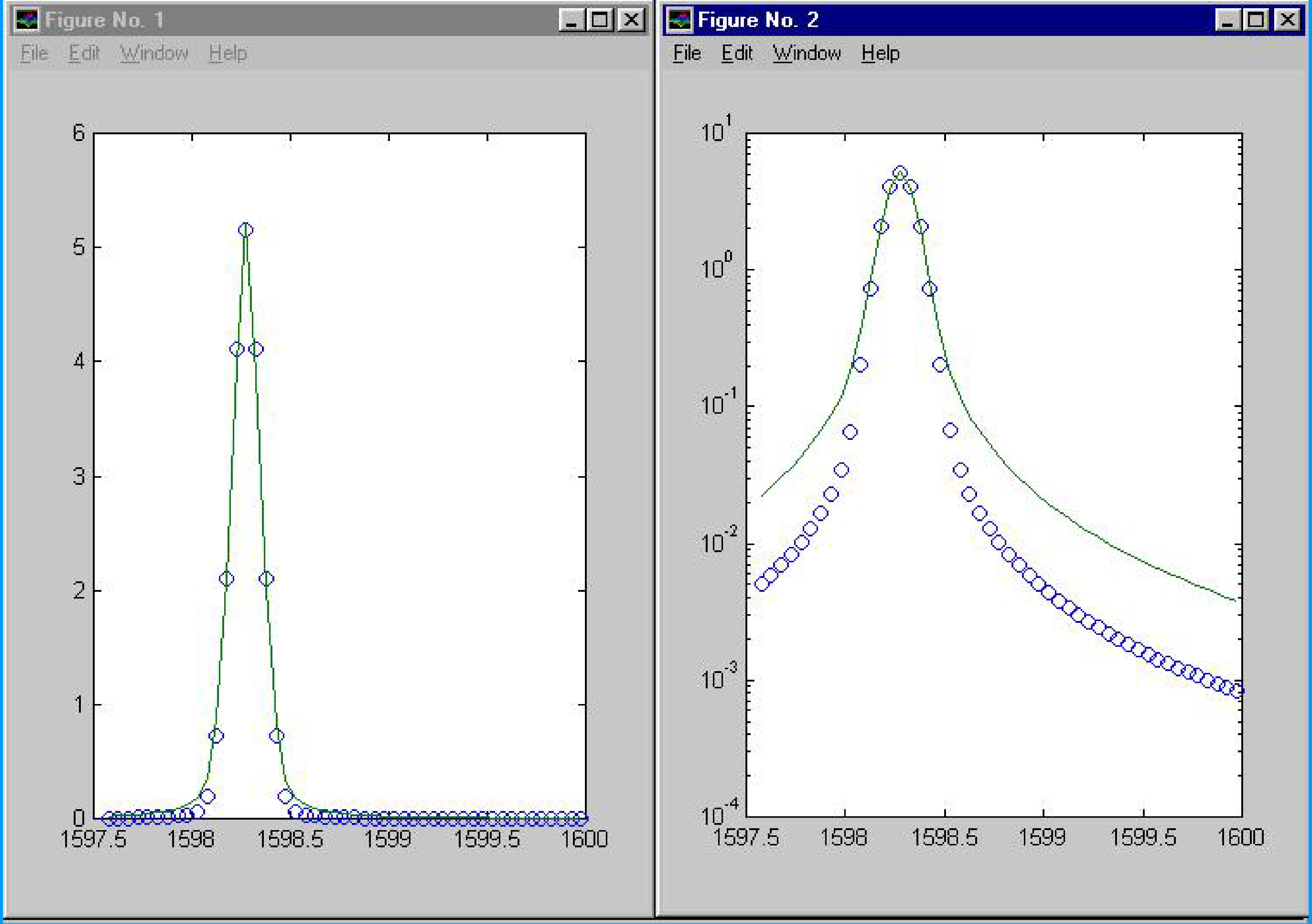
Parametrizing the database



Attempt to fit He_{α} by a Lorentzian (automatic fitter)



Attempt to fit He_{α} by a Gaussian (automatic fitter)



Attempt to fit He_{α} by a combined Lorentzian + Gaussian (automatic)

Conclusions

The database is useful as a source of data files for simulations

The work with automatic parametrization is promissing

The parametrization will greatly simplify the applications of the line data.