Stochastic processes applied to line shapes

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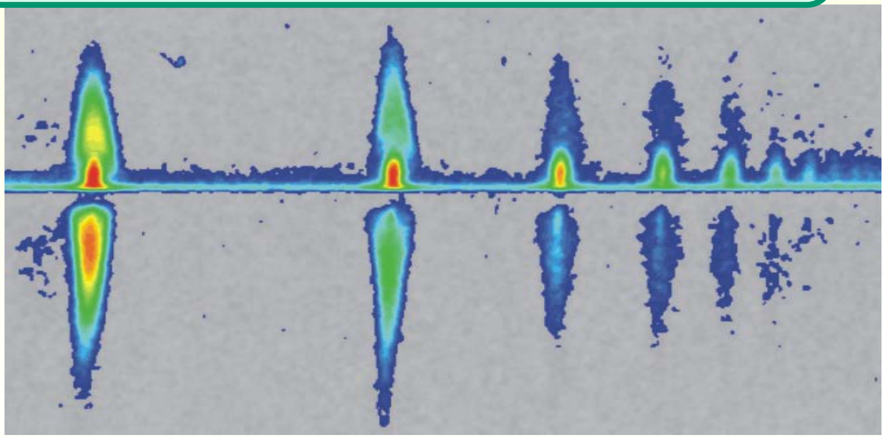
Modeling of radiative properties of plasmas

Line shapes for a plasma diagnostic

-Broadening : Doppler, Stark

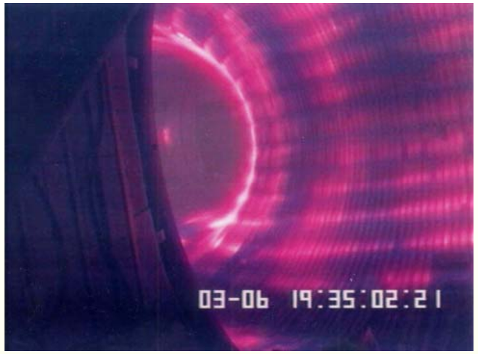
-Zeeman splitting



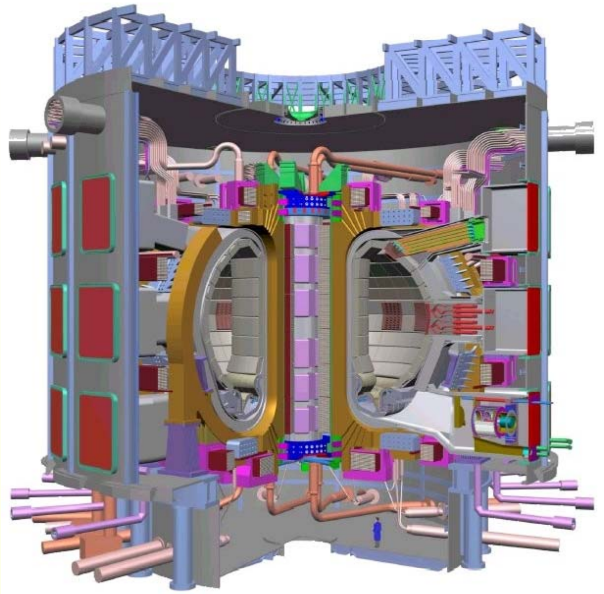
Laser plasma

Analysis results in the knowledge of plasma parameters, bulk motion, turbulence..

Applied to
-Laboratory plasmas
-Fusion
-Astrophysics



Tore-Supra (D_α)

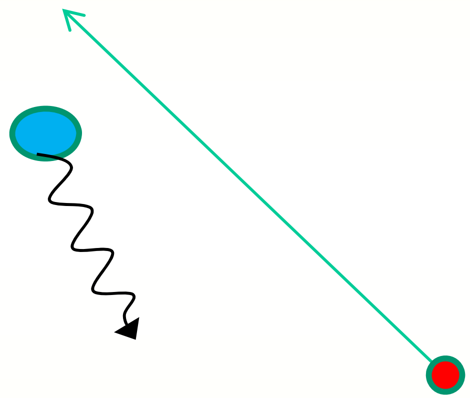


ITER

Lorentz (1906)

A model for binary collisions: one emitter and one perturber

The light wave is interrupted by the perturber



The times t between collisions are distributed with a Poisson law: $\nu \exp(-\nu t)$

$\tau=\nu^{-1}$ is the average time between collisions

The intensity is $$I(\Delta\omega) = \frac{1}{\pi}\frac{\nu}{(\Delta\omega^2+\nu^2)}$$

Outline

1. **Stark profile basics**
2. Non binary dynamic interactions, simulation
3. Stochastic processes for line shapes
4. Stochastic processes for level populations
5. Conclusions

Stark broadening : line shape

Fourier transform of the dipole autocorrelation function

$$L(\Delta\omega) = \frac{1}{\pi} \mathrm{Re} \int_0^\infty C(t) e^{i\Delta\omega t} dt$$

Time of interest: $\tau_i \approx 1/\Delta\omega_{1/2}$

dipole autocorrelation function

$$C(t) = Tr \left\langle \rho \, \vec{d}\,(0) \, \vec{d}\,(t) \right\rangle_{av}$$

$$\vec{d}\,(t) = U^{+}(t) \vec{d}(0) U(t)$$

U(t) is the emitter evolution operator

Stark broadening : Schrödinger equation and interaction potential

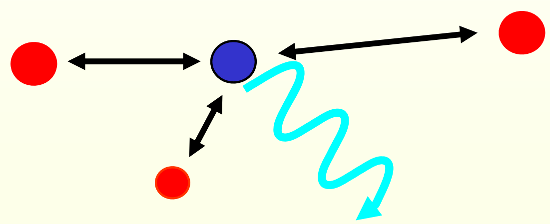
Schrödinger equation for the emitter

$$i\hbar \frac{dU}{dt}(t) = (H_0 + V(t))\, U(t)$$

$$V(t) = -\vec{d}.\vec{E}(t)$$

Stark effect in dipolar approximation

$\vec{E}(t)$ is the electric microfield created by the charged particles



Static and impact approximations

Stark effect in two limiting regimes

<u>Static</u> $\tau_i << \tau_c$

$\tau_i \approx 1/\Delta\omega$ Time of interest

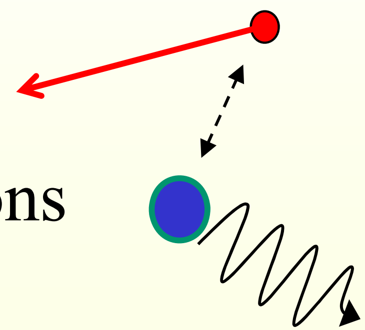
$\tau_c \approx r_0/\mathrm{v}$ Collision time

$\vec{\mathrm{E}}(\mathrm{t}) \approx \vec{\mathrm{E}}(0)$ In Schrödinger equation

Only the microfield probability density function P(E) is required

pdf

<u>Impact</u> $\tau_i >> \tau_c$ Binary collisions



Impact approximation

Hydrogen plasma with $N_e=10^{12}$ cm^{-3} or lower, T=1-100 eV
Impact binary approximation valid for both electrons and ions

H. Griem, A. Kolb, K. Shen
M. Baranger
Collision operator expressed with the S matrix

$$\Phi = N\int dv f(v) v \int d\rho 2\pi\rho \{1 - S(\rho, v)\}_{angle}$$

$$C(t)=\exp(-\Phi t) \quad \text{and} \quad L(\Delta\omega) = -\frac{1}{\pi}\mathrm{Re}\frac{1}{i\Delta\omega - \Phi}$$

Collision operator in second order

second order approximation

$$S = 1 + \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt V(t) + \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} dt' V(t) V(t') + \dots$$

$$\langle 1 - S_{\alpha\alpha} \rangle_{av} = \frac{1}{3\hbar^2} \sum_{\alpha\alpha'} \left| \vec{d}_{\alpha\alpha'} \right|^2 \int_{-\infty}^{+\infty} dt \int_{-\infty}^{t} dt' \langle \vec{E}(t) . \vec{E}(t') \rangle_{av}$$

The microfield autocorrelation fonction is an important statistical property for the line shape

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Strong simultaneous collisions

- Non binary collisions are common for ions

-They can be treated approximately by kinetic theory (analytic model by J. Dufty, particle point of view)

-A microfield field point of view has been more successful.

Two approaches:

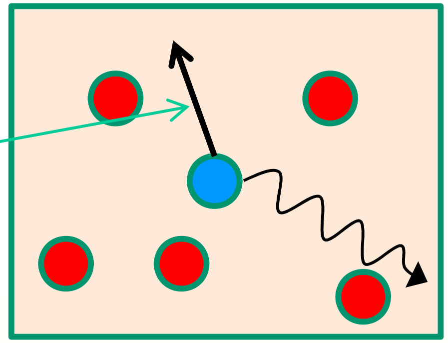
-Stochastic process for the microfield

-Ab initio simulation (intermediate between particle and microfield)

Non binary effects: numerical simulation

Many moving charged particles perturb simultaneously the emitter

i) Microfield simulation →E(t)

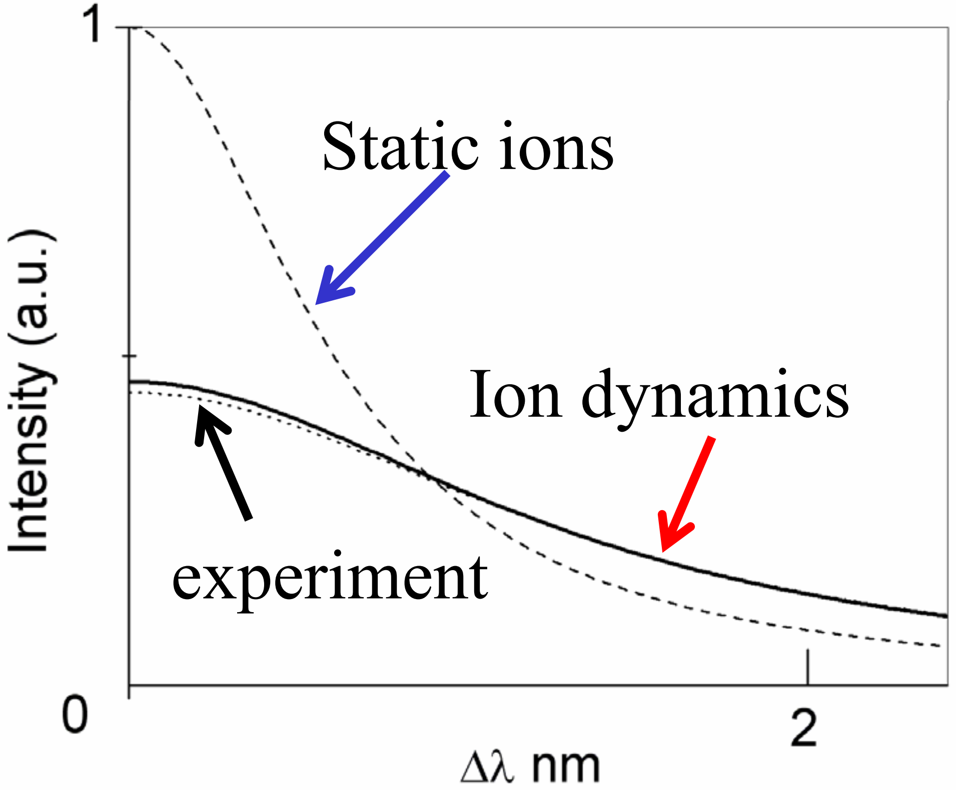


ii) Integration of Schrödinger equation→C(t) $U(t \rightarrow t + dt)$

iii) Fourier transform→line shape

Benchmark profiles by simulation: ion dynamics

Lyman alpha, N_e=2.10^{17} cm^{-3}, T=15 500 K,
Argon plasma containing traces of hydrogen



Experiment by Geisler et al.
Spectral Line Shapes vol. 1

Outline

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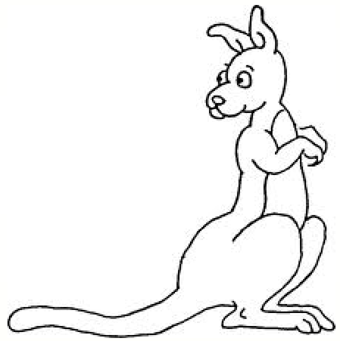
Stochastic processes for line shapes

Poisson process in nuclear magnetic resonance:
Anderson 1954, Kubo 1954



Model Microfield Method:
(Poisson Step and Kangaroo Process):
Brissaud and Frisch 1971
Seidel 1977
Frerichs 1989
Stehlé 1994, 1999, 2010

Statistical properties of the microfield are used:
Static microfield pdf $P(E)$

Microfield correlation function $\left\langle \vec{E}(0)\vec{E}(t) \right\rangle$

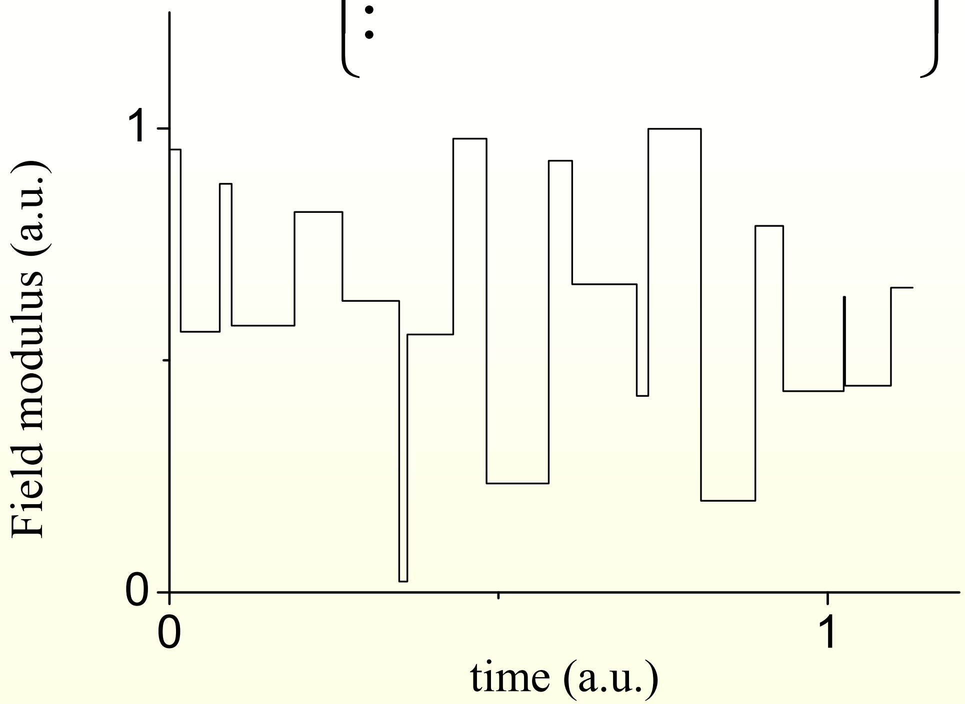
A renewal process: first step

The microfield is stepwise constant

$$\vec{E}(t) = \begin{cases} \vec{E}_1, & 0 \le t \le t_1 \\ \vec{E}_2, & t_1 \le t \le t_2 \\ \vdots & \\ \vec{E}_n, & t_{n-1} \le t \le t_n \\ \vdots & \end{cases}$$

First Step
-t=0 not a jumping time
-The microfield modulus is distributed with the pdf $P(\vec{E})$
-The waiting time obeys to a conditionnal pdf

$$v(t|\vec{E})$$



Renewal process: next steps

-The microfield modulus is distributed with the pdf $Q(\vec{E})$
-The waiting time for all but the first step obey to a pdf $w(t|\vec{E})$

How to obtain Q , v and w? We require the stationarity of the process, and find:

$$\begin{cases} Q(\vec{E}) = \dfrac{v(0|\vec{E})P(\vec{E})}{\langle v(0|\vec{E}\rangle_S} \\ w(t|\vec{E}) = \dfrac{-\dot{v}(t|\vec{E})}{v(t|\vec{E})} \end{cases}$$

where $<\ldots.>_S$ is a static average over P

The statistical properties of the process are given by P and v

Using the microfield correlation

The pdf P and v have to reflect the main statistical features of the microfield.
We suppose to have isotropic plasma, and use $\mathrm{P(E) = P(\vec{E})4\pi E^2}$
P(E) is known from kinetic theory (Hooper 1968)
We can relate the microfield autocorrelation function Γ_{RP} of the renewal process to v(t | E):

$$\Gamma_{RP}(t) = \int_0^\infty dE E^2 P(E) \int_t^\infty dt' \, \mathrm{v}(t' | E)$$

We can impose that Γ_{RP} is equal to the true microfield correlation:

$$\Gamma_{RP} = \left\langle \vec{E}(0)\vec{E}(t) \right\rangle$$

This expression is available from kinetic theory (Rosenbluth)

Choice of a stochastic process: Kangaroo Process (KP)

Brissaud and Frisch use the KP, a Markovian process losing its memory not only when a jump occurs, but at every time.
For the KP, one obtains that w=v, and

$$w(t|E) = v(E)\exp(-v(E)t)$$

Where v(E)=v(0 | E) is the jumping frequency

This leads to the solution for the KP evolution operator:

$$\left\langle \tilde{U}(\omega) \right\rangle_{KP} = \left\langle \tilde{U}(\omega'|E) \right\rangle_s + \left\langle v(E)\tilde{U}(\omega'|E) \right\rangle_s$$

Static average

$$\left[\left\langle v(E) \right\rangle_s - \left\langle v^2(E)\tilde{U}(\omega'|E) \right\rangle_s \right]^{-1} \left\langle v(E)\tilde{U}(\omega'|E) \right\rangle_s$$

with $\quad \omega' = \omega + iv(E)$

Simulation calculation of the stochastic process

Frerichs proposed in 1989 a simulation of the stochastic process. Applied to the KP, we generate a history of the microfield according to P(E) for the first step, and Q(E) for the following.
The waiting time distribution is

$$v(t \mid E)=v(E)\exp(-v(E)t)$$

At each step, the microfield is constant, and so is the evolution operator. The evolution operator may be written as:

$$U(t_n,0)=U(t_n, t_{n-1})\, U(t_{n-1}, t_{n-2})\ldots\ldots U(t_1,0)$$

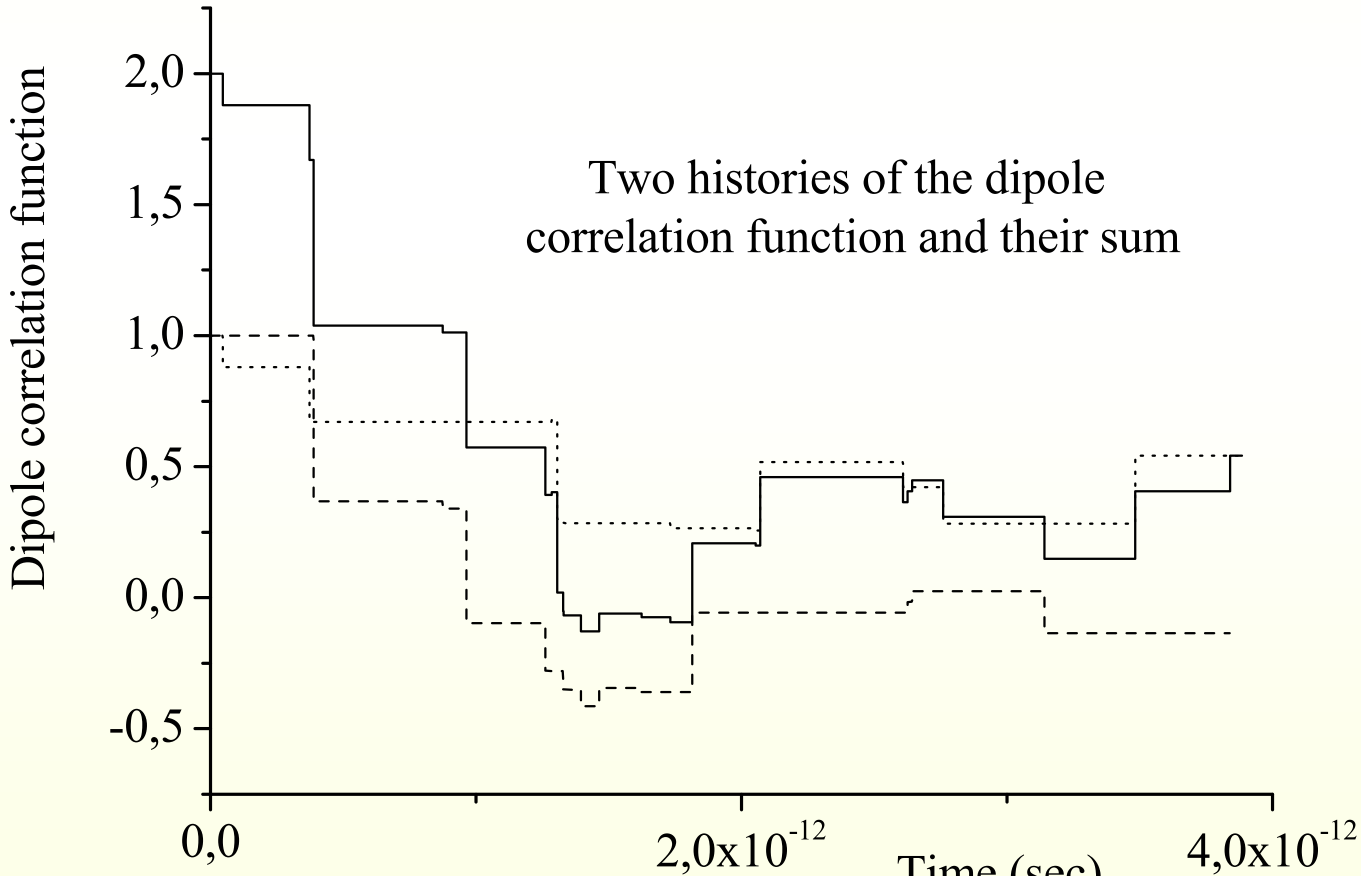
The solution for one history is a product of constant operators

Simulation of the stochastic process

We need to average over a large set of histories

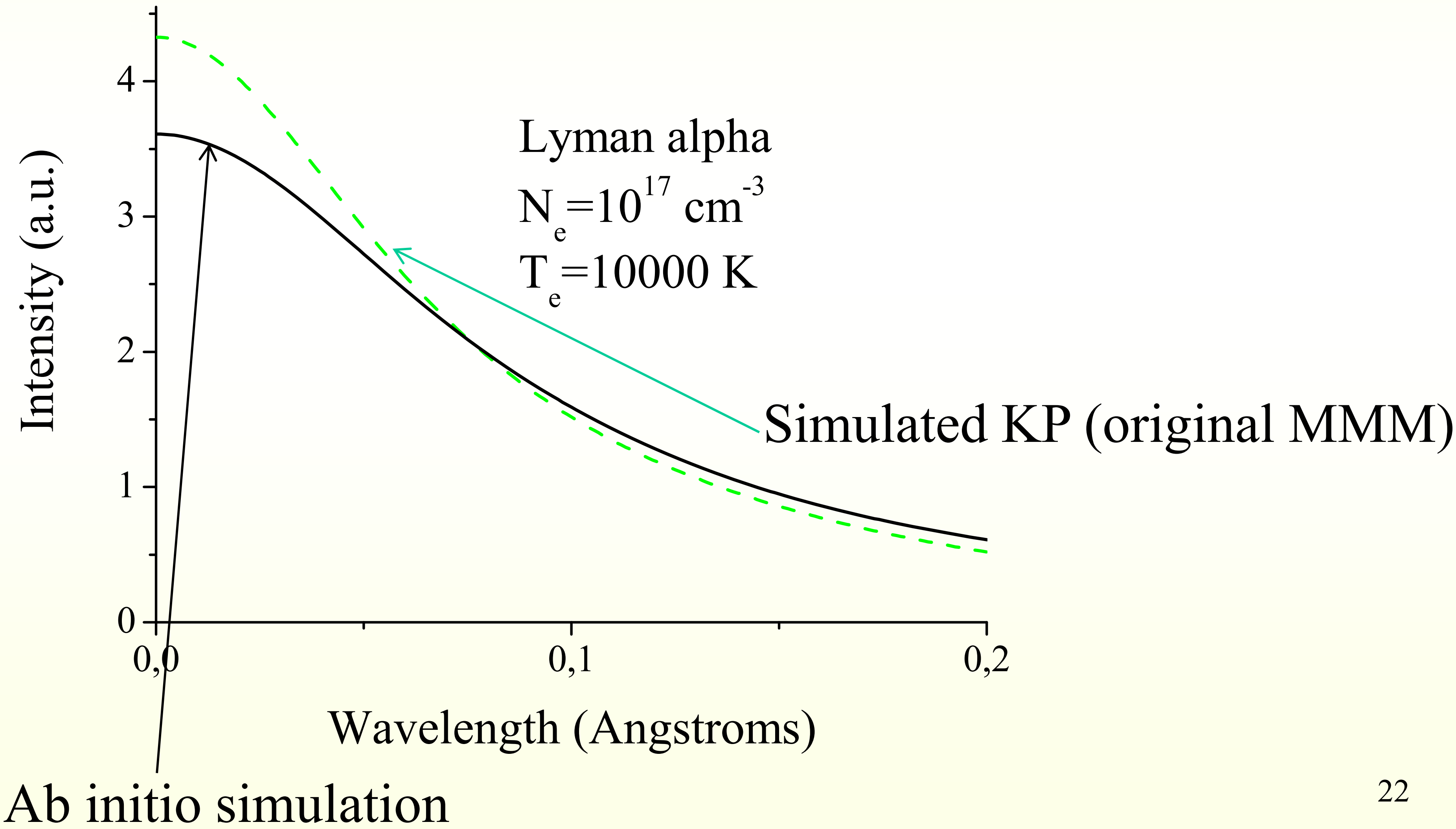
Let us illustrate this on the simple case of Lyman alpha

For each value of the microfield the dipole correlation function is constant



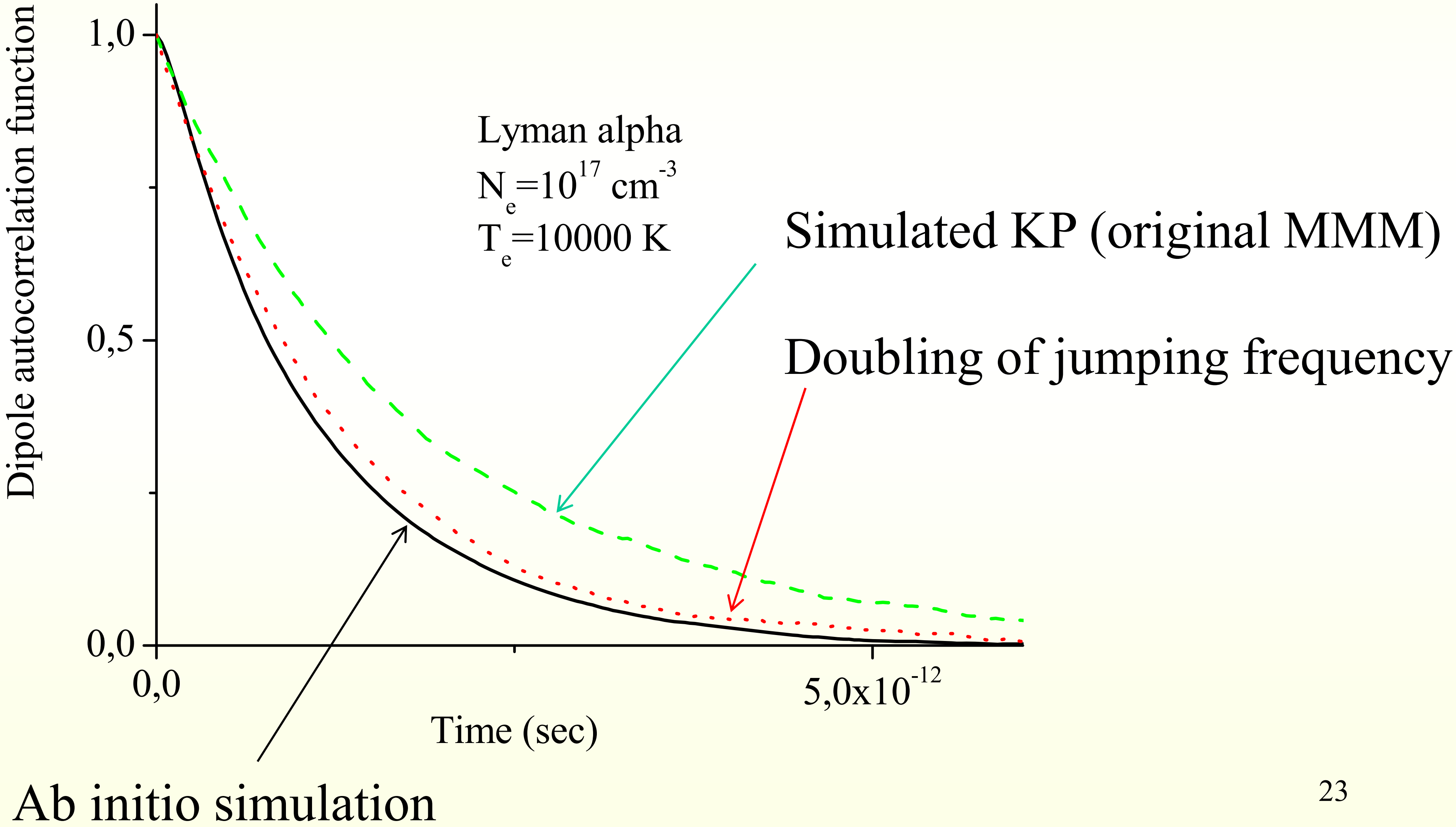
Results for Lyman α

Comparison of line profiles (ions and electrons)



Results for Lyman α

Comparison of dipole correlation functions (ions only)



Other stochastic process: Theta process, CTRW

Seidel proposed the theta process, with a persistent memory

$v(t \mid E)=\theta[T(E) - t]/T(E)$

$w(t \mid E) = \delta[t-T(E)]$

We are also using the continuous time random walk (CTRW) for including memory effects

Our aim is to investigate out of equilibrium plasma affected by turbulence (magnetic fusion, astrophysics)

Waiting time Pdf with long tails (Levy type distribution) are being tested

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Turbulent fluctuations may be represented by a stochastic process

-Atomic populations in presence of temperature fluctuations
-The pdf and correlation functions of the fluctuations are measured

We are looking for the solution of a collisional-radiative model, in presence of a time dependent fluctuation

Array of atomic populations for levels 1 to n;
$X(t)=\{x_1(t), x_2(t)\ldots\ldots x_n(t)\}$

Matrix $M(T(t))$ of transition rates between levels
Fluctuating fluid variable $T(t)$

$dX(t)/dt=M(T(t))\,X(t)$

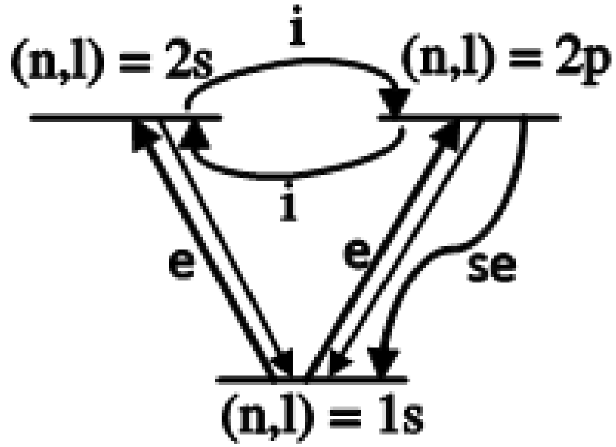
Solution of the kinetic equation

We use an exponential waiting time pdf with a jump frequency v
The Laplace transform $\widetilde{X}(s)$ of X(t) may be written after an average over the fluctuations:

$$\left\langle \widetilde{X}(s) \right\rangle = \left[I - v\widetilde{X}_S(s) \right]^{-1} \widetilde{X}_S(s)$$

Where $\widetilde{X}_S(s)$ is a static average over the fluctuating variable

Effect of fluctuations on the system 1s,2s,2p
-Increase of 2s and 2p populations
-Population of 2s increases by a factor 2 when going from a static regime ($t_{at} << t_{fl}$) to a diabatic one ($t_{at} >> t_{fl}$)



t_{at}: atomic relaxation time, t_{fl}: typical fluctuation time

Summary

-Accurate Stark profile need to retain the dynamics of the ionic field for many astrophysical and laboratory plasma

-Realistic models are provided by ab initio simulation or efficient stochastic processes

-The Kangaroo process may be improved by including memory effects

-Stochastic processes are flexible, and ready to treat several problems in turbulent plasmas