

Developments in beam models

Motion Stark Effect

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Max-Planck-Institut
für Plasmaphysik
EURATOM Assoziation



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The Motion Stark Effect (MSE)

In fusion devices, like tokamaks, Neutral Beam Injectors (NBI) insert high-energy neutral atoms inside the magnetic confined plasma.

As the atoms are neutrals, they do not react **as a hole system** to these magnetic fields, being able to penetrate deeply into the plasma until they are ionised.

Internally, the neutrals can feel simultaneous electric and magnetic fields, which disturb their electronic structure.

The atom is moving rapidly under an intense magnetic field, what causes a Lorentz electric field.

The atom is under the influence of simultaneous electric and magnetic fields.

MSE spectrum diagnostic

MSE spectroscopy to determine magnetic and electric fields in ASDEX-Upgrade Tokamak.

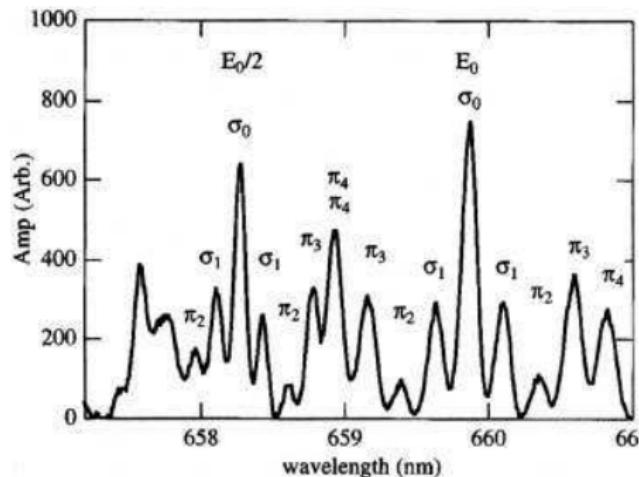


Figure: MSE spectrum of D_{α} line

Diagnostic setup overview

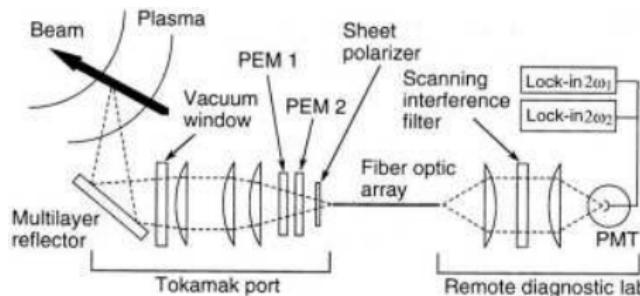


Figure: Schematic overview of MSE diagnostic in ASDEX-Upgrade Tokamak

MSE lines of sight

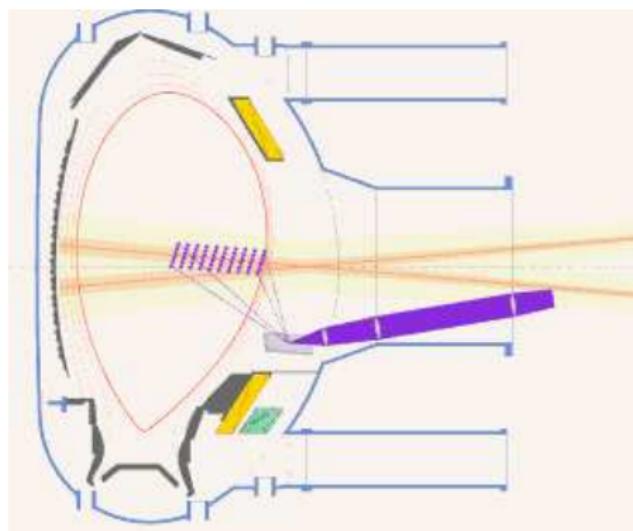


Figure: Poloidal overview of MSE sight lines

MSE diagnostic

MSE lines of sight

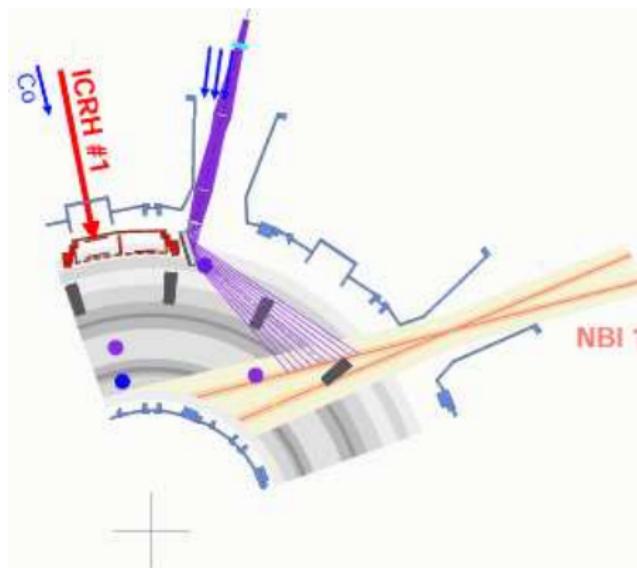


Figure: Toroidal overview of MSE sight lines

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ANNALEN DER PHYSIK.

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1. *Beobachtungen über den Effekt des elektrischen Feldes auf Spektrallinien. I. Quereffekt;¹⁾ von J. Stark.*
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PHYSICAL REVIEW A **88**, 022509 (2013)**Stark effect in neutral hydrogen by direct integration of the Hamiltonian in parabolic coordinates**L. Fernández-Menchero^{1,2} and H. P. Summers¹¹*Atomic Data and Analysis Structure, Department of Physics, University of Strathclyde,
107 Rottenrow East, Glasgow G4 0NG, United Kingdom*²*Max-Planck-Institut für Plasmaphysik, Boltzmannstraße 2, D-85748 Garching, Germany*

(Received 18 June 2013; published 19 August 2013)

We present a theoretical study to determine the energies, widths, and wave functions of the neutral hydrogen atom under a constant electric field by the direct integration of the Hamiltonian in parabolic coordinates. We work in terms of the complex coordinate rotation to distinguish the resonances from the continuum sea, and the wave functions are expanded in a basis set of Laguerre-mesh polynomials. We obtain *ab initio* results for the first five atomic shells of neutral hydrogen for a field intensity up to 10^9 V/m.

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- Inconsistencies of perturbation theory for Stark effect
- The complex coordinate rotation
- Basis set

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The Stark hydrogen atom

$$\begin{aligned}x &= \sqrt{\xi\eta} \cos\phi, & y &= \sqrt{\xi\eta} \sin\phi \\z &= \frac{\xi-\eta}{2}, & r &= \frac{\xi+\eta}{2}\end{aligned}$$

RHA Rydberg hydrogen atom: Solution to the Schrödinger equation for the unperturbed hydrogen atom. Usual wave functions in spherical coordinates and labeled by quantum numbers n , l and m .

SHA Stark hydrogen atom: Solution to the Schrödinger equation for the hydrogen atom under a constant electric field, which can tend to zero. Wave functions described in parabolic coordinates and labeled by quantum numbers n , k and m .

Bethe, H. A. and Salpeter, E. E., 1957, Quantum Mechanics of One- and Two-Electron Systems, New York: Academic Press

Inconsistencies of perturbation theory for Stark effect

Potential

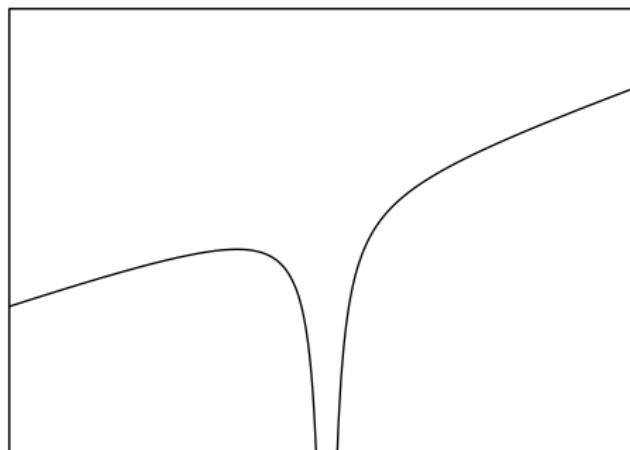


Figure: Diagram showing the behavior of a root in the Hydrogen atom under a constant electric field

Inconsistencies of perturbation theory for Stark effect

Potential

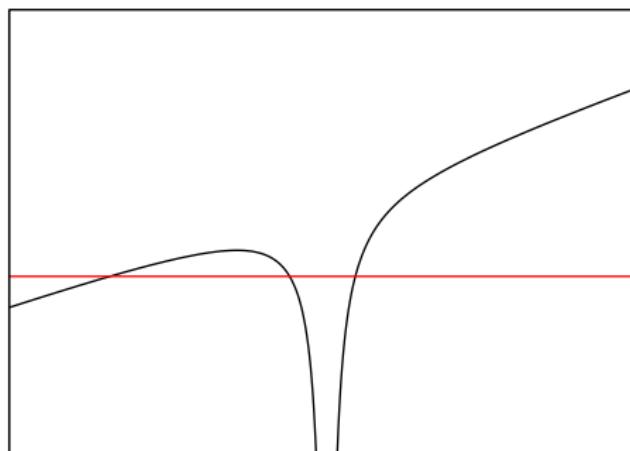


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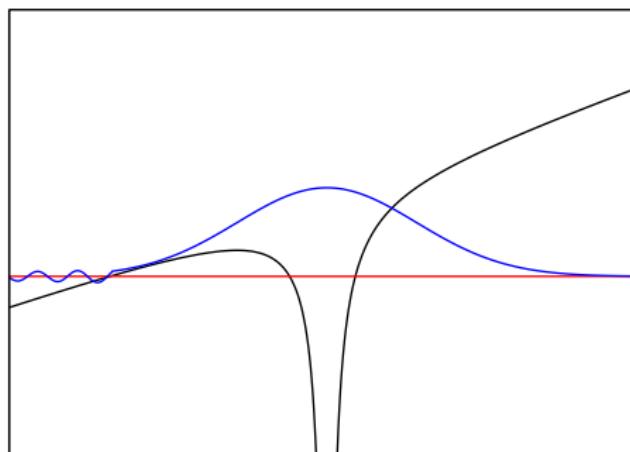


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Inconsistencies of perturbation theory for Stark effect

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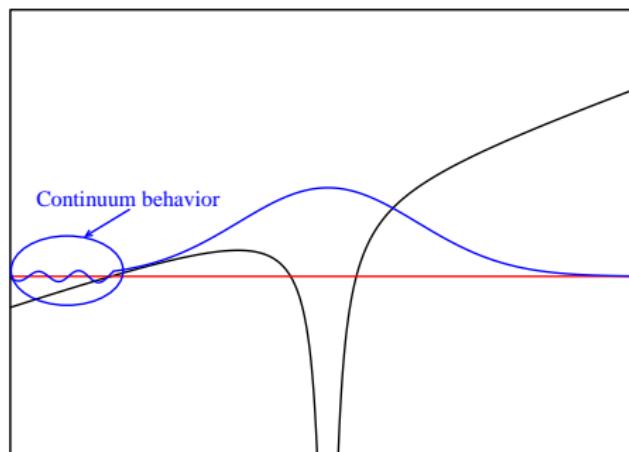


Figure: Diagram showing the behavior of a root in the Hydrogen atom under a constant electric field

Potential

Hydrogen atom under a constant electric field must be determined by any exact method beyond perturbation theory.

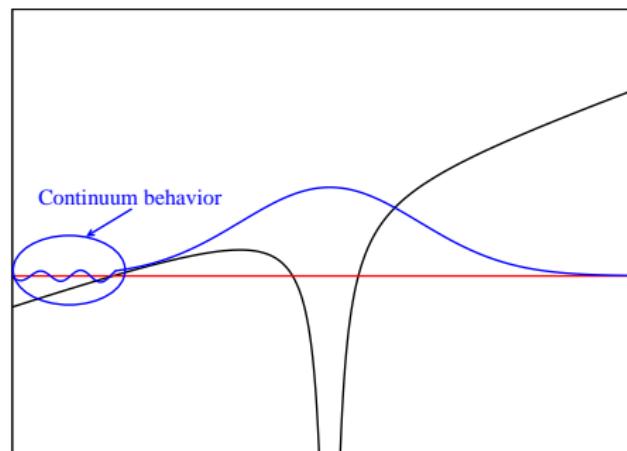


Figure: Diagram showing the behavior of a root in the Hydrogen atom under a constant electric field

The complex coordinate rotation

SHA Hamiltonian. The complex coordinate method.

$$\begin{aligned}H_0 &= -\frac{1}{2\mu} \nabla^2 - \frac{1}{r} + Fr \cos \theta \\&= \frac{2}{\xi + \eta} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) - \frac{2}{\xi + \eta} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) - \frac{1}{2\xi\eta} \frac{\partial^2}{\partial \varphi^2} \\&\quad - \frac{2}{\xi + \eta} + \frac{1}{2} F(\xi - \eta)\end{aligned}$$

The complex coordinate rotation

SHA Hamiltonian. The complex coordinate method.

$$\begin{aligned}H_0 &= -\frac{1}{2\mu} \nabla^2 - \frac{1}{r} + F r \cos \theta \\&= \frac{2}{\xi + \eta} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) - \frac{2}{\xi + \eta} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) - \frac{1}{2\xi\eta} \frac{\partial^2}{\partial \varphi^2} \\&\quad - \frac{2}{\xi + \eta} + \frac{1}{2} F (\xi - \eta)\end{aligned}$$

Complex coordinate rotation.

$$r' = r e^{i\vartheta}$$

The complex coordinate rotation

SHA Hamiltonian. The complex coordinate method.

$$\begin{aligned} H_0(\vartheta) &= -\frac{e^{-2i\vartheta}}{2\mu} \nabla^2 - \frac{e^{-i\vartheta}}{r} + e^{i\vartheta} F r \cos \theta \\ &= \frac{2e^{-2i\vartheta}}{\xi + \eta} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) - \frac{2e^{-2i\vartheta}}{\xi + \eta} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) - \frac{e^{-2i\vartheta}}{2\xi\eta} \frac{\partial^2}{\partial \varphi^2} \\ &\quad - \frac{2e^{-i\vartheta}}{\xi + \eta} + \frac{e^{i\vartheta}}{2} F (\xi - \eta) \end{aligned}$$

Complex coordinate rotation.

$$r' = r e^{i\vartheta}$$

Basis set

Variational method: basis set

$$\Psi(\xi, \eta, \varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} (\xi\eta)^{\frac{|m|}{2}} e^{-\frac{\xi+\eta}{2}} \sum_{k=1}^N \sum_{l=1}^N c_{klm} \Lambda_{Nk}(\xi) \Lambda_{Nl}(\eta)$$

Lagrange-Laguerre-mesh polynomials:

$$\Lambda_{Ni}(x) = (-1)^i \sqrt{x_i} \frac{L_N(x)}{x - x_i}$$

x_i : zeros of the Laguerre polynomial $L_N(x)$.

Secular equation

$$S_{klk'l'm} = \left\langle (\xi\eta)^{\frac{|m|}{2}} e^{-\frac{\xi+\eta}{2}} \Lambda_{Nk} \Lambda_{NI} \mid (\xi\eta)^{\frac{|m|}{2}} e^{-\frac{\xi+\eta}{2}} \Lambda_{Nk} \Lambda_{NI} \right\rangle$$

$$H_{klk'l'm}(\vartheta) = \left\langle (\xi\eta)^{\frac{|m|}{2}} e^{-\frac{\xi+\eta}{2}} \Lambda_{Nk} \Lambda_{NI} \mid \hat{H}(\vartheta) \mid (\xi\eta)^{\frac{|m|}{2}} e^{-\frac{\xi+\eta}{2}} \Lambda_{Nk} \Lambda_{NI} \right\rangle$$

Secular equation

$$(\mathbf{H} - \mathbf{E}\mathbf{S})\mathbf{C} = 0$$

For further detail:

L. F. Menchero and H. P. Summers, Max Planck Institute for Plasma Physics, Report No. IPP-10/49, 2013, internal report,
<http://edoc.mpg.de/display.epl?mode=doc&id=656145>.

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- Wave functions
- Derived quantities

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Energies and widths

Found eigenvalues

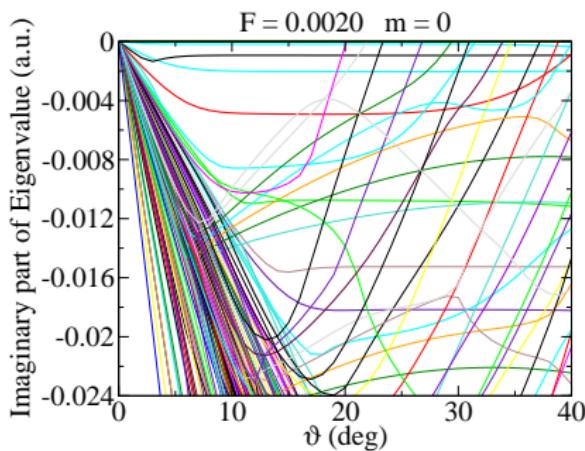
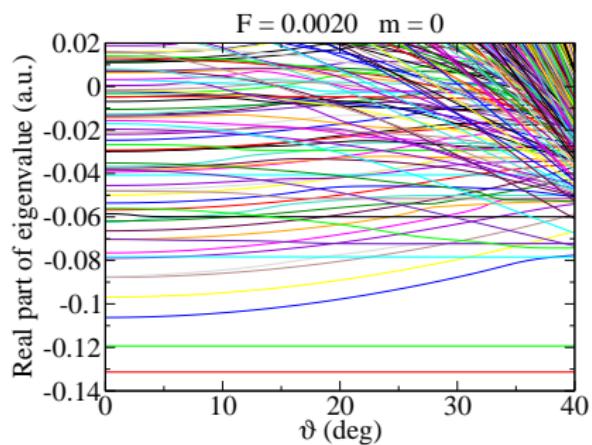


Figure: Obtained eigenvalues for a basis set $N = 30$ for $m = 0$ and a field intensity $F = 0.0020$ a.u. Marked some found resonances.

Energies and widths

Found eigenvalues

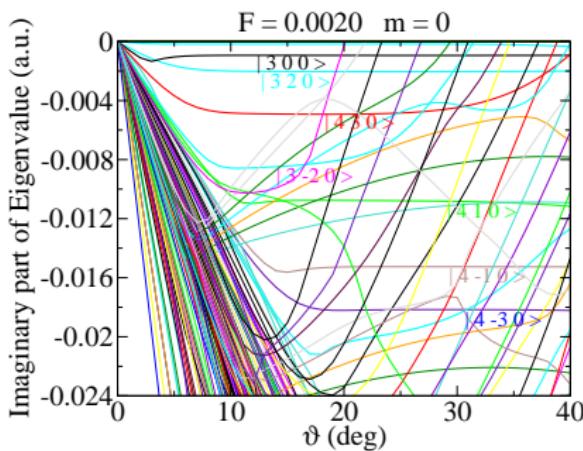
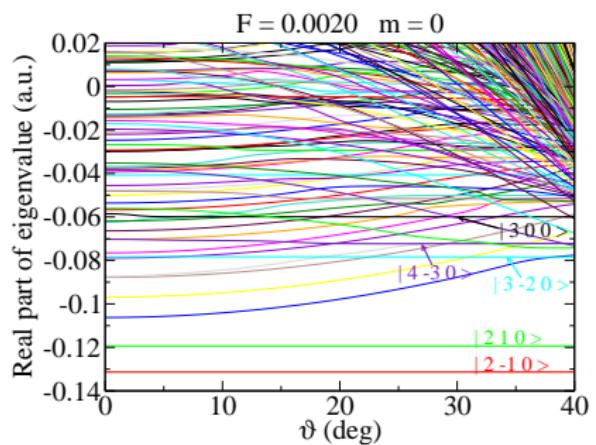


Figure: Obtained eigenvalues for a basis set $N = 30$ for $m = 0$ and a field intensity $F = 0.0020$ a.u. Marked some found resonances.

Energies and widths

Energies

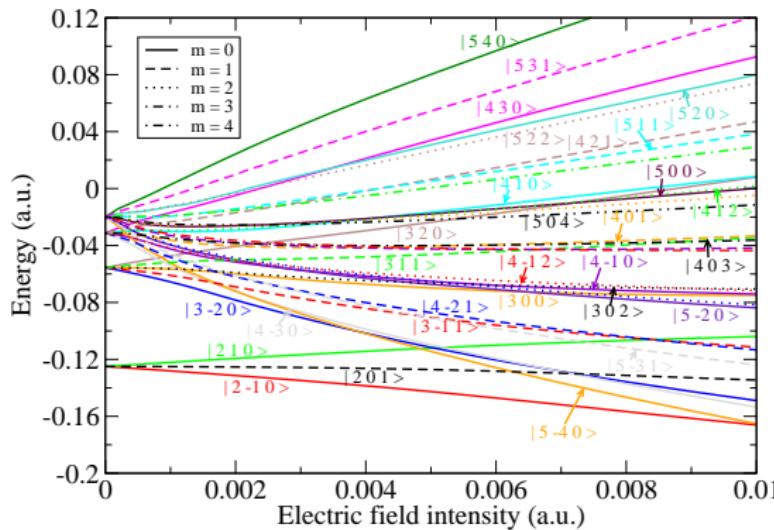


Figure: State energies of the H atom versus electric field intensity for $m = 0 - 4$.

Energies and widths

Widths

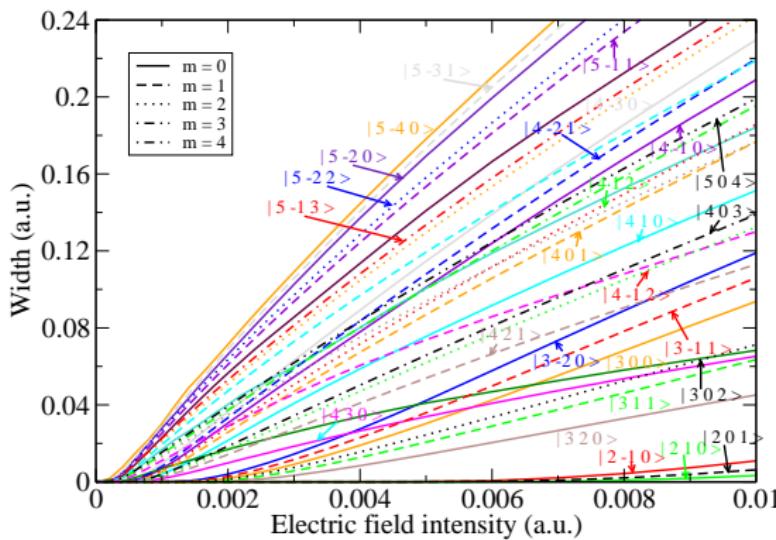


Figure: State widths of the H atom versus electric field intensity for $m = 0 - 4$.

Wave functions

Wave functions

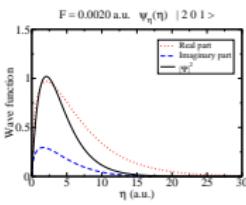
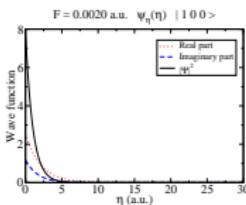
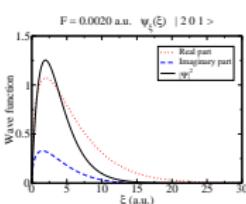
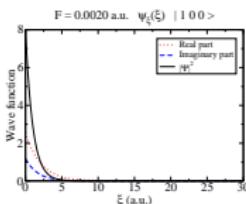
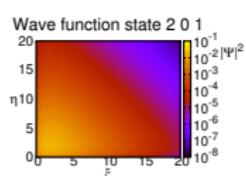
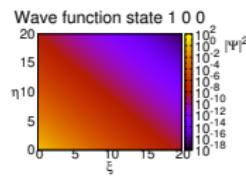


Figure: Wave function of the Stark states $|1\ 0\ 0\rangle$ and $|2\ 0\ 1\rangle$ for a field intensity of $F = 0.0020 \text{ a.u.}$

Wave functions

Wave functions

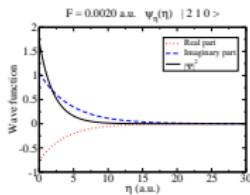
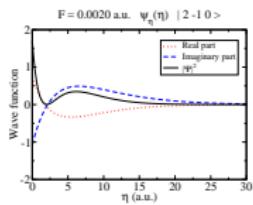
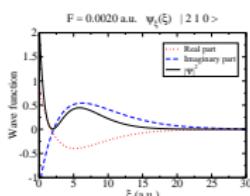
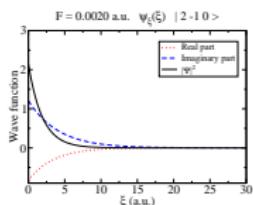
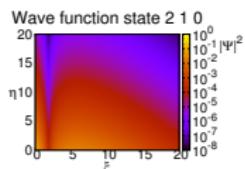
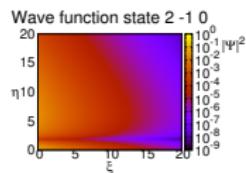


Figure: Wave function of the Stark states $|2-10\rangle$ and $|210\rangle$ for a field intensity of $F = 0.0020 \text{ a.u.}$

Derived quantities

Einstein transition coefficients

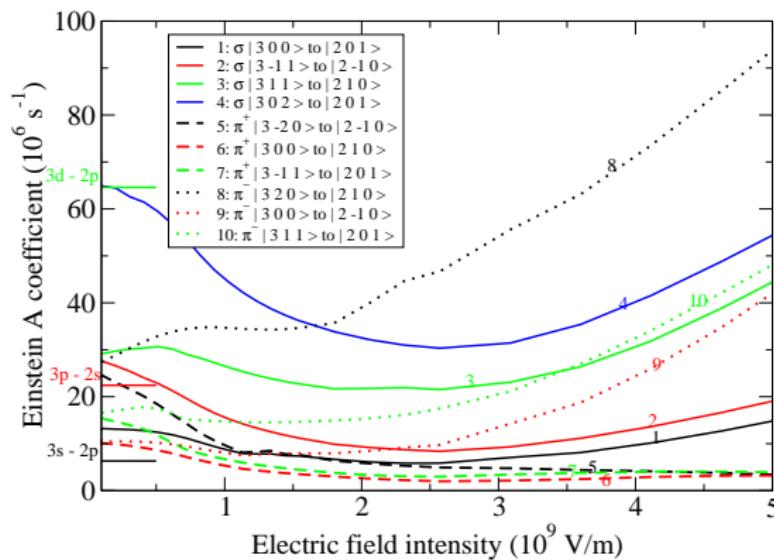


Figure: Einstein spontaneous emission coefficients of neutral hydrogen versus the electric field intensity. Marked the values for the Rydberg Hydrogen Atom for zero field intensity.

Derived quantities

Balmer D_α line splitting

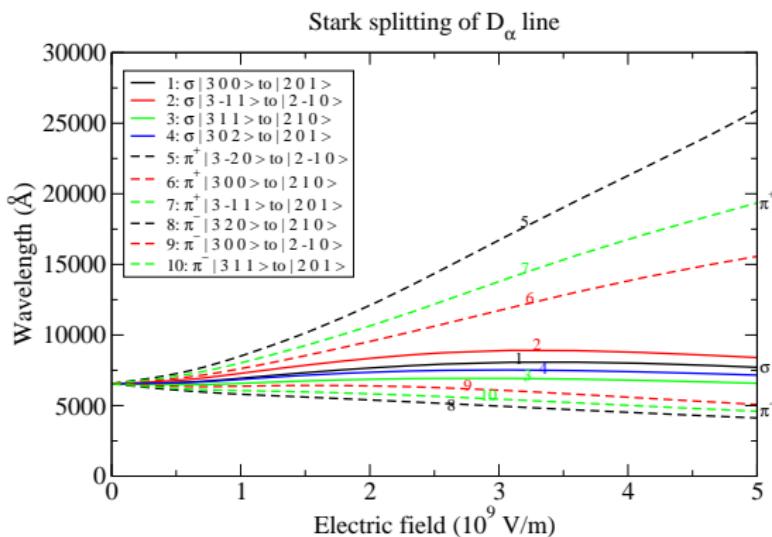


Figure: Stark splitting of the D_α line of deuterium versus the electric field intensity.

Derived quantities

Balmer D_{α} line splitting

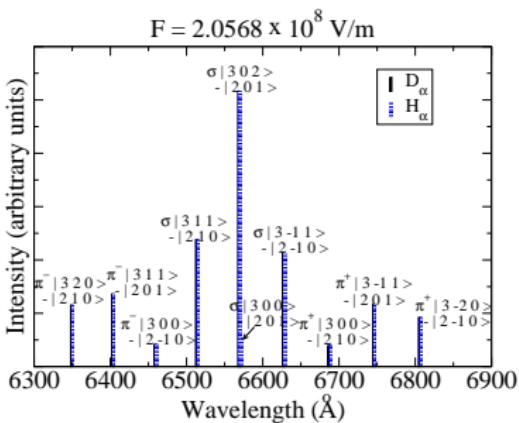
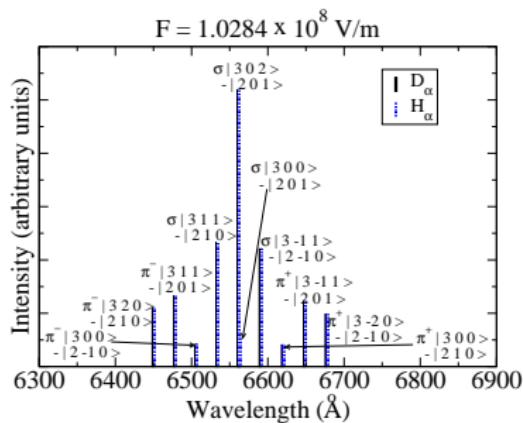


Figure: Emission profile of the Balmer D_{α} and H_{α} lines for two different field intensities in corona equilibrium.

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Conclusions

- A method to solve the hydrogen atom under a constant electric field has been developed beyond perturbation theory.
- Stark energies, widths and wave functions nkm have been determined up to $n = 5$.
- Wave functions can be used to get any physical observable.
- Further effects (fine structure, static magnetic field) can be added as perturbations of the Stark wave functions.
- A background has been prepared to develop a collision-radiative model for hydrogen atom under a constant electric field.
- Results are collected in [adf50](#) format.

Further work

- Use the obtained wave functions to calculate directional cross sections of collision with SHA: electron impact, ion impact, charge exchange.
- Include these cross sections and Einstein coefficients in the collision-radiative model for hydrogen atom under constant simultaneous electric and magnetic field.
- Collect all in a second version of [ADAS305](#).

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