

(Motion) Stark Effect models

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 EURATOM Association

University of
Strathclyde
 Science



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- 2 Solution of the Schorödinger Equation
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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.

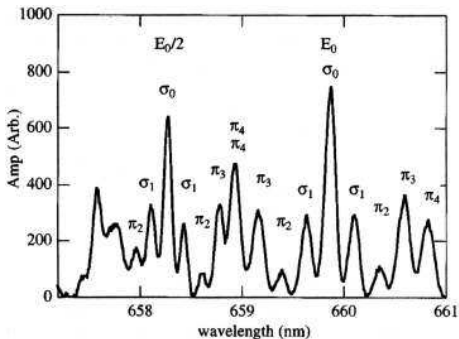


Figure: MSE spectrum of D α line

Diagnostic setup overview

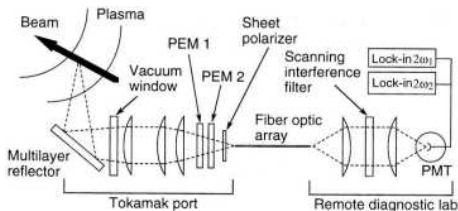


Figure: Schematic overview of MSE diagnostic in ASDEX-Upgrade Tokamak

MSE lines of sight

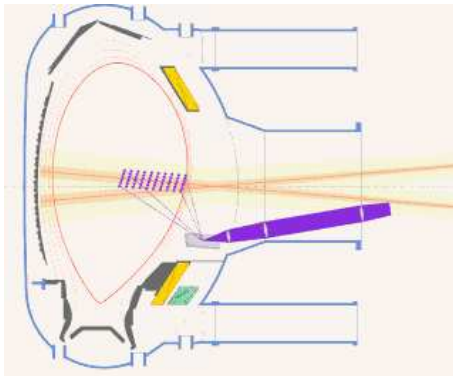


Figure: Poloidal overview of MSE sight lines

MSE lines of sight

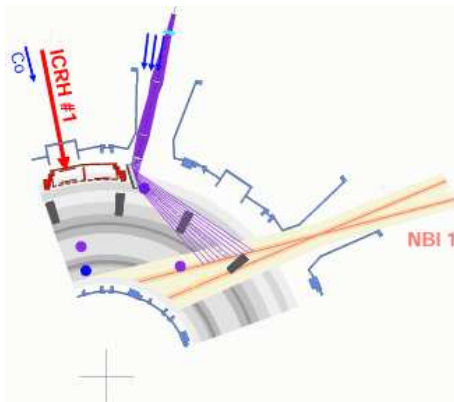


Figure: Toroidal overview of MSE sight lines

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Hamiltonian

- Zero order: Coulomb and external constant electric field.
- Perturbation: constant magnetic field and fine structure.

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

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

SHA Hamiltonian. The complex coordinate method.

Zero order Hamiltonian:

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

SHA Hamiltonian. The complex coordinate method.

Zero order Hamiltonian:

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 H_0 &= -\frac{1}{2\mu} \nabla^2 - \frac{1}{r} + F r \cos \theta \\
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 \end{aligned}$$

Complex coordinate rotation.

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

SHA Hamiltonian. The complex coordinate method.

Zero order Hamiltonian:

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

Complex coordinate rotation.

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

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

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

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

Secular equation

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

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Calculated eigenvalues

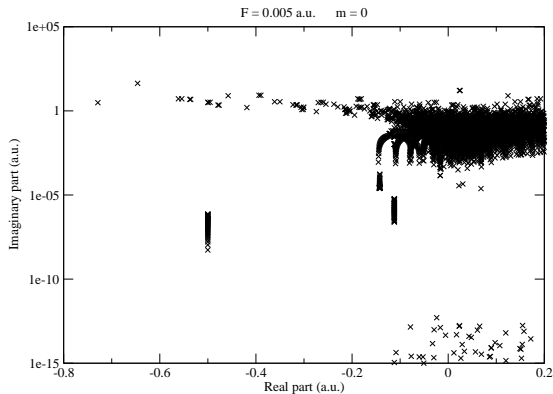


Figure: Calculated eigenvalues for H atom under a constant electric field for several values of the complex rotation angle ϑ .

Calculated eigenvalues

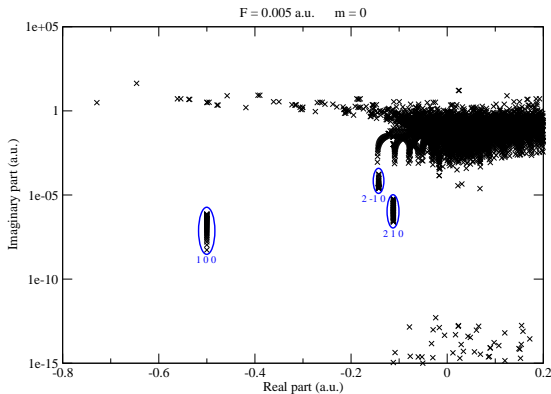


Figure: Calculated eigenvalues for H atom under a constant electric field for several values of the complex rotation angle ϑ .

Energies

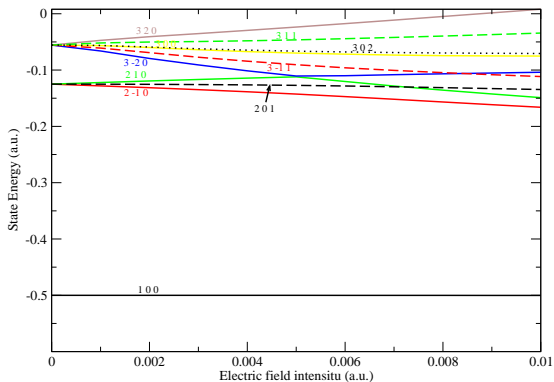


Figure: State energies of the H atom versus electric field intensity for $m = 0, 1, 2$.

Widths

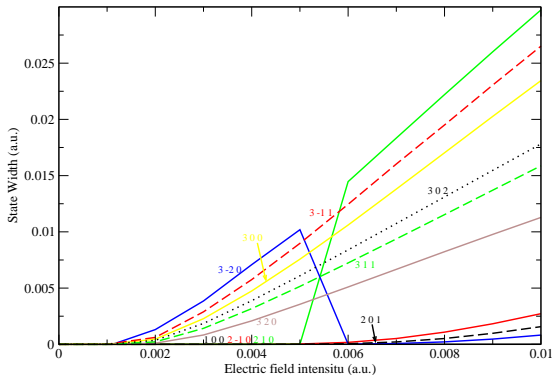


Figure: State widths of the H atom versus electric field intensity for $m = 0, 1, 2$.

Stark splitting of H_{α} line

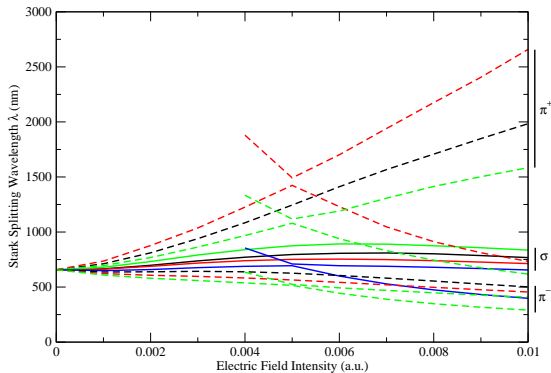


Figure: Stark splitting of H_{α} line versus electric field intensity.

Wave functions

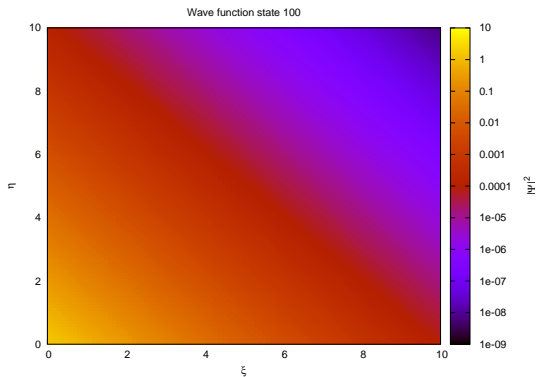


Figure: Wave function of the state 100 of the H atom under a constant electric field of 0.005 a.u..

Wave functions

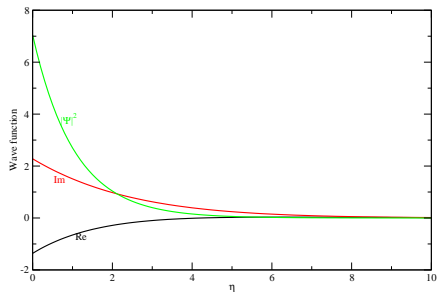
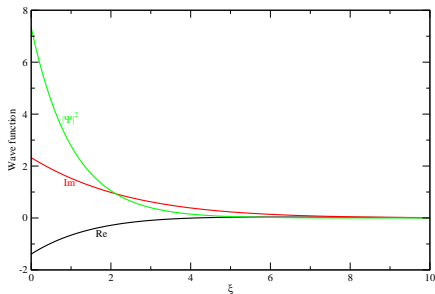


Figure: Wave function of the state 100 of the H atom under a constant electric field of 0.005 a.u..

Wave functions

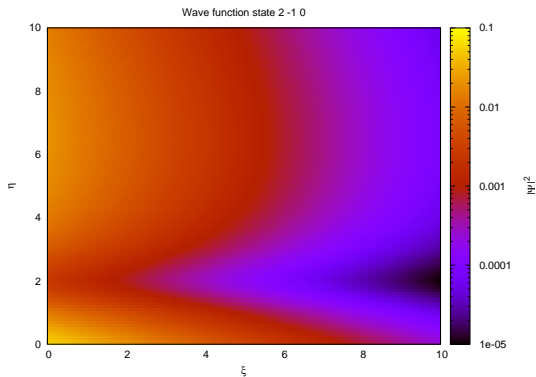


Figure: Wave function of the state 2 – 10 of the H atom under a constant electric field of 0.005 a.u..

Wave functions

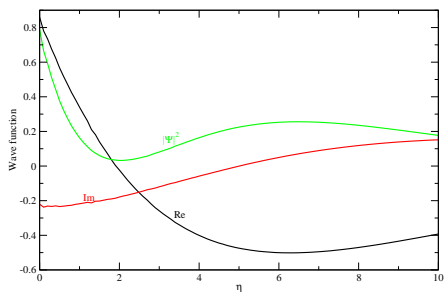
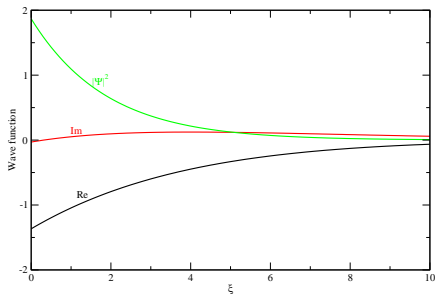


Figure: Wave function of the state 2 – 10 of the H atom under a constant electric field of 0.005 a.u..

Wave functions

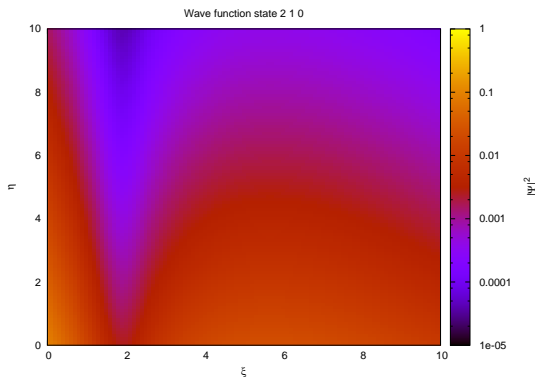


Figure: Wave function of the state 210 of the H atom under a constant electric field of 0.005 a.u..

Wave functions

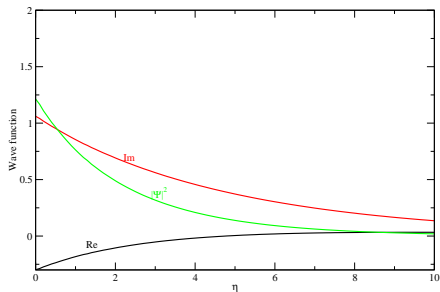
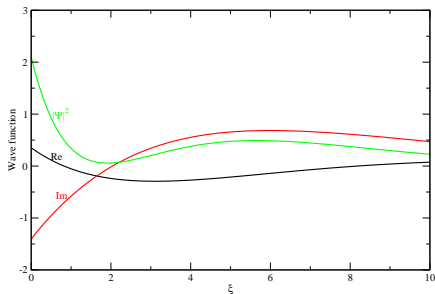


Figure: Wave function of the state 210 of the H atom under a constant electric field of 0.005 a.u..

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Conclusions

- Stark wave functions nkm should be determined.
- Cross sections and Einstein coefficients between Stark states.
- Include directionality.
- As “rough” approximation cross sections and Einstein coefficients for Rydberg states can be used.

Future work

- Use the obtained wave functions to calculate directional cross sections of collision with SHA: electron impact, ion impact, charge exchange.
- Obtain Einstein coefficients for SHA: directional emission.
- Include these cross sections and Einstein coefficients in the collision-radiative model of ADAS305.

Acknowledgments

Thanks to:

ASDEX-Upgrade MSE diagnosis team: M. Reich and J. Hobirk.