Developments in beam models

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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 fell 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.

$$\vec{F} = \frac{1}{c}\vec{v}\times\vec{B}$$

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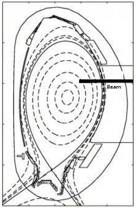
Hydrogen atom in motion under constant electric and magnetic fields

- Projectile momentum vector $\vec{K}$ z-axis.
- Magnetic field vector $\vec{B}$, zx-plane.
- External electric field vector $\vec{F}_{\rm ext}$, any direction.
- Lorenz electric field $\vec{F}_{\rm Lor}$, y-axis.



$$\begin{aligned}
\vec{K} &= K\,\hat{z} \\
\vec{B} &= B_z\,\hat{z} + B_x\,\hat{x} \\
\vec{F}_{\rm ext} &= F_z\,\hat{z} + F_x\,\hat{x} + F_y\,\hat{y} \\
\vec{F}_{\rm Lor} &= \frac{1}{Mc}\,K\,B_x\,\hat{y} \\
\vec{F} &= F_z\,\hat{z} + F_x\,\hat{x} + (F_y + \frac{1}{Mc}\,K\,B_x)\,\hat{y}
\end{aligned}$$

MSE spectrum diagnostic

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

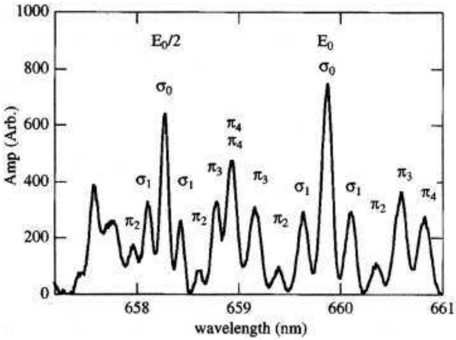


Figure: MSE spectrum of D_α line

Diagnostic setup overview

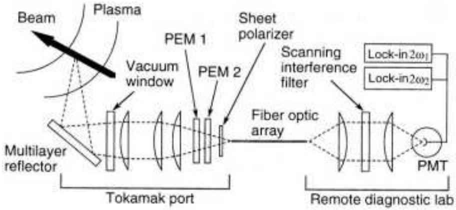


Figure: Schematic overview of MSE diagnostic in ASDEX-Upgrade Tokamak

MSE lines of sight

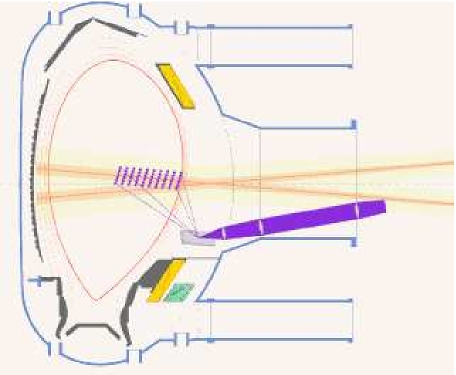


Figure: Poloidal overview of MSE sight lines

MSE lines of sight

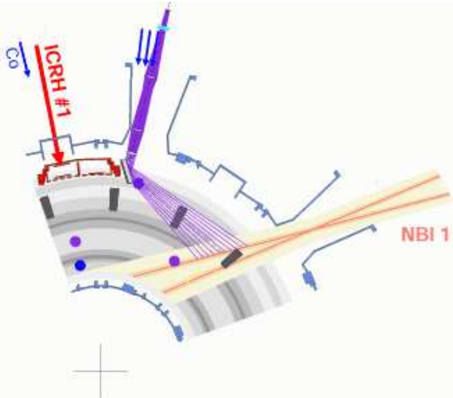


Figure: Toroidal overview of MSE sight lines

Hamiltonian

$$H = H_0 + H_F + H_B + H_{fe}$$

$$H_0 = -\frac{1}{2\mu}\nabla^2 - \frac{1}{r}$$

$$H_F = F\,z = F\,r\cos\theta$$

$$H_B = \frac{\mu_B}{\mu} B_z\left(L_z + g_e S_z\right) + \frac{\mu_B}{\mu} B_x\left(L_x + g_e S_x\right)$$

$$H_{fe} = -\frac{p^4}{8\mu^3 c^2} + \frac{1}{2}\frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r^3}\vec{L}\cdot\vec{S} + \frac{\hbar^2}{8\mu^2 c^2}\frac{Ze^2}{4\pi\epsilon_0}4\pi\delta^{(3)}(\vec{r})$$

Hamiltonian

Zero order Hamiltonian:

$$H_0 \; = \; -\frac{1}{2\mu}\,\nabla^2 \; - \; \frac{1}{r} \; + \; F\,r\,\cos\theta$$

Complex coordinate integration method.

$H_B + H_{fe}$ Perturbation theory.

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Field-free Stark Hydrogen Atom

Parabolic coordinates:

$$\begin{aligned} \xi &= r + z = r\,(1 + \cos\theta) \\ \eta &= r - z = r\,(1 - \cos\theta) \\ \tan\phi &= \frac{y}{x} \end{aligned}$$

Wave function

$$\Psi = \frac{1}{\sqrt{2\pi}}\, u(\xi)\, v(\eta)\, \mathrm{e}^{im\phi}$$

Schrödinger Equation:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\xi}\left(\xi\,\frac{\mathrm{d}u}{\mathrm{d}\xi}\right) + \left(E\,\frac{\xi}{2} + Z_1 - \frac{m^2}{4\xi} - F\,\frac{\xi^2}{4}\right) u &= 0 \\ \frac{\mathrm{d}}{\mathrm{d}\eta}\left(\eta\,\frac{\mathrm{d}v}{\mathrm{d}\eta}\right) + \left(E\,\frac{\eta}{2} + Z_2 - \frac{m^2}{4\eta} + F\,\frac{\eta^2}{4}\right) v &= 0\,. \end{aligned}$$

$$Z_1 + Z_2 = 1$$

Field-free Stark Hydrogen Atom

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$$Z_1 + Z_2 = 1$$

Field-free Stark Hydrogen Atom

Solution $F = 0$ bounded states:
Bethe, H. A. and Salpeter, E. E., 1957, Quantum Mechanics of One- and Two-Electron Systems, New York: Academic Press

$$
\begin{aligned}
Z_{1 n_1 n_2 m} &= \frac{2n_1 + m + 1}{2(n_1 + n_2 + m + 1)} \\
Z_{2 n_1 n_2 m} &= \frac{2n_2 + m + 1}{2(n_1 + n_2 + m + 1)} \\
E_{n_1 n_2 m} &= -\frac{1}{2\,(n_1 + n_2 + m + 1)^2}
\end{aligned}
$$

$$
\begin{aligned}
u_{n_1 n_2 m}(\xi) &= N_u \sqrt{\epsilon}\, \mathrm{e}^{-\frac{1}{2}\epsilon\xi} (\epsilon\xi)^{\frac{m}{2}}\, \mathrm{L}_{n_1}^{m}(\epsilon\xi) \\
v_{n_1 n_2 m}(\eta) &= N_v \sqrt{\epsilon}\, \mathrm{e}^{-\frac{1}{2}\epsilon\eta} (\epsilon\eta)^{\frac{m}{2}}\, \mathrm{L}_{n_2}^{m}(\epsilon\eta)
\end{aligned}
$$

$$
\begin{aligned}
\epsilon &= 2\sqrt{-E} \\
n &= n_1 + n_2 + m + 1 \\
k &= n_1 - n_2
\end{aligned}
$$

Perturbation Hamiltonian for SHA

$$H^{(0)} = \frac{\mathrm{d}}{\mathrm{d}x}\left(x\,\frac{\mathrm{d}u}{\mathrm{d}x}\right) + E\,\frac{x}{2} - \frac{m^2}{4x}$$

$$H^{(1)} = \mp F\,\frac{x^2}{4}\,,$$

with $x = \xi, \eta$.

$$Z^{(0)}_{(1,2)} = \frac{2n_{1,2} + m + 1}{2(n_1 + n_2 + m + 1)}$$

$$E^{(0)} = -\frac{1}{2(n_1 + n_2 + m + 1)^2}$$

$$u^{(0)}_{(1,2)}(x) = N\,\sqrt{\epsilon}\,\mathrm{e}^{-\frac{1}{2}\epsilon x}\,(\epsilon x)^{\frac{m}{2}}\,\mathrm{L}^{m}_{n_{(1,2)}}(\epsilon x)$$

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Perturbation Hamiltonian for SHA

First order perturbation theory

$$-Z^{(1)}_{(1,2)} = \frac{\left\langle u^{(0)} \left| \mp \frac{1}{4} F \xi^2 \right| u^{(0)} \right\rangle}{\left\langle u^{(0)} \mid u^{(0)} \right\rangle}$$

$$Z_1 + Z_2 = 1$$

$$u^{(1)}_{n_{(1,2)}}(\xi) = \pm \frac{F}{4\epsilon^2} \sum_{n' \neq n_{(1,2)}} \frac{1}{-Z^{(0)}_{1n'} + Z^{(0)}_{1n_{(1,2)}}} \frac{\left\langle u^{(0)}_{n'} \left| (\epsilon x)^2 \right| u^{(0)}_{n_{(1,2)}} \right\rangle}{\sqrt{\left\langle u^{(0)}_{n'} \middle| u^{(0)}_{n'} \right\rangle \left\langle u^{(0)}_{n_{(1,2)}} \middle| u^{(0)}_{n_{(1,2)}} \right\rangle}} u^{(0)}_{n'}$$

$$- \frac{F}{4\epsilon^2} \int_0^\infty \mathrm{d}k_{(1,2)} \frac{1}{-Z'^{(0)}_{(1,2)}(k_{(1,2)}) + Z^{(0)}_{1n_{(1,2)}}}$$

$$\times \frac{\left\langle u'(k_{(1,2)})^{(0)} \left| (\epsilon \xi)^2 \right| u^{(0)}_{n_{(1,2)}} \right\rangle}{\sqrt{\left\langle u'^{(0)}(k_{(1,2)}) \middle| u'^{(0)}(k_{(1,2)}) \right\rangle \left\langle u^{(0)}_{n_{(1,2)}} \middle| u^{(0)}_{n_{(1,2)}} \right\rangle}} u'^{(0)}(k_{(1,2)})$$

Perturbation Hamiltonian for SHA

First order perturbation theory

$$Z_1 + Z_2 = (n_1 + n_2 + m + 1)\left(\epsilon + \frac{3}{2}\frac{F}{\epsilon^2}(n_1 - n_2)\right)$$

$$E^{(0)} + E^{(1)} = -\frac{1}{2n^2} + \frac{3}{2} F\, n\, k + O(F^2)$$

$$\begin{aligned}
u^{(1)}_{n_{(1,2)}}(\xi) = {} & \frac{1}{4}\frac{F}{\epsilon^{(0)3}}\, \mathrm{e}^{-\frac{1}{2}\epsilon^{(0)}\xi}\, (\epsilon^{(0)}\xi)^{\frac{m}{2}} \\
& \Big[-\frac{1}{2}\sqrt{n_{(1,2)}(n_{(1,2)}-1)(n_{(1,2)}+m)(n_{(1,2)}+m+1)}\, \mathrm{L}^{|m|}_{n_{(1,2)}-2}(\epsilon^{(0)}\xi) \\
& + 2\sqrt{n_{(1,2)}(n_{(1,2)}+m)(2n_{(1,2)}+m)^2}\, \mathrm{L}^{|m|}_{n_{(1,2)}-1}(\epsilon^{(0)}\xi) \\
& - 2\sqrt{(n_{(1,2)}+m)(n_{(1,2)}+m+1)(2n_{(1,2)}+m+2)^2}\, \mathrm{L}^{|m|}_{n_{(1,2)}+1}(\epsilon^{(0)}\xi) \\
& + \frac{1}{2}\sqrt{(n_{(1,2)}+1)(n_{(1,2)}+2)(n_{(1,2)}+m+1)(n_{(1,2)}+m+2)}\, \mathrm{L}^{|m|}_{n_{(1,2)}+2}(\epsilon^{(0)}\xi)\Big]
\end{aligned}$$

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Perturbation Hamiltonian for SHA

First order perturbation theory

$$Z_1 + Z_2 = (n_1 + n_2 + m + 1)\left(\epsilon + \frac{3}{2}\frac{F}{\epsilon^2}(n_1 - n_2)\right)$$

$$E^{(0)} + E^{(1)} = -\frac{1}{2n^2} + \underbrace{\frac{3}{2} F\, n\, k}_{\text{Linear Stark Effect}} + O(F^2)$$

$$\begin{aligned}
u^{(1)}_{n_{(1,2)}}(\xi) = {} & \frac{1}{4}\frac{F}{\epsilon^{(0)3}}\, \mathrm{e}^{-\frac{1}{2}\epsilon^{(0)}\xi}\, (\epsilon^{(0)}\xi)^{\frac{m}{2}} \\
& \Big[-\frac{1}{2}\sqrt{n_{(1,2)}(n_{(1,2)}-1)(n_{(1,2)}+m)(n_{(1,2)}+m+1)}\, \mathrm{L}^{|m|}_{n_{(1,2)}-2}(\epsilon^{(0)}\xi) \\
& + 2\sqrt{n_{(1,2)}(n_{(1,2)}+m)(2n_{(1,2)}+m)^2}\, \mathrm{L}^{|m|}_{n_{(1,2)}-1}(\epsilon^{(0)}\xi) \\
& - 2\sqrt{(n_{(1,2)}+m)(n_{(1,2)}+m+1)(2n_{(1,2)}+m+2)^2}\, \mathrm{L}^{|m|}_{n_{(1,2)}+1}(\epsilon^{(0)}\xi) \\
& + \frac{1}{2}\sqrt{(n_{(1,2)}+1)(n_{(1,2)}+2)(n_{(1,2)}+m+1)(n_{(1,2)}+m+2)}\, \mathrm{L}^{|m|}_{n_{(1,2)}+2}(\epsilon^{(0)}\xi)\Big]
\end{aligned}$$

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Energies

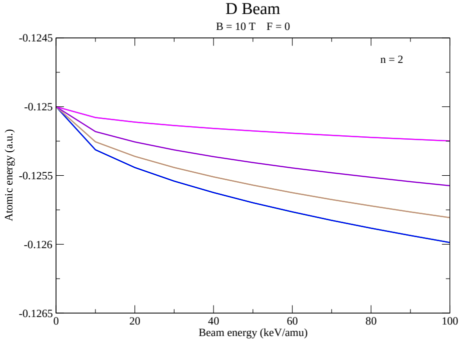
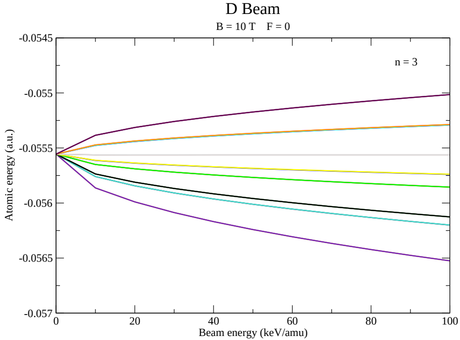


Figure: MSE energies for a D beam.

Energies



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Energies

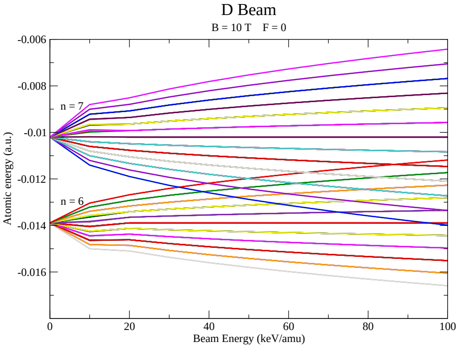


Figure: MSE energies for a D beam.

Wave functions

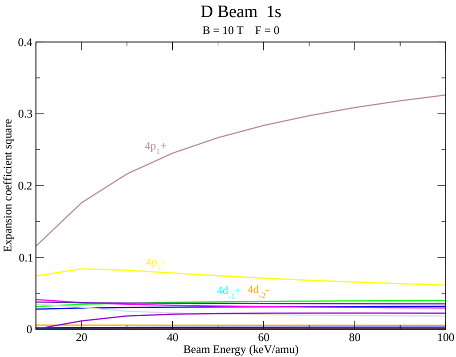
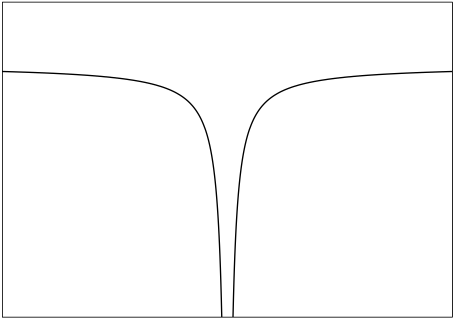
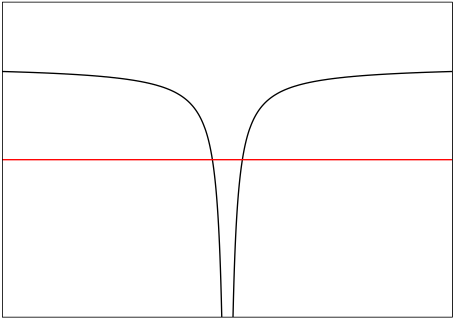


Figure: Coefficients of the expansion of the $|1\,0\,0\rangle$ Stark level of the D atom

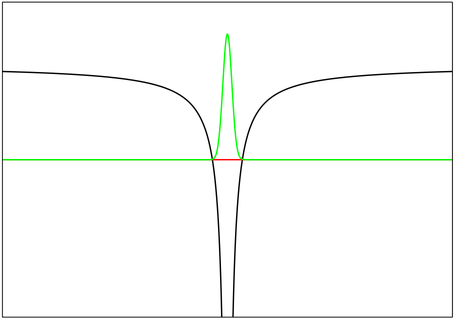
Field-free hydrogen atom



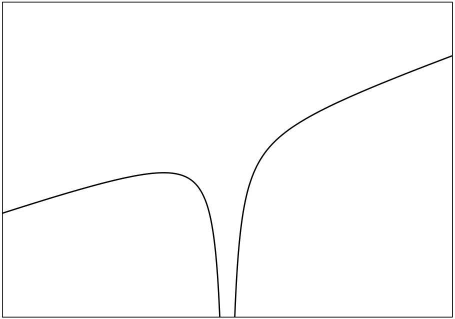
Field-free hydrogen atom



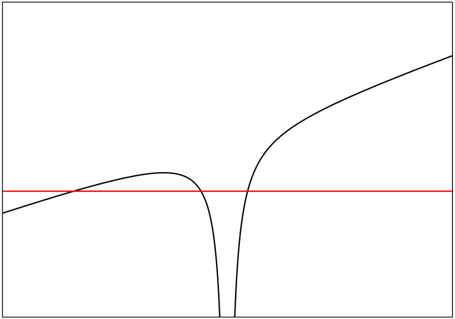
Field-free hydrogen atom



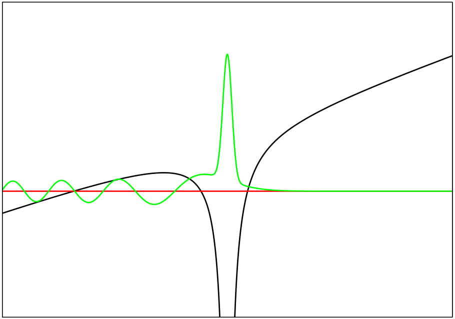
Hydrogen atom under a constant electric field



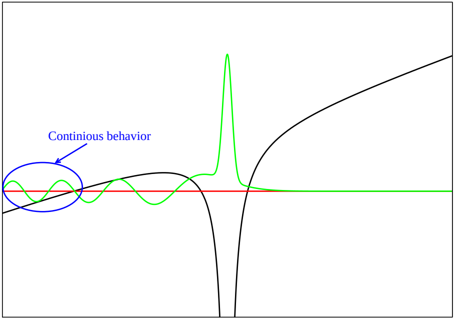
Hydrogen atom under a constant electric field



Hydrogen atom under a constant electric field



Hydrogen atom under a constant electric field



Problems with perturbation theory for Stark effect

- Perturbation does not tend to zero asymptotically.
  Perturbation dominates at long distances!
- Topology of the spectrum absolutely different.
  Any real number is eigenvalue of Stark Hamiltonian!
- Coupling bound–continuum, possibility of tunnel effect.
  States are not stable, even the ground state!

Conclusions about perturbation theory

Perturbation theory is not applicable to Stark effect.

Problems with perturbation theory for Stark effect

Look for alternative theories: complex coordinate integration.

A. Maquet, S. I. Chu, and W. P. Reinhardt. *Phys. Rev. A*. **27**: 2946. (1983).

D. Farrelly and W. P. Reinhardt. *J. Phys. B*. **16**: 2103. (1983).

C. Y. Lin and Y. K. Ho. *J. Phys. B*. **44**: 175001. (2011).

Complex coordinate method

Ho, Y. K., *Phys. Rep.*, **99**: 1 (1983).
Reinhardt, W. P., *Annu. Rev. Phys. Chem.*, **33**: 223 (1982).

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

Complex energy eigenvalues $E = E_r + i\frac{\Gamma}{2} = |E|\mathrm{e}^{i\beta}$

- Bounded states: energies remain unchanged ($\Gamma = 0$).
- Continuous states: eigenvalues are rotated an angle 2ϑ in complex plane.
- Resonances: their eigenvalues remain independent of ϑ if it is greater than the argument of the complex root β. In that case, asymptotically, their behavior is equivalent to the bounded states.

SHA Hamiltonian in complex coordinate

$$\left[\mathrm{e}^{-i\vartheta} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \left(\mathrm{e}^{i\vartheta} \frac{1}{2} E \xi + \mathrm{e}^{-i\vartheta} \frac{m^2}{4\xi} - \mathrm{e}^{2i\vartheta} \frac{1}{4} F \xi^2 + Z_1 \right) \right] u(\xi) = 0$$

$$\left[\mathrm{e}^{-i\vartheta} \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) + \left(\mathrm{e}^{i\vartheta} \frac{1}{2} E \eta + \mathrm{e}^{-i\vartheta} \frac{m^2}{4\eta} + \mathrm{e}^{2i\vartheta} \frac{1}{4} F \eta^2 + Z_2 \right) \right] v(\eta) = 0$$

$$Z_1 + Z_2 = 1$$

SHA Hamiltonian in complex coordinate

$$\left[e^{-i\vartheta} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \left(e^{i\vartheta} \frac{1}{2} E \xi + e^{-i\vartheta} \frac{m^2}{4\xi} - e^{2i\vartheta} \frac{1}{4} F \xi^2 + Z_1 \right) \right] u(\xi) = 0$$

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$$Z_1 + Z_2 = 1$$

Coupled system of two differential and one algebraic equations and three unknowns.

Solution

$Z_{1\tilde{n}_1\tilde{n}_2m}$, $Z_{2\tilde{n}_1\tilde{n}_2m}$, $E_{\tilde{n}_1\tilde{n}_2m}$, $u_{\tilde{n}_1\tilde{n}_2m}(\xi)$, $v_{\tilde{n}_1\tilde{n}_2m}(\eta)$ with

$$E_{\tilde{n}_1\tilde{n}_2m} = E^{\mathrm{R}}_{\tilde{n}_1\tilde{n}_2m} + i\,\frac{1}{2}\,\Gamma_{\tilde{n}_1\tilde{n}_2m}$$

Approximate quantum numbers $\tilde{n}_1\tilde{n}_2$ are identified for the nodes of the wave function.

$$\begin{aligned} \tilde{n} &= \tilde{n}_1 + \tilde{n}_2 + m + 1 \\ \tilde{k} &= \tilde{n}_1 - \tilde{n}_2 \end{aligned}$$

Contents

Cross sections

$$\sigma_{i\to f} = \langle \psi_i \,|\, T \,|\, \psi_f \rangle$$

$$\psi_{(i,f)} = \psi_{nkm}^{\mathrm{Stark}} = \sum_{n'l'} c_{nkn'l'}\, \psi_{n'l'm}^{\mathrm{Rydberg}}$$

Einstein coefficients

$$A_{i\to f} = cte \langle \psi_i \,|\, r \,|\, \psi_f \rangle$$

$$B_{i\to f} = cte \langle \psi_i \,|\, r \,|\, \psi_f \rangle$$

$$\psi_{(i,f)} = \psi_{nkm}^{\text{Stark}} = \sum_{n'l'} c_{nkn'l'} \psi_{n'l'm}^{\text{Rydberg}}$$

Directional cross sections and Einstein coefficients

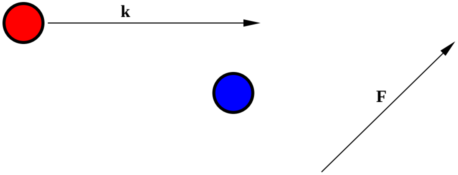

Figure: Ion-atom collision under a constant electric field

The electric field vector points to a privileged direction.
$\sigma_{i\to f}(E, \vec{F})$, $A_{i\to f}(\vec{F})$, $B_{i\to f}(\vec{F})$.
Wave functions are also non-spherically symmetric.
In an usual tokamak Lorentz field is much higher as pure electric field, so $\vec{F}$ vector is very approximately perpendicular to $\vec{K}$.

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.