Comments on capture of electrons by ions

Ladislav Kocbach

University of Bergen, Norway

Comments on capture of electrons by ions in ion-atom and ion-ion collisions

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Workshop “Ultrashort pulse laser-plasma interactions”, Prague, September 24-27, 2003

Capture of electrons by ions in ion-atom and ion-ion collisions

Electron Capture

Electron Transfer

Charge Exchange **Charge Exchange Processes**

Charge Transfer

Electron capture
by bare carbon
from doubly ionized carbon

Selective population of the n=3 level of hydrogen-like carbon in two colliding laser-produced plasmas

F. Ruhl, L. Aschke and H.-J. Kunze

Phys. Lett. A 225 (1997) 107-112

The possibility is investigated that charge exchange collisions between ions of a hot plasma (C^{6+}) and a cold plasma (C^{2+}) is responsible for selectively enhanced emission of the C^{5+} Balmer-alpha line emitted from the interaction zone of the two colliding laser-produced plasmas.

Electron capture
by bare carbon
from doubly ionized carbon

X-Ray lasers employing capillary discharges

H.-J. Kunze

Institut für Experimentalphysik

Ruhr-Universität Bochum

Collision of special interest:

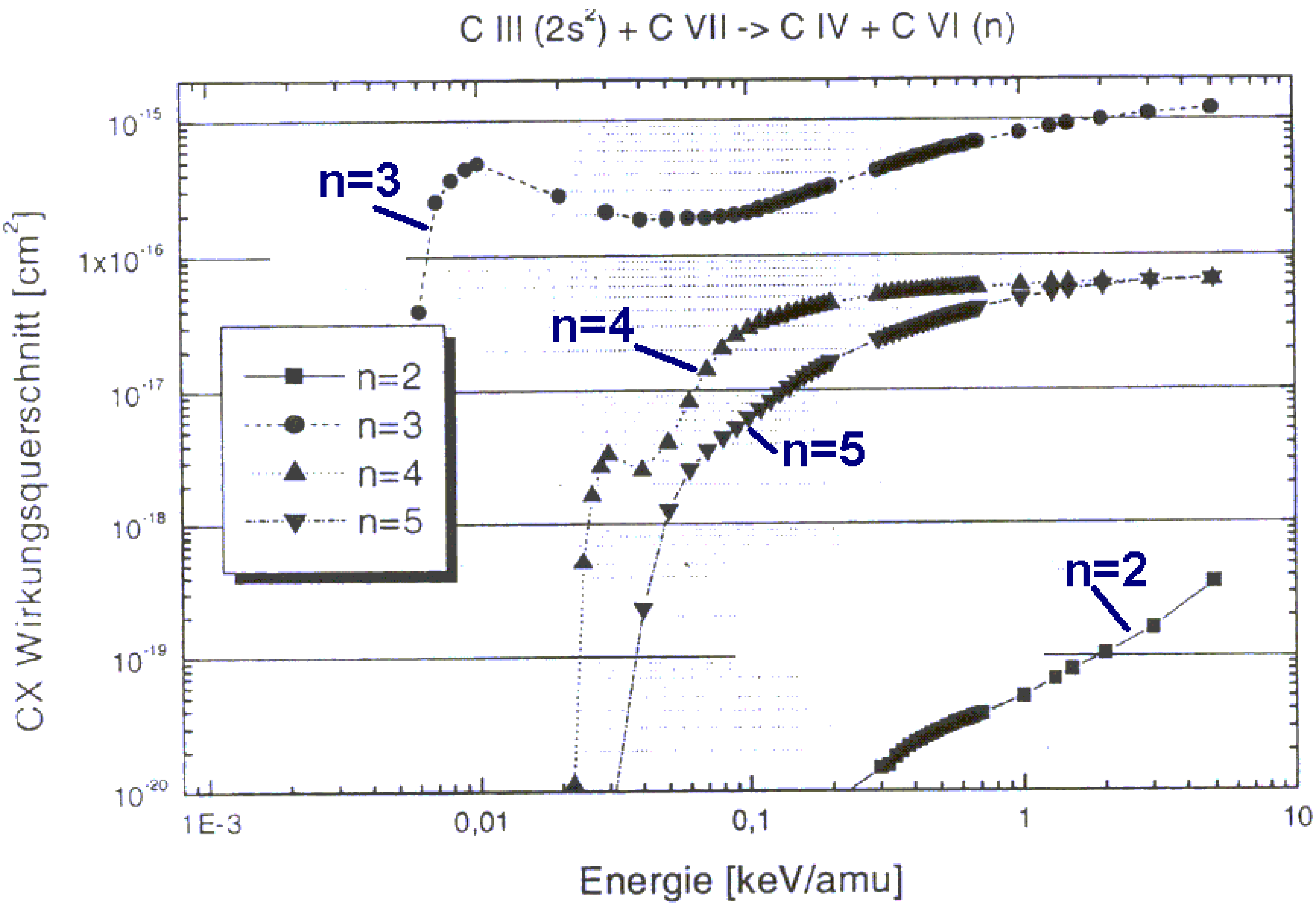
$$C^{6+} + C^{2+} \rightarrow C^{5+}(n=3) + C^{3+}$$

Theoretical calculations yielded cross sections

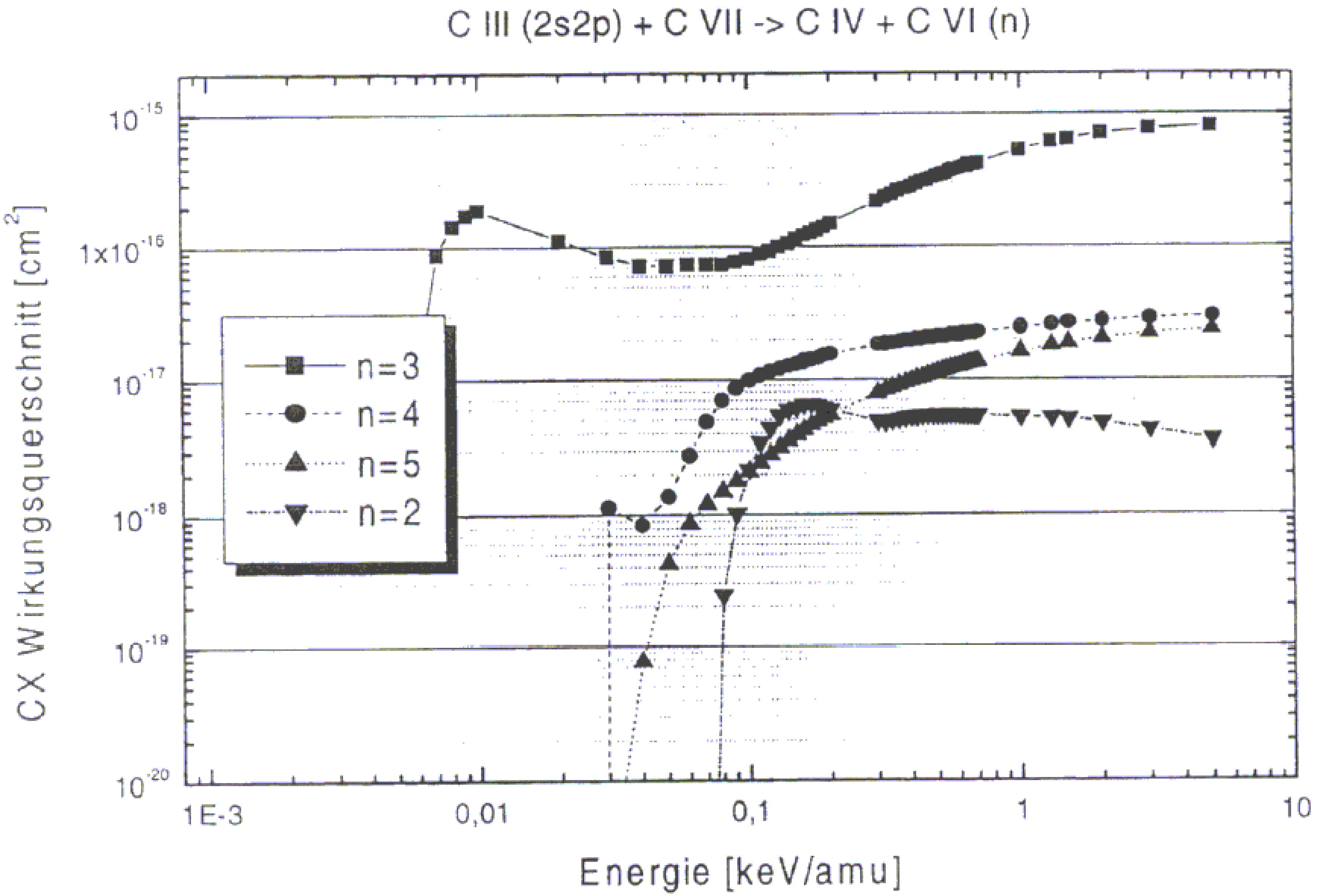
$$\sigma \geq 10^{-15}\ \mathrm{cm}^2$$

at velocities of about 10^7 cm/s

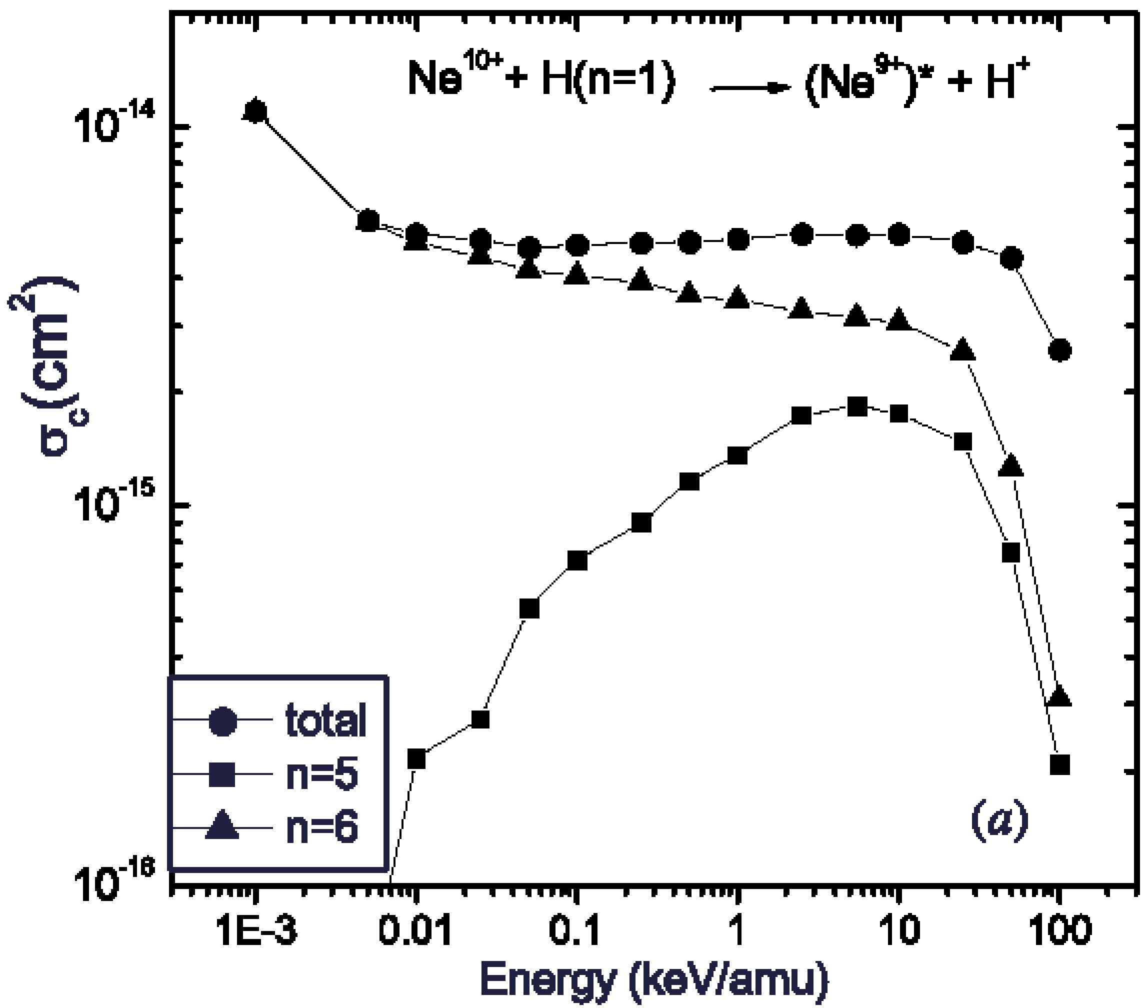
Electron capture by bare carbon from doubly ionized carbon



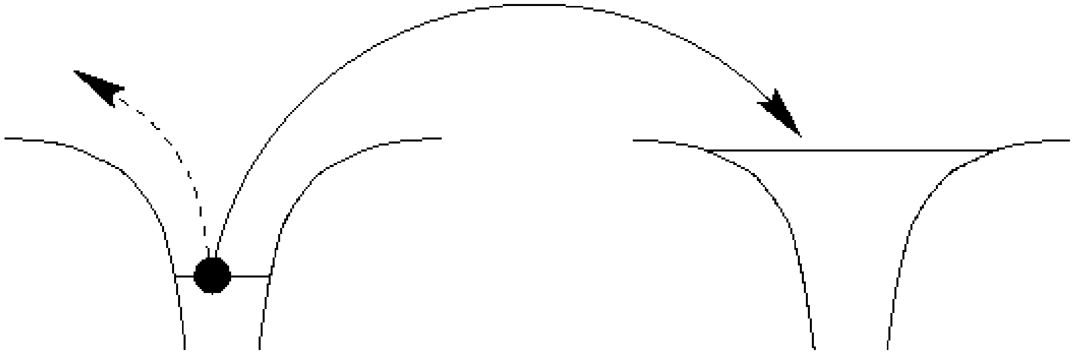
Electron capture by bare carbon from doubly ionized carbon

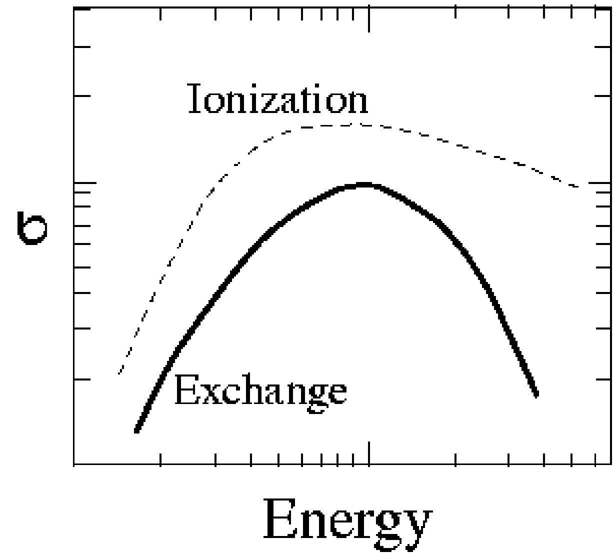


Electron capture by bare neon from neutral (atomic) hydrogen (THEORY)

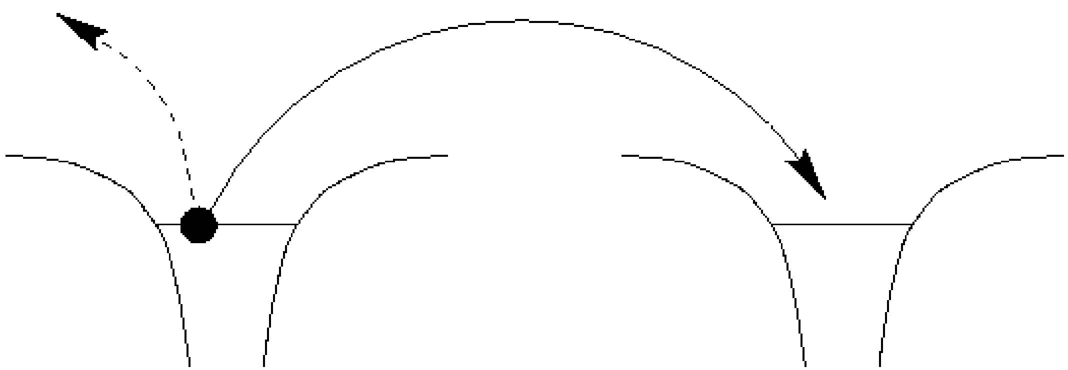


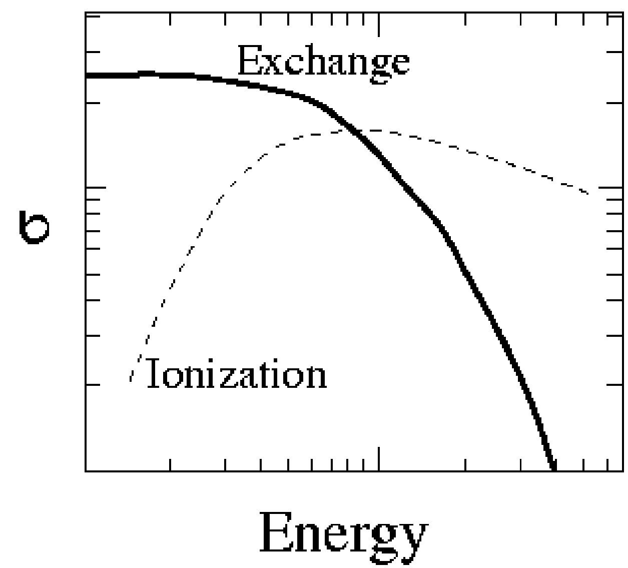
Nonresonant Exchange

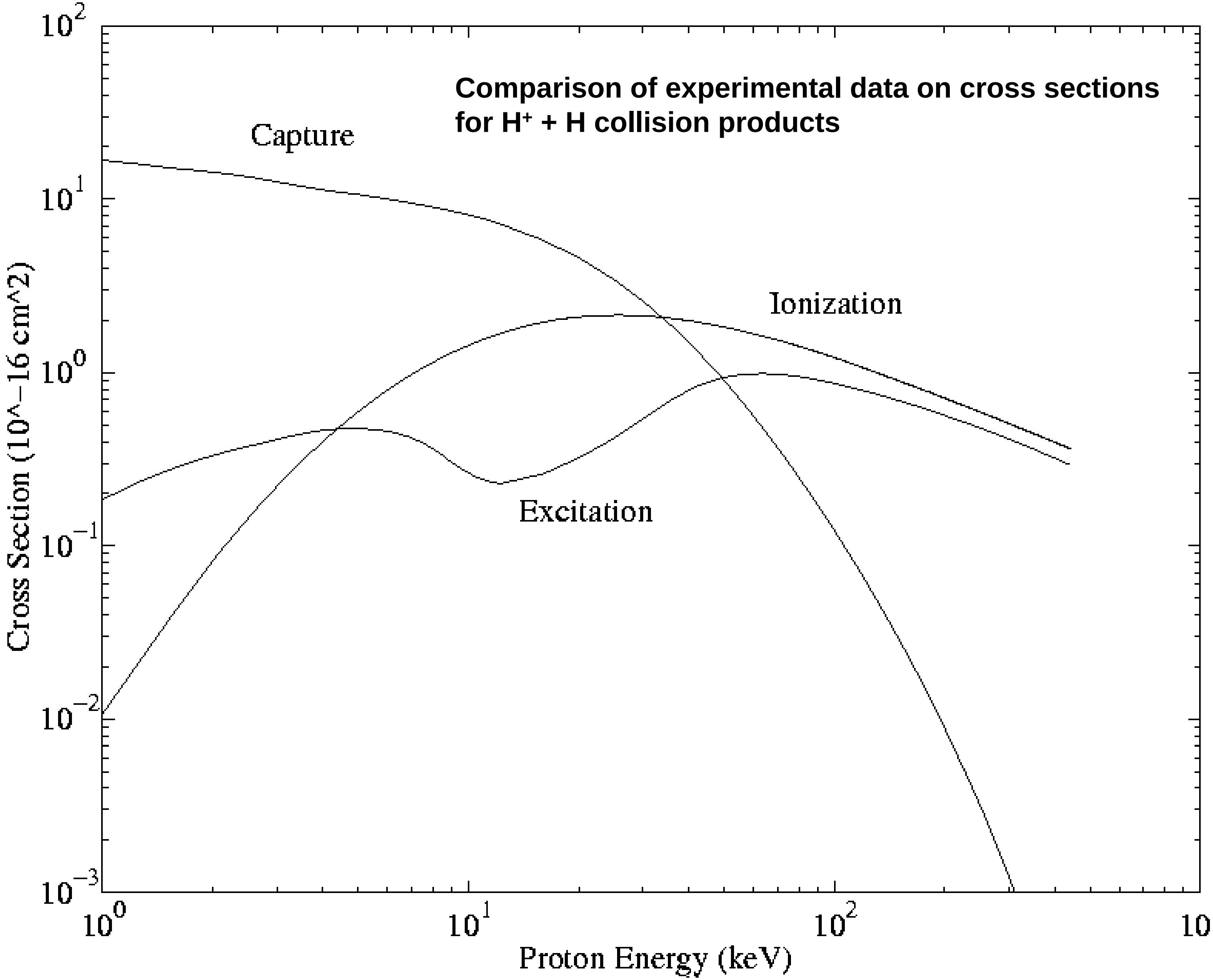




Resonant Exchange







Workshop “Ultrashort pulse laser-plasma interactions”, Prague, September 24-27, 2003

Electron capture by proton from neutral (atomic) oxygen (important in aurora physics)

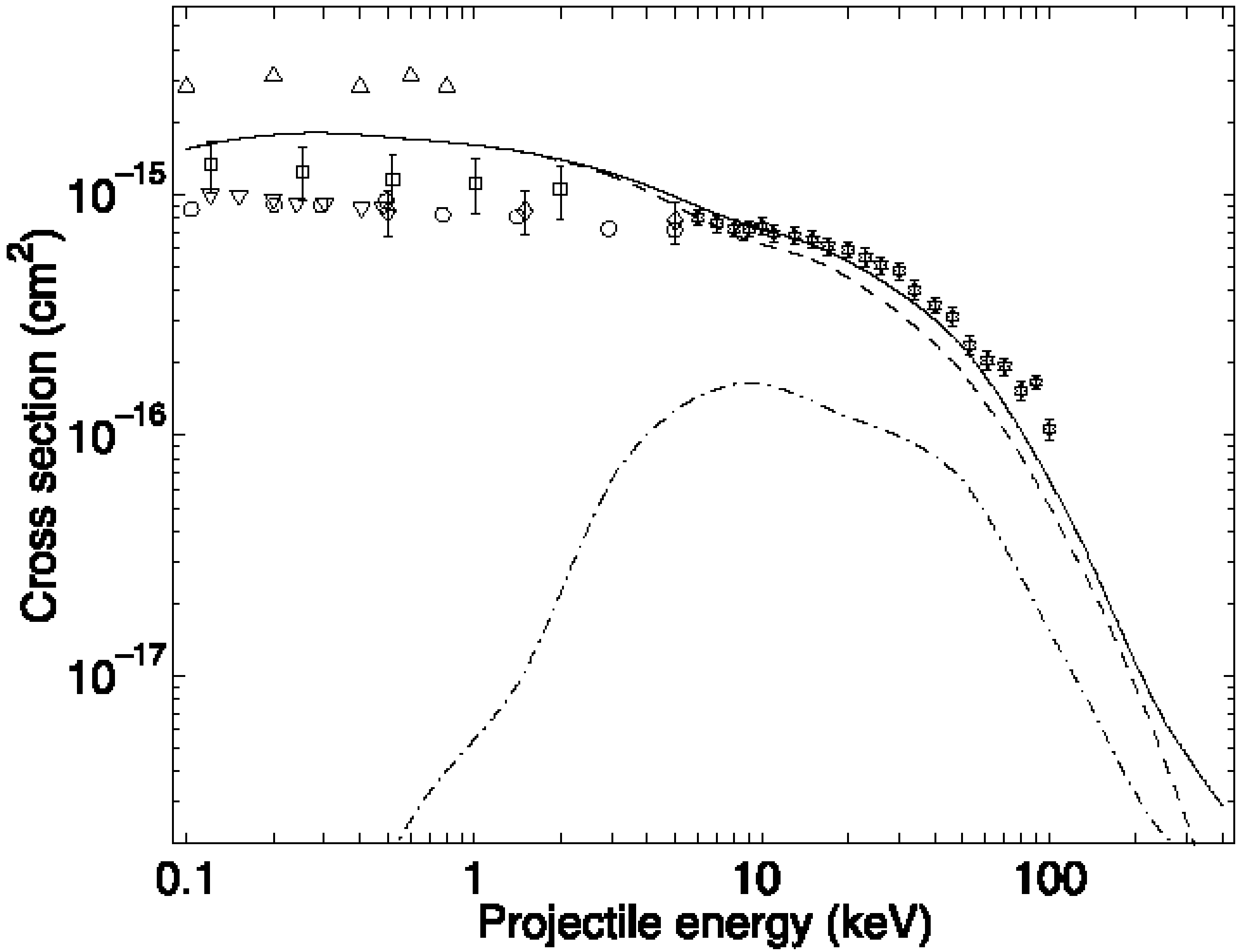
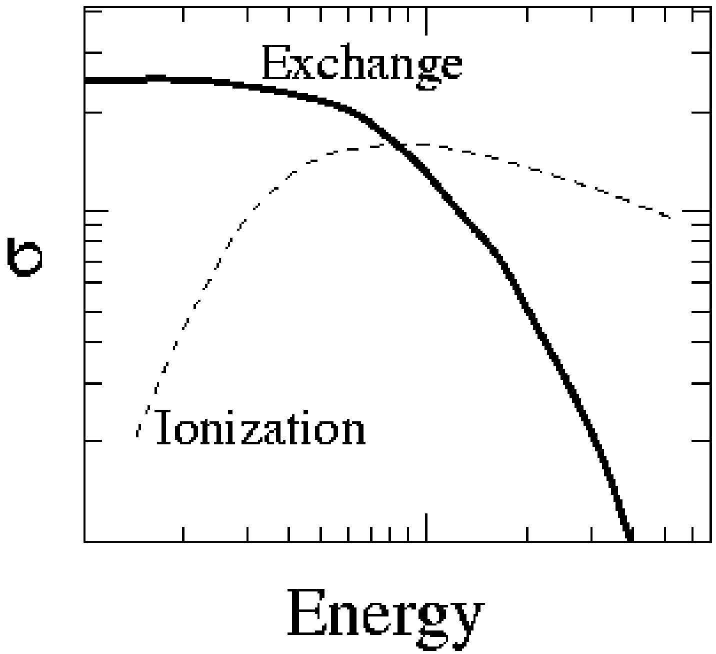
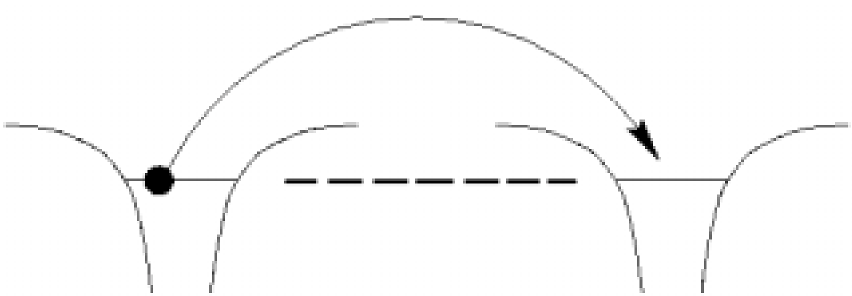


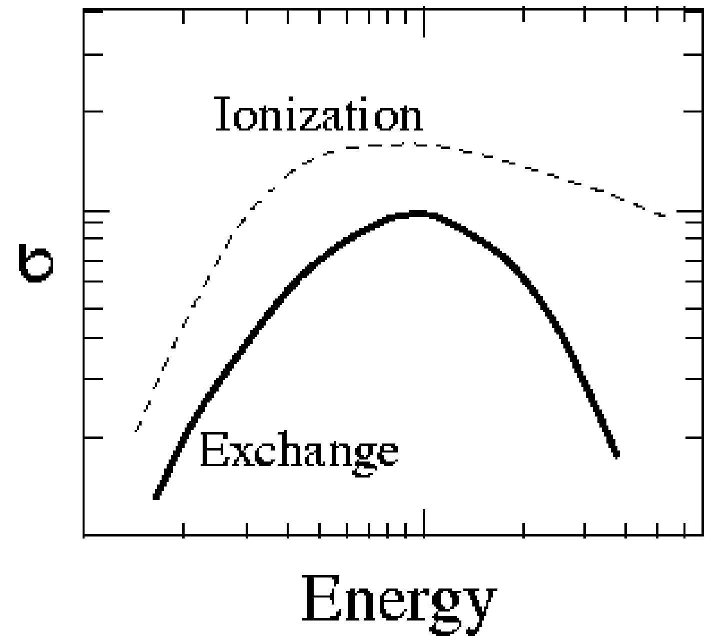
Figure 1. Total cross sections for electron capture. Theory: ——, total capture; - - - -, capture from 2p; — · —, capture from 2s; △, Kimura [3]. Experiment: □, Van Zyl and Steven [9]; ✡, Thompson *et al* [6]; ○, Stebbings *et al* [4]; ◇, Lindsay *et al* [5]; ▽, Rutherford and Vroom [8].

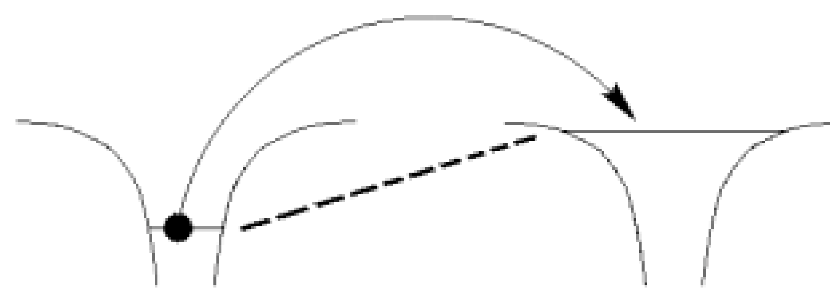
resonant charge exchange



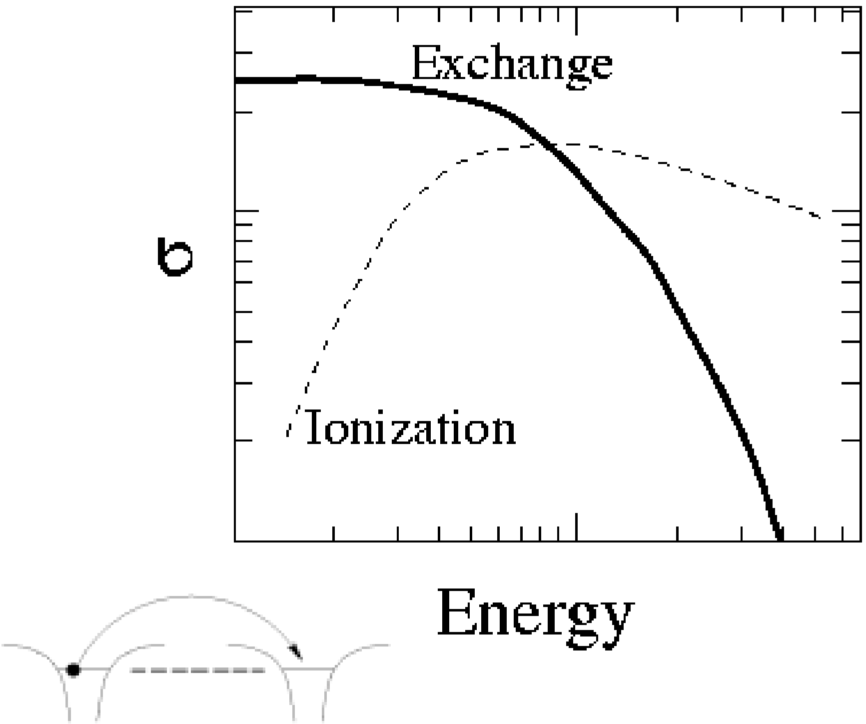


normal charge exchange

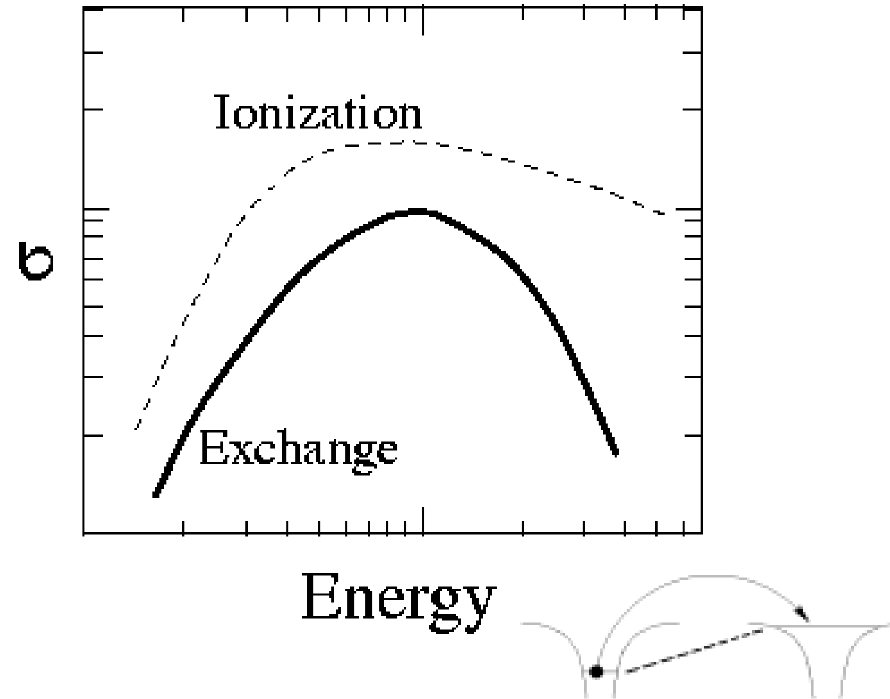




resonant charge exchange

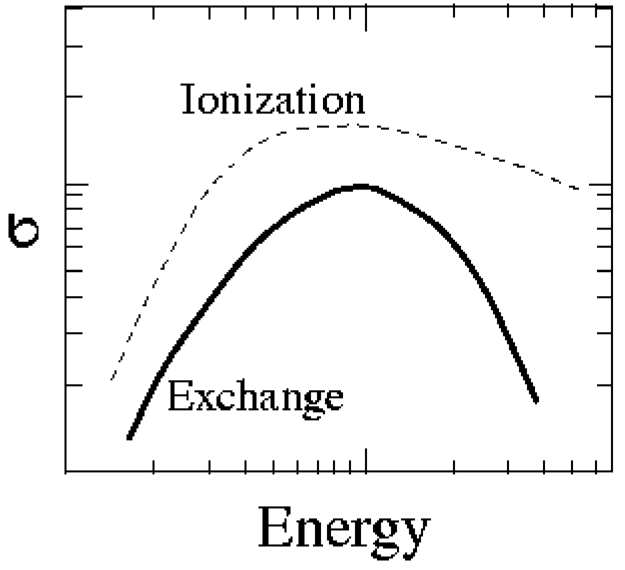


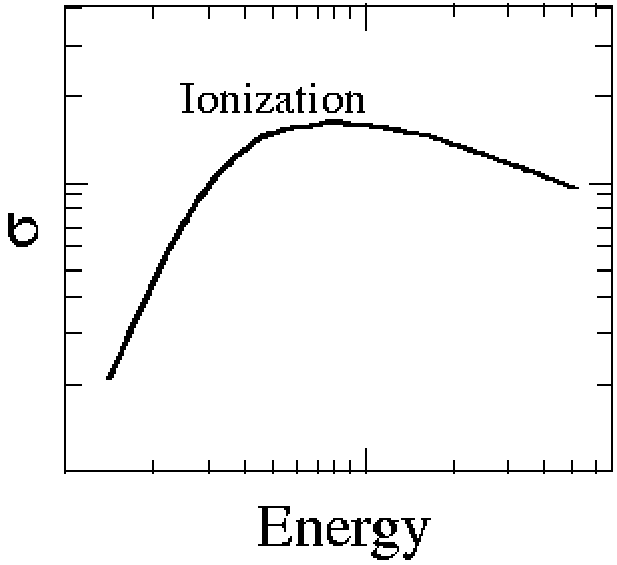
normal charge exchange



We shall explain the three features:

1. why does excitation/ionization remain large
2. Why the charge exchange is ‘narrower’
3. The behaviour of the resonant cross section


Ionization
Exchange
σ
Energy

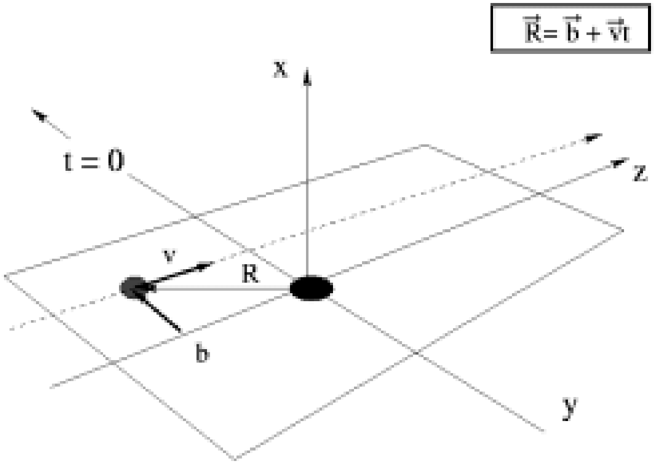


Ionization
σ
Energy

Ionization and Excitation Theories

Atomic collisions
classical trajectory

$$\vec{R}(t) = \vec{b} + \vec{v}t$$



Hamiltonian for Schrödinger equation

$$H_0 = H_{atom}$$

Total hamiltonian

$$H(t) = H_0 - \frac{Z_1 e^2}{\left|\vec{r} - \vec{R}(t)\right|}$$

$$\boxed{\sigma = \int d^2\vec{b} \left|a_{fi}(\vec{b})\right|^2}$$

Important frequency

$$\omega_{fi} = \frac{\Delta E_{fi}}{\hbar} = \frac{E_f - E_i}{\hbar}$$

Time-Dependent Schrödinger Equation

$$i \frac{\partial}{\partial \mathrm{t}} | \psi(t) \rangle = \hat{H}(t) \; | \psi(t) \rangle$$

$$| \psi(t) \rangle = \sum \alpha_i(t) | \phi_i \rangle$$

$$i \frac{\mathrm{d}}{\mathrm{dt}} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ . \\ \alpha_n \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} & ... & H_{1n} \\ H_{21} & H_{22} & ... & H_{2n} \\ ... & ... & ... & ... \\ H_{n1} & H_{n2} & ... & H_{nn} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ . \\ \alpha_n \end{bmatrix}$$

Perturbation Theory

First order theory

$$a_{fi}(\vec{b}) = \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt\ e^{i\omega_{fi}t} \int d^3\vec{r}\ \Phi_f^*(\vec{r})\ \frac{Z_1 e^2}{\left|\vec{r}-\vec{R}(t)\right|}\ \Phi_i(\vec{r})$$

has thus a form

$$a_{fi}(\vec{b}) \to \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt\ e^{i\omega_{fi}t} G_{fi}(\vec{R}(t))$$

The last expression is usually converted by using Fourier methods

$$\int dt\ e^{i\omega t} \int\ d^3\vec{s}\ e^{i\vec{s}.\vec{R}(t)}\ F(\vec{s})$$

take out integration along the velocity direction

$$\int dt\ e^{i\omega t} \int\ d^3\vec{s} e^{i\vec{s}.\vec{R}(t)} F(\vec{s}) \to \int dt\ e^{i\omega t} \int\ ds_z d^2\vec{s}_\perp e^{i\vec{s}.\vec{R}(t)} F(\vec{s})$$

evaluate the time integration as an extra integral along z-direction

$$\int ds_z \int dt\ e^{i\omega t} e^{-is_z vt} \int d^2\vec{s}_\perp e^{-i\vec{s}_\perp . \vec{b}} F(\vec{s})$$

Dirac delta representation

$$\int dt\ e^{i\omega t - is_z vt} = \frac{1}{v} \int dT\ e^{i\frac{\omega}{v}T - is_z T} \rightarrow \frac{1}{v} 2\pi\delta\left(q - s_z\right)$$

The most important characteristic variable

$$q = \frac{\omega}{v} = \frac{\Delta E}{\hbar v}$$

$$a_{fi}(\vec{b}) \propto \frac{C}{v} \int \; ds_z \delta(q - s_z) \int \; d^2\vec{s}_\perp e^{-i\vec{s}_\perp.\vec{b}} F(\vec{s})$$

$$a_{fi}(\vec{b}) \propto \frac{C}{v} \int \; d^2\vec{s}_\perp e^{-i\vec{s}_\perp.\vec{b}} F(\vec{s} = \{\vec{s}_\perp, s_z = q\})$$

$$\sigma = \int d^2\vec{b} \left| a_{fi}(\vec{b}) \right|^2$$

for s-states isotropic, otherwise slightly more complicated:

$$a_{fi}(\vec{b}) \propto \frac{C}{v} \int \; d^2\vec{s}_\perp e^{-i\vec{s}_\perp.\vec{b}} F(\sqrt{(\vec{s}_\perp)^2 + q^2})$$

$$\sigma \propto \frac{1}{v^2}\int d^2 s_\perp \int d^2\vec{s}\,'_\perp \left(\int d^2\vec{b} e^{i\vec{s}_\perp.\vec{b}} e^{-i\vec{s}\,'_\perp.\vec{b}}\right) F^*\left(\vec{s}_\perp, q\right) F\left(\vec{s}\,'_\perp, q\right)$$

$$\int d^2\vec{b} e^{i\vec{s}_\perp.\vec{b}} e^{-i\vec{s}\,'_\perp.\vec{b}} = (2\pi)^2\,\delta^2\left(\vec{s}_\perp - \vec{s}\,'_\perp\right)$$

$$\sigma \propto \int_{s_{\min}}^{\infty} d^2\vec{s}_\perp\ \left|F\left(\vec{s}_\perp, q\right)\right|^2$$

for s-states isotropic

$$\sigma \propto \int_{s_{\min}}^{\infty} s\,ds\ \left|F\left(\sqrt{\left(\vec{s}_\perp\right)^2 + q^2}\right)\right|^2$$

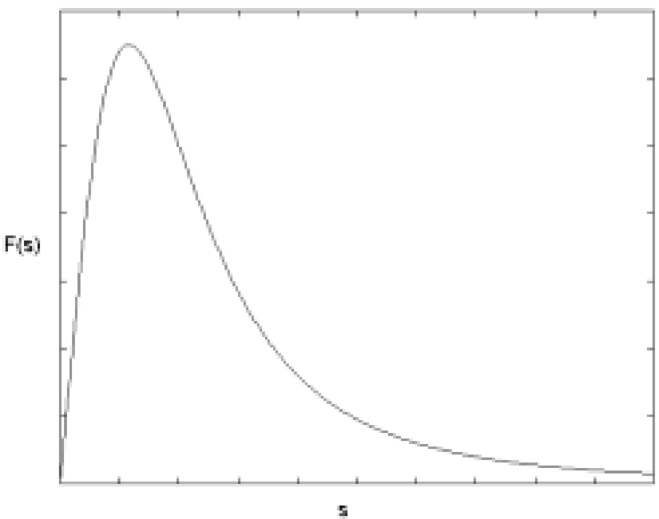
$$s_{\min} = q \qquad q = \frac{\omega}{v} \qquad s_{\min} = \frac{\Delta E}{\hbar v}$$

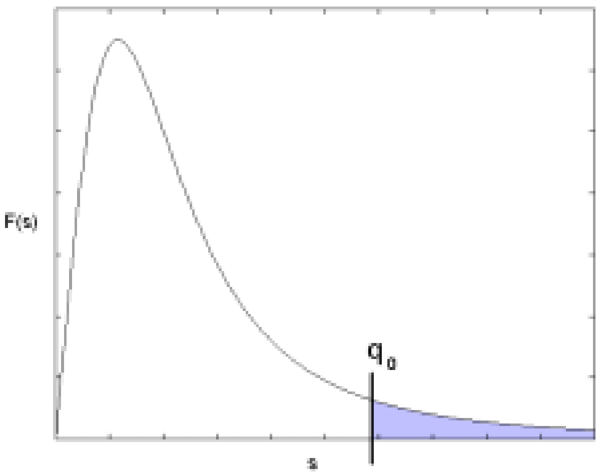
$$\left(\frac{Z_1 e^2}{\hbar v}\right)^2$$

large velocity behaviour

$$\left(\frac{Z_1 e^2}{\hbar v}\right)^2 \propto \frac{1}{E_1}$$

The typical shape of the F(s)





$$\sigma \propto \int_{s_{\min}}^{\infty} d^2\vec{s}_\perp \; \left| F\left(\vec{s}_\perp, q\right) \right|^2$$

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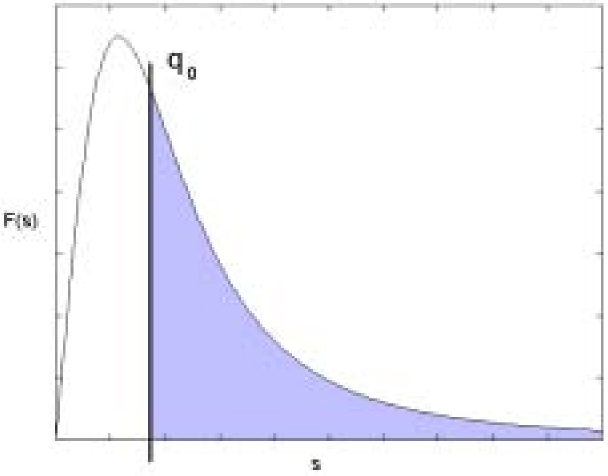
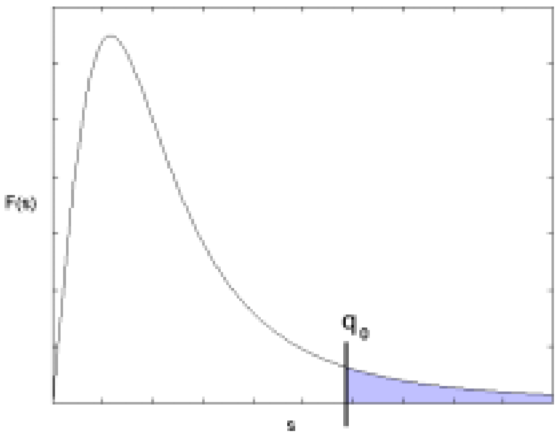
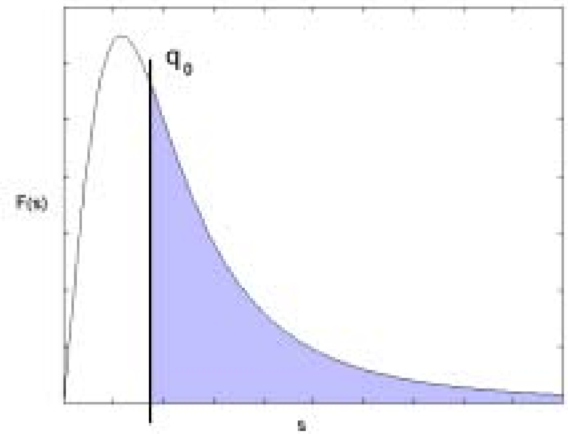
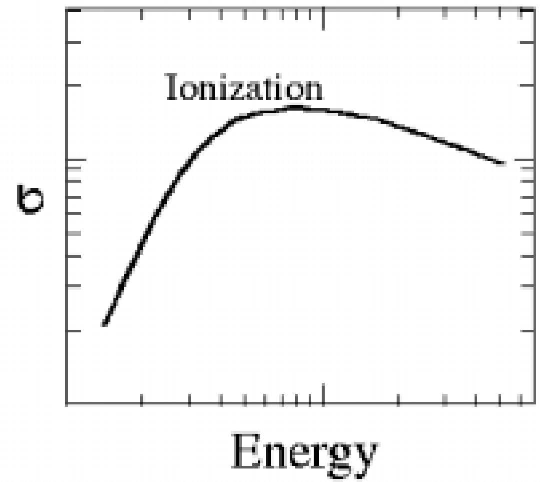


Understanding the shape F(s) of excitation cross sections







$$\sigma \propto \int_{s_{\min}}^{\infty} d^2\vec{s}_\perp \ \left|F\left(\vec{s}_\perp, q\right)\right|^2$$

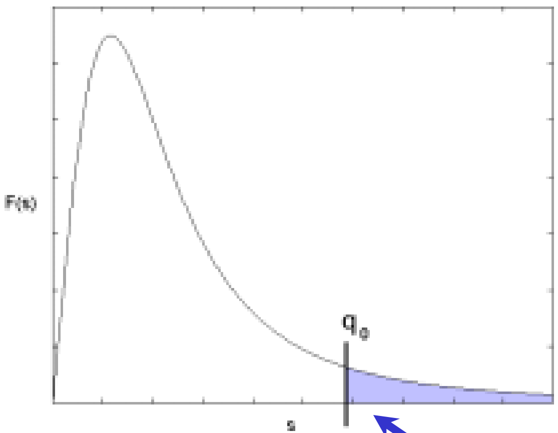
$$\left(\frac{Z_1 e^2}{\hbar v}\right)^2$$

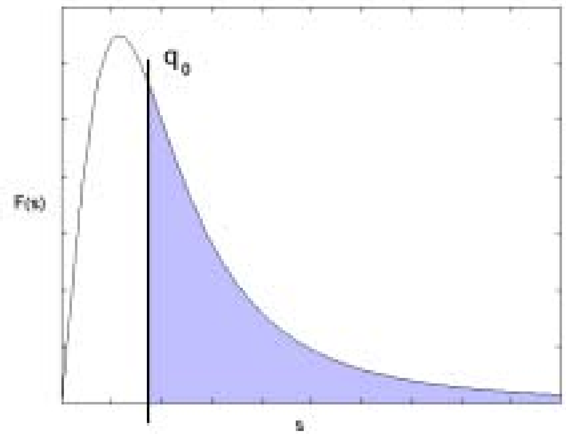
for s-states isotropic

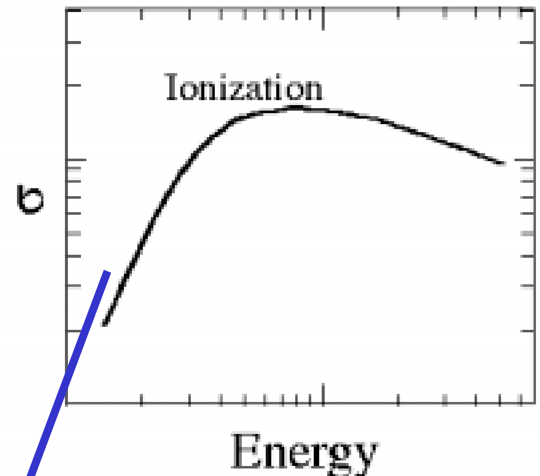
$$\sigma \propto \int_{s_{\min}}^{\infty} s\,ds \ \left|F\left(\sqrt{\left(\vec{s}_\perp\right)^2 + q^2}\right)\right|^2$$

$$s_{\min} = q \qquad q = \frac{\omega}{v} \qquad s_{\min} = \frac{\Delta E}{\hbar v}$$

Understanding the shape F(s) of excitation cross sections







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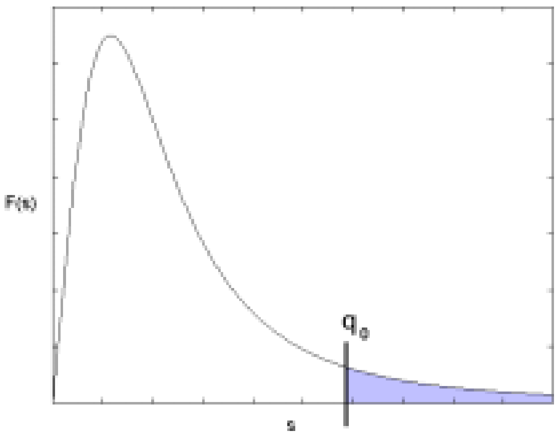
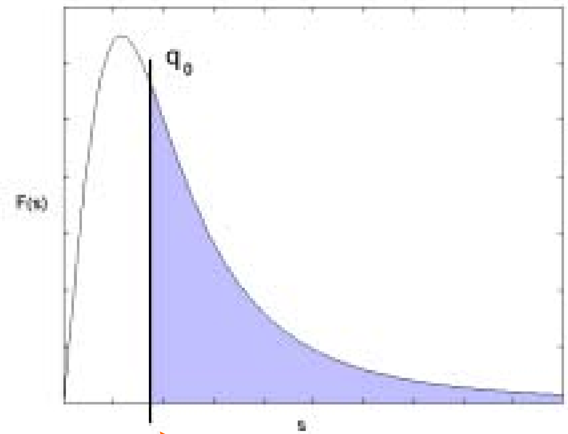
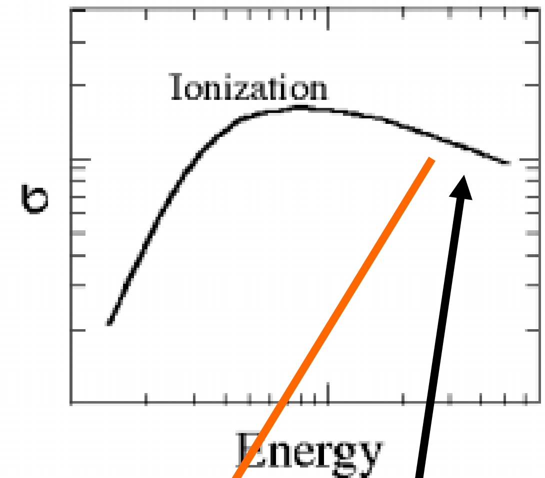
Understanding the shape F(s) of excitation cross sections







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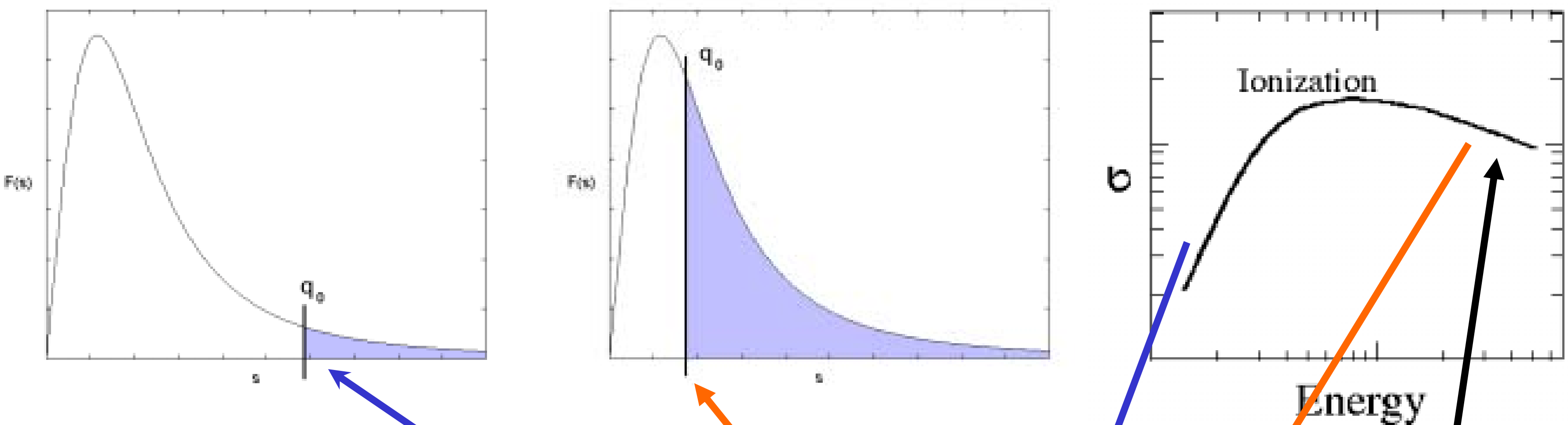
Understanding the shape F(s) of excitation cross sections



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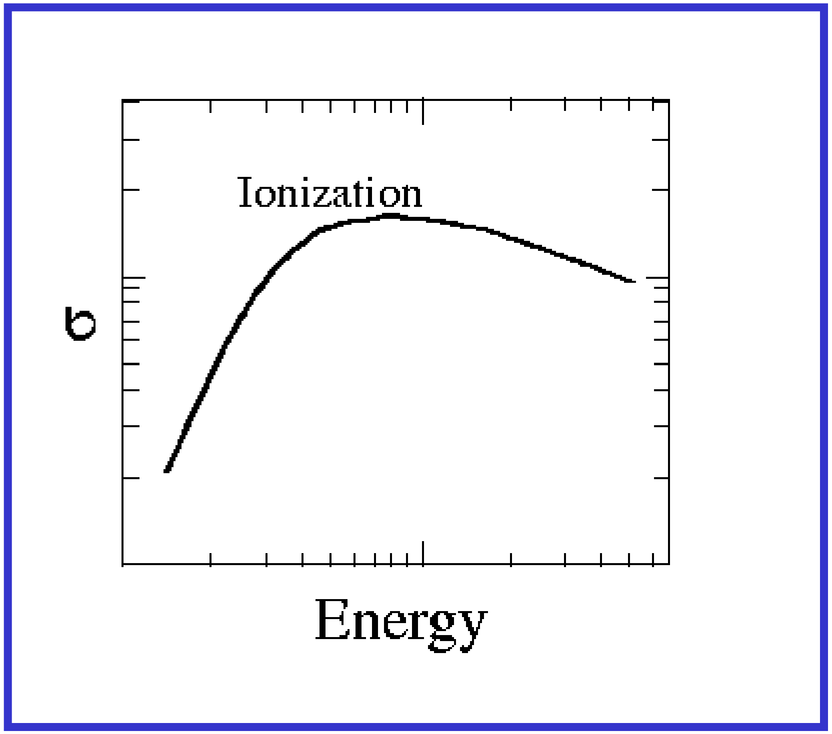
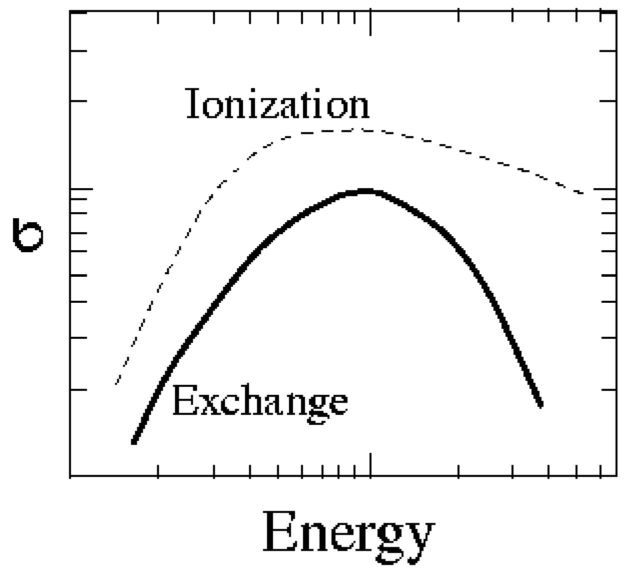

Ionization
σ
Energy



Ionization
σ
Exchange
Energy

Charge exchange theory

$$a_{fi}(\vec{b}) \propto \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt \quad \int d^3\vec{r}\, \Phi_f^*\left(\vec{r}_B, t\right) \; \frac{Z_1 e^2}{\left|\vec{r}_A - \vec{R}(t)\right|} \; \Phi_i\left(\vec{r}_A, t\right)$$

The main difference the Galilean trasformation factor

$$\vec{r}_B = \vec{r}_A - \vec{R}(t)$$

$$\vec{r}_B = \vec{r}_A - \vec{v}t$$

$$\Phi_f\left(\vec{r}_B, t\right) \rightarrow \varphi_f\left(\vec{r}_A - \vec{v}t\right) e^{i\,\frac{m}{\hbar}v.r} e^{-i\,\frac{m}{2\hbar}v^2 t} e^{-i\,\frac{E_f}{\hbar}t}$$

$$\Phi_f(\vec{r}_B, t) \to \varphi_f(\vec{r}_A - \vec{v}t)\, e^{i\frac{m}{\hbar}\vec{v}.\vec{r}} e^{-i\frac{m}{2\hbar}v^2 t} e^{-i\frac{E_f}{\hbar}t}$$

$$E_f \to E_f + \frac{1}{2}mv^2$$

Ionization, excitation

$$s_{\min} = q \qquad q = \frac{\omega}{v} \qquad \boxed{s_{\min} = \frac{\Delta E}{\hbar v}}$$

Charge Exchange

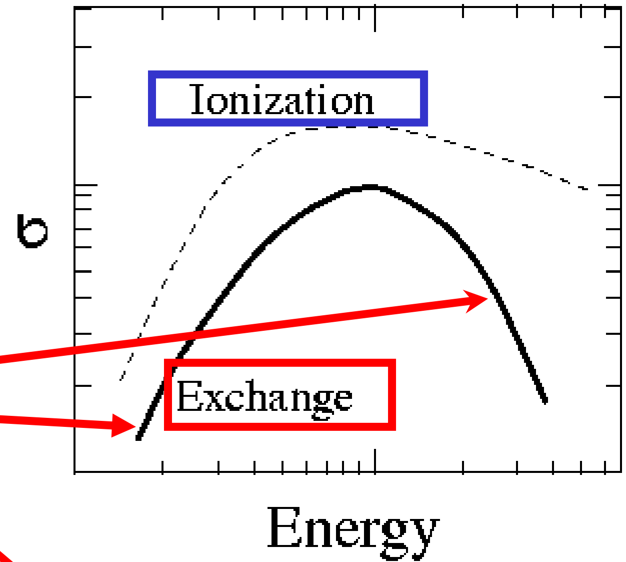
$$s_{\min} = q \qquad q = \frac{\omega}{v} + \frac{1}{2}\frac{m}{\hbar}v \qquad \boxed{s_{\min} = \frac{\Delta E}{\hbar v} + \frac{1}{2}\frac{m}{\hbar}v}$$

Discuss the charge exchange minimum momentum

$$\boxed{s_{\min} = \frac{\Delta E}{\hbar v} + \frac{1}{2}\frac{m}{\hbar}v}$$

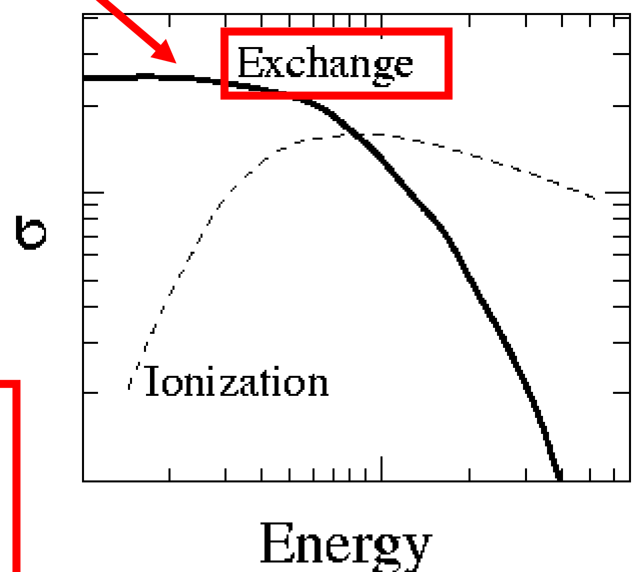
$$s_{\min} = \frac{\Delta E}{\hbar v}$$

$$\boxed{s_{\min} = \frac{\Delta E}{\hbar v} + \frac{1}{2}\frac{m}{\hbar}v}$$



$$\left(\frac{Z_1 e^2}{\hbar v}\right)^2$$

$$q = \frac{\omega}{v} = \frac{\Delta E}{\hbar v}$$



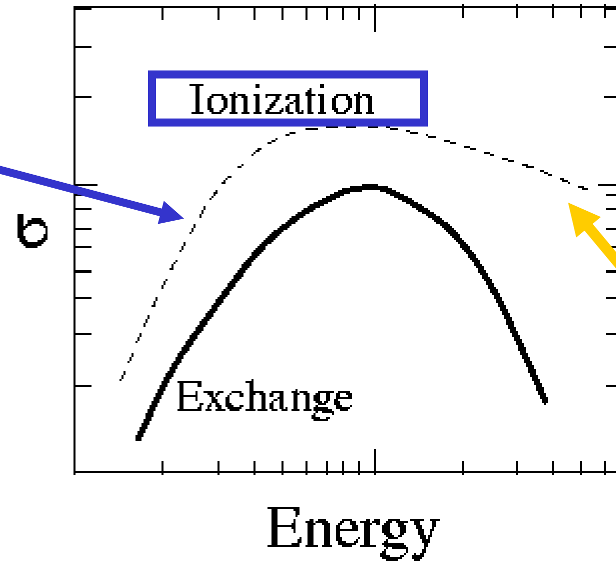
$$\sigma = \int d^2\vec{b}\left|a_{fi}(\vec{b})\right|^2$$

$$s_{\min} = \frac{\Delta E}{\hbar v}$$

$$\boxed{\sigma \propto \int_{s_{\min}}^{\infty} s\,ds\,\left|F\left(\sqrt{(\vec{s}_\perp)^2 + q^2}\right)\right|}$$

$$s_{\min} = \cancel{\frac{\Delta E}{\hbar v}} + \frac{1}{2}\frac{m}{\hbar}v$$

$$s_{\min} = \frac{\Delta E}{\hbar v}$$



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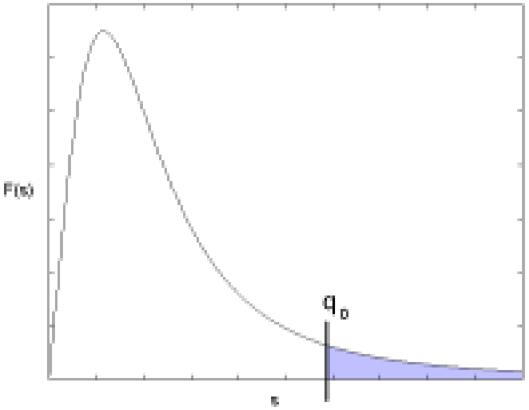

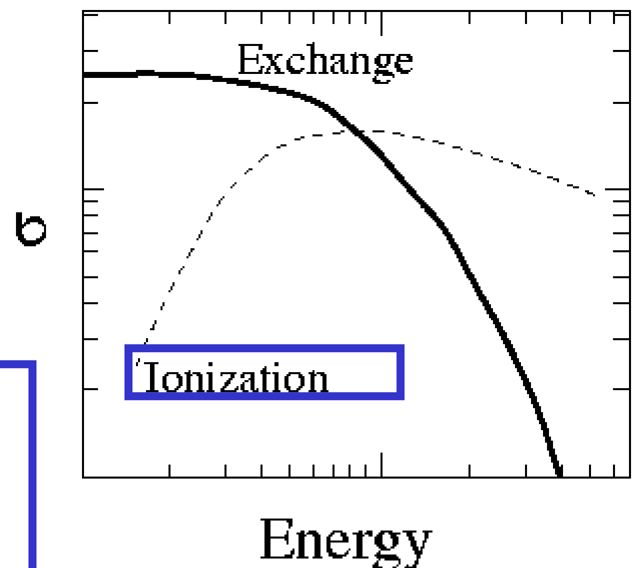

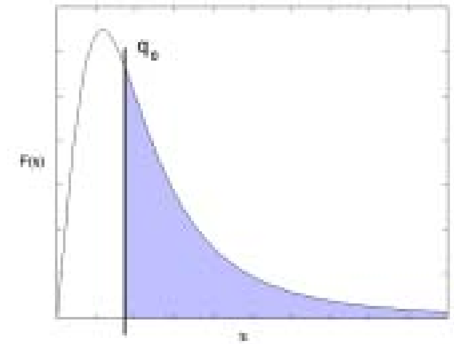

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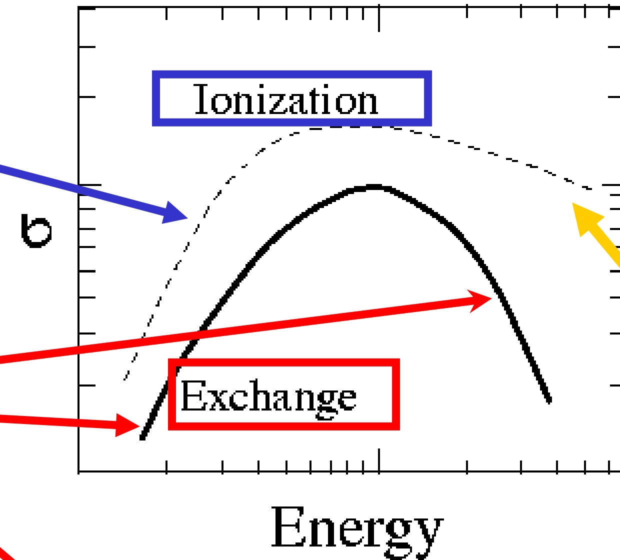
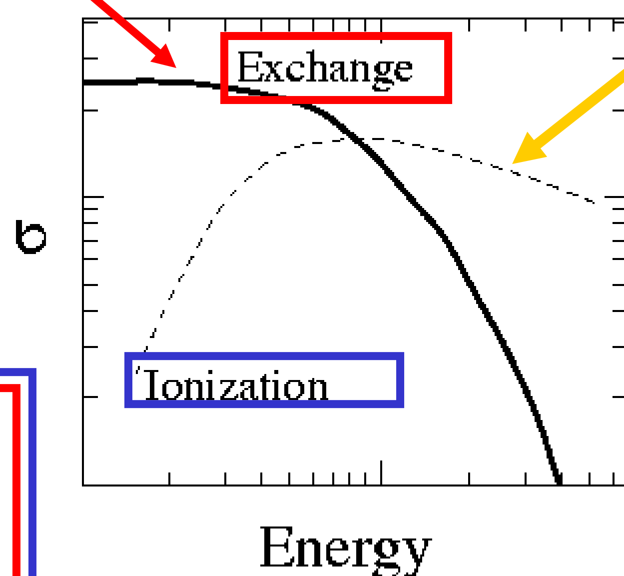
$$\sigma \propto \int_{s_{\min}}^{\infty} s\,ds\,\left|F\left(\sqrt{(\vec{s}_\perp)^2 + q^2}\right)\right.$$

$$\boxed{s_{\min} = \frac{\Delta E}{\hbar v}}$$

$$\boxed{s_{\min} = \frac{\Delta E}{\hbar v} + \frac{1}{2}\frac{m}{\hbar}v}$$



$$\boxed{\left(\frac{Z_1 e^2}{\hbar v}\right)^2}$$



$$\boxed{q = \frac{\omega}{v} = \frac{\Delta E}{\hbar v}}$$

$$\sigma = \int d^2\vec{b}\left|a_{fi}(\vec{b})\right|^2$$

$$s_{\min} = \frac{\Delta E}{\hbar v}$$

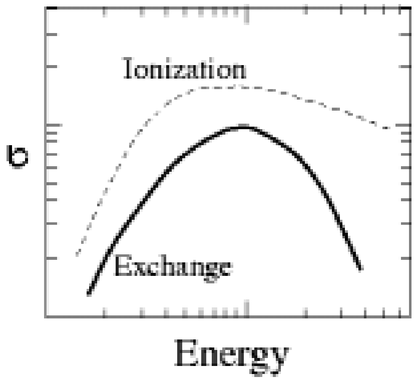
$$s_{\min} = \cancel{\frac{\Delta E}{\hbar v}} + \frac{1}{2}\frac{m}{\hbar}v$$

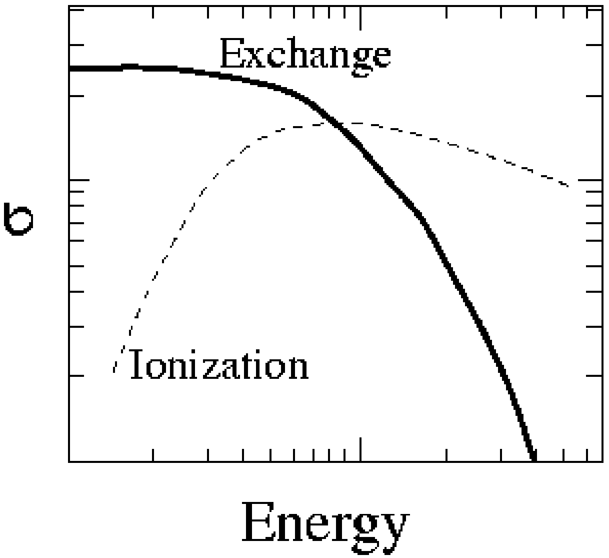
$$\boxed{\sigma \propto \int_{s_{\min}}^{\infty} s\,ds\,\left|F\left(\sqrt{(\vec{s}_\perp)^2 + q^2}\right)\right|}$$

The decrease at large projectile velocities explained.

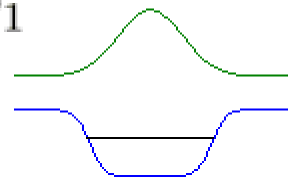
The resonant property associated with $\Delta E = 0$

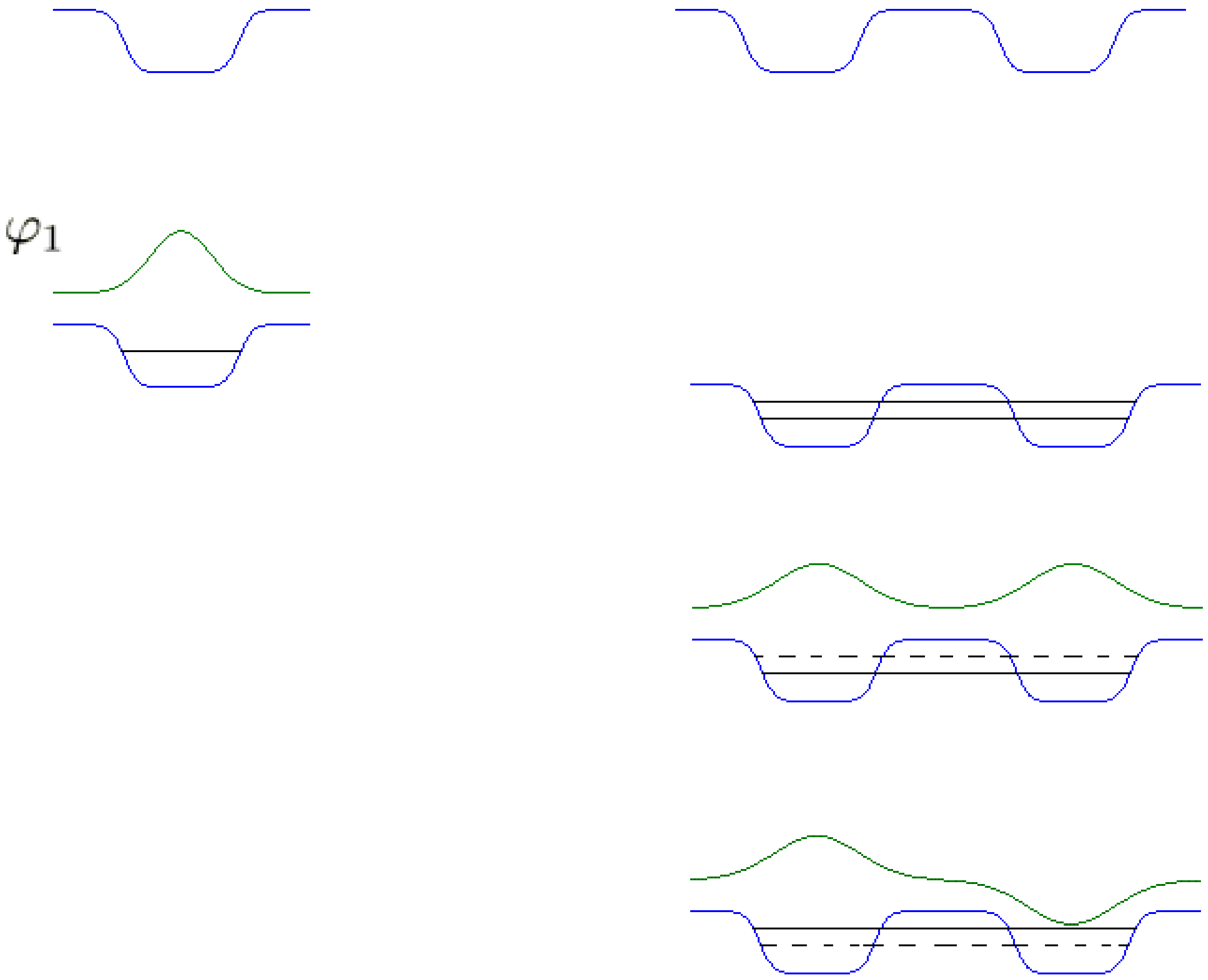
Alternative, Nonperturbative explanation

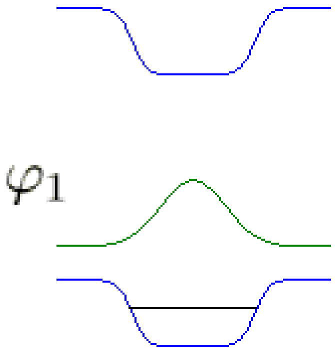


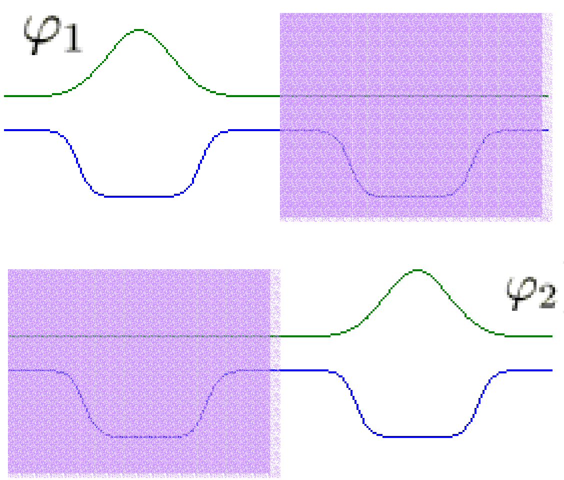


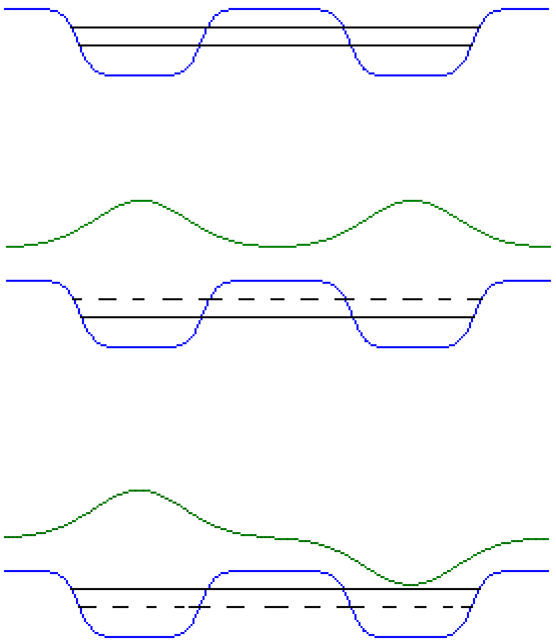
φ_1

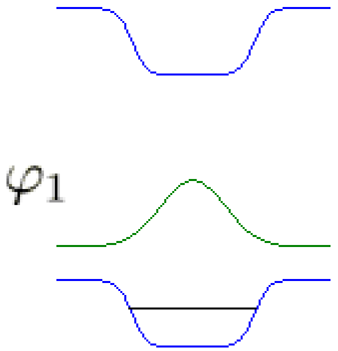


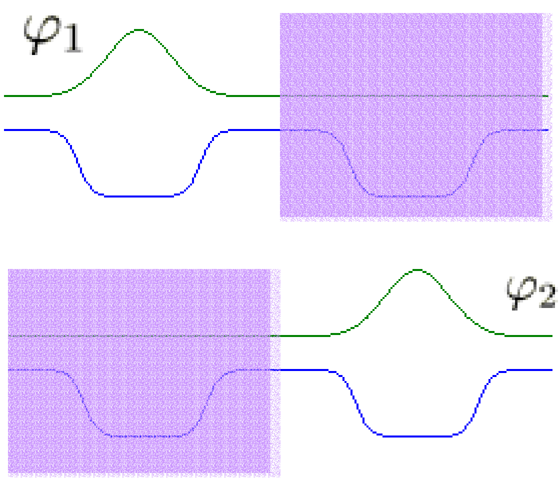

φ_1

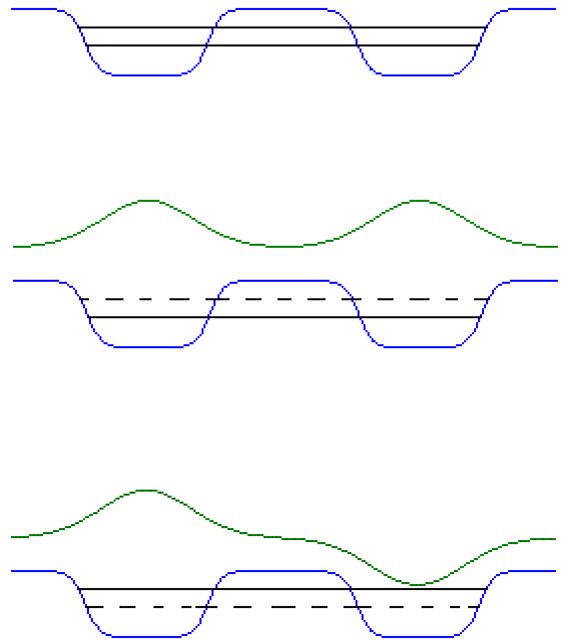

φ_1


φ_1
φ_2



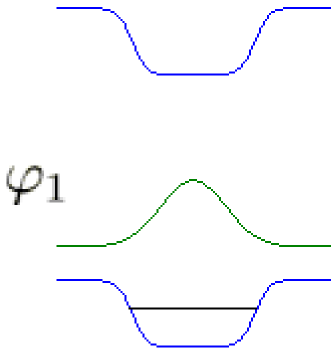


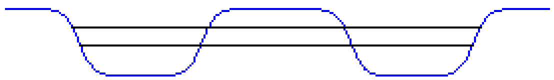


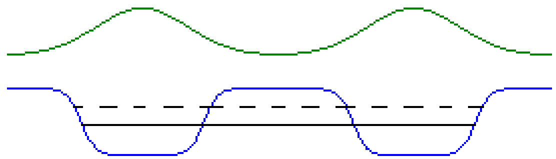


$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$$

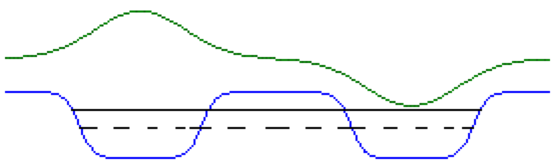
$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2)$$



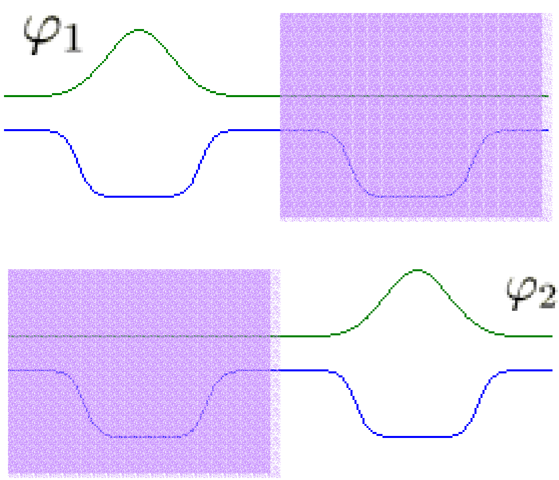




$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$$



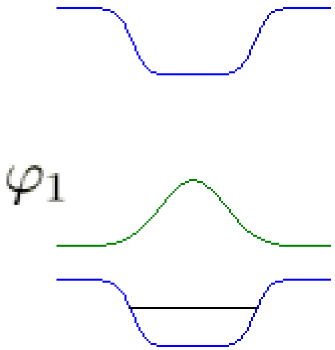
$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2)$$

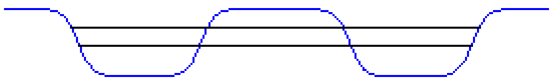


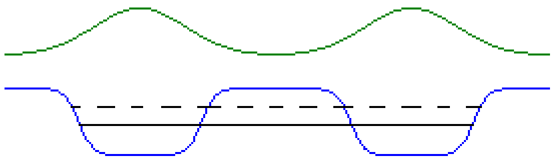
$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2) \qquad \varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2) \qquad \varphi_2 = \frac{1}{\sqrt{2}}(\psi_+ - \psi_-)$$

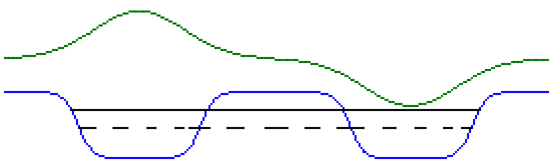
Place the electron in one well: Time development



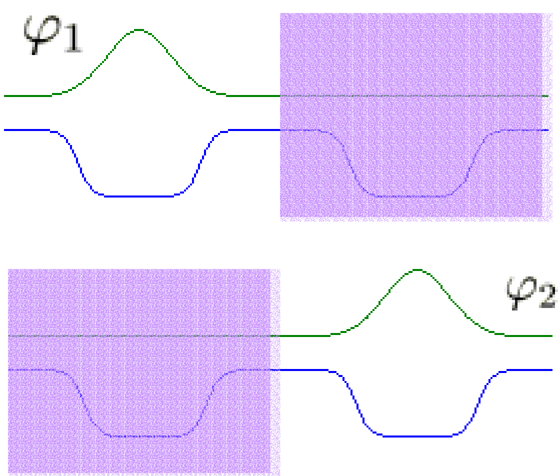




$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$$



$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2)$$



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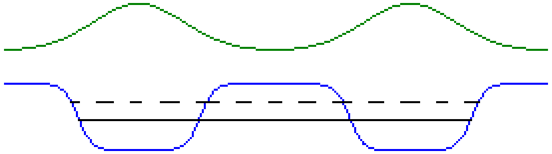
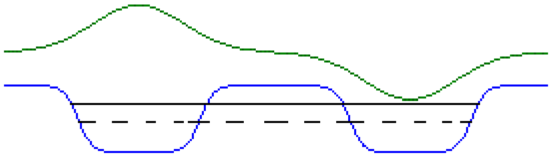
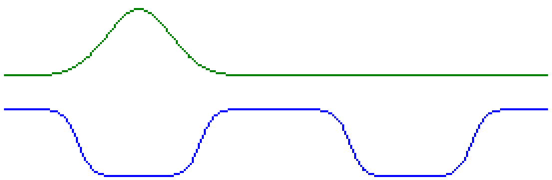


$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2) \qquad \varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

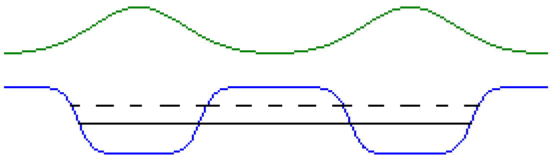


$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2) \qquad \varphi_2 = \frac{1}{\sqrt{2}}(\psi_+ - \psi_-)$$

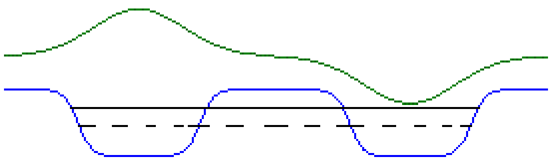


Place the electron in one well

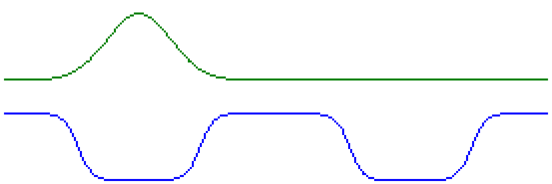
Time development



$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2) \qquad \varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

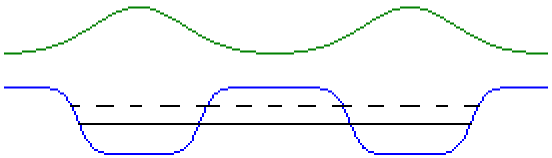


$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2) \qquad \varphi_2 = \frac{1}{\sqrt{2}}(\psi_+ - \psi_-)$$

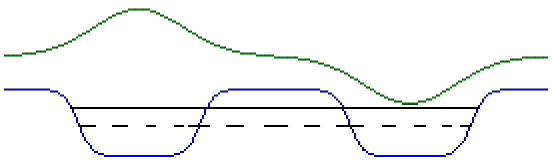


$$\Psi(t=0) = \varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

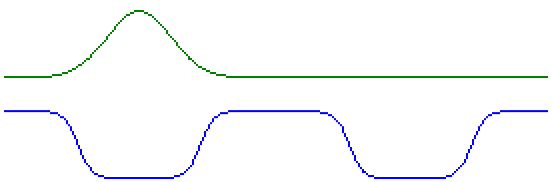
Time development



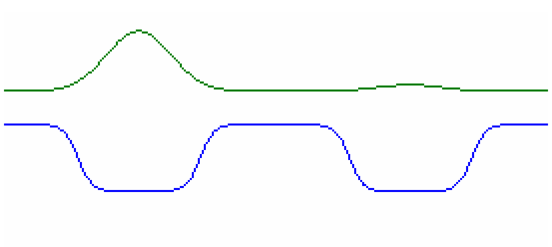
$$\psi_+ \approx \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_2) \qquad \varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$



$$\psi_- \approx \frac{1}{\sqrt{2}}(\varphi_1 - \varphi_2) \qquad \varphi_2 = \frac{1}{\sqrt{2}}(\psi_+ - \psi_-)$$



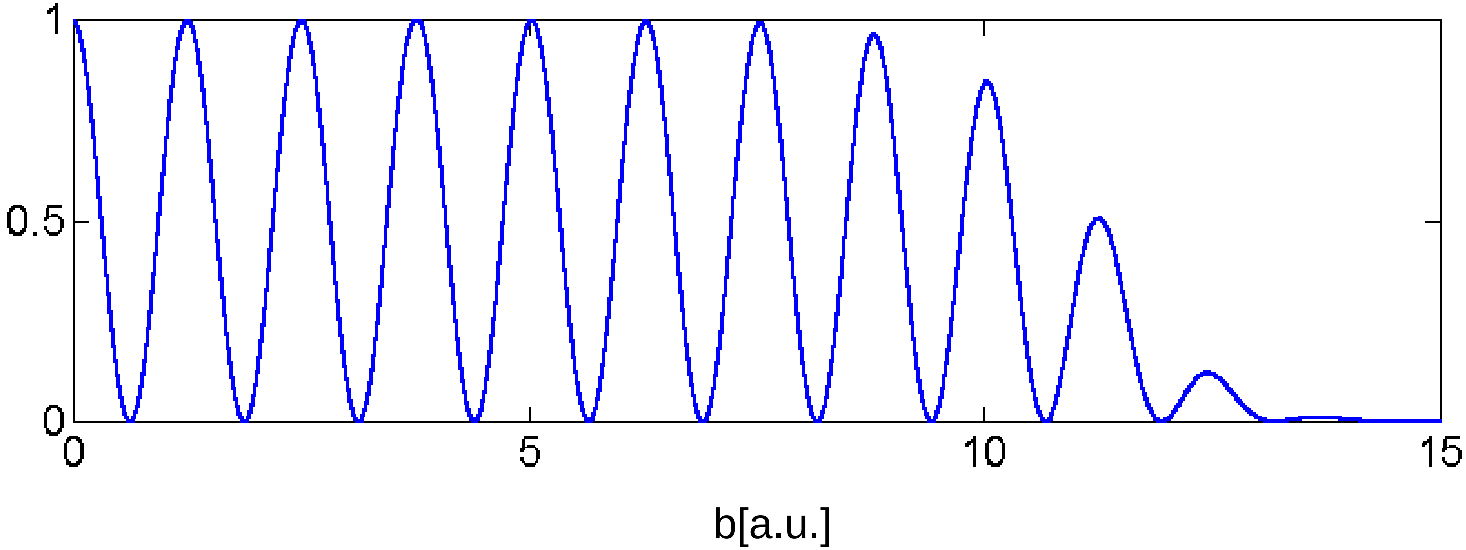
$$\Psi(t=0) = \varphi_1 = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$



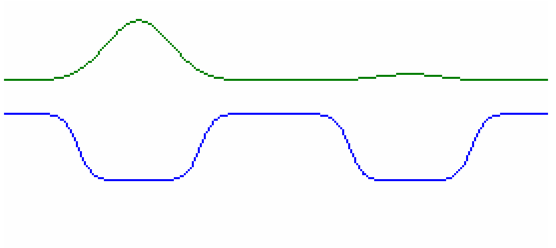
$$\Psi(t) = \frac{1}{\sqrt{2}}\left(\psi_+ e^{iE_+ t/\hbar} + \psi_- e^{iE_- t/\hbar}\right)$$

$$\Psi(t) = e^{i\,C(t)}\;\left(\;\psi_+\;+\;e^{i\omega t}\;\psi_-\;\right)$$

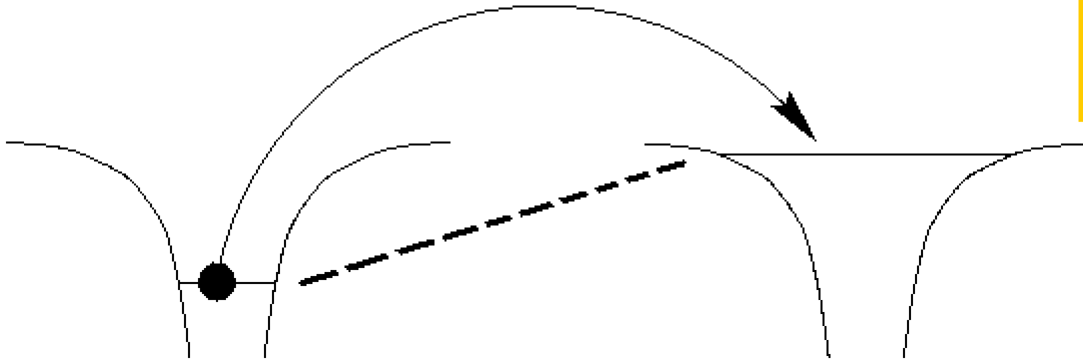
Probability as function of impact parameter



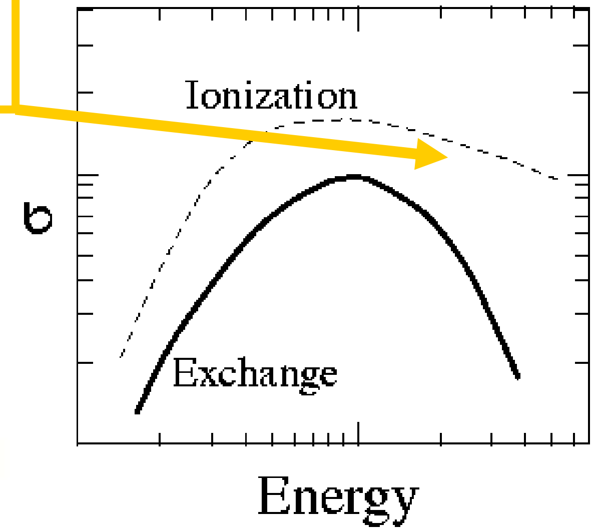
$$\sigma = \int d^2\vec{b}\left|a_{fi}(\vec{b})\right|^2$$



$\sigma \sim 0.5\ \pi\,(b_{max})^2$

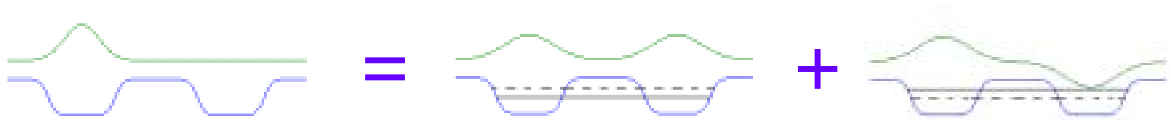


$$\left(\frac{Z_1 e^2}{\hbar v}\right)^2$$

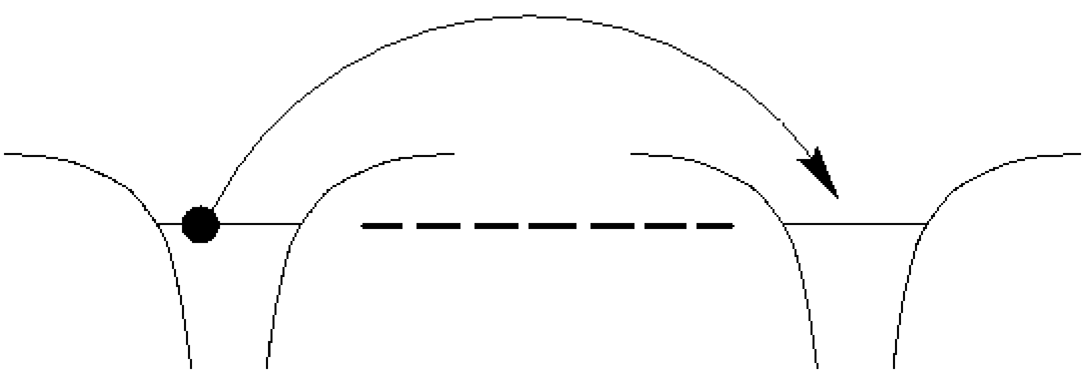


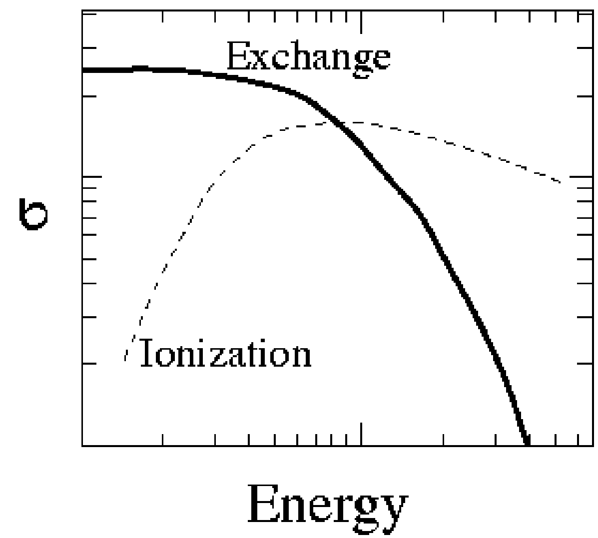
$$s_{\min} = \frac{\Delta E}{\hbar v}$$

$$\sigma \propto \int_{s_{\min}}^{\infty} s\,ds \left| F\left(\sqrt{(\vec{s}_{\perp})^2 + q^2}\right)\right|^2$$

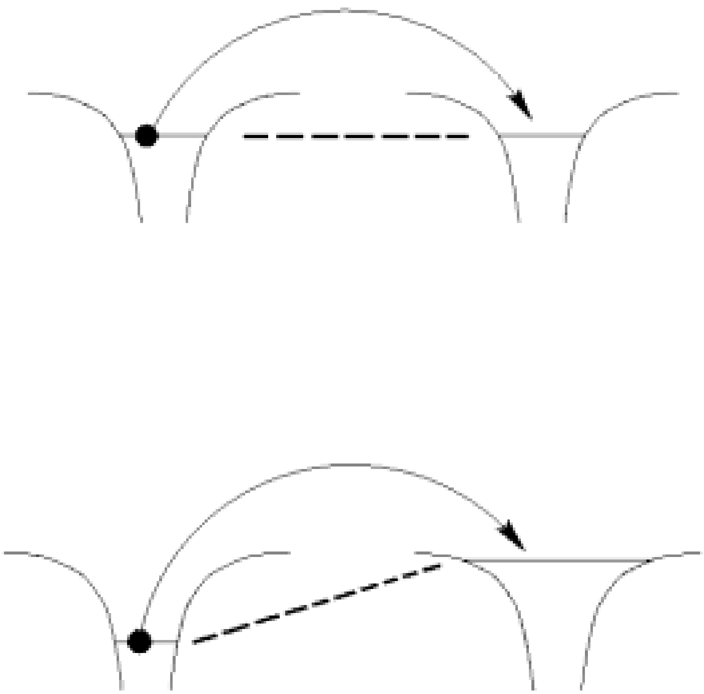


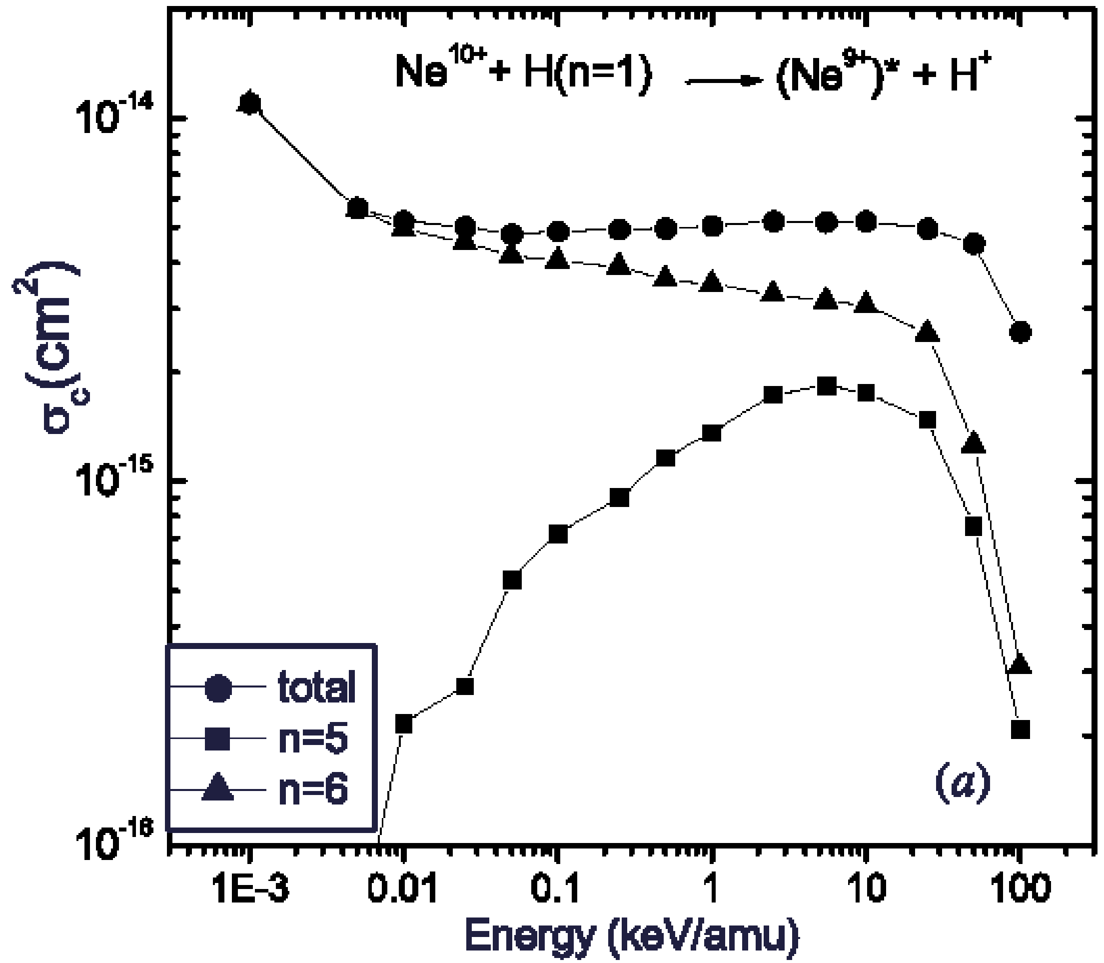
$$s_{\min} = \frac{\Delta E}{\hbar v} + \frac{1}{2}\frac{m}{\hbar}v$$





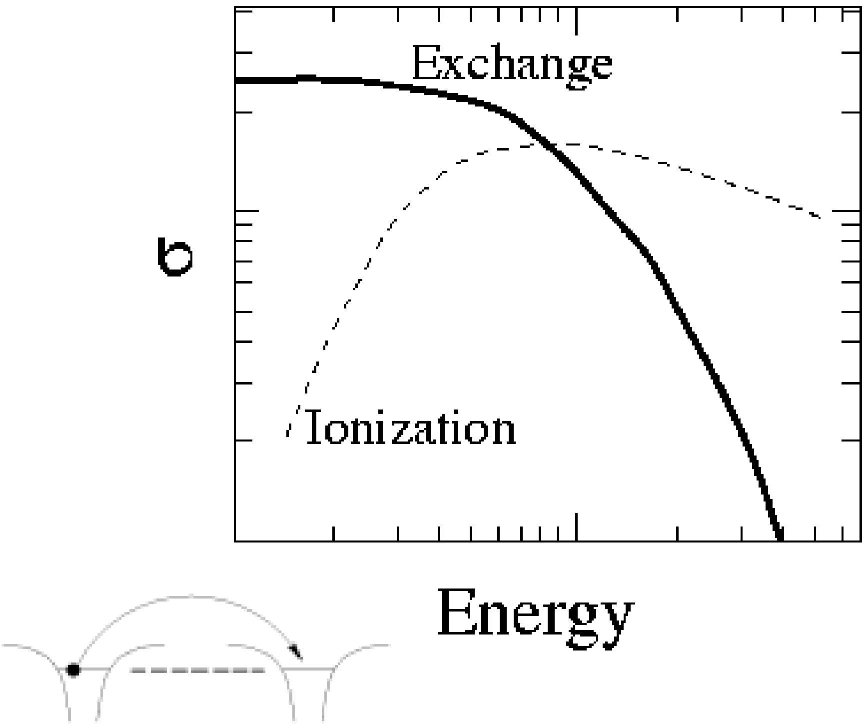
Electron capture by bare neon from neutral (atomic) hydrogen (THEORY)

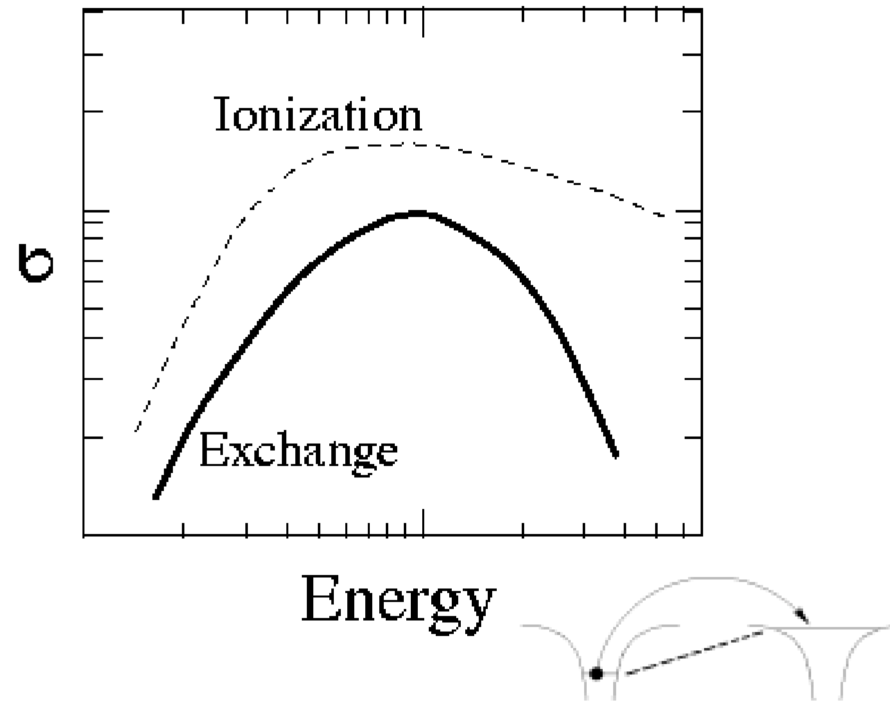




If there is any resonant or quasi-resonant process, it will dominate

resonant charge exchange **normal charge exchange**





We have explained these three features:

1. excitation/ionization remain large at large energies
2. the charge exchange is ‘narrower’
3. The behaviour of the resonant cross section