ELECTRON-HYDROGEN COMPTON SCATTERING at HIGH MOMENTUM TRANSFER:
Calculations of Second Born Singular Integrals

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INTRODUCTIVE REMARKS

In the report we consider the quasielastic collisions of electrons with hydrogen and helium atoms at large momentum transfer. Elastic and quasi-elastic reactions are well studied. Recently they have attracted a new interest of scientists. Last time these reactions are called like electron compton scattering, what is a little strange :)

Why is it interesting? A few keV electrons at back scattering cause the nucleus motion after a kick, what leads to unexpected effects in shapes of differential cross sections, calculated within the first and second Born approximations.

We consider the reaction

$$e + A \to e + A^*$$

and present below a typical loss spectrum for He atom.

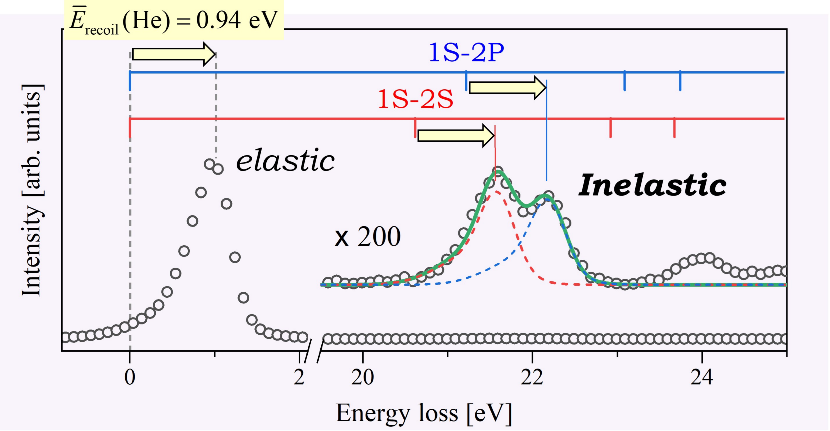

Figure 1: Energy loss spectrum for He. Electron energy = 2 keV, scattering angle = 135°

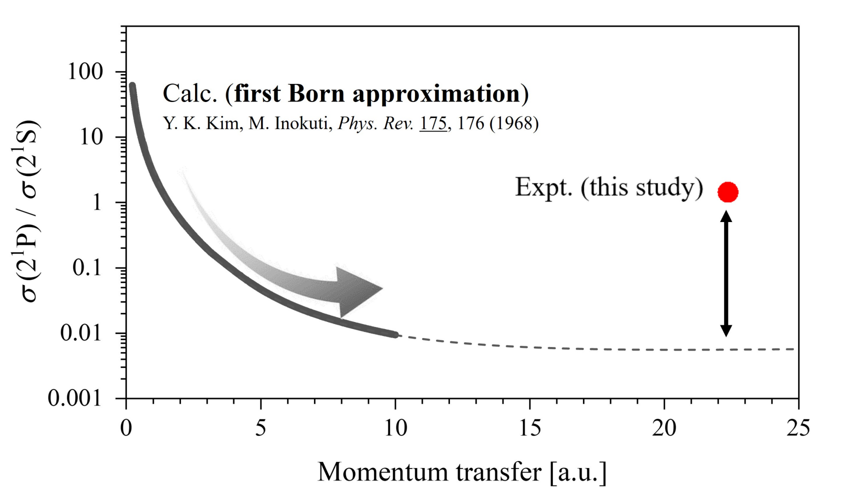

Figure 2: FBA at large momentum transfer $Q = |\vec{k}_i - \vec{k}_f|$. Here nuclear mass $m_{He} = \infty$ au. Red point is the experiment, which about 100 times bigger than FBA.

Table 1: Comparison of energies of trial wf constructed using HF and CF basis functions $Y_{lm}(\vec{r}_1)\exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}), \quad l = 0, 1.$

	1^1S	2^1S	2^1P
HF	-2.86167	-2.16940	-2.12715
CF	-2.90371	-2.14594	-2.12381
Ext	-2.90372	-2.14597	-2.12384

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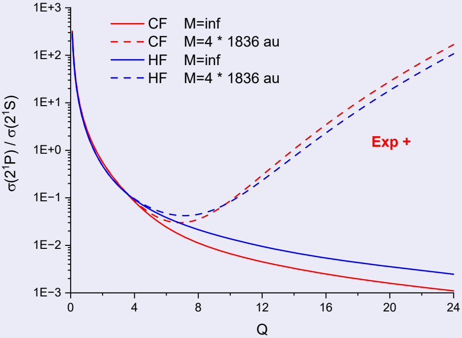

Figure 3: Comparison of FBA with $m_{He} = \infty$ au and $m_{He} = 4 \times 1836$ au nuclear masses. Experiment is approximately 55–85 times smaller than the FBA with a finite nuclear mass, depending on the trial wavefunctions.

Conclusion on He atom

1. It is necessary to take into account the finite nuclear mass of the He atom for large momentum transfer and large projectile energies.

2. Ratio of the cross sections for He depends on the choice of the trial wavefunctions, especially at large momentum transfer.

3. The FBA doesn't describe these experiments well, and calculation of SBA is needed. For helium it is more complicated than for hydrogen.

Theory. differential cross section for hydrogen: First Born Approximation

We mainly use the atomic system of units: $m_e = \hbar = |e| = 1$. In these units, the speed of light is $c = 137$.

First Born approximation

$$\langle \vec{k}_f, \varphi_f | T^{FBA} | \vec{k}_i, \varphi_i \rangle = \frac{4\pi}{Q^2} \int d^3\rho_2 \varphi_f(\vec{\rho}_2) \left(e^{i\vec{Q}\cdot\vec{\rho}_2} - e^{-i[1/(m_N)]\vec{Q}\cdot\vec{\rho}_2} \right) \varphi_{1s}(\rho_2). \quad (1)$$

Consequently

$$\frac{d\sigma(1s)}{d\Omega_f} = \frac{4}{Q^4} \frac{k_f}{k_i} \left| \int d^3\rho_2 \varphi_{1s}(\vec{\rho}_2) \left(e^{i\vec{Q}\cdot\vec{\rho}_2} - e^{-i([1/(m_N)\vec{Q}\cdot\vec{\rho}_2} \right) \varphi_{1s}(\rho_2) \right|^2 . \quad (1.1)$$

$$\frac{d\sigma(2s)}{d\Omega_f} = \frac{4}{Q^4} \frac{k_f}{k_i} \left| \int d^3\rho_2 \varphi_{2s}(\vec{\rho}_2) \left(e^{i\vec{Q}\cdot\vec{\rho}_2} - e^{-i([1/(m_N)\vec{Q}\cdot\vec{\rho}_2} \right) \varphi_{1s}(\rho_2) \right|^2 . \quad (1.2)$$

$$\frac{d\sigma(2p)}{d\Omega_f} = \frac{4}{Q^4} \frac{k_f}{k_i} \sum_{m=-1}^{1} \left| \int d^3\rho_2 \varphi_{2p}(\vec{\rho}_2) \left(e^{i\vec{Q}\cdot\vec{\rho}_2} - e^{-i(1/(m_N)\vec{Q}\cdot\vec{\rho}_2} \right) \varphi_{1s}(\rho_2) \right|^2 ; \quad (1.3)$$

$$\frac{d\sigma(1s)}{d\Omega_f} = \frac{4}{Q^4}\,\frac{k_f}{k_i}\left|\frac{16}{(4+Q^2)^2} - \frac{16}{(4+Q^2/m_N^2)^2}\right|^2. \tag{2.1}$$

$$\frac{d\sigma(2s)}{d\Omega_f} = \frac{8}{Q^4}\,\frac{k_f}{k_i}\left|\frac{256Q^2}{(9+4Q^2)^3} - \frac{256Q^2/m_N^2}{(9+4Q^2/m_N^2)^3}\right|^2. \tag{2.2}$$

$$\frac{d\sigma(2p)}{d\Omega_f} = \frac{18}{Q^4}\,\frac{k_f}{k_i}\left|\frac{256Q}{(9+4Q^2)^3} + \frac{256Q/m_N}{(9+4Q^2/m_N^2)^3}\right|^2, \tag{2.3}$$

$$\frac{d\sigma(1s)}{d\Omega_f} = \frac{4}{Q^4}\,\frac{k_f}{k_i}\left|\frac{16}{(4+Q^2)^2} - \frac{16}{(4+Q^2/m_N^2)^2}\right|^2. \tag{2.1}$$

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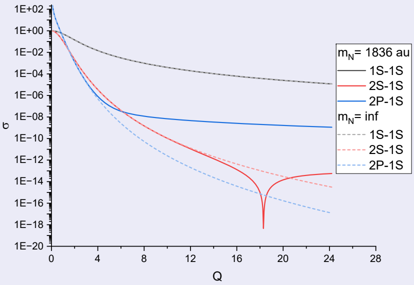

Figure 4: Comparison of FBA with $m_N = \infty$ au and $m_N = 1836$ au nuclear masses.

1. Despite the large mass $m_N = m_p = 1836$ au, the behavior of cross-sections in Eqs. (2.2) and (2.3) are different for the large momentum transfer Q and $d\sigma(2s)$ is zero at $Q \sim 17$.

2. Note that the elastic $1s \to 1s$ transition (2.1) doesn't depend on the finite and infinite nucleus masses.

Here we calculate the ratio

$$R = \frac{d\sigma(2p)}{d\sigma(2s)}, \quad (3)$$

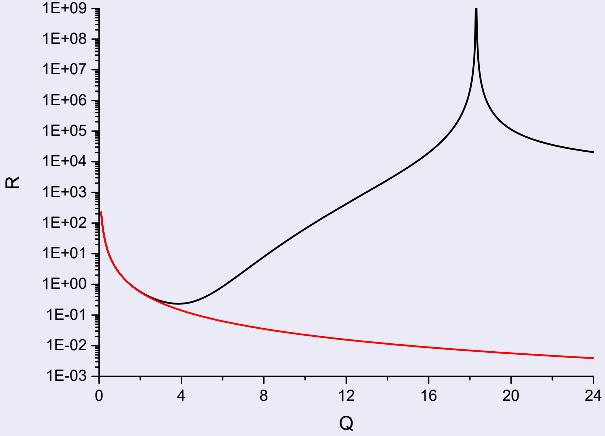

Figure 5: Ratio R of the cross sections. Black curve: $m_N = 1836$ au. Red curve: $m_H = \infty$ au.

Theory. differential cross section for hydrogen: Second Born Approximation

SBA takes the form

$$\langle \vec{k}_f, \varphi_f | T^{SBA} | \vec{k}_i, \varphi_i \rangle = \sum_{\alpha} \int \frac{d^3 k_s}{(2\pi)^3} \frac{\langle \vec{k}_f, \varphi_f | V | \vec{k}_s, \varphi_\alpha^- \rangle \langle \vec{k}_s, \varphi_\alpha^- | V | \vec{k}_i, \varphi_i \rangle}{k_i^2/2 + \varepsilon_i - k_s^2/2 - \varepsilon_\alpha + i0}. \quad (4)$$

Here

$$\langle \vec{k}_f, \varphi_f | V | \vec{k}_s, \varphi_\alpha^- \rangle = \frac{4\pi}{(\vec{k}_s - \vec{k}_f)^2}$$

$$\times \int d^3 \rho_2 \varphi_\alpha^{-*}(\vec{\rho}_2) \left(e^{i(\vec{k}_s - \vec{k}_f)\cdot\vec{\rho}_2} - e^{-i(1/(m_N)(\vec{k}_s - \vec{k}_f)\cdot\vec{\rho}_2} \right) \varphi_i(\rho_2), \quad (5.1)$$

$$\langle \vec{k}_s, \varphi_\alpha^- | V | \vec{k}_i, \varphi_i \rangle = \frac{4\pi}{(\vec{k}_i - \vec{k}_s)^2}$$

$$\times \int d^3 \rho_2 \varphi_f(\vec{\rho}_2) \left(e^{i(\vec{k}_i - \vec{k}_s)\cdot\vec{\rho}_2} - e^{-i(1/(m_N)(\vec{k}_i - \vec{k}_s)\cdot\vec{\rho}_2} \right) \varphi_\alpha^-(\vec{\rho}_2), \quad (5.2)$$

Summation is over the whole Coulomb spectrum, both bound and continuum.

The "closure approximation" means the replacement in (4)

$$\varepsilon_\alpha - \varepsilon_i \to \overline{\varepsilon} > 0.$$

In this case

$$\sum_\alpha |\varphi_\alpha^-\rangle\langle\varphi_\alpha^-| = \hat{I},$$

(density condition) and we have from (4)

$$\langle \vec{k}_f, \varphi_f | T^{SBA} | \vec{k}_i, \varphi_i \rangle = \int \frac{d^3 k_s}{(2\pi)^3} \, \frac{4\pi}{(\vec{k}_i - \vec{k}_s)^2} \frac{4\pi}{(\vec{k}_f - \vec{k}_s)^2} \, \frac{1}{[k_i^2/2 - k_s^2/2 - \overline{\varepsilon} + i0]}$$

$$\times \int d^3\rho_2 \varphi_f(\vec{\rho}_2) W(\rho_2) \varphi_i(\vec{\rho}_2), \qquad (6)$$

$$W(\rho_2) = e^{i\vec{Q}\cdot\vec{\rho}_2} + e^{-i(1/m_N)\vec{Q}\cdot\vec{\rho}_2} - e^{i[\vec{k}_i - \vec{k}_s + (1/m_N)(\vec{k}_f - \vec{k}_s)]\cdot\vec{\rho}_2} - e^{-i[\vec{k}_f - \vec{k}_s + (1/m_N)(\vec{k}_i - \vec{k}_s)]\cdot\vec{\rho}_2}$$

The FBA + closure SBA cross section takes the form

$$\frac{d\sigma_f}{d\Omega} = \frac{1}{(2\pi)^2} \, \frac{k_f}{k_i} \, \left| \langle \vec{k}_f, \varphi_f | T^{FBA} | \vec{k}_i, \varphi_i \rangle + \langle \vec{k}_f, \varphi_f | T^{SBA} | \vec{k}_i, \varphi_i \rangle \right|^2 . \qquad (7)$$

Here $f = 2s,\ 2p$ and $i = 1s$.

How to numerical integrate 6D singular integral (6)?

The Laplace transform: J_1

$$J_1 = \int \frac{d^3k_s}{k_s^2} \frac{1}{(\vec{Q}-\vec{k}_s)^2} \frac{1}{[k_i^2 - (\vec{k}_s+\vec{k}_f)^2 - 2\bar{\varepsilon} + i0]}$$
$$= -\imath \lim_{\lambda\to 0+} \int \frac{d^3k_s}{k_s^2} \frac{1}{(\vec{Q}-\vec{k}_s)^2} \frac{1}{\lambda - \imath(k_i^2 - (\vec{k}_s+\vec{k}_f)^2 - 2\bar{\varepsilon})}$$
$$= -\imath \lim_{\lambda\to 0+} \int_0^\infty d\alpha \int_0^\infty d\beta \int \frac{d^3k_s}{k_s^2}\, e^{-\alpha(\vec{Q}-\vec{k}_s)^2 - \beta(\lambda - \imath(k_i^2-(\vec{k}_s+\vec{k}_f)^2 - 2\bar{\varepsilon}))}$$
$$= -\imath \lim_{\lambda\to 0+} \int_0^\infty d\alpha \int_0^\infty d\beta \int \frac{d^3k_s}{k_s^2}\, e^{-Xk_s^2 + 2\vec{Y}\vec{k}_s - Z} \qquad (8)$$

$$X = \alpha + \imath\beta, \quad \vec{Y} = \alpha\vec{Q} - \imath\beta\vec{k}_f,$$
$$Z(\lambda) = \alpha Q^2 + \beta\left(\lambda - \imath\left(k_i^2 - k_f^2 - 2\bar{\varepsilon}\right)\right) \qquad (9)$$

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$$= -\imath \lim_{\lambda\to 0+} \int \frac{d^3k_s}{k_s^2} \frac{1}{(\vec{Q}-\vec{k}_s)^2} \frac{1}{\lambda - \imath(k_i^2 - (\vec{k}_s+\vec{k}_f)^2 - 2\bar{\varepsilon})}$$

$$= -\imath \lim_{\lambda\to 0+} \int_0^\infty d\alpha \int_0^\infty d\beta \int \frac{d^3k_s}{k_s^2}\, e^{-\alpha(\vec{Q}-\vec{k}_s)^2 - \beta(\lambda - \imath(k_i^2 - (\vec{k}_s+\vec{k}_f)^2 - 2\bar{\varepsilon}))}$$

$$= -\imath \lim_{\lambda\to 0+} \int_0^\infty d\alpha \int_0^\infty d\beta \int \frac{d^3k_s}{k_s^2}\, e^{-Xk_s^2 + 2\vec{Y}\vec{k}_s - Z} \qquad (8)$$

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$$Z(\lambda) = \alpha Q^2 + \beta\left(\lambda - \imath\left(k_i^2 - k_f^2 - 2\bar{\varepsilon}\right)\right) \qquad (9)$$

$$J_1 = -2\imath\pi^{3/2} \lim_{\lambda\to 0+} \int_0^\infty d\alpha \int_0^\infty d\beta \frac{e^{-Z}}{X^{1/2}}\, {}_1F_1\left(\frac{1}{2}, \frac{3}{2}, \frac{Y^2}{X}\right) \qquad (10)$$

How to numerical integrate 6D singular integral (6)?

The Laplace transform: J_1

$$\alpha = \rho x, \quad \beta = \rho(1-x) \tag{11}$$

$$\begin{aligned} J_1 &= -2\imath\pi^{3/2} \lim_{\lambda\to 0+} \int_0^1 dx \frac{1}{\tilde{X}^{1/2}} \int_0^\infty d\rho \rho^{1/2} e^{-\rho\tilde{Z}} {}_1F_1\left(\frac{1}{2}, \frac{3}{2}, \rho\frac{\tilde{Y}^2}{\tilde{X}}\right) \\ &= -2\imath\pi^{3/2}\Gamma(3/2) \int_0^1 dx \frac{1}{\tilde{Z}^{3/2}\tilde{X}^{1/2}} {}_2F_1\left(\frac{3}{2}, \frac{1}{2}; \frac{3}{2}, \frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right) \\ &= -\imath\pi^2 \int_0^1 dx \frac{1}{\tilde{Z}^{3/2}\tilde{X}^{1/2}} \left(1 - \frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right)^{-1/2} = -\imath\pi^2 \int_0^1 dx \frac{1}{\tilde{Z}} \left(\tilde{Z}\tilde{X} - \tilde{Y}^2\right)^{-1/2} \end{aligned} \tag{12}$$

$$\tilde{X} = X/\rho, \quad \tilde{Z} = Z(\lambda = 0)/\rho \tag{13}$$

How to numerical integrate 6D singular integral (6)?

The Laplace transform: J_2

$$J_2(\nu, a, \vec{b}, c) = \int \frac{d^3k_s}{k_s^2}\frac{1}{(\vec{Q}-\vec{k}_s)^2}\,\frac{1}{[k_i^2-(\vec{k}_s+\vec{k}_f)^2-2\overline{\varepsilon}+i0]}\,\frac{1}{(a^2+(\vec{b}-c\vec{k}_s)^2)^\nu}$$

$$= -\frac{\imath}{\Gamma(\nu)}\lim_{\lambda\to 0+}\int_0^\infty d\alpha\int_0^\infty d\beta\int_0^\infty d\gamma\gamma^{\nu-1}\int\frac{d^3k_s}{k_s^2}\,e^{-Xk_s^2+2\vec{Y}\vec{k}_s-Z}$$

$$= -\frac{2\imath\pi^{3/2}}{\Gamma(\nu)}\lim_{\lambda\to 0+}\int_0^\infty d\alpha\int_0^\infty d\beta\int_0^\infty d\gamma\gamma^{\nu-1}\frac{e^{-Z}}{X^{1/2}}{}_1F_1\left(\frac{1}{2},\frac{3}{2},\frac{Y^2}{X}\right) \qquad (14)$$

$$X = \alpha+\imath\beta+\gamma c^2,\quad \vec{Y} = \alpha\vec{Q}-\imath\beta\vec{k}_f+\gamma c\vec{b},$$

$$Z(\lambda) = \alpha Q^2+\beta\left(\lambda-\imath\left(k_i^2-k_f^2-2\overline{\varepsilon}\right)\right)+\gamma(a^2+b^2) \qquad (15)$$

How to numerical integrate 6D singular integral (6)?

The Laplace transform: J_2

$$J_2(\nu,a,\vec{b},c)=\int\frac{d^3k_s}{k_s^2}\frac{1}{(\vec{Q}-\vec{k}_s)^2}\,\frac{1}{[k_i^2-(\vec{k}_s+\vec{k}_f)^2-2\bar{\varepsilon}+i0]}\,\frac{1}{(a^2+(\vec{b}-c\vec{k}_s)^2)^\nu}$$

$$=-\frac{\imath}{\Gamma(\nu)}\lim_{\lambda\to0+}\int_0^\infty d\alpha\int_0^\infty d\beta\int_0^\infty d\gamma\gamma^{\nu-1}\int\frac{d^3k_s}{k_s^2}\,e^{-Xk_s^2+2\vec{Y}\vec{k}_s-Z}$$

$$=-\frac{2\imath\pi^{3/2}}{\Gamma(\nu)}\lim_{\lambda\to0+}\int_0^\infty d\alpha\int_0^\infty d\beta\int_0^\infty d\gamma\gamma^{\nu-1}\frac{e^{-Z}}{X^{1/2}}{}_1F_1\left(\frac{1}{2},\frac{3}{2},\frac{Y^2}{X}\right)\quad(14)$$

$$X=\alpha+\imath\beta+\gamma c^2,\quad \vec{Y}=\alpha\vec{Q}-\imath\beta\vec{k}_f+\gamma c\vec{b},$$

$$Z(\lambda)=\alpha Q^2+\beta\left(\lambda-\imath\left(k_i^2-k_f^2-2\bar{\varepsilon}\right)\right)+\gamma(a^2+b^2)\quad(15)$$

$$\alpha=\rho xy,\quad \beta=\rho(1-x)y,\quad \gamma=\rho(1-y).\quad(16)$$

$$J_2(\nu,a,\vec{b},c)=-\frac{2\imath\pi^{3/2}\Gamma(3/2+\nu)}{\Gamma(\nu)}\int_0^1dx\int_0^1dy\,\frac{y(1-y)^{\nu-1}}{\tilde{Z}^{3/2+\nu}\tilde{X}^{1/2}}\left(1-\frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right)^{-\nu-1/2}$$

$$\times{}_2F_1\left(-\nu,1;\frac{3}{2},\frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right),\quad \tilde{X}=X/\rho,\ \vec{\tilde{Y}}=\vec{Y}/\rho,\ \tilde{Z}=Z(\lambda=0)/\rho\quad(17)$$

How to numerical integrate 6D singular integral (6)?

The Laplace transform: J_3

$$J_3(a,\vec{b},c) = \int \frac{d^3k_s}{k_s} \frac{1}{(\vec{Q}-\vec{k}_s)^2} \frac{1}{[k_i^2-(\vec{k}_s+\vec{k}_f)^2-2\overline{\varepsilon}+i0]} \frac{Y_{1m}(\vec{k}_s)}{(a^2+(\vec{b}-c\vec{k}_s)^2)^3}$$

$$= -\frac{\imath}{2}\lim_{\lambda\to 0+}\int_0^\infty d\alpha \int_0^\infty d\beta \int_0^\infty d\gamma\gamma^2 \int \frac{d^3k_s}{k_s}\ e^{-Xk_s^2+2\vec{Y}\vec{k}_s-Z}\, Y_{1m}(\vec{k}_s) \qquad (18)$$

How to numerical integrate 6D singular integral (6)?

The Laplace transform: J_3

$$J_3(a,\vec{b},c) = \int \frac{d^3k_s}{k_s} \frac{1}{(\vec{Q}-\vec{k}_s)^2} \frac{1}{[k_i^2-(\vec{k}_s+\vec{k}_f)^2-2\bar{\varepsilon}+i0]} \frac{Y_{1m}(\vec{k}_s)}{(a^2+(\vec{b}-c\vec{k}_s)^2)^3}$$
$$= -\frac{\imath}{2}\lim_{\lambda\to 0+}\int_0^\infty d\alpha\int_0^\infty d\beta\int_0^\infty d\gamma\gamma^2\int \frac{d^3k_s}{k_s}\, e^{-Xk_s^2+2\vec{Y}\vec{k}_s-Z}\,Y_{1m}(\vec{k}_s) \qquad (18)$$

$$J_3(a,\vec{b},c) = -\frac{\imath\pi^{3/2}}{3}\lim_{\lambda\to 0+}\int_0^\infty d\alpha\int_0^\infty d\beta\int_0^\infty d\gamma\gamma^2\frac{e^{-Z}Y}{X^{\frac{3}{2}}}Y_{1m}(\vec{Y})\,{}_1F_1\left(\frac{3}{2},\frac{5}{2};\frac{Y^2}{X}\right)$$
$$= -\frac{35\imath\pi^2}{16}\int_0^1 dx\int_0^1 dy\,\frac{y(1-y)^2}{\tilde{Z}^{9/2}\tilde{X}^{3/2}}\,{}_2F_1\left(\frac{9}{2},\frac{3}{2};\frac{5}{2};\frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right)\tilde{\vec{Y}}Y_{1m}(\tilde{\vec{Y}})$$
$$= -\frac{35\imath\pi^2}{16}\int_0^1 dx\int_0^1 dy\,\frac{y(1-y)^2}{\tilde{Z}^{9/2}\tilde{X}^{3/2}}\left(1-\frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right)^{-7/2}{}_2F_1\left(-2,1;\frac{5}{2};\frac{\tilde{Y}^2}{\tilde{Z}\tilde{X}}\right)\tilde{\vec{Y}}Y_{1m}(\tilde{\vec{Y}})$$
$$(19)$$

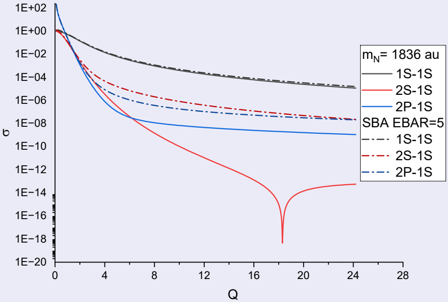
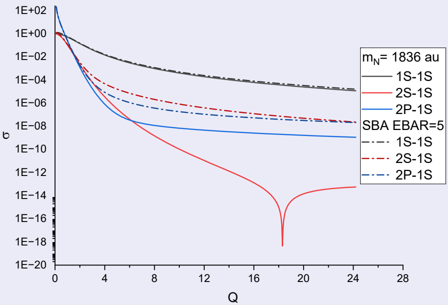


Figure 6: Contribution of SBA is rather significant at large momentum transfers for $1s \to 2s$ and $1s \to 2p$ transitions.



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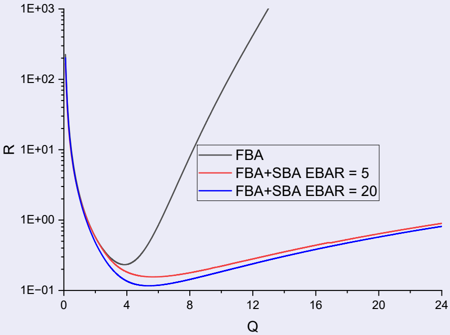

Figure 7: If the value of $\bar{\varepsilon}$ is in the region of a continuous spectrum, then the ratio is weakly dependent on this value.

Conclusion on the hydrogen

1. Contribution of SBA is rather significant at large momentum transfers.

2. The ratio depends weakly on the fitting parameter $\bar{\varepsilon}$ if it is in the continuous spectrum region.

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1. Contribution of SBA is rather significant at large momentum transfers.

2. The ratio depends weakly on the fitting parameter $\bar{\varepsilon}$ if it is in the continuous spectrum region.

Thank you for your attention !