Fully differential cross sections for single ionizing 1-MeV *p*+He collisions at small momentum transfer

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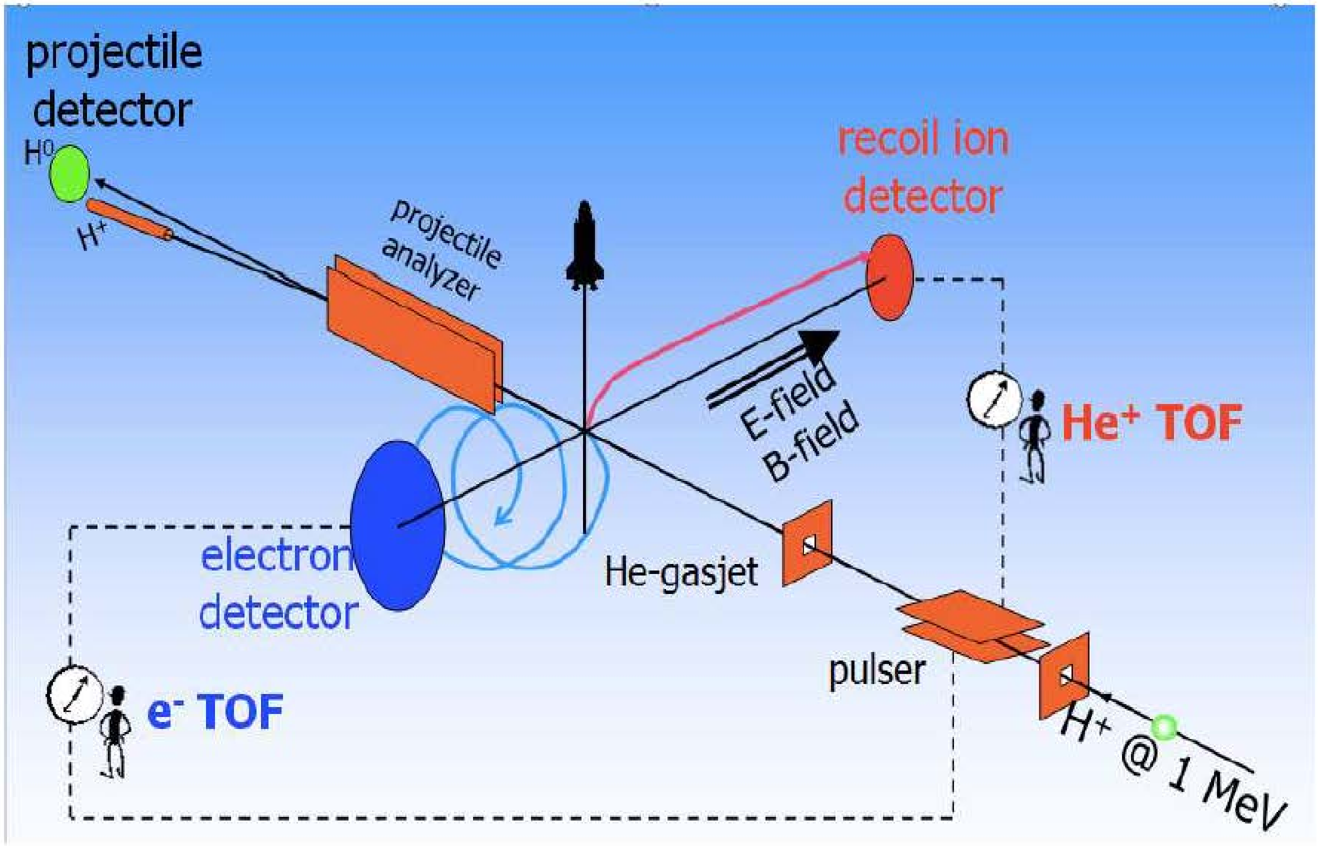
CONTENT

- Experiment
- Matrix element and cross section
- Results of calcs
- Numerical details of calculations
- Conclusions

Experiment: He + p -> He+ + p + e



Theory: matrix element

$$T_{fi}^{3C} = \sqrt{2}\int d^3R d^3r_1 d^3r_2 \; e^{i\vec{R}\vec{p}_i}\Psi_f^{(-*)}(\vec{R},\vec{r}_1,\vec{r}_2;\vec{p}_s,\vec{k}_e)\Phi_0^{\rm He}(\vec{r}_1,\vec{r}_2) \times \left[\frac{2}{R} - \frac{1}{|\vec{R}-\vec{r}_1|} - \frac{1}{|\vec{R}-\vec{r}_2|}\right],$$

$$T_{fi} = A_1 + A_2 + A_3$$

Theory: matrix element, 3C final wf

$$\Psi_f^{-*}(\vec{R},\vec{r}_1,\vec{r}_2) = e^{-i\vec{R}\vec{p}_s}\varphi_0^{\mathrm{He}^+}(\vec{r}_2)\phi^{-*}(\vec{k}_e,\vec{r}_1;-1)\exp\left(\frac{\pi}{2|\vec{v}_p-\vec{k}_e|}\right)\Gamma\left(1-i\frac{1}{|\vec{v}_p-\vec{k}_e|}\right)$$
$$\times {}_1F_1\left[i\frac{1}{|\vec{v}_p-\vec{k}_e|},1;i(|\vec{R}-\vec{r}_1||\vec{v}_p-\vec{k}|+(\vec{R}-\vec{r}_1)\cdot(\vec{v}_p-\vec{k}_e))\right]$$
$$\times\exp\left(-\frac{\pi}{2v_p}\right)\Gamma\left(1+i\frac{1}{v_p}\right){}_1F_1\left[-i\frac{1}{v_p},1;i(Rp_r+\vec{R}\cdot\vec{p}_r)\right].$$

$$\frac{d^3\sigma}{dE_e d\Omega_e d\Omega_s} = k_e\frac{m_p^2}{(2\pi)^5}|T_{fi}|^2$$

(θ_s is the scattering angle of the proton)

Theory: matrix element, momentum space

$$A_1 = 2\sqrt{2}\int \frac{d^3p}{(2\pi)^3}\,\tilde{\phi}^{-*}(\vec{v}_p - \vec{k}_e, \vec{p}; -1) I(\vec{p}_r, \vec{Q} + \vec{p}_r + \vec{v}_p - \vec{k}_e - \vec{p}; 1) G(\vec{k}_e, \vec{p} - \vec{v}_p + \vec{k}_e, 0)$$

$$A_2 = -\sqrt{2}\int \frac{d^3p}{(2\pi)^3}\, I(\vec{v}_p - \vec{k}_e, \vec{p}; -1)\tilde{\phi}^{-*}(\vec{p}_r, \vec{Q} + \vec{p}_r + \vec{v}_p - \vec{k}_e - \vec{p}; 1) G(\vec{k}_e, \vec{p} - \vec{v}_p + \vec{k}_e, 0)$$

$$A_3 = -4\pi\sqrt{2}\int \frac{d^3p_1}{(2\pi)^3}\frac{d^3p_2}{(2\pi)^3 p_2^2}\,\tilde{\phi}^{-*}(\vec{v}_p - \vec{k}_e, \vec{p}_1; -1)\times$$

$$\tilde{\phi}^{-*}(\vec{p}_r, \vec{Q} + \vec{p}_r + \vec{v}_p - \vec{k}_e - \vec{p}_1 - \vec{p}_2; 1) G(\vec{k}_e, \vec{p}_1 - \vec{v}_p + \vec{k}_e, \vec{p}_2).$$

Theory: matrix element, momentum space

$$G(\vec{k},\vec{q}_1,\vec{q}_2) = \int d^3r_1 d^3r_2\ \phi^{-*}(\vec{k},\vec{r}_1;-1)e^{i\vec{q}_1\cdot\vec{r}_1}\varphi_0^{He^+}(\vec{r}_2)e^{i\vec{q}_2\cdot\vec{r}_2}\Phi_0^{He}(\vec{r}_1,\vec{r}_2)$$

$$I(\vec{p},\vec{q};Z,\lambda) = \int \frac{d^3r}{r} e^{-\lambda r}\phi^{-*}(\vec{p},\vec{r};Z)e^{i\vec{q}\cdot\vec{r}} = 4\pi\ e^{-\pi\xi/2}\Gamma(1+i\xi)\frac{[q^2-(p+i\lambda)^2]^{i\xi}}{[(\vec{q}-\vec{p})^2+\lambda^2]^{(1+i\xi)}}$$

$$\tilde{\phi}^{-*}(\vec{p},\vec{q};Z,\lambda) = -\frac{\partial}{\partial\lambda}I(\vec{p},\vec{q};Z,\lambda)$$

$$\tilde{\phi}^{-*}(\vec{p},\vec{q};Z) = -8\pi(p\xi)\ e^{-\pi\xi/2}\ \Gamma(1+i\xi)\frac{(q^2-p^2-i0)^{(-1+i\xi)}}{|\vec{q}-\vec{p}|^{2(1+i\xi)}}. \qquad \lambda\to+0$$

$p\xi = Zp/v_p = Z\mu$, and μ is the reduced mass of colliding particles.

Theory: matrix element, initial states

$$\Psi(r_1, r_2, r_{12}) = \sum_{j=1}^{N} D_j \left[\exp(-\alpha_j r_1 - \beta_j r_2) + \exp(-\alpha_j r_2 - \beta_j r_1)\right] \exp(-\gamma_j r_{12})$$

$E_0^{CF} = -2.903724$ au

O. Chuluunbaatar *et al.*, Phys. Rev. A **74**, 014703, (2006)

[Silverman, Platas and Matsen (SPM)] [50] includes angular correlations

$E_{He}^{SPM} = -2.8952$

J.N. Silverman *et al.* J. Chem. Phys. **32**, 1402, (1960)

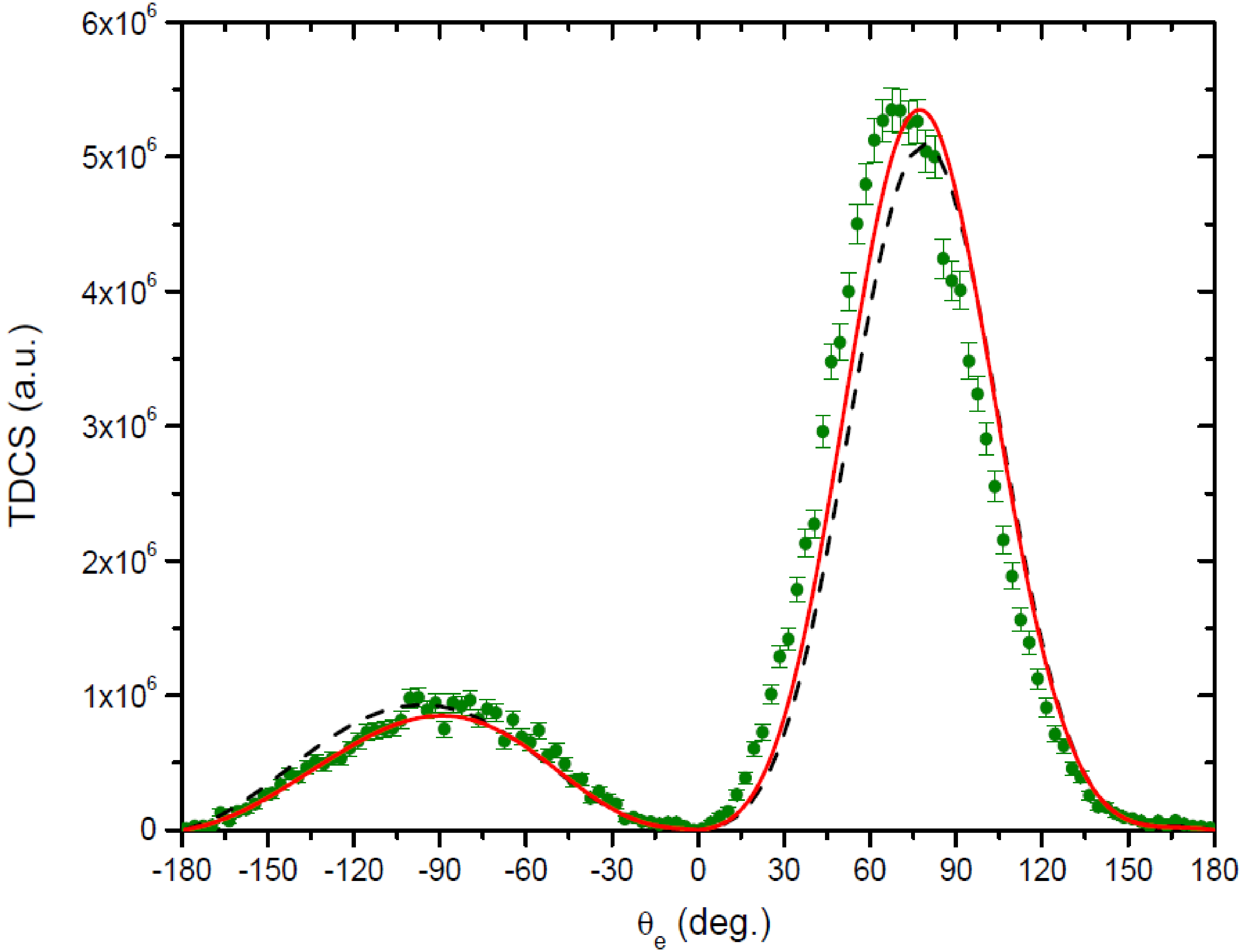
loosely correlated $1s^2$ Roothaan-Hartree-Fock (RHF) wave function

$E_{He}^{RHF} = -2.8617$ a.u.

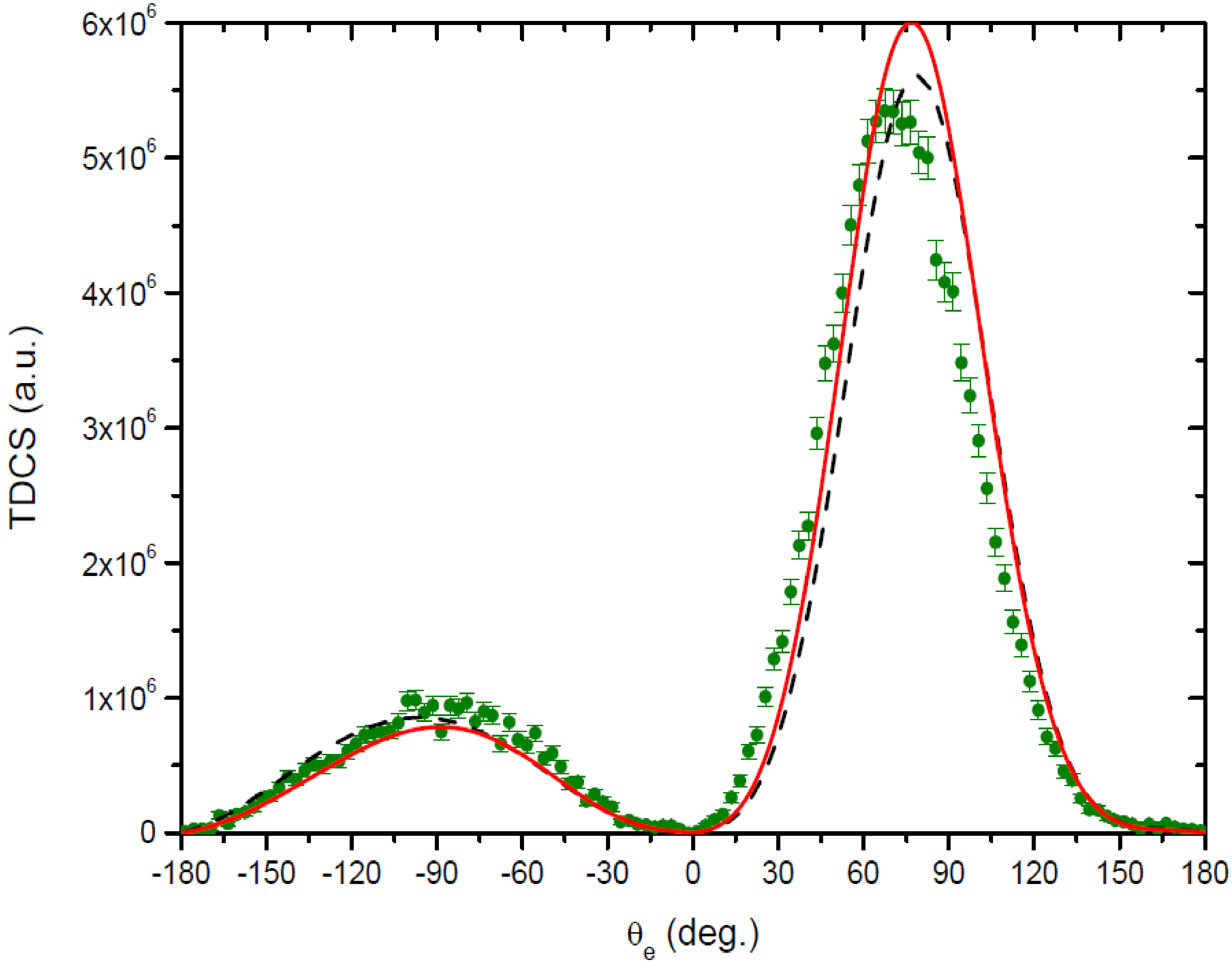
E. Clementi and C. Roetti. Atomic Data and Nuclear Data Tables 14, 177, (1974)

$E_0^{He} = -2.903724377034$

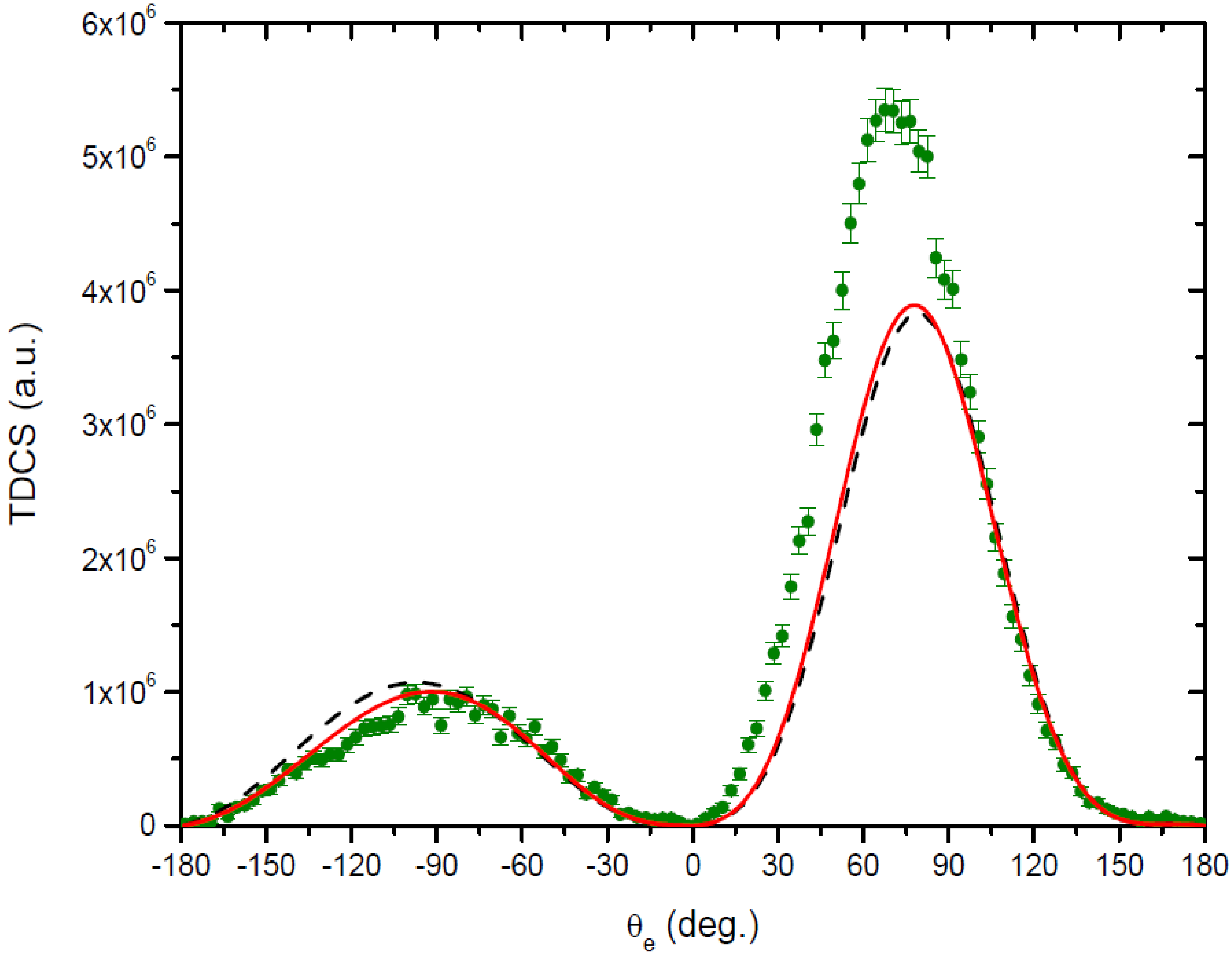
Experiment vs theory: CF-function



Experiment vs theory: SPM-function



Experiment vs theory: HF-function



Numerics: details

Weak singulary points of the integrand functions at $\lambda \to 0$:

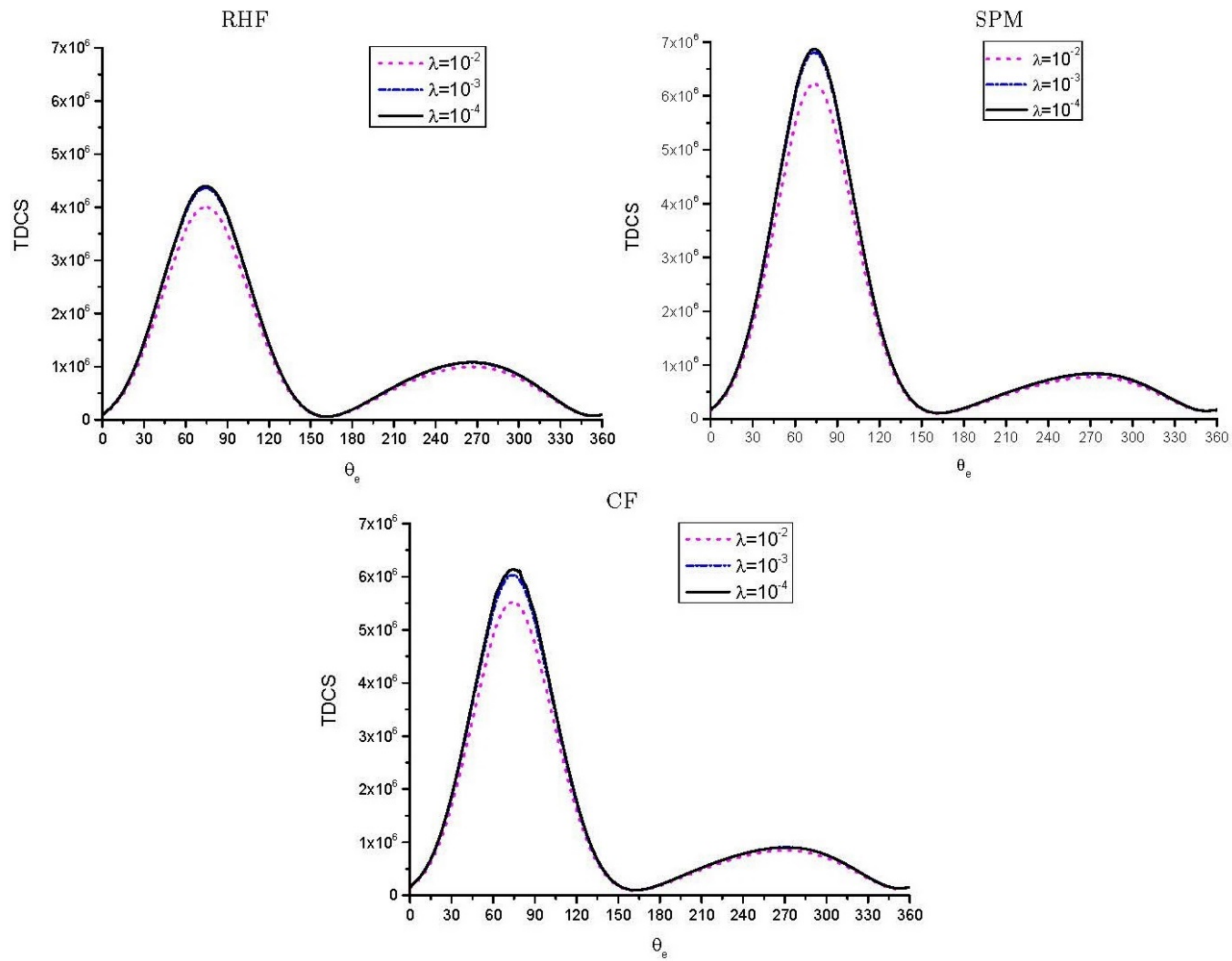
$$A_1\,,A_2: \quad \frac{\lambda}{(\lambda^2+p^2)^2}\frac{1}{(\lambda^2+(\vec{p}+\vec{Q})^2)},$$
$$A_3: \quad \frac{\lambda}{(\lambda^2+p_1^2)^2}\frac{1}{p_2^2}\frac{\lambda}{(\lambda^2+(\vec{p}_1+\vec{p}_2+\vec{Q})^2)^2}$$

$$A_1\,,A_2: \quad \vec{p}=\vec{0}, \quad \vec{p}+\vec{Q}=\vec{0},$$
$$A_3: \quad \vec{p}_1=\vec{0}, \quad \vec{p}_2=-\vec{p}_1-\vec{Q}$$

3D integrations in vicinity of singular points at $\lambda \to 0$: A_1 and A_2:

$$\int_{\Omega_0} d^3p\frac{\lambda}{(\lambda^2+p^2)^2} = 2\pi\left(\arctan\left(\frac{P}{\lambda}\right)-\frac{\lambda\,P}{\lambda^2+P^2}\right) \to \pi^2, \quad p \le P \ll 1,$$
$$\int_{\Omega_Q} d^3p\frac{1}{(\lambda^2+(\vec{p}+\vec{Q})^2)} = 4\pi\left(P-\lambda\arctan\left(\frac{P}{\lambda}\right)\right) \to 4\pi P, \quad |\vec{p}+\vec{Q}| \le P \ll 1$$

Convergence of the matrix elements



Conclusions

- **Physics.** The highly correlated ground wf gives the best binary/recoil ratio close to the experiment.

- **Physics**. The recoil peak has no deal to the ee-correlations in the initial state (another mechanism of its formation).

- **Numerics.** We observe quite wide domain of small parameters, when the results of calcs remain stable.

КОНЕЦ

Спасибо за внимание !

Calculation of the matrix element A_3

Term A_3 was obtained using 2 Fourier transforms for

$$ {}_1F_1\left[i\frac{1}{|\vec{v}_p-\vec{k}_e|},1;i(|\vec{R}-\vec{r}_1||\vec{v}_p-\vec{k}_e|+(\vec{R}-\vec{r}_1)\cdot(\vec{v}_p-\vec{k}_e))\right], \quad \text{and} \quad \frac{1}{|\vec{R}-\vec{r}_2|}. $$

Changing order of integration in T^{3C}_{fi} and using some analytic integrations

$$ \int d^3r_2\frac{e^{-ar_2}}{|\vec{R}-\vec{r}_2|}=4\pi\left[\frac{2}{a^3}\left(\frac{1}{R}-\frac{e^{-aR}}{R}\right)-\frac{e^{-aR}}{a^2}\right], $$

$$ \int d^3r_2\frac{e^{-ar_2}}{|\vec{R}-\vec{r}_2|}(\vec{r}_2\cdot\vec{r}_1)=\frac{32\pi}{a^2}(\vec{R}\cdot\vec{r}_1)\left(\frac{1}{a^3R^3}-\frac{e^{-aR}}{a^3R^3}-\frac{e^{-aR}}{a^2R^2}-\frac{e^{-aR}}{2aR}-\frac{e^{-aR}}{8}\right), $$

$$ \int d^3r_2\frac{e^{-Br_2-cr_{12}}}{|\vec{R}-\vec{r}_2|}=(4\pi)^3\frac{\partial^2}{\partial c\partial B}\int\frac{d^3p_2}{(2\pi)^3}\int\frac{d^3p}{(2\pi)^3}\frac{1}{p_2^2}\frac{e^{i\vec{p}_2\cdot\vec{R}}}{(B^2+(\vec{p}+\vec{p}_2)^2)}\frac{e^{i\vec{p}\cdot\vec{r}_1}}{(c^2+p^2)}, $$

$$ \int\frac{d^3p_2}{(2\pi)^3}\frac{8\pi\nu}{(\nu^2+p_2^2)^2}W_2(\zeta,\vec{p}_r,\vec{q}-\vec{p}_2,\lambda)=W_2(\zeta,\vec{p}_r,\vec{q},\lambda+\nu), $$

$$ W_1(\zeta,\mathbf{k},\mathbf{s},\lambda)=\int\frac{\mathbf{dr}}{r}\exp(-\imath\mathbf{sr}-\lambda r)\,{}_1F_1(-\imath\zeta,1,\imath[kr+\mathbf{kr}])=\frac{4\pi}{(s^2+\lambda^2)}(1-x)^{i\zeta}, $$

$$ W_2(\zeta,\mathbf{k},\mathbf{s},\lambda)=-\frac{\partial W_1(\zeta,\mathbf{k},\mathbf{s},\lambda)}{\partial\lambda}, \quad x=2\frac{\mathbf{sk}+\imath\lambda k}{\lambda^2+s^2}, $$

the term A_3 comes to the 3D, 4D and 7D integrals, respectively for RHF, SPM, and CF.

The integrand functions have the weak singular points $\vec{p}=\vec{0}$ and $\vec{Q}+\vec{p}=\vec{0}$ as A_1 and A_2.