Gailitis-Damburg oscillations in the three-body atomic systems

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Plan of the talk

1. Dipole interaction in the three-body system with Coulomb interaction, Gailitis-Damburg oscillations
2. Computational experiment: the Merkuriev-Faddeev equations in total orbital momentum representation
3. Corrected incoming and outgoing waves
4. Results: low-energy scattering processes in $e^+e^-\bar{p}$, e^-H, $\mu p \mu$ systems

Three-body system with Coulomb interaction

The 3-body Hamiltonian in the center of mass frame:

$$H = H_0 + V \equiv -\Delta_{\boldsymbol{X}} + \sum_{\alpha=1}^{3} V_\alpha(\boldsymbol{x}_\alpha),$$

$\boldsymbol{X} = \{\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha\} \in \mathbb{R}^6$ is the set of standard mass-weighted Jacobi coordinates, $\boldsymbol{x}_\alpha \in \mathbb{R}^3$ is the two-body relative coordinate

$V_\alpha(\boldsymbol{x}_\alpha)$ are two body Coulomb potentials:

$$V_\alpha(\boldsymbol{x}_\alpha) = \frac{q_\beta q_\gamma \sqrt{2\mu_\alpha}}{|\boldsymbol{x}_\alpha|}, \qquad \mu_\alpha = \frac{m_\beta m_\gamma}{m_\beta + m_\gamma}.$$

(a short-range potential $V^s_\alpha(\boldsymbol{x}_\alpha) \sim O\left(\frac{1}{|\boldsymbol{x}_\alpha|^{2+\mu}}\right)$, $\mu > 0$ can be added)
$\{\alpha, \beta, \gamma\}$ runs over $\{1, 2, 3\}$ cyclically.

Two-body sectors

$|\boldsymbol{x}_1| \ll |\boldsymbol{y}_1|$

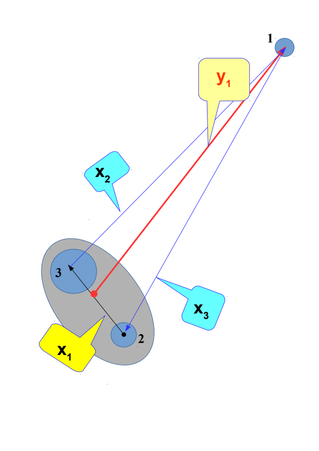


Figure: The configuration of bound state of particles (2,3) as a target and particle 1 as a spectator

The particle 1 — atom (23) interaction in the two-body sector $|\boldsymbol{x}_1| \ll |\boldsymbol{y}_1|$

Multipole expasion of Coulomb interactions:

$$\sum_{\beta=2}^{3} \frac{q_1 q_\gamma \sqrt{2\mu_\beta}}{|\boldsymbol{x}_\beta|} = \sum_{\beta=2}^{3} \frac{q_1 q_\gamma \sqrt{2\mu_\beta}}{|c_{\beta 1}\boldsymbol{x}_1 + s_{\beta 1}\boldsymbol{y}_1|} =$$

$$= \sum_{\beta=2}^{3} q_1 q_\gamma \sqrt{2\mu_\beta} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{(-1)^\ell 4\pi}{2\ell+1} \frac{(|c_{\beta 1}\boldsymbol{x}_1|)^\ell}{(|s_{\beta 1}\boldsymbol{y}_1|)^{\ell+1}} Y_{\ell m}(\hat{\boldsymbol{x}}_1) Y^*_{\ell m}(\hat{\boldsymbol{y}}_1) =$$

$$= \frac{1}{|\boldsymbol{y}_1|} \sum_{\beta=2}^{3} \frac{q_1 q_\gamma \sqrt{2\mu_\beta}}{|s_{\beta 1}|} - \frac{1}{|\boldsymbol{y}_1|^2} \sum_{\beta=2}^{3} q_1 q_\gamma \sqrt{2\mu_\beta} \frac{|c_{\beta 1}\boldsymbol{x}_1|}{|s_{\beta 1}|^2} P_1(\hat{\boldsymbol{x}}_1 \cdot \hat{\boldsymbol{y}}_1) + O(|\boldsymbol{y}_1|^{-3})$$

Result:

$$V_2 + V_3 \sim \frac{C}{|\boldsymbol{y}_1|} + \frac{A(\boldsymbol{x}_1, \hat{\boldsymbol{y}}_1)}{|\boldsymbol{y}_1|^2} + O(|\boldsymbol{y}_1|^{-3}), \quad |\boldsymbol{y}_1| \to \infty$$

CCE approach to scattering of a charged particle 1 on a bound pair of charged particles 2,3

The typical approach is the close coupling expansion (CCE) (Seaton, Burke, Gailitis...) within R-matrix formalism

CCE for wave function

$$\Psi(x_1, y_1) = \sum_{n\mathfrak{a}} \frac{\Psi_{n\mathfrak{a}}(y_1)}{x_1 y_1} \phi_{n\ell}(x_1) \mathcal{Y}_{\mathfrak{a}}(\hat{x}_1, \hat{y}_1), \quad \mathfrak{a} = LM\ell\lambda$$

where $\phi_{n\ell}$ is radial wave function of Coulomb bound state with the energy ϵ_n, $\mathcal{Y}_{\mathfrak{a}}$ are bispherical harmonics corresponding to the total orbital momentum L.

CCE equations as $y_1 \to \infty$

$$\left(-\frac{d^2}{dy_1^2} + \frac{C}{y_1} + \frac{\lambda(\lambda+1) + \mathbf{A}}{y_1^2} - \mathbf{p}^2\right) \Psi(y_1) = O(y_1^{-3}), \quad p_n^2 = E - \epsilon_n.$$

CCE equations for a long time were the main and ONLY tool for analyzing scattering of a charged particle on a two-body target bound by Coulomb potential (e^-–H, e^-–He^+, e^+–H, ...)

Two main known features of scattering of charged particles on two-body Coulomb target:

- Under threshold resonances
- Above threshold oscillations (GD = Gailitis, Damburg)

These features are derived from the solution of model CCE equations within the requirements that the dipole potential matrix $\mathbf{A}$ has the same block structure as the matrix $\mathbf{p}^2$, i.e. $A_{n\ell,n'\ell'} = A_{n,\ell\ell'}\delta_{nn'}$, i.e. by neglecting dipole coupling of target states with $n \neq n'$.

Gailitis-Damburg oscillations

Gailitis, Damburg *Sov. Phys. JETP*, 17:1107–1110, 1963
Proc. Phys. Soc., 82:192–200, 1963

Yakovlev, Gradusov *Theor. Math. Phys.* 217:2 416-429, 2023

Model CCE equations for $e^- H$ scattering:

Main consequence of diagonality of $\mathbf{A}$ is $[\mathbf{A}, \mathbf{p^2}] = 0$ and hence the diagonalising matrix $\mathbf{V}$ such that $\mathbf{V}^\dagger[\lambda(\lambda+1) + \mathbf{A}]\mathbf{V} = \mathbf{D}$, $\mathbf{D}_{(n\ell\lambda)(n'\ell'\lambda')} = d_{(n\ell\lambda)}\delta_{n\ell\lambda,n'\ell'\lambda'}$ commutes with $\mathbf{p}^2$, i.e. $[\mathbf{V}, \mathbf{p}^2] = 0$. This allows to diagonalize the CCE equations:

$$\left(-\frac{d^2}{dy_1^2} + \frac{\mathbf{D}}{y_1^2} - \mathbf{p}^2\right)\mathbf{V}^\dagger\Psi(y_1) = 0$$

$$\mathbf{D} = \mathcal{L}(\mathcal{L}+1), \quad \mathcal{L}_{(n\ell\lambda)(n'\ell'\lambda')} = \mathcal{L}_{(n\ell\lambda)}\delta_{n\ell\lambda,n'\ell'\lambda'},$$

$$\mathcal{L}_{(n\ell\lambda)} = -1/2 \pm \sqrt{1/4 + d_{(n\ell\lambda)}}$$

Two possibilities for $\mathbf{D}$:

1. $d_{(n\ell\lambda)} \geq 0$ then $\mathcal{L}_{(n\ell\lambda)} \geq 0$.
2. there is $n\ell\lambda$ such that $d_{(n\ell\lambda)} < 0$ then
   - the equation

     $$\left(-\frac{d^2}{dy_1^2} + \frac{d_{(n\ell\lambda)}}{y_1^2} - E\right)[\mathbf{V}^\dagger\Psi]_{n\ell\lambda}(y_1) = 0$$

     supports infinitely many bound states accumulating to the threshold ϵ_n from below
   - the scattering amplitude has the anomalous threshold behavior since if $d_{(n\ell\lambda)} < -1/4$ then $\mathcal{L}_{(n\ell\lambda)}$ is complex
     $\mathcal{L}_{(n\ell\lambda)} = -1/2 \pm i\sqrt{|d_{(n\ell\lambda)}| - 1/4}$
     T-matrix p_n dependence: $p_n^{\mathcal{L}_{(n\ell\lambda)}+1/2} = \exp\{i\Im\mathrm{m}(\mathcal{L}_{(n\ell\lambda)})\ln(p_n)\} \Rightarrow$

     $$\sigma_{n\ell,n_0\ell_0} = A + B\cos(2\Im\mathrm{m}(\mathcal{L}_{(n\ell\lambda)})\ln(p_n) + \phi),$$

     which gives rise to an infinite number of oscillations in the cross section as the energy tends to threshold from above (GD oscillations formula).

Solution (asymptote): $[\mathbf{V}^\dagger\Psi(y_1)]_{n\ell\lambda} = h^{\pm}_{\mathcal{L}_{(n\ell\lambda)}}(p_n y_1)$.

Corrected incoming and outgoing waves

Gradusov, Yakovlev *Theor. Math. Phys. 2024 to appear*

$$\psi^{\pm}_{(n\ell\lambda)(n'\ell'\lambda')}(y_1, p_{n'}) = \\ = \left[W^{(0)}_{(n\ell\lambda)(n'\ell'\lambda')} + \frac{1}{y_1^2} W^{(1)}_{(n\ell\lambda)(n'\ell'\lambda')} \right] u^{\pm}_{\mathcal{L}_{(n'\ell'\lambda')}}(\eta_{n'}, p_{n'} y_1). \quad (1)$$

$$\begin{aligned} W^{(0)}_{(n\ell\lambda)(n'\ell'\lambda')} &= \delta_{nn'} V_{(n\ell\lambda)(n\ell'\lambda')}, \\ W^{(1)}_{(n\ell\lambda)(n'\ell'\lambda')} &= (1-\delta_{nn'}) \frac{\sum_{\ell'',\lambda''} A_{(n\ell\lambda)(n'\ell''\lambda'')} V_{(n'\ell''\lambda'')(n'\ell'\lambda')}}{(p_n^2 - p_{n'}^2)}, \end{aligned} \quad (2)$$

$$\mathcal{L}_{(n\ell\lambda)}(\mathcal{L}_{(n\ell\lambda)} + 1) = d_{(n\ell\lambda)} \quad (3)$$

$d_{(n'\ell'\lambda')}$ and $V_{(n'*)(n'\ell'\lambda')}$ are eigen values and eigen vectors of the matrix

$$\lambda(\lambda+1)\delta_{\ell\lambda,\ell'\lambda'} + A_{(n'\ell\lambda)(n'\ell'\lambda')}.$$

The Merkuriev-Faddeev equations in total orbital momentum representation

Merkuriev *Ann. Phys.* 130 395–426, 1980
Kostrykin, Kvitsinsky, Merkuriev *Few Body Syst.* 6 97–113, 1989

Gradusov et al. *Commun. Comput. Phys.* 30 255–287, 2021

The Merkuriev-Faddeev equations

$$\{T_\alpha + V_\alpha(x_\alpha) + \sum_{\beta\neq\alpha} V_\beta^{(\mathrm{l})}(x_\beta) - E\}\psi_\alpha(\boldsymbol{x}_\alpha, \boldsymbol{y}_\alpha) = -V_\alpha^{(\mathrm{s})}(x_\alpha) \sum_{\beta\neq\alpha} \psi_\beta(\boldsymbol{x}_\beta, \boldsymbol{y}_\beta),$$

$T_\alpha \equiv -\Delta_{\boldsymbol{x}_\alpha} - \Delta_{\boldsymbol{y}_\alpha}$, potential splitting $V_\alpha(x_\alpha) = V_\alpha^{(\mathrm{s})}(x_\alpha) + V_\alpha^{(\mathrm{l})}(x_\alpha)$.
Total orbital momentum representation

$$\psi_\alpha(X_\alpha, \Omega_\alpha) = \sum_{LM\tau} \sum_{M'} (1 - z_\alpha^2)^{M'/2} \times \frac{\psi^{L\tau}_{\alpha MM'}(X_\alpha)}{x_\alpha y_\alpha} F^{L\tau}_{MM'}(\Omega_\alpha),$$

$F^{L\tau}_{MM'}$ — common eigenfunction of the total orbital momentum squared, its projection and the spatial inversion operators.
$X_\alpha = \{x_\alpha, y_\alpha, z_\alpha \equiv \cos\theta_\alpha = \hat{\boldsymbol{x}}_\alpha \cdot \hat{\boldsymbol{y}}_\alpha\}$, Ω_α — Euler angles.

Partial equations:

A set of 3D MFE for given $LM\tau$

$$\left[T^{L\tau}_{\alpha M M'} + V_\alpha(x_\alpha) + \sum\nolimits_{\beta\neq\alpha} V^{(1)}_\beta(x_\beta,y_\beta) - E\right]\psi^{L\tau}_{\alpha M M'}(X_\alpha)$$

$$+T^{L\tau-}_{\alpha M, M'-1}\psi^{L\tau}_{\alpha M, M'-1}(X_\alpha) + T^{L\tau+}_{\alpha M,M'+1}\psi^{L\tau}_{\alpha M,M'+1}(X_\alpha)$$

$$= -\frac{V^{(s)}_\alpha(x_\alpha,y_\alpha)}{(1-z_\alpha^2)^{\frac{M'}{2}}}\sum\nolimits_{\beta\neq\alpha}\frac{x_\alpha y_\alpha}{x_\beta y_\beta}\sum\nolimits_{M''}\frac{(-1)^{M''-M'}2}{\sqrt{2+2\delta_{M''0}}}$$

$$\times F^{L\tau}_{M''M'}(0,w_{\beta\alpha},0)(1-z_\beta^2)^{\frac{M''}{2}}\psi^{L\tau}_{\beta M M''}(X_\beta).$$

Partial component asymptote **with correction** (neutral atom $\beta\gamma$):

$$\psi^{L\tau}_{\alpha M M'}(X_\alpha) \sim \frac{1}{\sqrt{2+2\delta_{M'0}}}\sum\nolimits_{n\ell}\sqrt{2\ell+1}\,\phi_{n\ell}(x_\alpha)$$

$$\times\sum\nolimits_{\lambda} C^{LM'}_{\lambda M'\ell 0}\left(1+\tau(-1)^{\ell+\lambda-L}\right)\frac{Y_{\lambda M'}(\theta_\alpha,0)}{(1-z_\alpha^2)^{M'/2}}$$

$$\times\sum\nolimits_{n'\ell'\lambda'}\left[\delta_{\alpha\alpha_0}\delta_{n'n_0}\mathrm{e}^{\mathrm{i}\pi\lambda_0/2}\left(V^{L\tau}_{\alpha(n_0\ell_0\lambda_0)(n_0\ell'\lambda')}\right)^*\psi^{L\tau-}_{\alpha(n\ell\lambda)(n_0\ell'\lambda')}(y_\alpha)\right.$$

$$\left.+\frac{1}{\sqrt{4\pi}}\sqrt{\frac{p_{n_0}}{p_{n'}}}\,\mathfrak{S}^{L\tau}_{(\alpha n'\ell'\lambda')(\alpha_0 n_0\ell_0\lambda_0)}\psi^{L\tau+}_{\alpha(n\ell\lambda)(n'\ell'\lambda')}(y_\alpha)\right].$$

Partial equations:

Partial component asymptote **with correction** (neutral atom $\beta\gamma$):

$$\psi^{L\tau}_{\alpha M M'}(X_\alpha) \sim \frac{1}{\sqrt{2+2\delta_{M'0}}} \sum_{n\ell} \sqrt{2\ell+1}\phi_{n\ell}(x_\alpha)$$
$$\times \sum_\lambda C^{LM'}_{\lambda M' \ell 0}(1+\tau(-1)^{\ell+\lambda-L}) \frac{Y_{\lambda M'}(\theta_\alpha,0)}{(1-z_\alpha^2)^{M'/2}}$$
$$\times \sum_{n'\ell'\lambda'} \left[\delta_{\alpha\alpha_0}\delta_{n'n_0} \mathrm{e}^{\mathrm{i}\pi\lambda_0/2} \left(V^{L\tau}_{\alpha(n_0\ell_0\lambda_0)(n_0\ell'\lambda')} \right)^* \psi^{L\tau-}_{\alpha(n\ell\lambda)(n_0\ell'\lambda')}(y_\alpha) \right.$$
$$\left. + \frac{1}{\sqrt{4\pi}} \sqrt{\frac{p_{n_0}}{p_{n'}}} \mathfrak{S}^{L\tau}_{(\alpha n'\ell'\lambda')(\alpha_0 n_0 \ell_0 \lambda_0)} \psi^{L\tau+}_{\alpha(n\ell\lambda)(n'\ell'\lambda')}(y_\alpha) \right].$$

Connection to physical amplitude:

$$S^{L\tau}_{(\alpha n\ell\lambda)(\alpha_0 n_0\ell_0\lambda_0)} = \frac{\mathrm{i}}{2\sqrt{2\ell_0+1}} \sum_{\ell'\lambda'} V^{L\tau}_{\alpha(n\ell\lambda)(n\ell'\lambda')} \mathfrak{S}^{L\tau}_{(\alpha n\ell'\lambda')(\alpha_0 n_0\ell_0\lambda_0)}.$$

G-D oscillations in $e^+e^-\bar{p}$ system, above Ps(2) threshold

V. Gradusov, S. Yakovlev, JETP Letters 2024, 119:3, 151-157

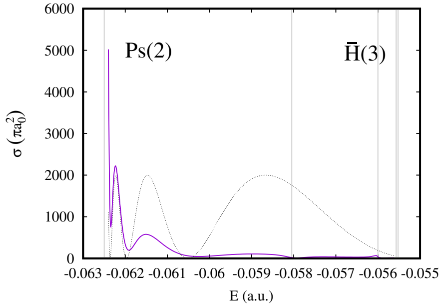


Figure: Ps(2s) $\rightarrow$ Ps(2s) cross section, $L = 0$.

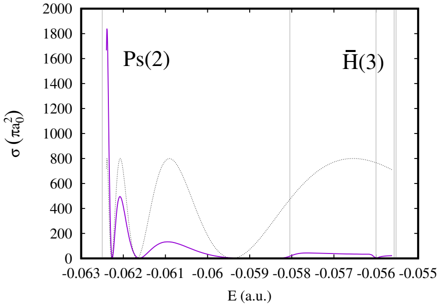


Figure: Ps(2s) $\rightarrow$ Ps(2p) cross section, $L = 0$.

G-D oscillations in $e^+e^-\bar{p}$ system, above Ps(2) threshold

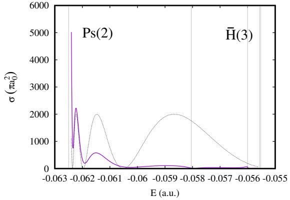


Figure: Ps(2s) → Ps(2s) cross section, $L = 0$.

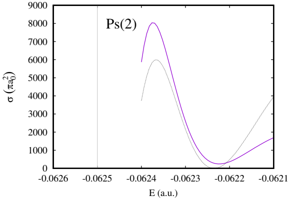


Figure: same, $L = 1$.

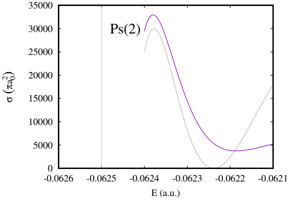


Figure: same, $L = 2$.

G-D oscillations in $e^+e^-\bar{p}$ system, above $\overline{\mathrm{H}}(2)$ threshold

V. Gradusov, S. Yakovlev, JETP Letters 2024, 119:3, 151-157

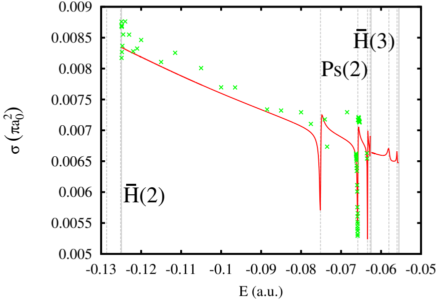


Figure: Antihydrogen formation cross section Ps(1)→ $\overline{\mathrm{H}}(1)$, $L = 0$.

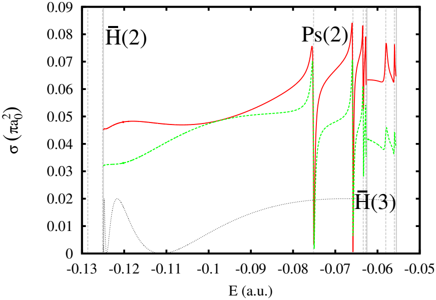


Figure: Antihydrogen formation cross sections Ps(1)→ $\overline{\mathrm{H}}$(2s) (solid) and Ps(1)→ $\overline{\mathrm{H}}$(2p) (dashed line), $L = 0$.

G-D oscillations in $e^+e^-\bar{p}$ system, above $\overline{\mathrm{H}}(3)$ threshold

V. Gradusov, S. Yakovlev, JETP Letters 2024, 119:3, 151-157

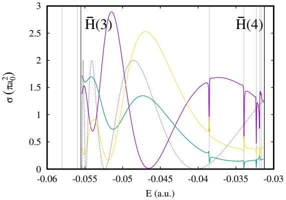


Figure: $L = 0$

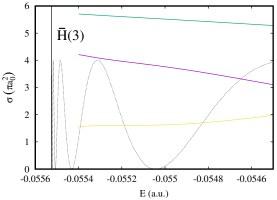


Figure: $L = 1$.

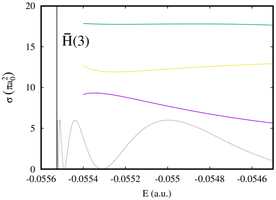


Figure: $L = 2$.

Antihydrogen formation cross sections Ps(2p)→ $\overline{\mathrm{H}}$(3s) (solid), Ps(2p)→ $\overline{\mathrm{H}}$(3p) (dashed) and Ps(2p)→ $\overline{\mathrm{H}}$(3d) (dash-dotted line).

G-D oscillations in e^--H and μ-(μp) collision

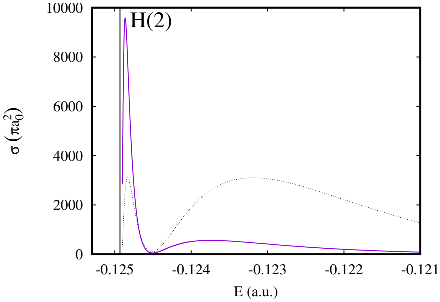


Figure: H(2s)-H(2s) cross section, $L = 0$.

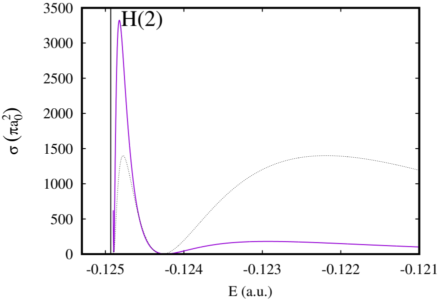


Figure: H(2s)-H(2p) cross section, $L = 0$.

G-D oscillations in e^--H and μ-(μp) collision

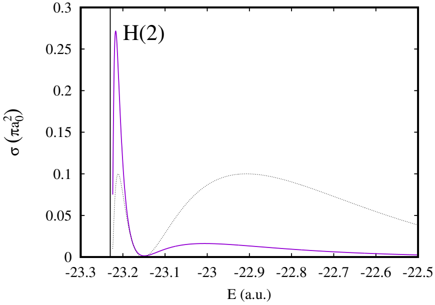


Figure: (μp)(2s)-(μp)(2s) cross section, $L = 0$.

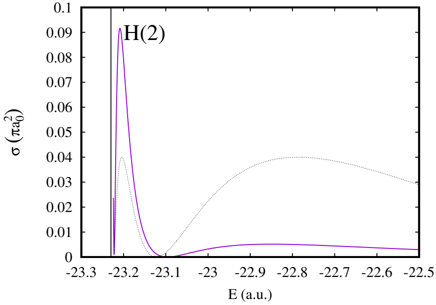


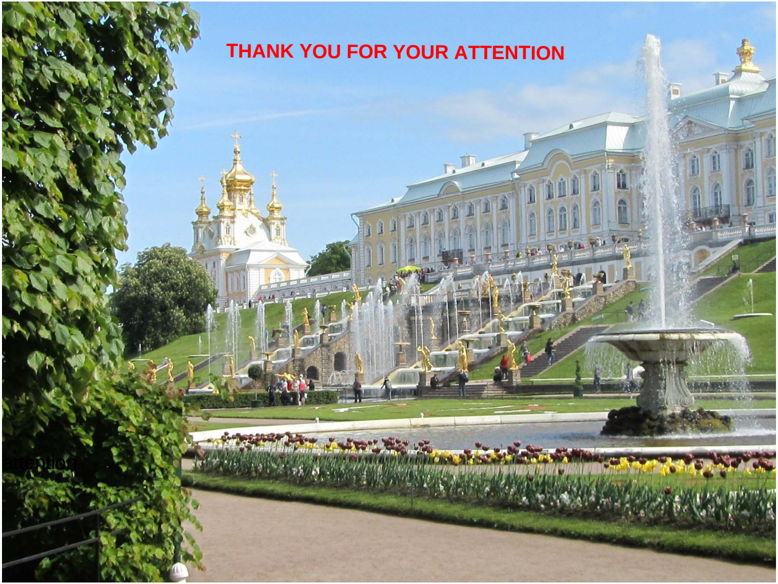
Figure: (μp)(2s)-(μp)(2p) cross section, $L = 0$.

Conclusion

- The induced dipole interaction plays an important role in the three-body collision processes generating multiple resonances and specific oscillations of cross sections in Coulomb systems.
- Taking into account the contribution of the dipole interaction potential into the asymptotic boundary condition is decisive for correct treatment of the scattering problem in the three-body Coulomb systems.

Collaborants

This report is based on joint work with
E.A. Yarevsky (SPbSU)
V.A. Roudnev (SPbSU)


THANK YOU FOR YOUR ATTENTION
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