Ab initio scattering calculation in three-body Coulomb systems: $e^- - \bar{\mathrm{H}}$ $(e^+ - \mathrm{H})$ and $e^+ - \mathrm{He}^+$

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Plan of the talk

1. Theory of Faddeev-Merkuriev equations
2. Solution method
3. Results for $e^- e^+ \bar{p}$
4. Results for $e^+ e^- \mathrm{He}^{++}$
5. Summary

Scattering processes

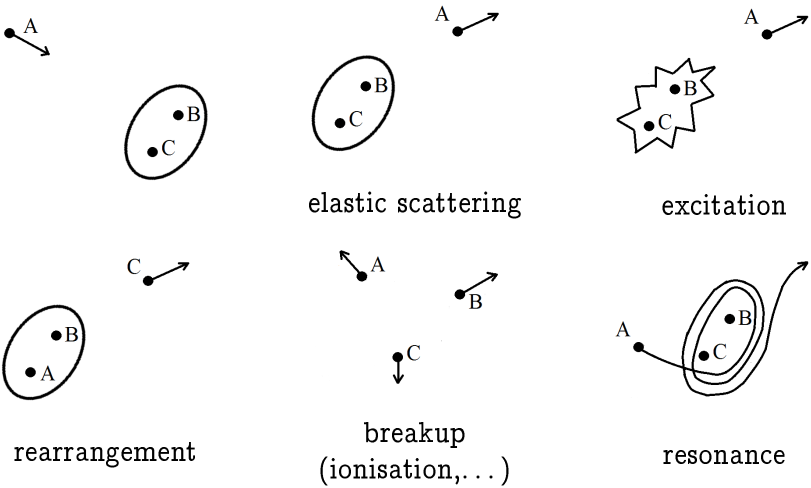


Figure: Scattering processes in a three-body system.

Schrödinger equation

The nonrelativistic Schrödinger equation ($\hbar = 1$)

$$\Big(-\frac{\Delta_{\boldsymbol{r}_1}}{2m_1}-\frac{\Delta_{\boldsymbol{r}_2}}{2m_2}-\frac{\Delta_{\boldsymbol{r}_3}}{2m_3}+V_1(r_{23})+V_2(r_{13})+V_3(r_{12})-E\Big)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3)=0.$$

In the center of mass coordinate frame and reduced Jacobi coordinates $\boldsymbol{x}_1 \to \sqrt{2m_{23}}\boldsymbol{x}_1$, $\boldsymbol{y}_1 \to \sqrt{2m_{1,23}}\boldsymbol{y}_1$:

$$\Big(-\Delta_{\boldsymbol{x}_1}-\Delta_{\boldsymbol{y}_1}+V_1(x_1)+V_2(x_2)+V_3(x_3)-E\Big)\psi(\boldsymbol{x}_1,\boldsymbol{y}_1)=0.$$

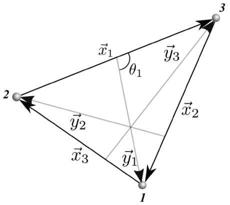


Figure: Jacobi coordinates

Schrödinger equation

The nonrelativistic Schrödinger equation ($\hbar = 1$)

$$\Big(-\frac{\Delta_{\mathbf{r_1}}}{2m_1}-\frac{\Delta_{\mathbf{r_2}}}{2m_2}-\frac{\Delta_{\mathbf{r_3}}}{2m_3}+V_1(r_{23})+V_2(r_{13})+V_3(r_{12})-E\Big)\Psi(\mathbf{r_1},\mathbf{r_2},\mathbf{r_3}) = 0.$$

In the center of mass coordinate frame and reduced Jacobi coordinates $\mathbf{x_1} \to \sqrt{2m_{23}}\mathbf{x_1}$, $\mathbf{y_1} \to \sqrt{2m_{1,23}}\mathbf{y_1}$:

$$\Big(-\Delta_{\mathbf{x_1}} - \Delta_{\mathbf{y_1}} + V_1(x_1) + V_2(x_2) + V_3(x_3) - E\Big)\psi(\mathbf{x_1},\mathbf{y_1}) = 0.$$

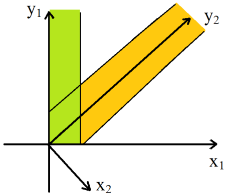


Figure: The wave function

+ complicated boundary conditions on ψ at infinity, in different parts of the configuration space:

$$\begin{cases} y_\alpha \to \infty, \\ x_\alpha \text{ fixed} \end{cases} \text{ or } \begin{cases} y_1 \to \infty, \\ x_1 \to \infty \end{cases}$$

(describe different configurations after collision - e.g. rearrangement, breakup)

Faddeev equations

The system of Faddeev equations

$$\begin{cases} \Big(-\Delta_{\boldsymbol{x}_1} - \Delta_{\boldsymbol{y}_1} + V_1(x_1) - E\Big)\psi_1(\boldsymbol{x}_1, \boldsymbol{y}_1) = -V_1(x_1)\Big(\psi_2 + \psi_3\Big), \\ \Big(-\Delta_{\boldsymbol{x}_2} - \Delta_{\boldsymbol{y}_2} + V_2(x_2) - E\Big)\psi_2(\boldsymbol{x}_2, \boldsymbol{y}_2) = -V_2(x_2)\Big(\psi_1 + \psi_3\Big), \\ \Big(-\Delta_{\boldsymbol{x}_3} - \Delta_{\boldsymbol{y}_3} + V_3(x_3) - E\Big)\psi_3(\boldsymbol{x}_3, \boldsymbol{y}_3) = -V_3(x_3)\Big(\psi_1 + \psi_2\Big). \end{cases}$$

Asymptotic uncoupling of components!

$\psi = \psi_1 + \psi_2 + \psi_3$

The r.h.s.'s — "sources".

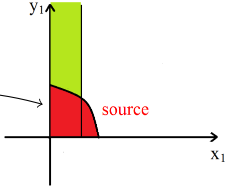


Figure: The ψ_1 component.

In the case of charged particles $V_\alpha(x_\alpha) = \sqrt{2\mu_\alpha} Z_\beta Z_\gamma / x_\alpha$ the square integrability of sources breaks!

Faddeev equations

The system of Faddeev equations

$$\begin{cases} \Big(-\Delta_{\boldsymbol{x}_1} - \Delta_{\boldsymbol{y}_1} + V_1(x_1) - E \Big)\psi_1(\boldsymbol{x}_1, \boldsymbol{y}_1) = -V_1(x_1)\Big(\psi_2 + \psi_3\Big), \\ \Big(-\Delta_{\boldsymbol{x}_2} - \Delta_{\boldsymbol{y}_2} + V_2(x_2) - E \Big)\psi_2(\boldsymbol{x}_2, \boldsymbol{y}_2) = -V_2(x_2)\Big(\psi_1 + \psi_3\Big), \\ \Big(-\Delta_{\boldsymbol{x}_3} - \Delta_{\boldsymbol{y}_3} + V_3(x_3) - E \Big)\psi_3(\boldsymbol{x}_3, \boldsymbol{y}_3) = -V_3(x_3)\Big(\psi_1 + \psi_2\Big). \end{cases}$$

Modification in the charged particles case — the system of Faddeev-Merkuriev equations, $V_\alpha(x_\alpha) = V_\alpha^{(s)}(x_\alpha, y_\alpha) + V_\alpha^{(l)}(x_\alpha, y_\alpha)$:

$$\Big(-\Delta_{\boldsymbol{x}_1} - \Delta_{\boldsymbol{y}_1} + V_1(x_1) + \sum_{\beta\neq 1} V_\beta^{(l)} - E \Big)\psi_1(\boldsymbol{x}_1, \boldsymbol{y}_1) = -V_1^{(s)}\Big(\psi_2 + \psi_3\Big),$$

$$\Big(-\Delta_{\boldsymbol{x}_2} - \Delta_{\boldsymbol{y}_2} + V_2(x_2) + \sum_{\beta\neq 2} V_\beta^{(l)} - E \Big)\psi_2(\boldsymbol{x}_2, \boldsymbol{y}_2) = -V_2^{(s)}\Big(\psi_1 + \psi_3\Big),$$

$$\Big(-\Delta_{\boldsymbol{x}_3} - \Delta_{\boldsymbol{y}_3} + V_3(x_3) + \sum_{\beta\neq 3} V_\beta^{(l)} - E \Big)\psi_3(\boldsymbol{x}_3, \boldsymbol{y}_3) = -V_3^{(s)}\Big(\psi_1 + \psi_2\Big).$$

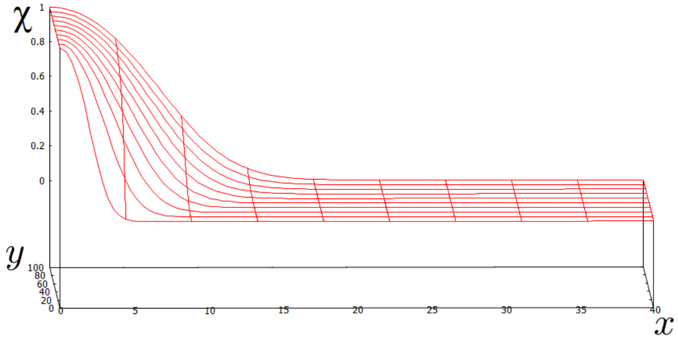
The cut-off function

$$V_\alpha(x_\alpha) = V_\alpha^{(s)}(x_\alpha, y_\alpha) + V_\alpha^{(l)}(x_\alpha, y_\alpha), \quad V_\alpha^{(s)}(x_\alpha, y_\alpha) = \chi_\alpha(x_\alpha, y_\alpha) V_\alpha(x_\alpha).$$

The Merkuriev cut-off function ($\nu_\alpha > 2$):

$$\chi_\alpha(x_\alpha, y_\alpha) = \frac{2}{1 + e^{(x_\alpha/x_{0\alpha})^{\nu_\alpha}/(1+y/y_{0\alpha})}}$$

Plotted in the case $\nu_\alpha = 2.01$, $x_{0\alpha} = 2.0$, $y_{0\alpha} = 8.0$:



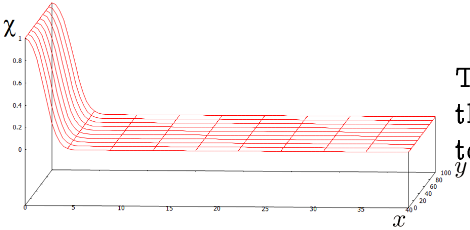
The cut-off function

We use a cut-off function $\chi_\alpha(x_\alpha)$ in the two-body configuration space:

$$V_\alpha(x_\alpha) = V_\alpha^{(s)}(x_\alpha) + V_\alpha^{(l)}(x_\alpha), \quad V_\alpha^{(s)}(x_\alpha) = \chi_\alpha(x_\alpha)\, V_\alpha(x_\alpha),$$

$$\chi_\alpha(x_\alpha) = \frac{2}{1 + e^{(x_\alpha/x_{0\alpha})^{\nu_\alpha}}}.$$

Plotted in the case $\nu = 2.01$, $x_0 = 5.0$:



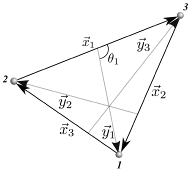
There is an algorithm of choosing the cut-off function parameter $x_{0\alpha}$ to minimize computational efforts.

Total angular momentum representation

The components expansion in terms of the eigenstates with total angular momentum J, its projection M and parity τ
$F^{J\tau}_{MM'} = (D^J_{M,M'} + \tau(-1)^{M'} D^J_{M,-M'})/\sqrt{2+2\delta_{M'0}}$:

$$\psi_\alpha(x_\alpha, y_\alpha) = \sum_{J,\tau,M,M'} \psi^{J\tau}_{\alpha MM'}(x_\alpha, y_\alpha, \theta_\alpha) F^{J\tau}_{MM'}(\Omega_\alpha),$$

Ω_α — 3 Euler angles, $x_\alpha, y_\alpha, \theta_\alpha$ — coordinates in a plane containing particles, $D^J_{M,M'}$ — Wigner D-functions.



J, M, τ are the integrals of motion.
Projecting the equations onto a subspace of given J, M and τ we get a set of independent systems of 3d equations connecting $\psi^{J\tau}_{\alpha MM'}$ with different M' and α.

The $J = 0$ case

We consider the case $J = 0$: $\psi_\alpha(x_\alpha, y_\alpha) = \psi_\alpha(X_\alpha)$, $X_\alpha = \{x_\alpha, y_\alpha, \theta_\alpha\}$.

The Faddeev-Merkuriev equations (α=1,2,3):

$$\{T_\alpha + V_\alpha(x_\alpha) + \sum_{\beta\neq\alpha} V_\beta^{(l)}(x_\beta) - E\}\psi_\alpha(X_\alpha) = -V_\alpha^{(s)}(x_\alpha) \sum_{\beta\neq\alpha} \psi_\beta(X_\beta),$$

where the kinetic energy operator:

$$T_\alpha = -\frac{\partial^2}{\partial y_\alpha^2} - \frac{2}{y_\alpha}\frac{\partial}{\partial y_\alpha} - \frac{\partial^2}{\partial x_\alpha^2} - \frac{2}{x_\alpha}\frac{\partial}{\partial x_\alpha} - \left(\frac{1}{y_\alpha^2} + \frac{1}{x_\alpha^2}\right)\frac{\partial}{\partial z_\alpha}(1 - z_\alpha^2)\frac{\partial}{\partial z_\alpha}, \quad z_\alpha \equiv \cos(\theta_\alpha)$$

The $J = 0$ case

We consider the case $J=0$: $\psi_\alpha(x_\alpha, y_\alpha) = \psi_\alpha(X_\alpha)$, $X_\alpha = \{x_\alpha, y_\alpha, \theta_\alpha\}$.

Boundary conditions:

$$\psi_\alpha(X_\alpha) \sim -\frac{\phi_{n_0\ell_0}(x_\alpha)}{x_\alpha y_\alpha} Y_{\ell_0 0}(\theta_\alpha, 0) e^{-i\vartheta_{\ell_0}(y_\alpha, p_{n_0})}\delta_{\alpha,\alpha_0} + \sum_{n\ell} \frac{\phi_{n\ell}(x_\alpha)}{x_\alpha y_\alpha} Y_{\ell 0}(\theta_\alpha, 0)\sqrt{\frac{p_{n_0}}{p_n}} S_{n\ell, n_0\ell_0}\, e^{+i\vartheta_\ell(y_\alpha, p_n)},$$

where

- The indices $\{n, \ell\}$ and wave functions $\phi_{n\ell}(x_\alpha)$ specify various two-body Coulombic bound states of particles of pairing α with energy $\varepsilon_n = E - p_n^2$ (i.e., binary scattering channels).
- The Coulomb distorted phase $\vartheta_\ell(y_\alpha, p_n) \equiv p_n y_\alpha - \eta_n \ln(2p_n y_\alpha) - \ell\pi/2 + \sigma_n$, $\sigma_n = \arg\Gamma(1 + i\eta_n)$, the Sommerfeld parameter $\eta_n \equiv Z_\alpha(\sum_{\beta\neq\alpha} Z_\beta)\sqrt{2m_{\alpha(\beta\gamma)}}/(2p_n)$.
- $S_{n\ell, n_0\ell_0}$ are the S-matrix elements ($\Rightarrow$ cross sections).

Numerical solution

Few modifications:

- V_3 repulsive, can be included in the left-hand side of equations by choosing $\chi_3 = 0$ ($\Rightarrow$ two equations).
- the asymptotic particle-atom Coulomb potential $V_\alpha^{\rm eff}(y_\alpha) = 2p_n\eta_n/y_\alpha$ introduced explicitly in equations ($\Rightarrow$ Coulomb singularity can be effectively inverted).
- introduce $\widetilde{\psi_\alpha}(X_\alpha) = x_\alpha y_\alpha \psi_\alpha(X_\alpha)$ ($\Rightarrow$ zero boundary conditions on the lines $x_\alpha = 0$, $y_\alpha = 0$).

$$\{\widetilde{T_\alpha} + V_\alpha(x_\alpha) + V_\alpha^{\rm eff}(y_\alpha) - E\}\widetilde{\psi_\alpha}(X_\alpha) = -\frac{x_\alpha y_\alpha}{x_\beta y_\beta} V_\alpha^{(s)}(x_\alpha)\widetilde{\psi_\beta}(X_\beta) - \left[V_\beta^{(l)}(x_\beta) + V_3(x_3) - V_\alpha^{\rm eff}(y_\alpha)\right]\widetilde{\psi_\alpha}(X_\alpha), \quad \alpha = 1, 2,$$

with $\widetilde{T_\alpha} = -\frac{\partial^2}{\partial y_\alpha^2} - \frac{\partial^2}{\partial x_\alpha^2} - \left(\frac{1}{y_\alpha^2} + \frac{1}{x_\alpha^2}\right)\frac{\partial}{\partial z_\alpha}(1 - z_\alpha^2)\frac{\partial}{\partial z_\alpha}$.

Numerical solution

- real asymptotic boundary conditions ($\Rightarrow$ real solutions $\widetilde{\psi_\alpha}$):

$$\widetilde{\psi_\alpha}(X_\alpha) \sim -\phi_{n_0\ell_0}(x_\alpha)\, Y_{\ell_0 0}(\theta_\alpha, 0) \sin\left(\vartheta_{\ell_0}(y_\alpha, p_{n_0})\right) \delta_{\alpha,\alpha_0} + \sum_{n\ell} \phi_{n\ell}(x_\alpha)\, Y_{\ell 0}(\theta_\alpha, 0) \sqrt{\frac{p_{n_0}}{p_n}} K_{n\ell,n_0\ell_0} \cos\left(\vartheta_\ell(y_\alpha, p_n)\right),$$

The matrix relation between the S- and K-matrices:

$$S = (iI + K)^{-1} \cdot (iI - K).$$

Numerical solution

Parallel object-oriented program.

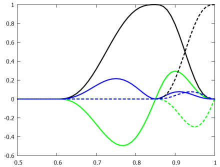


Figure: Hermite basis S_5^3 splines

Basic ideas:

- Products of Hermite basis S_5^3 splines (local!) in each coordinate for expanding the components $\widetilde{\psi_\alpha}$; collocation method $\Rightarrow$ sparse discretized version of operators of the r.h.s of the system of equations.
- The left-hand side matrix is used for preconditioning in the GMRES variant of Arnoldi iterations.
- The left-hand side matrix is (almost) a sum of tensor products of "one-dimensional" matrices of splines and their second derivatives values $\Rightarrow$ inverted using the "tensor trick".

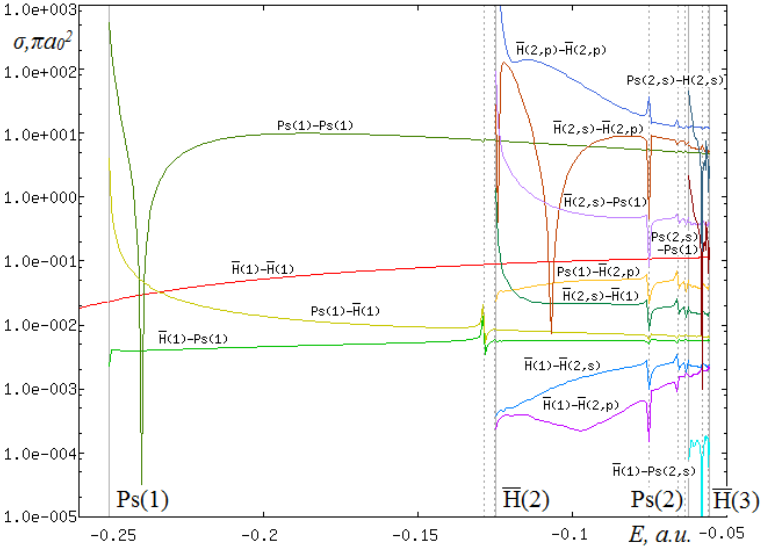
$e^+e^-\bar{\text{p}}$ system

waves	$\bar{\text{H}}$(n=1)	Ps(n=1)	$\bar{\text{H}}$(n=2) s, p	Ps(n=2) s, p	$\bar{\text{H}}$(n=3) s, p, d
a.u.	-0.4997	-0.250	-0.1249	-0.0625	-0.0555
eV	-13.6	-6.80	-3.40	-1.70	-1.51

Table: Energy thresholds of $e^+e^-\bar{\text{p}}$ binary channels

6 open channels between Ps(n=2) and $\bar{\text{H}}$(n=3) thresholds.
All K-matrix elements calculation for one value of E:
(r.h.s.) matrix linear size 3,241,020 with 432 nonzero elements in a row ($\approx$ 20 Gb), $\approx$ 3 hours (32 cores).

Cross sections $e^+e^-\bar{p}$



Ramsauer effect

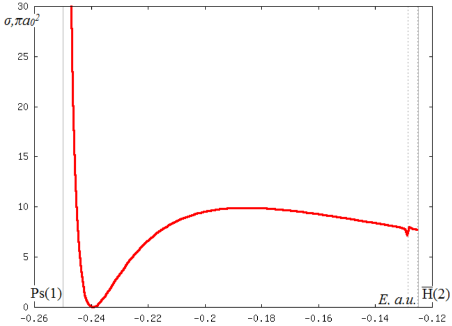


Figure: Ps(1, s)→Ps(1, s) cross section

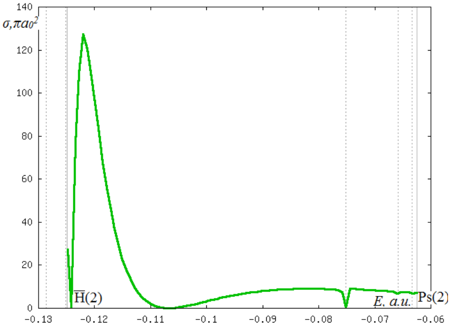
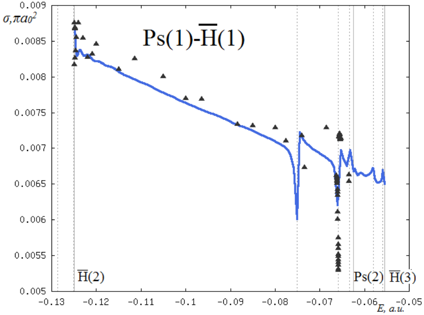
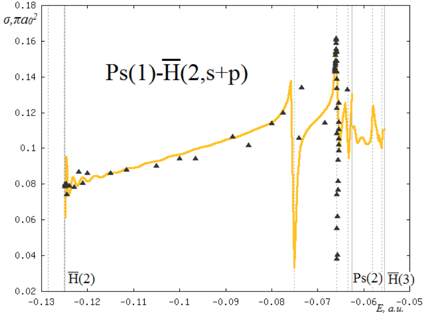
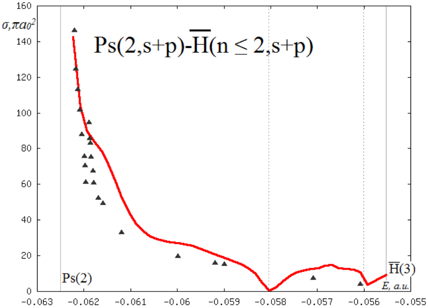


Figure: $\bar{\mathrm{H}}(2, \mathrm{s}) \rightarrow \bar{\mathrm{H}}(2, \mathrm{p})$ cross section

Antihydrogen formation



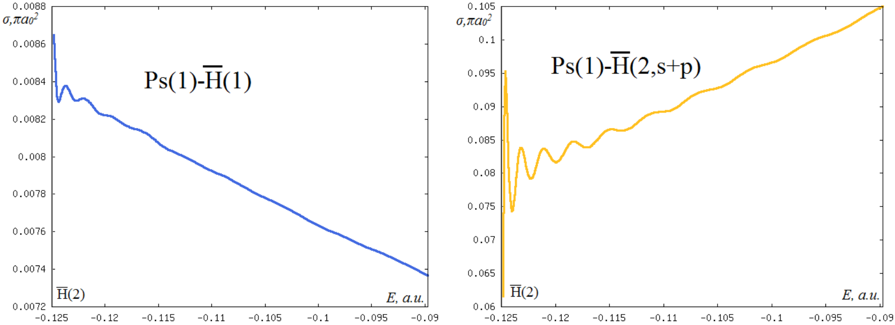




Gravitational Behaviour of Antihydrogen at Rest (experiment on antimatter at CERN).

▲ M. Valdes, M. Dufour, R. Lazauskas, and P.-A. Hervieux. *Phys. Rev. A*, 97:012709, 2018.

Gailitis-Damburg oscillations



Predicted: $\boxed{\log(E_n - E_{\text{th}}) = An + B}$

where E_n — the energy of the position cross section's nth maximum,

E_{th} — the threshold energy,

A and B — constants.

M. Gailitis and R. Damburg. *Proc. Phys. Soc.*, 82:192–200, 1963.

Gailitis-Damburg oscillations

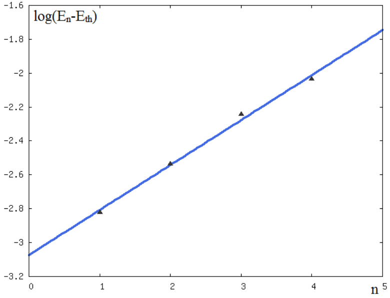


Figure: Maxima of Ps(1)→$\bar{\mathrm{H}}$(1) cross section positions

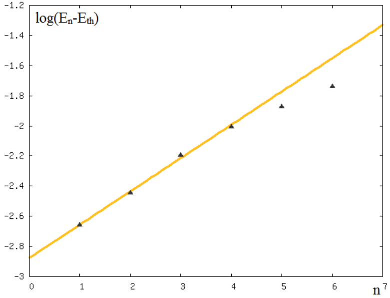


Figure: Maxima of Ps(1)→$\bar{\mathrm{H}}$(2, *s*) cross section positions

Predicted: $$\boxed{\log(E_n - E_{\text{th}}) = An + B}$$

where E_n — the energy of the position cross section's nth maximum,

E_{th} — the threshold energy,

A and B — constants.

M. Gailitis and R. Damburg. *Proc. Phys. Soc.*, 82:192–200, 1963.

Gailitis-Damburg oscillations

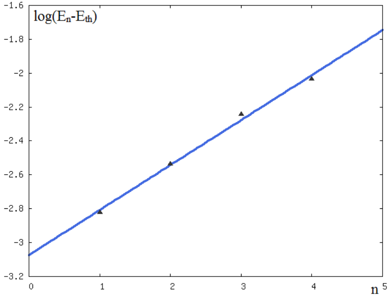


Figure: Maxima of Ps(1)→$\bar{\mathrm{H}}$(1) cross section positions

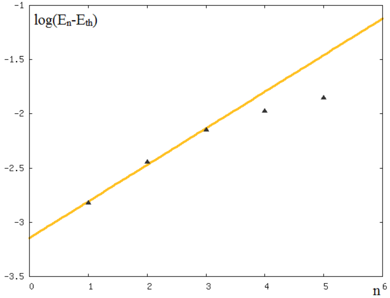


Figure: Maxima of Ps(1)→$\bar{\mathrm{H}}(2, p)$ cross section positions

Predicted: $$\log(E_n - E_{\mathrm{th}}) = An + B$$

where E_n — the energy of the position cross section's nth maximum,

E_{th} — the threshold energy,

A and B — constants.

M. Gailitis and R. Damburg. *Proc. Phys. Soc.*, 82:192–200, 1963.

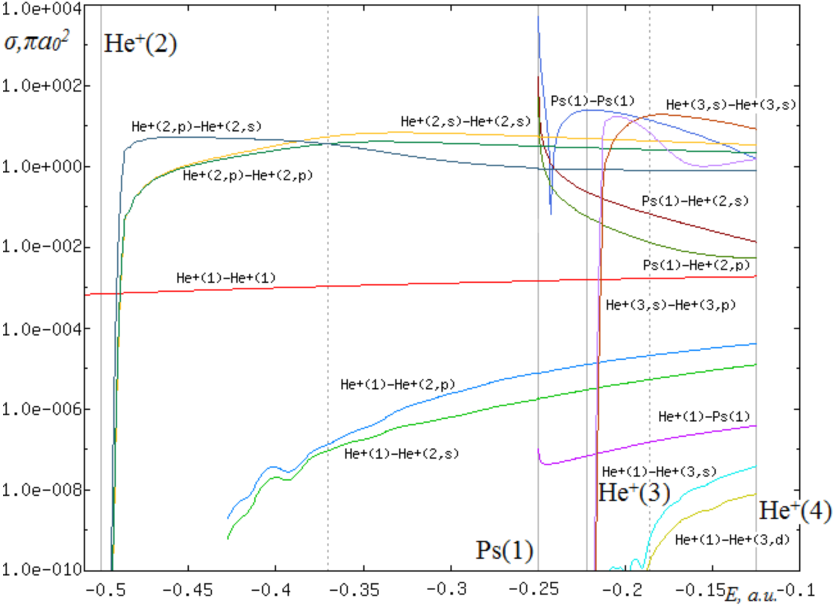
$e^+e^-\mathrm{He}^{++}$ system

waves	He^+(n=1)	He^+(n=2) s, p	Ps(n=1)	He^+(n=3) s, p, d	He^+(n=4) s, p, d, f
a.u.	-1.9997	-0.4999	-0.25	-0.2222	-0.1250
eV	-54.4	-13.6	-6.80	-6.05	-3.40

Table: Energy thresholds of $e^+e^-\mathrm{He}^{++}$ binary channels

7 open channels between He^+(n=3) and He^+(n=4) thresholds.

Cross sections $e^+e^-\mathrm{He}^{++}$

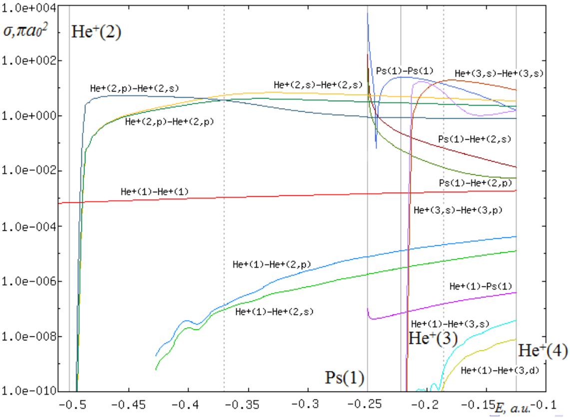


$e^+e^-\mathrm{He}^{++}$ resonances

(-0.3705, 0.1294)	(-0.250014, $7.4 \cdot 10^{-6}$)	(-0.1856, 0.0393)

Table: Known resonance energies (E_r, Γ) (in a.u.)

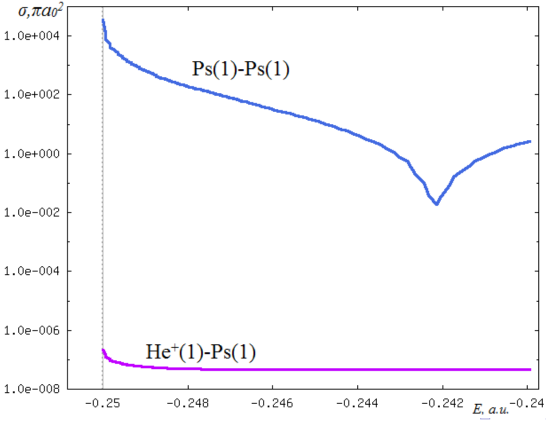
A. Igarashi and I. Shimamura. *Phys. Rev. A*, 70:012706, 2004



$e^+e^-\mathrm{He}^{++}$ resonances

Process:	not charged	charged
elastic	const	$1/p^2$
slow→fast rearrangement	$1/p$	$1/p^2$
fast→slow rearrangement	p	const

$$p \equiv \sqrt{E - E_{th}}$$



$e^+e^-He^{++}$ resonances

Complex rotation method applied to the Schrödinger equation: broad resonances exist!

Present work	(-0.3704, 0.1297)	(-0.1857, 0.0395)
*	(-0.3705, 0.1294)	(-0.1856, 0.0393)

Table: Broad resonance in the $e^+e^-He^{++}$ system energies (E_r, Γ) (in a.u.)

* A. Igarashi and I. Shimamura. *Phys. Rev. A*, 70:012706, 2004

SUMMARY

1. High precision method of solving three-body Coulomb scattering problem for $J=0$ on the base of 3D FM equations without partial waves decomposition is developed.
2.
   - All 36 cross sections of scattering in $e^- e^+ \bar{p}$ below the $\bar{\mathrm{H}}(n=3)$ threshold are calculated with high resolution in energy, reproducing all known Feshbach resonances.
   - The Ramsauer minima in cross sections are reproduced.
   - The just above the $\bar{\mathrm{H}}(2)$ threshold Gailitis-Damburg oscillations of 2 rearrangement cross sections are discovered for the first time.
3.
   - All 49 cross sections of scattering in $e^+ e^- \mathrm{He}^{++}$ systems are calculated below the He^+(n=4) threshold.
   - Two known resonances are confirmed by complex rotation approach. Broad resonances do not contribute in cross section profiles.
   - The narrow resonance at the Ps(1) threshold leads to the threshold anomaly in He^+(1)-Ps(1) rearrangement cross section.
4. The extension of current approach for $J>0$ case is in progress.

Publications

- Algorithm
  V. Roudnev, S. Yakovlev *Improved tensor-trick: application to helium trimer*/ Computer Physics Communications, V. 126, (2000), 162-164
- Cut-off function
  Vitaly A. Gradusov, Vladimir A. Roudnev and Sergey L. Yakovlev *Merkuriev cut-off in* $e^+ - \mathrm{H}$ *multichannel scattering calculations*/ Atoms 2016, 4(1), 9
- Results
  V. A. Gradusov, V. A. Roudnev, E. A. Yarevsky and S. L. Yakovlev *High resolution calculation of low energy scattering in* $e^-e^+\bar{p}$ and $e^+e^-\mathrm{He}^{++}$ *systems via Faddeev-Merkuriev equations*/ arXiv:1810.11123

Thank you
for your attention!