#### <span id="page-0-0"></span>Scattering in Three-body Coulomb System

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### Plan of the talk

- I. Scattering processes in three-body system
- II. Effective interaction in two-body sector of the three-body system with Coulomb interaction. CCE approach
- III. Dipole interaction in CCE
- IV. Model free formalism for Three Body Coulomb Scattering Problem
- V. Ab initio calculation of the scattering problem in  $e^-e^-p^+,$  $e^-e^+p^-~{\rm and}~e^-{\rm He^+~ systems}$
- IV. Conclusion



#### I. Scattering Processes in Three-Body System



### I. Scattering Processes in Three-Body System



#### Jacobi vectors for three-body system



Figure: Jacobi coordinates



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## II. Effective Interaction in Two-Body Sector of the Three-Body System with Coulomb Interaction

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

$$
H=H_0+V\equiv -\Delta_{\bm{x}_1}-\Delta_{\bm{y}_1}+\sum_{a=1}^3V_a(\bm{x}_a),
$$

 ${x_a, y_a}$  is the set of standard mass-weighted Jacobi coordinates:  $x_a = \sqrt{\mu_{bc}} \text{x}_a, y_a = \sqrt{\mu_{a,bc}} \text{y}_a.$ 

 $V_a(x)$  are two body potentials:

$$
V_a(x)=\frac{q_bq_c}{|x|}
$$

 ${a, b, c}$  runs over  ${1, 2, 3}$  cyclically.  $\hbar = 1$  throughout.



#### II.1. Two-body sectors



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

II.2. Interactions of particle 1 with particles 2 and 3 in the two-body sector  $|x_1|\ll |y_1|$ 

Multipole expasion of Coulomb interactions:

$$
\begin{aligned}\n\sum_{a=2}^3 \frac{q_1 q_a}{|x_a|} &= \sum_{a=2}^3 \frac{q_1 q_a}{|c_{a1} x_1 + s_{a1} y_1|} = \\
&= \sum_{a=2}^3 q_1 q_a \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell (-1)^\ell \frac{4\pi}{2\ell+1} \frac{(|c_{a1} x_1|)^\ell}{(|s_{a1} y_1|)^{\ell+1}} Y_{\ell m}(\hat{x}_1) Y_{\ell m}^*(\hat{y}_1) = \\
&= \frac{1}{|y_1|} \sum_{a=2}^3 \frac{q_1 q_a}{|s_{a1}|} - \frac{1}{|y_1|^2} \sum_{a=2}^3 q_1 q_a \frac{|c_{a1} x_1|}{|s_{a1}|} P_1(\hat{x}_1 \cdot \hat{y}_1) + O(|y_1|^{-3})\n\end{aligned}
$$

Result:

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

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### II.3. 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) (if rearrangement process are not taken into account) (Seaton, Burke, Gailitis...) within R-matrix formalism

CCE for wave function

$$
\Psi(x_1,y_1)=\sum_{n\alpha}\frac{\Psi_{n\alpha}(y_1)}{x_1y_1}\phi_{n\ell}(x_1)\mathcal{Y}_{\alpha}(\hat{x}_1,\hat{y}_1),\ \ \alpha=LM\ell\ell_1
$$

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

Or

$$
\Psi(\boldsymbol{x}_1,\boldsymbol{y}_1)=\sum_{n\alpha}\frac{\Psi_{n\alpha}(y_1)}{x_1y_1}|n\alpha\rangle
$$

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CCE representation of the Schrödinger equation

$$
\langle n\alpha|[H_0+V_1+\sum_{b=2}^3V_b-E]\sum_{n'\alpha'}|n'\alpha'\rangle\frac{\Psi_{n'\alpha'}}{x_1y_1}=0
$$

Or

$$
p_n^2 = E - \epsilon_n
$$

$$
\left(-\frac{d^2}{dy_1^2} + \frac{C}{y_1} + \frac{\ell_1(\ell_1 + 1)}{y_1^2} - p_n^2\right) \Psi_{n\alpha} + \sum_{n'\alpha'} \langle n\alpha| \frac{A}{y_1^2} + ... |n'\alpha'\rangle \Psi_{n'\alpha'} = 0
$$
(1)

Asymptotic matrix form when  $y_1 \to \infty$ 

$$
\left(-\frac{d^2}{dy_1^2}+\frac{C}{y_1}+\frac{\text{I}_1(\text{I}_1+1)+\textbf{A}}{y_1^2}-\textbf{p}^2\right)\Phi(y_1)=O(y_1^{-3})
$$

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<span id="page-10-0"></span>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  $(e^--{\rm H},\,e^--{\rm He}^+,\,e^+-{\rm H},\,...)$ 

Two main 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 A has the same block structure than the matrix  $\mathbf{p}^2,$  i.e.

$$
\mathbf{p}^2 \sim p_n^2 \delta_{n n'} \delta_{\alpha \alpha'} \;\; \mathbf{A} \propto \langle n \alpha | A | n \alpha' \rangle \delta_{n n'},
$$

i.e. by neglecting dipole coupling of target states with  $n\neq n'$  .

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#### III. Dipole interaction in CCE Gailitis 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  ${\bf A}$  is  $[{\bf A},{\bf p^2}]=0$  and hence the diagonalizing matrix  $\mathbf{W}$  such that  $\mathbf{W}^\dagger [\mathbf{l}_1 (\mathbf{l}_1 + 1) + \mathbf{A}] \mathbf{W} = \mathbf{D},$  $\mathbf{D}_{n\alpha,n'\alpha'}=d_{n\ell}\delta_{n\alpha,n'\alpha'}$  commutes with  $\mathbf{p}^2,$  i.e.  $[\mathbf{W},\mathbf{p}^2]=0.$  This allows to diagonalize the CCE equations:

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

<span id="page-11-0"></span>
$$
[\mathbf{W}^{\dagger} \Phi^{\pm}(y_1)]_{n\alpha} = H^{\pm}_{\mathcal{L}_{n\alpha}}(p_n y_1) \delta_{nn'} \delta_{\alpha \alpha'}
$$
(2)  

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

$$
\mathcal{L}_{n\alpha} = -1/2 \pm \sqrt{1/4 + d_{n\alpha}} \delta_{n\alpha, n'\alpha'}
$$

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### III.1 Two possibilities for D:

- <span id="page-12-0"></span> $\bullet$   $d_{n\alpha} \geq 0$  then with  $\mathcal{L}_{n\alpha} \geq 0$  two solutions are given by [\(2\)](#page-11-0) **2** there is  $n\alpha$  such that  $d_{n\alpha} < 0$  then
	- if  $|d_{n\alpha}| < 1/4$  the new momenta  $\mathcal{L}_{n\alpha}$  are real, the solutions are given by [\(2\)](#page-11-0). For this case the equation

<span id="page-12-1"></span>
$$
\left(-\frac{d^2}{dy_1^2} + \frac{C}{y_1} + \frac{d_{n\alpha}}{y_1^2} - E + \epsilon_n\right) [\mathbf{W}^\dagger \Phi]_{n\alpha}(y_1) = 0 \tag{3}
$$

supports finite number of bound states. For full equation [\(1\)](#page-9-0) where the coupling between channels with different  $n$  are not zero these bound states transforms into resonances (called as Feshbach resonances).

if  $|d_{n\alpha}| > 1/4$  then new momenta are complex  ${\cal L}_{n\ell} = -1/2 \pm i\sqrt{|d_{n\ell}| - 1/4},$  the equation [\(3\)](#page-12-1) supports infinitely many bound states accumulating to the threshold  $\epsilon_n$  from below. For full equation [\(1\)](#page-9-0) where the coupling between channels with different *n* are not zero these bound states transforms into series of resonances accumulating to the thresholds (called as Feshbach resonances).  $\left\{ \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \end{array} \right.$ **E**  $\Omega$ 

# III. 2 Asymptotic boundary conditions for full CCE equations [\(1\)](#page-9-0). Oscillation of cross section when  $|d_{n,\alpha}| > 1/4$

Standard boundary conditions for full CCE equations have the form

$$
\Psi_{n\alpha}(y_1) \sim H_{\ell_1}^-(\eta_n, p_n y_1) \delta_{n n'} \delta_{\alpha \alpha'} - H_{\ell_1}^+(\eta_n, p_n y_1) S_{n n', \alpha \alpha'} \qquad (4)
$$

where  $H^{\pm}_{\ell}=G_{\ell}\pm iF_{\ell},\,\eta_n=C/(2p_n)$  and  $S_{nn',\alpha\alpha'}$  is S-matrix. Set of asymptotic solutions [\(2\)](#page-11-0) provides more sophisticated asymptotic condition that compensates as  $y_1 \to \infty$  the diagonal blocks of dipole coupling matrix:

$$
\Psi_{n\alpha}(y_1) \sim W_{n\alpha,\alpha'} \delta_{nn'} H_{\mathcal{L}_{n'\alpha'}}^{-}(\eta'_n, p'_n y_1) -
$$
  
- 
$$
\sum_{\alpha''} W_{n\alpha,\alpha''} H_{\mathcal{L}_{n\alpha''}}^{+}(\eta_n, p_n y_1) \hat{S}_{nn',\alpha''\alpha'}.
$$
 (5)

The original S-matrix S then is calculated from renormalized one  $\hat{S}$  by similarity transformation

$$
S = W J \hat{S} J^{\dagger} W^{\dagger}.
$$

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Oscillation of cross section when  $|d_{n,q}|>1/4$ 

If  $d_{n\alpha}< -1/4$  then  $\mathcal{L}_{n,\alpha}$  is complex  $\mathcal{L}_{n\alpha}=-1/2 \pm i\surd |d_{n\alpha}|-1/4$  and the T matrix p-dependence  $(iT = S - 1)$ 

 $T_{n\alpha,n_0\alpha_0}\sim p_n^{2\mathcal{L}_{n,\alpha}+1} = \exp\{i2\mathfrak{Sm}(\mathcal{L}_{n\alpha})\ln(p_n)\},$ 

leads to the specific anomalous cross section oscillations

$$
\sigma_{n\alpha,n_0\alpha_0}=A+B\cos[2\Im{\mathrm{m}}\mathcal{L}_{n\alpha}\ln(p_n)+\phi],
$$

which gives rise to an infinite number of oscillations in the cross section as the energy approaches the threshold from above (GD oscillations formula 1963).



 $\left\{ \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \end{array} \right.$ 

#### III.1. Importance of account for the dipole interaction in practical calculations

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

CCE model  $Ps(n = 2) - \bar{p}$  scattering

$$
\begin{aligned}\n&\left[-\frac{d^2}{dy^2}-p^2+\frac{1}{\rho^2(y)}\left(\begin{array}{cc} 24.9947 & 0 \\ 0 & -22.9947 \end{array}\right)\right]\Psi =\\ \n&\left[-\frac{d^2}{dy^2}-p^2+\frac{1}{\rho^2(y)}\Lambda(\Lambda+1)\right]\Psi=0\\ \n&\Lambda=diag[4.52441,i4.76914],\Psi=[\Psi_1,\Psi_2]^T\\ \rho(y)=6\ a.u.\ \text{if}\ y\leq 6\ a.u.,\ \rho(y)=y,\ \text{if}\ y>6\ a.u.\n\end{aligned}
$$



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Figure: Squared  $\Psi_2$  component of wave functions for different values of p: solid line corresponds to  $p=0.006\,a_0^{-1},$  dashed line corresponds to  $p=0.02\,a_0^{-1}.$ 

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## IV. Model free formalism for three-body Coulomb scattering problem

Merkuriev-Faddeev equations (MFE)

$$
\begin{aligned}&\left(-\Delta_{\bm{x_1}}-\Delta_{\bm{y_1}}+V_1(\bm{x_1})+\sum\limits_{b\neq 1}V_b^{(l)}-\bm{E}\right)\psi_1(\bm{x_1},\bm{y_1})=-V_1^{(s)}\left(\psi_2+\psi_3\right),\\&\left(-\Delta_{\bm{x_2}}-\Delta_{\bm{y_2}}+V_2(\bm{x_2})+\sum\limits_{b\neq 2}V_b^{(l)}-\bm{E}\right)\psi_2(\bm{x_2},\bm{y_2})=-V_2^{(s)}\left(\psi_1+\psi_3\right),\\&\left(-\Delta_{\bm{x_3}}-\Delta_{\bm{y_3}}+V_3(\bm{x_3})+\sum\limits_{b\neq 3}V_b^{(l)}-\bm{E}\right)\psi_3(\bm{x_3},\bm{y_3})=-V_3^{(s)}\left(\psi_1+\psi_2\right).\end{aligned}
$$

Splitting of Coulomb potential

$$
V_a(x)=V^{(s)}_a(x)+V^{(l)}_a(x)\quad
$$

 $V^{(l)}_a(x) = \frac{q_bq_c}{x} \theta_s(r-R),~~~\theta_s-\text{smoothed out theta function}.$ 



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#### Stucture of the r.h.s. of MFE





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Asymptotic decoupling of MFE as  ${x_a, y_a} \rightarrow \infty$ 

$$
\Big( -\Delta_{\bm{x_1}} - \Delta_{\bm{y_1}} + V_1(\bm{x_1}) + \sum_{b \neq 1} V_b^{(l)} - E \Big) \psi_1(\bm{x_1},\bm{y_1}) = 0, \\ \Big( -\Delta_{\bm{x_2}} - \Delta_{\bm{y_2}} + V_2(\bm{x_2}) + \sum_{b \neq 2} V_b^{(l)} - E \Big) \psi_2(\bm{x_2},\bm{y_2}) = 0, \\ \Big( -\Delta_{\bm{x_3}} - \Delta_{\bm{y_3}} + V_3(\bm{x_3}) + \sum_{b \neq 3} V_b^{(l)} - E \Big) \psi_3(\bm{x_3},\bm{y_3}) = 0. \\ \psi_a(\bm{x}_a,\bm{y}_a) = \sum_{n\alpha} \frac{\psi_{a(n\alpha)}(y_a)}{x_a y_a} |n\alpha\rangle
$$

Asymptotic equation for partial wave of MF component  $\psi_a$ 

$$
\left(-\frac{d^2}{dy_a^2} + \t+\frac{\ell_1(\ell_1+1)}{y_a^2} - p_{an}^2\right)\psi_{a(n\alpha)} + \sum_{n'\alpha'} \langle n\alpha|\sum_{b\neq a} V_b^{(l)}|n'\alpha'\rangle \psi_{a(n'\alpha')} = 0
$$

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### Asymptotic boundary conditions for MF

Asymptotic waves which take into account full dipole coupling. Gradusov Yakovlev Theor. Math. Phys. 2024

$$
\phi^\pm_{a(n\alpha)(n'\alpha')} (y_a,p_{n'})=\left[W^{a(0)}_{(n\alpha)(n'\alpha')}+\frac{1}{y_a^2}W^{a(1)}_{(n\alpha)(n'\alpha')}\right]H^\pm_{\mathcal{L}_{a(n'\alpha')}}(\eta_{n'},p_{n'}y_a).
$$

$$
\begin{array}{ccc} W^{a(0)}_{(n\alpha)(n'\alpha')} & = & \delta_{n n'} W^a_{n\alpha\alpha'},\\[2ex] W^{a(1)}_{(n\alpha)(n'\alpha')} & = & (1-\delta_{n n'}) \frac{\sum_{\alpha''} A^a_{(n\alpha)(n'\alpha'')} W^a_{n'\alpha''\alpha'}}{(p_n^2-p_{n'}^2)}, \end{array}
$$

$$
\mathcal{L}_{a(n\alpha)}(\mathcal{L}_{a(n\alpha)}+1)=q_{a(n\alpha)}
$$

 $q_{a(n\alpha)}$  and  $W^a_{n\alpha\alpha'}$  are eigen values and eigen vectors of the block matrix  $\ell_1(\ell_1 + 1)\delta_{\alpha\alpha'} + A^a_{(n\alpha)(n\alpha')} .$ 4 D F

### MF partial wave asymptotic for scattering problem

Standard boundary conditions for MF, incident channel  $a(n'\alpha')$ 

$$
\psi_{a(n\alpha)}(y_a) \sim H_{\ell_1}^-(\eta_{an},p_{an}y_a)\delta_{nn'}\delta_{\alpha\alpha'} - H_{\ell_1}^+(\eta_{an},p_{an}y_a)S_{a(n\alpha),a(n'\alpha')}
$$
  

$$
\psi_{b(n\alpha)}(y_b) \sim -H_{\ell_1}^+(\eta_{bn},p_{bn}y_b)S_{b(n\alpha),a(n'\alpha')}
$$

Advanced boundary conditions, incident channel  $a(n'\alpha')$ 

$$
\begin{aligned} \psi_{a(n\alpha)}(y_a) &\sim \phi^-_{a(n\alpha)(n'\alpha')} (y_a,p_{an'}) - \\ &\quad - \sum_{n''\alpha''} \phi^+_{a(n''\alpha'')(n'\alpha')} (y_a,p_{an'}) S(a(n''\alpha'')|a(n'\alpha')) \\ \psi_{b(n\alpha)}(y_b) &\sim - \sum_{n''\alpha''} \phi^+_{b(n''\alpha'')(n'\alpha')} (y_b,p_{bn'}) S(b(n''\alpha'')|a(n'\alpha')) \end{aligned}
$$

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V. Ab initio calculation of the scattring problem  $\mathrm{in} \,\, e^-e^-p^+,\, e^-e^+p^- \,\, \mathrm{and} \,\, e^- \mathrm{He^+ \,\, systems}$ 

- 3D tree-body MF equations in total orbital momentum representation
- Advanced asymptotic boundary conditions, which compensate long-range Coulomb and dipole interactions
- Quintic splines expansion of the solution
- Tensor trick preconditioning procedure for solving discretized MFE
- Complex rotation method for 3D Schrödinger equation



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V.1. Calculation of  $e^-$ -H and  $e^-$ -He<sup>+</sup> Scattering-Resonances  $L = 0$ 



Figure: Left: The singlet 1s  $\rightarrow$  1s, 2s, 3s, 4s cross sections for the e–H scattering as a function of the incident electron energy. The thresholds are 0, 0.375, 0.444 and 0.469 a.u., respectively. Right: The singlet  $1s \rightarrow 1s$ , 2s, 3s, 4s cross sections for the e–He<sup>+</sup> scattering as a function of the incident electron energy. The thresholds are 0, 1.5, 1.778 and 1.87 5a.u., respectively.

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# V.2.  $e^+e^-\bar{p}$  system

Gradusov, Roudnev, Yarevsky, Yakovlev J. Phys. B: At. Mol. Opt. Phys. 52(2019) 055202



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

6 open channels between  $Ps(n=2)$  and  $\overline{H}(n=3)$  thresholds.



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 $\mathcal{A} \cap \mathcal{B} \rightarrow \mathcal{A} \supseteq \mathcal{B} \rightarrow \mathcal{A} \supseteq \mathcal{B}$ 

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



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#### Ramsauer effect



Figure:  $Ps(1, s) \rightarrow Ps(1, s)$  cross section Figure:  $\overline{H}(2, s) \rightarrow \overline{H}(2, p)$  cross section



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## V.3. Realistic Calculations of Multiconfiguration Colision in  $e^+e^-\bar{p}$  system  $L=0$  via MFE

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



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#### GD oscillations in  $Ps \rightarrow Ps$  collision



Figure:  $\text{Ps}(2\text{s}) \rightarrow \text{Ps}(2\text{s})$  cross section  $\text{Figure: Ps}(2\text{s}) \rightarrow \text{Ps}(2\text{p})$  cross section for  $L = 0$ for  $L = 0$ 



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#### GD oscillations in  $Ps \rightarrow Ps$  collision



Figure: Antihydrogen formation cross sections  $Ps(1) \rightarrow \overline{H}(1)$ .

Figure: Antihydrogen formation cross sections  $Ps(1) \rightarrow \overline{H}(2s)$  (solid) and  $Ps(1) \rightarrow \overline{H}(2p)$  (dashed line)

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## G-D oscillations of  $Ps \rightarrow \overline{H}$  production cross sections above  $\overline{H}(3)$  threshold



Figure: Fig. 5 Antihydrogen formation cross sections  $Ps(2s) \rightarrow \overline{H}(3s)$  (red),  $Ps(2s) \rightarrow \overline{H}(3p)$  (green) and  $Ps(2s) \rightarrow \overline{H}(3d)$  (blue).

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### G-D oscillations in  $e^-$ -H collision



Figure: H(2s)-H(2s) cross section. Figure: H(2s)-H(2p) cross section.

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## $V.4.$   $e^+e^-He^{++}$  system.

Gradusov, Roudnev, Yarevsky, Yakovlev J. Phys. B: At. Mol. Opt. Phys. 52(2019) 055202



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

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



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## Cross sections  $e^+e^-$ He<sup>++</sup>



## $e^+e^-{\rm He}^{++}$  resonances

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

Table: Known resonance energies  $(E_r, \Gamma)$  (in a.u.)

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



## $e^+e^-{\rm He}^{++}$  resonances





# $e^+e^-{\rm He}^{++}$  resonances

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

$$
\begin{array}{c|c|c|c|c} * & (-0.3704, 0.1297) & (-0.1857, 0.0395) \\ * & (-0.3705, 0.1294) & (-0.1856, 0.0393) \end{array}
$$

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

\* Gradusov, Roudnev, Yarevsky, Yakovlev J. Phys. B: At. Mol. Opt. Phys. 52(2019) 055202

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



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## VI. 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)



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