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 $e^-e^-p^+$, $e^-e^+p^-$ and $e^-\text{He}^+$ 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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3B Scattering

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:

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

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

 $V_a(x)$ are two body potentials:

$$V_a(x) = rac{q_b q_c}{|x|}$$

 $\{a, b, c\}$ 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

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II.2. Interactions of particle 1 with particles 2 and 3 in the two-body sector $|m{x}_1| \ll |m{y}_1|$

Multipole expasion of Coulomb interactions:

$$\begin{split} \sum_{a=2}^{3} \frac{q_1 q_a}{|\boldsymbol{x}_a|} &= \sum_{a=2}^{3} \frac{q_1 q_a}{|\boldsymbol{c}_{a1} \boldsymbol{x}_1 + \boldsymbol{s}_{a1} \boldsymbol{y}_1|} = \\ &= \sum_{a=2}^{3} q_1 q_a \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^{\ell} \frac{4\pi}{2\ell+1} \frac{(|\boldsymbol{c}_{a1} \boldsymbol{x}_1|)^{\ell}}{(|\boldsymbol{s}_{a1} \boldsymbol{y}_1|)^{\ell+1}} Y_{\ell m}(\hat{\boldsymbol{x}}_1) Y_{\ell m}^*(\hat{\boldsymbol{y}}_1) = \\ &= \frac{1}{|\boldsymbol{y}_1|} \sum_{a=2}^{3} \frac{q_1 q_a}{|\boldsymbol{s}_{a1}|} - \frac{1}{|\boldsymbol{y}_1|^2} \sum_{a=2}^{3} q_1 q_a \frac{|\boldsymbol{c}_{a1} \boldsymbol{x}_1|}{|\boldsymbol{s}_{a1}|} P_1(\hat{\boldsymbol{x}}_1 \cdot \hat{\boldsymbol{y}}_1) + O(|\boldsymbol{y}_1|^{-3}) \end{split}$$

Result:

$$V_2+V_3\sim rac{C}{|m{y}_1|}+rac{m{A}(m{x}_1,m{\hat{y}}_1)}{|m{y}_1|^2}+O(|m{y}_1|^{-3}), \ \ |m{y}_1|
ightarrow\infty$$

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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

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

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

Or

$$\Psi(m{x}_1,m{y}_1) = \sum_{nlpha} rac{\Psi_{nlpha}(m{y}_1)}{m{x}_1m{y}_1} |nlpha
angle$$

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CCE representation of the Schrödinger equation

$$\langle nlpha|[H_0+V_1+\sum\limits_{b=2}^3V_b-E]\sum\limits_{n'lpha'}|n'lpha'
anglerac{\Psi_{n'lpha'}}{x_1y_1}=0$$

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

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

Asymptotic matrix form when $y_1
ightarrow \infty$

$$\left(-rac{d^2}{dy_1^2}+rac{C}{y_1}+rac{\mathbf{l}_1(\mathbf{l}_1+1)+\mathbf{A}}{y_1^2}-\mathbf{p}^2
ight)\Phi(y_1)=O(y_1^{-3})$$

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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 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 p^2 , i.e.

$$\mathbf{p}^2 \sim p_n^2 \delta_{nn'} \delta_{lpha lpha'} ~~ \mathbf{A} \propto \langle n lpha | \mathbf{A} | n lpha'
angle \delta_{nn'},$$

i.e. by neglecting dipole coupling of target states with n
eq 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 A is $[\mathbf{A}, \mathbf{p}^2] = 0$ and hence the diagonalizing matrix 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:

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

$$[\mathbf{W}^{\dagger} \Phi^{\pm}(y_1)]_{n\alpha} = H^{\pm}_{\mathcal{L}_{n\alpha}}(p_n y_1) \delta_{nn'} \delta_{\alpha \alpha'}$$
(2)

$$egin{aligned} \mathrm{D} &= \mathcal{L}(\mathcal{L}+1), \ \ \mathcal{L}_{nlpha,n'lpha'} &= \mathcal{L}_{nlpha}\delta_{nlpha,n'lpha'}, \ \mathcal{L}_{nlpha} &= -1/2\pm\sqrt{1/4+d_{nlpha}} \end{aligned}$$

III.1 Two possibilities for D:

- d_{nα} ≥ 0 then with L_{nα} ≥ 0 two solutions are given by (2)
 there is nα such that d_{nα} < 0 then
 - if |d_{nα}| < 1/4 the new momenta L_{nα} are real, the solutions are given by (2). For this case the equation

$$\left(-\frac{d^2}{dy_1^2} + \frac{C}{y_1} + \frac{d_{n\alpha}}{y_1^2} - E + \epsilon_n\right) [\mathbf{W}^{\dagger}\Phi]_{n\alpha}(y_1) = 0$$
(3)

supports finite number of bound states. For full equation (1) 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 $\mathcal{L}_{n\ell} = -1/2 \pm i\sqrt{|d_{n\ell}| - 1/4}$, the equation (3) supports infinitely many bound states accumulating to the threshold ϵ_n from below. For full equation (1) where the coupling between channels with different *n* are not zero these bound states transforms into series resonances accumulating to the thresholds (called as Feshbach resonances).

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III. 2 Asymptotic boundary conditions for full CCE equations (1). Oscillation of cross section when $|d_{n\alpha}|>1/4$

Standard boundary conditions for full CCE equations have the form

$$\Psi_{nlpha}(y_1) \sim H^-_{\ell_1}(\eta_n, p_n y_1) \delta_{nn'} \delta_{lpha lpha'} - H^+_{\ell_1}(\eta_n, p_n y_1) S_{nn', lpha lpha'}$$

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

$$\Psi_{nlpha}(y_1) \sim W_{nlpha,lpha'} \delta_{nn'} H^-_{\mathcal{L}_{n'lpha'}}(\eta'_n, p'_n y_1) - \sum_{lpha''} W_{nlpha,lpha''} H^+_{\mathcal{L}_{nlpha''}}(\eta_n, p_n y_1) \hat{S}_{nn',lpha''lpha'}.$$
(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 $|d_{n\alpha}| > 1/4$

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

 $T_{nlpha,n_0lpha_0}\sim p_n^{2\mathcal{L}_{n,lpha}+1}=\exp\{i2\Im\mathrm{m}(\mathcal{L}_{nlpha})\ln(p_n)\},$

leads to the specific anomalous cross section oscillations

$$\sigma_{nlpha,n_0lpha_0} = A + B \cos[2\Im m \mathcal{L}_{nlpha} \ln(p_n) + \phi],$$

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).



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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

$$egin{split} & \left[-rac{d^2}{dy^2}-p^2+rac{1}{
ho^2(y)}\left(egin{array}{cc} 24.9947 & 0 \ 0 & -22.9947 \end{array}
ight)
ight]\Psi=\ & \left[-rac{d^2}{dy^2}-p^2+rac{1}{
ho^2(y)}\Lambda(\Lambda+1)
ight]\Psi=0\ & \Lambda=diag[4.52441,i4.76914],\Psi=\left[\Psi_1,\Psi_2
ight]^T\ &
ho(y)=6\ a.u.\ ext{if}\ y\leq 6\ a.u.,\
ho(y)=y,\ ext{if}\ y>6\ a.u. \end{split}$$





Figure: Squared Ψ_2 component of wave functions for different values of p: solid line corresponds to $p = 0.006 a_0^{-1}$, dashed line corresponds to $p = 0.02 a_0^{-1}$.

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

Merkuriev-Faddeev equations (MFE)

$$igg(- \Delta_{m{x_1}} - \Delta_{m{y_1}} + V_1(m{x_1}) + \sum\limits_{b
eq 1} V_b^{(l)} - E igg) \psi_1(m{x_1},m{y_1}) = -V_1^{(s)}igg(\psi_2 + \psi_3igg), \ igg(- \Delta_{m{x_2}} - \Delta_{m{y_2}} + V_2(m{x_2}) + \sum\limits_{b
eq 2} V_b^{(l)} - E igg) \psi_2(m{x_2},m{y_2}) = -V_2^{(s)}igg(\psi_1 + \psi_3igg), \ igg(- \Delta_{m{x_3}} - \Delta_{m{y_3}} + V_3(m{x_3}) + \sum\limits_{b
eq 3} V_b^{(l)} - E igg) \psi_3(m{x_3},m{y_3}) = -V_3^{(s)}igg(\psi_1 + \psi_2igg).$$

Splitting of Coulomb potential

$$V_a(x) = V_a^{(s)}(x) + V_a^{(l)}(x)$$

 $V_a^{(l)}(x)=rac{q_bq_c}{x} heta_s(r-R), \;\; heta_s- ext{smoothed out theta function.}$



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Stucture of the r.h.s. of MFE





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

$$egin{aligned} &igl(-\Delta_{m{x_1}} -\Delta_{m{y_1}} + V_1(m{x_1}) + \sum\limits_{b
eq 1} V_b^{(l)} - Eigr) \psi_1(m{x_1},m{y_1}) = 0, \ &igl(-\Delta_{m{x_2}} -\Delta_{m{y_2}} + V_2(m{x_2}) + \sum\limits_{b
eq 2} V_b^{(l)} - Eigr) \psi_2(m{x_2},m{y_2}) = 0, \ &igl(-\Delta_{m{x_3}} -\Delta_{m{y_3}} + V_3(m{x_3}) + \sum\limits_{b
eq 3} V_b^{(l)} - Eigr) \psi_3(m{x_3},m{y_3}) = 0. \ &igl(\psi_a(m{x_a},m{y_a}) = \sum\limits_{nlpha} rac{\psi_{a(nlpha)}(m{y_a})}{m{x_a}m{y_a}} |nlpha
angle \end{aligned}$$

Asymptotic equation for partial wave of MF component ψ_a

$$\left(-rac{d^2}{dy_a^2}++rac{\ell_1(\ell_1+1)}{y_a^2}-p_{an}^2
ight)\psi_{a(nlpha)}+\sum_{n'lpha'}\langle nlpha|\sum_{b
eq a}V_b^{(l)}|n'lpha'
angle\psi_{a(n'lpha')}=0$$

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Asymptotic boundary conditions for MF

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

$$\phi^{\pm}_{a(nlpha)(n'lpha')}(y_{a},p_{n'}) = \left[W^{a(0)}_{(nlpha)(n'lpha')} + rac{1}{y^{2}_{a}} W^{a(1)}_{(nlpha)(n'lpha')}
ight] H^{\pm}_{\mathcal{L}_{a(n'lpha')}}(\eta_{n'},p_{n'}y_{a}).$$

$$egin{array}{rcl} W^{a(0)}_{(nlpha)(n'lpha')}&=&\delta_{nn'}W^a_{nlphalpha'},\ W^{a(1)}_{(nlpha)(n'lpha')}&=&(1-\delta_{nn'})rac{\sum_{lpha''}A^a_{(nlpha)(n'lpha'')}W^a_{n'lpha''lpha'}}{(p_n^2-p_{n'}^2)}, \end{array}$$

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

 $q_{a(n\alpha)}$ and $W^a_{n\alpha\alpha'}$ are eigen values and eigen vectors of the block matrix

$$\ell_1(\ell_1+1)\delta_{\alpha\alpha'}+A^a_{(n\alpha)(n\alpha')}.$$



MF partial wave asymptotic for scattering problem

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

$$egin{aligned} &\psi_{a(nlpha)}(y_a)\sim H^-_{\ell_1}(\eta_{an},p_{an}y_a)\delta_{nn'}\delta_{lphalpha'}-H^+_{\ell_1}(\eta_{an},p_{an}y_a)S_{a(nlpha),a(n'lpha')}\ &\psi_{b(nlpha)}(y_b)\sim -H^+_{\ell_1}(\eta_{bn},p_{bn}y_b)S_{b(nlpha),a(n'lpha')} \end{aligned}$$

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

$$egin{aligned} &\psi_{a(nlpha)}(y_{a})\sim\phi_{a(nlpha)(n'lpha')}^{-}(y_{a},p_{an'})-\ &-\sum\limits_{n''lpha''}\phi_{a(n''lpha'')(n'lpha')}^{+}(y_{a},p_{an'})S(a(n''lpha'')|a(n'lpha'))\ &\psi_{b(nlpha)}(y_{b})\sim-\sum\limits_{n''lpha''}\phi_{b(n''lpha'')(n'lpha')}^{+}(y_{b},p_{bn'})S(b(n''lpha'')|a(n'lpha')) \end{aligned}$$

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



V.1. Calculation of e^- -H and e^- -He⁺ 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⁺ 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

	$\bar{H}(n=1)$	Ps(n=1)	$\overline{H}(n=2)$	Ps(n=2)	H (n=3)
waves			s, p	s, p	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 $e^+e^-\bar{p}$ binary channels

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



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



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

for L = 0



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)



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).



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. $e^+e^-\text{He}^{++}$ system.

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

	$He^+(n=1)$	$He^+(n=2)$	Ps(n=1)	$He^+(n=3)$	$He^+(n=4)$
waves		s, p		s, p, d	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 $e^+e^-\text{He}^{++}$ binary channels

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



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



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



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

Process:	not charged	charged	
elastic	const	$1/p^2$	$n = \sqrt{E - E_{\rm eff}}$
$slow{\rightarrow} fast\ rearrangement$	1/p	$1/p^2$	$p \equiv \sqrt{E} - E_{th}$
$fast \rightarrow slow \ rearrangement$	p	const	



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

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

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



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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