Scattering in the system of three charged particles
Treatment by potential splitting approach

Sergey L. Yakovlev

International Conference
Nuclear Theory in the Supercomputing Era – 2016
Khabarovsk, September 19 – 23, 2016

Department of Computational Physics,
St. Petersburg State University, Russia

September 22, 2016

COULOMB INTERACTION
1785

$$V_C(r) = \frac{q_1 q_2}{r}$$

One of the most simple interaction
One of the most complicated dynamics

Three-body short-range (non Coulomb) case

Two-body level

Solve two body problems for bound states and T-matrices

Three-body level

- Solve three-body Faddeev equation
- Calculate wave function, transition amplitudes, cross sections ... *etc.*

Three-body Coulomb case

Two-body level

Solve the two body Coulomb problem analytically

Three-body level

- the original Faddeev integral equations cannot be used since the strong singularities of the two-body Coulomb T-matrices in the kernel
- Faddeev-Noble integral equations are well behaved for repulsive Coulomb plus short-range potentials but require the three-body Coulomb Green's function
- Faddeev-Merkuriev integral and differential equations with splitting of the Coulomb potentials into long-range and short-range parts are well defined for both repulsive and attractive Coulomb potentials but still contain complicated three-body Green's function

Screening in the Three-body Coulomb Scattering problem (Alt, Sandhas, Ziegelmann 1978)

Two-body level

- Solve the two-body problem with screened Coulomb potentials (Yukawa and cut off screening possess analytic solution)
- Renormalize the t-matrix for the screened Coulomb potential to have the finite limit when the screening radius tends to ∞

Three-body level

- Insert renormalised t-matrices into short-range Faddeev equations and solve with increasing the screening radius as long as the results get stability
- Calculate wave function, transition amplitudes, cross sections
- Declare that these quantities ARE THE SOLUTION of the three-body Coulomb problem

Screening in the Three-body Coulomb Scattering problem (Alt, Sandhas, Ziegelmann 1978)

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Three-body level

- Insert renormalised t-matrices into short-range Faddeev equations and solve with increasing the screening radius as long as the results get stability

- Interpretation of the solution is problematic:when screening radius tends to infinity the limiting Faddeev eqution become bad defined and do not generate the solution to the tree-body Coulomb problem

Coulomb scattering problem

What to do

Search for such a formalism for solving the three-body Coulomb scattering problem which treats properly the two specific Coulomb features

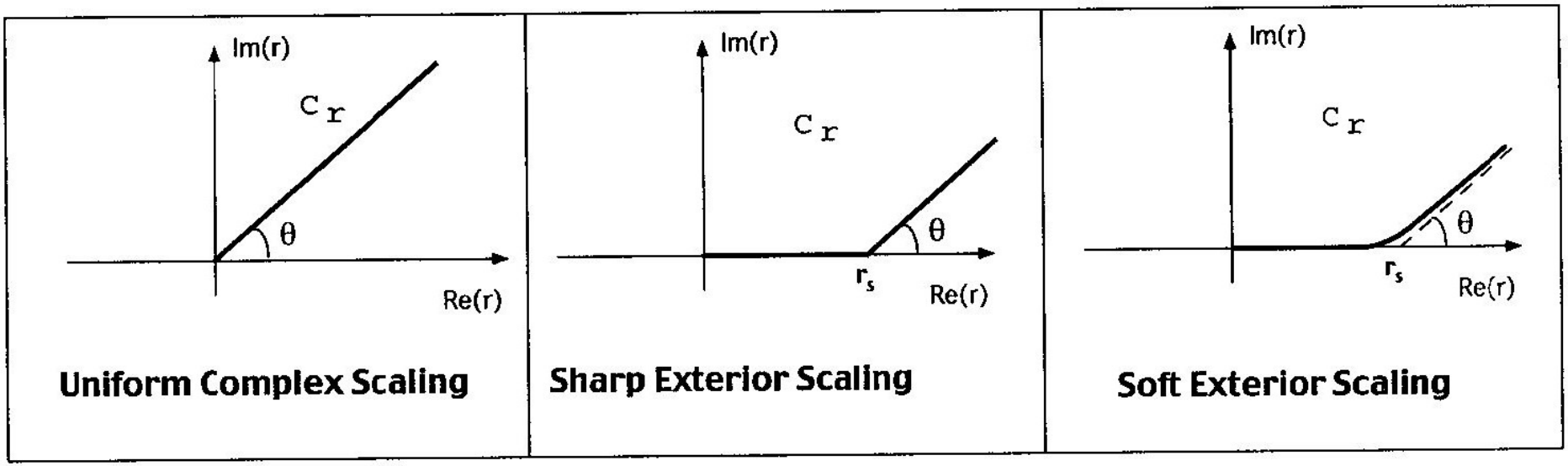
- Long-range character of the Coulomb potentials
- Infinite number of Coulomb excitations of two-body subsystems which leads to the asymptotic representation of the wave-function with infinite number of terms

Complex scaling method allows to avoid the use explicitly the asymptotic form of the wave function

I. Complex scaling (rotation) method

Complex scaling transformation $(W^\theta u)(x) = J(\theta)^{1/2} u[\phi_\theta(x)]$.

The transformed Hamiltonian $H(\theta) = W^\theta \; H \; (W^\theta)^{-1}$.



The spectrum of $H(\theta)$:

- All branches of continuous spectrum H are rotated on 2θ
- Bound states energies remain unchanged
- New complex eigenvalues may appear. Those which are independent on θ (after some minimal critical angle) are resonances.

I. Solution of the scattering problem with the complex scaling

The problem: complicated boundary conditions.

A solution: the complex scaling.

The rotated variable

$$\phi_\theta(r) \sim \text{const} + r\exp(i\theta) \quad \text{at} \quad r \to \infty.$$

gives for the wave e^{ikr} at the complex argument $\phi_\theta(r)$

$$e^{ik\phi_\theta(r)} \sim \text{const}\ e^{ikr\exp(i\theta)} = \text{const}\ e^{ikr\cos\theta} e^{-kr\sin\theta}.$$

e^{-ikr} **grows** exponentially at large distances on $\phi_\theta(r)$.

I. Driven equation in the two body case

Following the representation of the Hamiltonian $H = H^{as} + V^{res}$ the total w.f. Ψ is represented as

$$\Psi = \Psi^{in} + \Phi.$$

If an incident wave Ψ^{in} obeys $(H^{as} - E)\Psi^{in} = 0$ then

$$(H^{as} + V - E)\,\Phi = -V^{res}\Psi^{in}$$

and asymptotically Φ behaves as outgoing $\Phi \propto e^{+ikr}$ wave.
Application of the CS:

$$H(\theta)(W^{\theta}\Phi) = -W^{\theta}V^{res}\Psi^{in}.$$

Under which conditions can this equation be solved ?
1) $W^{\theta}\Phi$ is square integrable (goes to zero at infinity).
2) The R.H.S. goes to zero at infinity.

It depends on both V^{res} and Ψ^{in}.

I. The driven equation

1) Exponentially decreasing potentials (J. Nuttall et al. 1969).
$(H_0 - E)\Psi^{in} = 0$, and

$$(H_0 + V - E)\Phi = -V\Psi^{in}$$

After CS, Φ decreases exponentially. Ψ^{in} can grow as long as V can compensate this growth.

2) Long range (but not Coulomb) potentials (T.N.Rescigno et al. 1997)
Cut-off the potential: $V \to V_R$,

$$V_R(r) = \begin{cases} V(r), & r \le R \\ 0, & r > R, \end{cases}$$

V_R is not analytic for $r \le R \to$ the exterior CS is required with $Q \ge R$.
Then

$$W^{\theta}\left[V_R\Psi^{in}\right](r) = 0 \quad \text{at} \quad r \to \infty.$$

I. Splitting approach for Coulomb potential

(the original idea by S.P. Merkuriev 1978..., implementation by S.L. Yakovlev et al. 2009...)

A. Splitting the Coulomb potential

$$V^C = V_R + V^R$$

into core V_R and tail $V^R = V^C - V_R$ parts.

B. Solving *analytically* the Schrödinger equation for the tail part of the potential

$$(H_0 + V^R - E)\Psi^{inR} = 0$$

in order to construct the distorted incident wave Ψ^{inR}.

C. Solving the inhomogeneous (driven) Schrödinger equation for Φ

$$(H_0 + V^C - E)\Phi = -V_R\Psi^{inR}$$

by exterior complex scaling with boundary condition $W^\theta\Phi \to 0$ as $r \to \infty$ and the driven term such that $W^\theta V_R\Psi^{inR} \to 0$ as $r \to \infty$.

II. Three-Body Problem

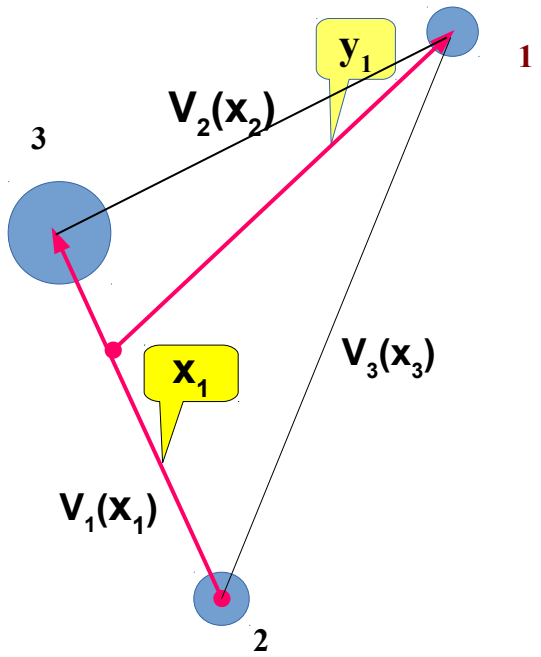


Figure: Three-body Jacobi coordinates and potentials

II. Three-Body Problem

Three-body Hamiltonian has the form

$$H = H_0 + V_1(x_1) + V_2(x_2) + V_3(x_3)$$

H_0 is the kinetic energy operator

$$H_0 = -\frac{1}{2\mu_\alpha}\Delta_{\mathbf{x}_\alpha} - \frac{1}{2\nu_\alpha}\Delta_{\mathbf{y}_\alpha}$$

with reduced masses defined as

$$\mu_\alpha = \frac{m_\beta m_\gamma}{m_\beta + m_\gamma} \qquad \nu_\alpha = \frac{m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}$$

$V_\alpha(x_\alpha)$ are the Coulomb potentials

$$V_\alpha(x_\alpha) = \frac{q_\beta q_\gamma}{|\mathbf{x}_\alpha|}$$

Convention:

$$\{\alpha, \beta, \gamma\} \text{ is any ciclic pemutation of } \{1, 2, 3\}$$

II. Incident configuration for three-Body scattering problem

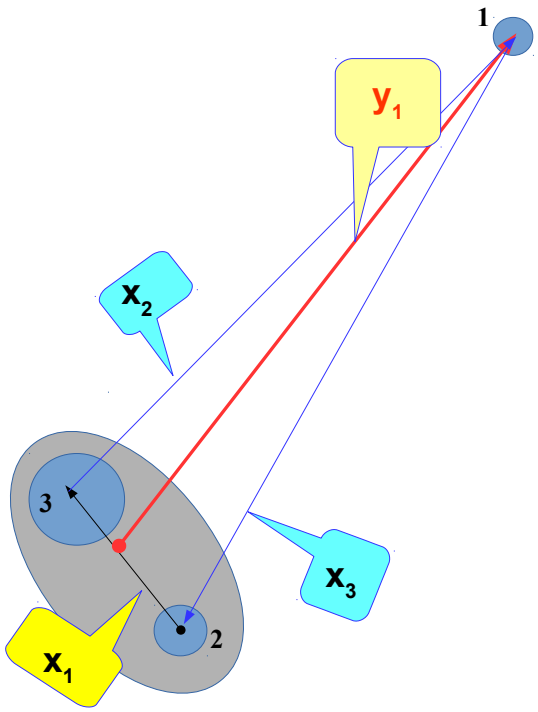


Figure: The incident configuration of bound state of particles (2,3) as a target and particle 1 as a spectator

II. Incident channel attributes

The incident channel Hamiltonian

$$H_1 = H_0 + V_1(x_1) + V_{\text{eff}}(y_1), \qquad \boxed{V_{\text{eff}}(y_1) = \frac{q_1(q_2+q_3)}{|\mathbf{y}_1|}}$$

dictates the incident channel wave function of the form

$$\Psi_{A_0}(\mathbf{x}_1, \mathbf{y}_1) = \phi_{A_0}(\mathbf{x}_1)\psi_C(\mathbf{p}_{A_0}, \mathbf{y}_1)$$

where
$\phi_{A_0}(\mathbf{x})$ is the two body bound state wave function with quantum numbers $A_0 = n_0, \ell_0$
$\psi_C(\mathbf{p}, \mathbf{y})$ is the two-body Coulomb scattering state for the potential $V_{\text{eff}}(y_1)$

II. Three-body scattering problem

Solve the Schrödinger equation

$$[H_0 + V(x,y)]\Psi \equiv (H_0 + V_1(x_1) + V_2(x_2) + V_3(x_3))\Psi(\mathbf{x},\mathbf{y}) = E\Psi(\mathbf{x},\mathbf{y})$$

with the asymptotic boundary conditions: 1) for the incident configuration

$$\Psi(\mathbf{x},\mathbf{y}) \sim \Psi_{A_0}(\mathbf{x}_1,\mathbf{y}_1) + \sum_A F_{A,A_0}\phi_A(\mathbf{x}_1)\exp\{i[p_A y_1 - \eta_A \log(2p_A y_1)]\}/y_1,$$

when $x_1 < const$ and $y_1 \to \infty$, 2) for the rearrangement configuration

$$\Psi(\mathbf{x},\mathbf{y}) \sim \sum_B F_{B,A_0}\phi_B(\mathbf{x}_\beta)\exp\{i[p_B y_\beta - \eta_B \log(2p_B y_\beta)]\}/y_\beta, \quad \beta = 2,3,$$

when $x_\beta < const$ and $y_\beta \to \infty$, 3) for the breakup channel with hyper radius definition $\rho^2 = \frac{1}{2}(\frac{x^2}{\mu} + \frac{y^2}{\nu})$

$$\Psi(\mathbf{x},\mathbf{y}) \sim F_{br,A_0}\exp\{i[\sqrt{E}\rho - \frac{\rho}{2\sqrt{E}}V(x,y)\log(2\sqrt{E}\rho)]\}/\rho^{5/2},$$

when $x, y \to \infty$.

II. The main asymptotic features of the three-body Coulomb scattering problem

1.

Asymptotic form is different in different arrangements $\Omega_\alpha = \{x_\alpha < const,\ y_\alpha \to \infty\},\ \alpha = 1,2,3$ of the configuration space

2.

Asymptotic boundary conditions contain infinitely many terms for energies above the break up threshold, since all Coulomb excitation channels are open!

These "1. and 2." require to search

for a new formulation, which solves both of these problems

II. "Minimal" potential splitting approach algorithm

A) Split the reaction potential in the incident channel into the sum of **the core** V_R and **the tail** V^R parts

$$V_2(\mathbf{x}_2) + V_3(\mathbf{x}_3) \equiv V(\mathbf{x},\mathbf{y}) = V_R(\mathbf{x},\mathbf{y}) + V^R(\mathbf{x},\mathbf{y}),$$

where

$$V_R = V,\ y_1 \le R, \quad V_R = 0,\ y_1 > R, \quad V^R = V - V_R$$

B) Define the distorted incident wave $\Psi^R(\mathbf{x},\mathbf{y})$:

$$\left[H_0 + V_1(x_1) + V^R(\mathbf{x},\mathbf{y}) - E\right]\Psi^R(\mathbf{x},\mathbf{y}) = 0.$$

C) Solve for $\Phi \equiv \Psi - \Psi^R$ the driven Schrödinger equation

$$(\mathbf{H_0} + \mathbf{V} - \mathbf{E})\,\mathbf{\Phi} = -V_R\Psi^R.$$

with boundary conditions containing only outgoing waves and with R.H.S. of the finite range with respect to the variable y_1.

Potential splitting approach

How to construct Ψ^R?

At the first stage we take the leading term of $V^R(\mathbf{x},\mathbf{y})$ in the incident configuration $V_C^R(y_1) = (q_2+q_3)/y_1$ (or 0) when $y_1 > R$ (or $\leq R$) and define the wave function

$$\Psi_0^R(\mathbf{x}_1,\mathbf{y}_1) = \varphi_{A_0}(\mathbf{x}_1)\psi_C^R(\mathbf{y}_1,\mathbf{p}_{A_0})$$

where $\psi_C^R(\mathbf{y},\mathbf{p}_{A_0})$ is found analytically (Yakovlev et al. 2010). In the region $(y \leq R)$ it is given by

$$\psi_C^R(\mathbf{y}) = \frac{4\pi}{p_{A_0} y}\sum_{\ell,m} a_\ell^R i^\ell \hat{j}_\ell(p_{A_0} y) Y_{\ell,m}(\hat{p}_{A_0}) Y_{\ell,m}(\hat{y})$$

with

$$a_\ell^R = e^{i\sigma_\ell} W_R(F_\ell, u_\ell^+)/W_R(\hat{j}_\ell, u_\ell^+),$$

$$u_\ell^+ = e^{-i\sigma_\ell}(G_\ell + iF_\ell)$$

.

Potential splitting approach

The full distorted wave Ψ^R is then represented as

$$\Psi^R = \Psi_0^R + \Psi_1^R.$$

with Ψ_1^R satisfying the inhomogeneous equation:

$$\left(H_0 - V_1(\mathbf{x}_1) + V^R - E\right)\Psi_1^R = -(V^R - V_C^R)\Psi_0^R.$$

In the region where $\varphi_{A_0}(\mathbf{x}_1)$ is not negligible one obtains

$$V^R(\mathbf{x}_1, \mathbf{y}_1) - V_C^R(y_1) \sim O\left(y_1^{-2}\right) \quad y_1 > R$$

therefore

$$|V^R(\mathbf{x}_1, \mathbf{y}_1) - V_C^R(y_1)| \leq const \times R^{-2}$$

and as the consequence this therm can be treated perturbatively if R is large.

Potential splitting approach

The solution Φ of the problem

$$\Phi = \Phi_0 + \Phi_1,$$

where the functions Φ_0, Φ_1 are the solutions to the equations

$$\left(H_0 - V_1(\mathbf{x}_1) + V^R - E\right)\Phi_i = (H - E)\,\Phi_i = -V_R\Psi_i^R, \quad i = 0, 1.$$

The total wave function Ψ

$$\Psi = \Psi_0^R + \Phi_0 + \Psi_1^R + \Phi_1.$$

The two last terms vanish when $R \to \infty$.
For moderate values of R, their contributions might not be negligible.

Wave function asymptotic behavior

$$\Phi \sim \sum_{n,\ell} \left[\frac{R_{n,\ell}(x_\alpha)}{x_\alpha} Y_{\ell,0}(\theta, 0) \right] u_\ell^+(y_\alpha, p_n) \tilde{F}_{n,\ell} + B(x, y, \theta).$$

The total state-to-state $(n_0, \ell_0) \to (n, \ell)$ scattering amplitude $F_{n,\ell}$ is split into terms

$$F_{n,\ell} = [F_0^R]_{n,\ell} + [F_1^R]_{n,\ell} + \tilde{F}_{n,\ell}.$$

The term $[F_0^R]_{n,\ell}$ corresponds to the function Ψ_0^R and is calculated explicitly.
The terms $[F_1^R]_{n,\ell}$ and $\tilde{F}_{n,\ell}$ correspond to the functions Ψ_1^R and $\Phi = \Phi_0 + \Phi_1$, respectively.
The local representation for the partial amplitudes $\tilde{F}_{n,\ell}$

$$\tilde{F}_{n,\ell} \approx \frac{(u_\ell^+)^{-1}(y_\alpha, p_n)}{2\pi} \int_0^\infty dx \int_0^\pi \sin\theta d\theta x R_{n,\ell}(x) \Phi(x, y, \theta) Y_{\ell,0}(\theta, 0).$$

Solution of the scattering problem

Two-step process:

1. Solution of the driven equation
2. Calculation of the scattering amplitudes

Step 1

The exterior complex rotation of the driven equation:

$$H(\theta)(W^{\theta}\Phi) = W^{\theta}[\mathrm{RHS}].$$

Zero boundary conditions at infinity, original b.c. are not used!

Step 2

Calculation of amplitudes inside the non-rotated region.
original b.c. are used!

Unified approach for scattering and resonances

- Mathematically correct platform for treating scattering processes and resonances
- The same numerical approach for both problems
- The same parameters of the numerical approach
- Natural parameter-free correspondence between resonances and peculiarities of scattering data

Numerical approach: FEM

- Finite element method: $\Phi(\mathbf{x},\mathbf{y}) = \sum_i v_i f_i(x,y,\cos\theta)$
- Spatial elements: rectangular elements in xy plane, Legendre polynomials in $\cos\theta$
- Local basis: projection of $f_i(x,y,\cos\theta)$ on each element

$$f_i(x,y,\cos\theta)|_{\Omega_m} = f_{im}^{(x)}(x) f_{im}^{(y)}(y) f_{im}^{(z)}(\cos\theta)$$

The Schrödinger equation is written as the linear system for the scattering problem:

$$(\tilde{H} - z\tilde{S})v = f \ ,$$

and as the generalized matrix eigenvalue problem (GEP) for resonances:

$$\tilde{H}\ v = z\tilde{S}v \ .$$

Here

$$(\tilde{H})_{i,j} = \langle f_i|H|f_j\rangle, \qquad (\tilde{S})_{i,j} = \langle f_i|f_j\rangle.$$

$\tilde{H}$ is complex symmetric.

Computational approach

General structure of the problem:

- matrices $\tilde{H}$ are $\tilde{S}$ are (relatively) sparse
- complex symmetric matrices of dimension from 10^5 to 10^6
- direct PARDISO and MUMPS solvers of algebraic linear equation systems
- GEP solution: shift-invert approach and the Arnoldi method

Parallel calculation:

- computation of the matrix elements over finite elements (MPI)
- parallel solvers for the system of linear equations and GEP

Parallelization

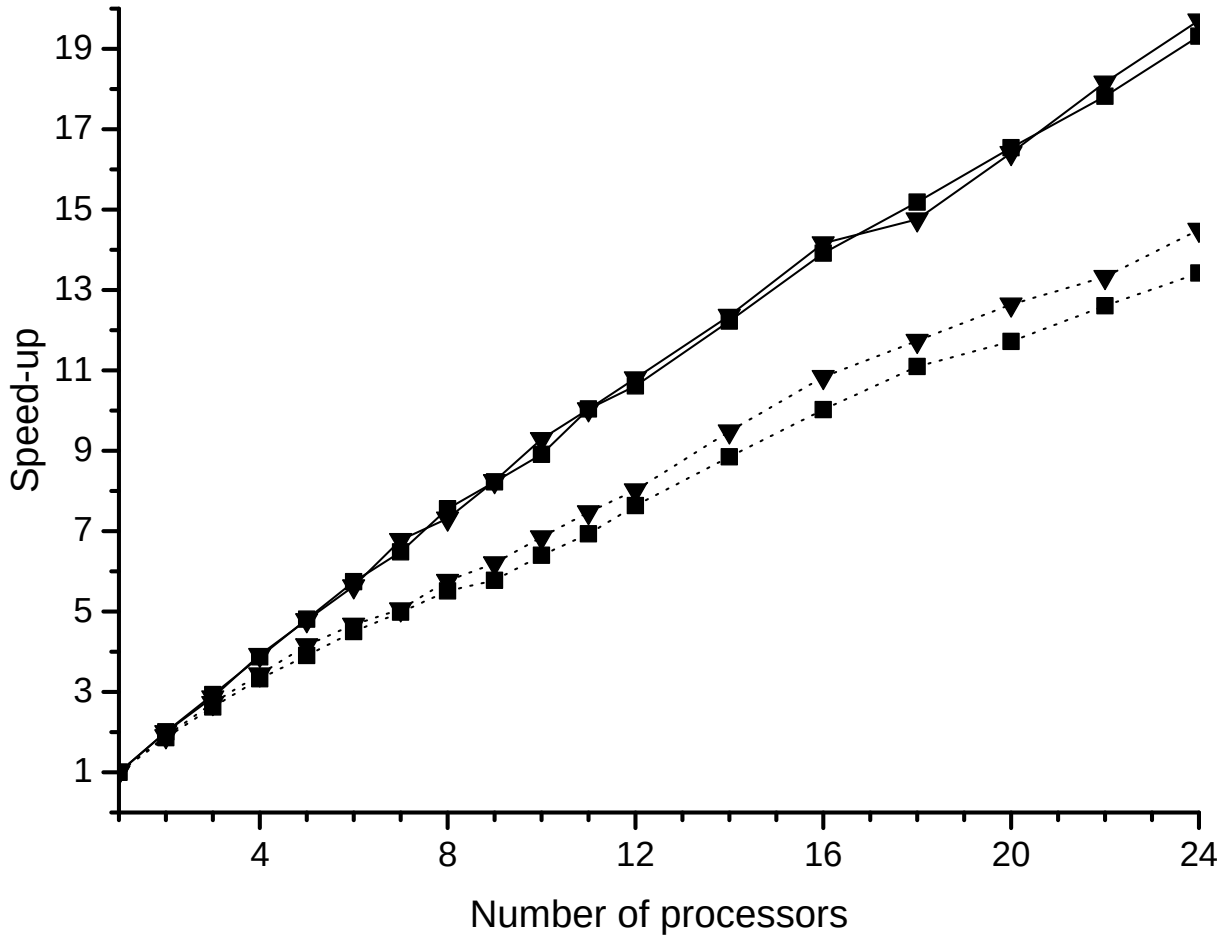


Figure: Calculation speed-up as a function of the number of processors. The squares and triangles are the results for the FEM degree of 7 and 9, respectively. The solid line corresponds to the matrix elements of the Hamiltonian, and the dot line does to the r.h.s.

Electron-H and electron-He^+ scattering

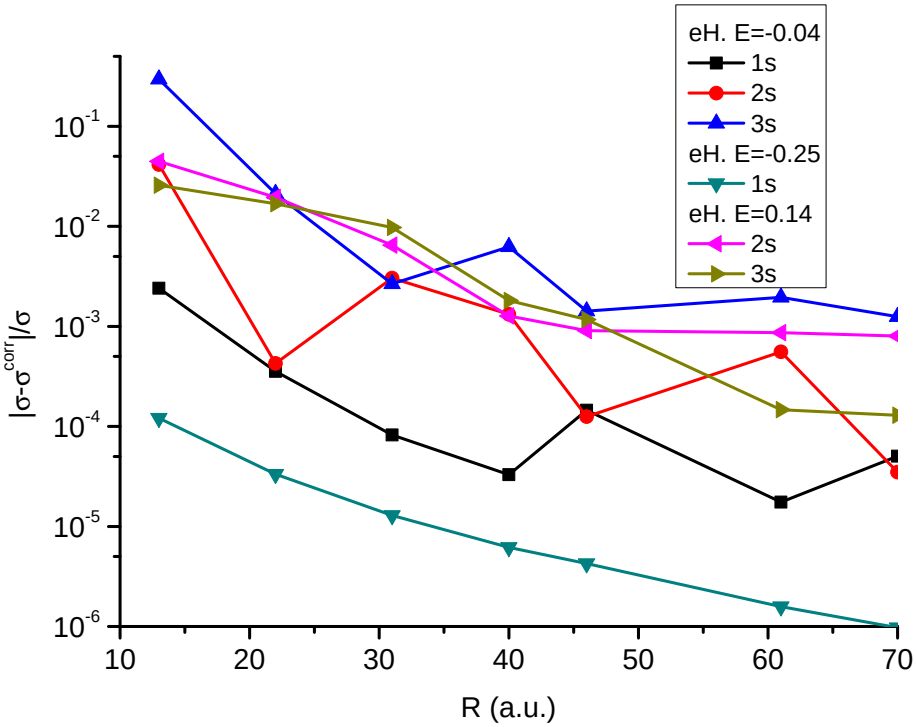


Figure: The relative difference $|\sigma - \sigma^{\text{corr}}|/\sigma$ for the 1s→ns cross sections for the e-H scattering as a function of the splitting radius R. The ECS radius Q=121 a.u.

Electron-H and electron-He$^+$ scattering

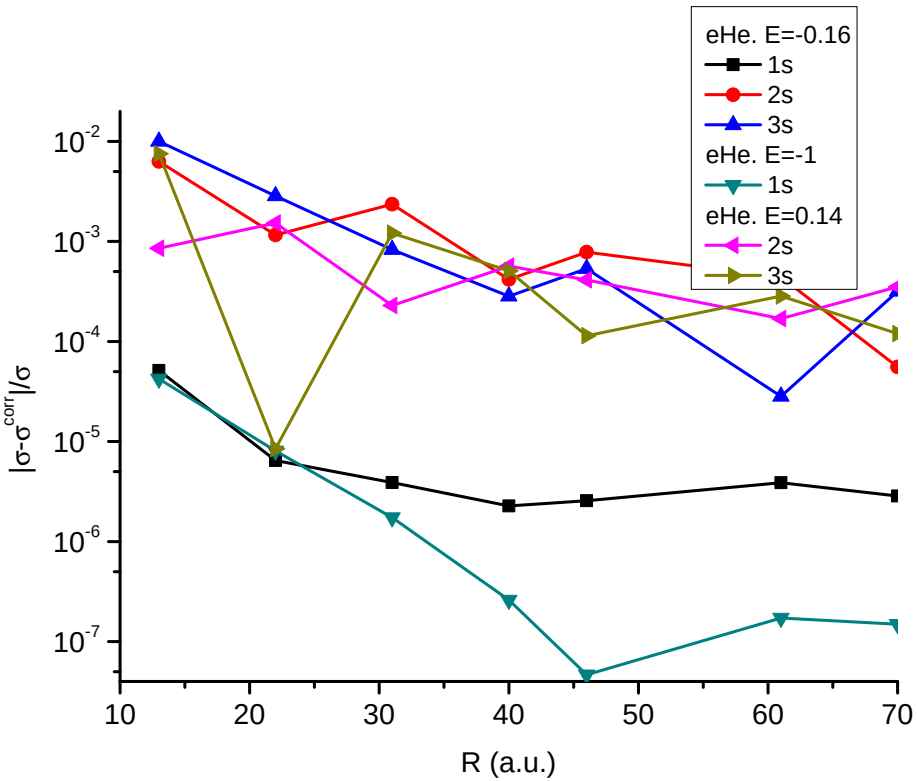


Figure: The relative difference $|\sigma - \sigma^{\text{corr}}|/\sigma$ for the 1s→ns cross sections for e-He$^+$ scattering as a function of the splitting radius R. The ECS radius Q=121 a.u.

Corrections for the Temkin-Poet model

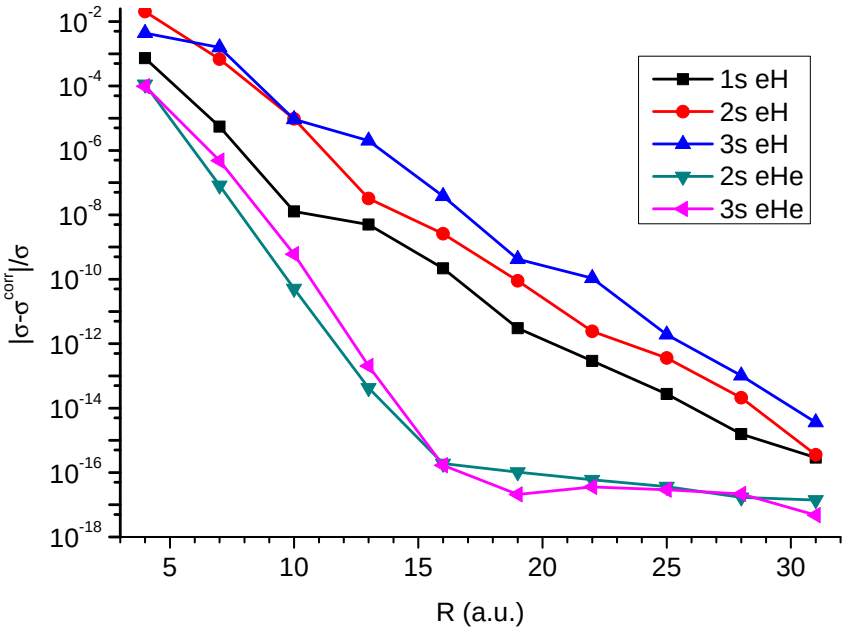


Figure: The relative difference $|\sigma - \sigma^{\text{corr}}|/\sigma$ for the 1s→ns cross sections for the Temkin-Poet model as a function of the splitting radius R. The energy E=0.147 a.u. above the ionization threshold, the ECS radius Q=121 a.u.

Electron-H and electron-He^+ scattering

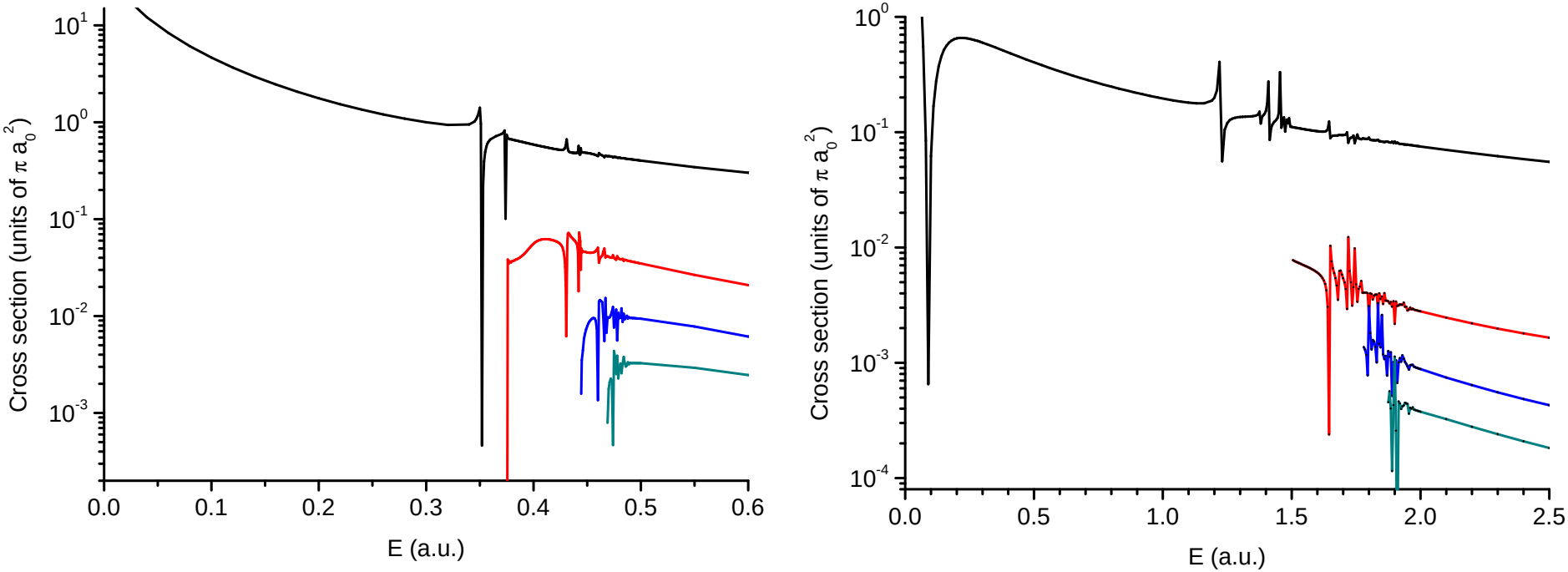


Figure: The singlet e-H (left) and e-He^+ (right) cross sections. Ionization thresholds are 0.5 a.u. for e-H and 2.0 a.u. for e-He^+ scattering.

Resonances in the three-body Coulomb system

Three-body resonances are calculated as the complex eigenvalues of the rotated Hamiltonian $H(\theta)$ which do not change its position with variation of the rotation angle θ. As an example, in the table the first deepest resonances for He are given. They fit perfectly the peaks in the e-He^+ cross section below the first excitation threshold of He^+.

Table: First deepest resonances of He atom below the first excitation threshold of He^+

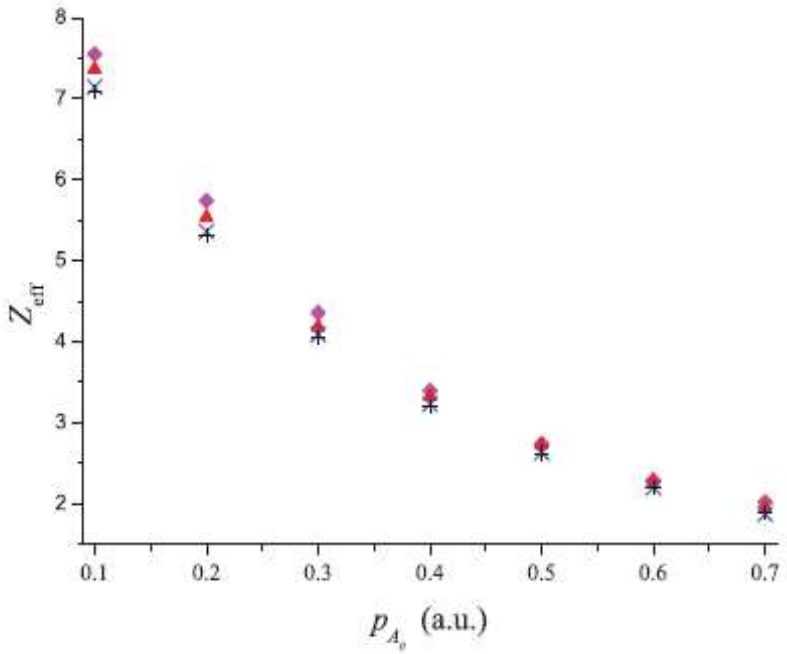
1.22214 -i 2.27(-3)
1.37839 -i 1.09(-4)
1.39742 -i 3.33(-6)
1.41011 -i 6.83(-4)
1.44026 -i 1.30(-7)
1.45195 -i 3.82(-5)

Positron Hydrogen scattering and annihilation

The effective annihilation rate parameter Z_{eff} is defined through the wave function as

$$Z_{\text{eff}} = \int dx dy |\Psi(x, y)|^2 \delta(x_3)$$

assuming that the particle 1 is the positron, particle 2 is the electron and particle 3 is the proton.



Conclusions

- Mathematically well defined approach for calculations both scattering and resonances
- The same numerical approach for both problems: easy comparison
- Future: incorporate the potential splitting into Faddeev type equation in order to have as much as optimal Faddeev equation formalism for the three-body Coulomb scattering

Acknowledgements

This work has been done in collaboration with

- Evgeny A. Yarevsky (St. Petersburg State University)
- Mikhail V. Volkov (St. Petersburg State University)
- Nils Elander (Stockholm University)

The work was supported by Russian Foundation for Basic Research grant No 14-02-00326 and by St Petersburg State University within the project No. 11.38.241.2015.

arXiv:1606.03228

Potential splitting approach to e-H and e-He^+ scattering with zero total angular momentum

EPJ Web of Conferences, 108 (2016) 02046

Scattering Problem and Resonances for Three-Body Coulomb Quantum Systems: Parallel Calculations

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THANK YOU
FOR YOUR ATTENTION