THREE-BODY SCATTERING IN THE TOTAL ANGULAR MOMENTUM REPRESENTATION

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Few-body Coulomb scattering problem

Systems with Coulomb interactions: nuclear, atomic, and molecular systems

The complicated boundary conditions at large distances are a major difficulty for this kind of problems

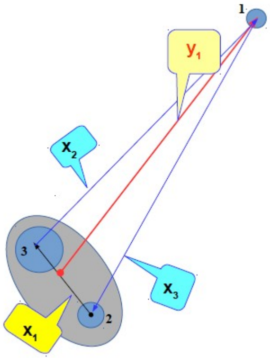
Several methods have been developed for constructing solutions to the three-body scattering problem

Some of these avoid using the explicit form of the asymptotic nature of the wave function

Three-body systems

$$H = T_{\mathbf{x}_\alpha} + T_{\mathbf{y}_\alpha} + V(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$$

An equation and boundary conditions $\rightarrow$ solutions



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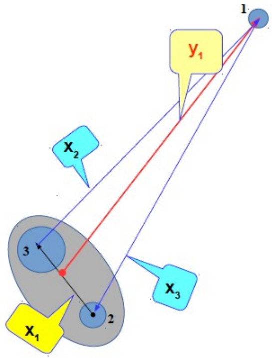

Complex rotation (scaling) method

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

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

Solution of the scattering problem with the complex scaling

The problem: complicated boundary conditions.
A solution: the complex scaling.
For 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 $\phi_\theta(r)$.

Solution of the scattering problem with the complex scaling: driven equation

The total w.f. Ψ is represented as

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

Ψ^{in} is **AN** incoming wave.

$$\left(H^K + V - E\right)\Phi = -V^{resid}\Psi^{in}.$$

Application of the CS:

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

Under what 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^{resid} and Ψ^{in}.

The driven equation

1) Exponentially decreasing potentials

J. Nuttall and H.L. Cohen, Phys. Rev. **188**, 1542 (1969).

$(H_0 - E)\Psi^{in} = 0$, and

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

After CS, Φ decreases exponentially. The R.H.S. can grow depending on $V(x)$.

2) Long range (but not Coulomb!) potentials

T.N.Rescigno, M.Baertschy, D.Byrum, C.W.McCurdy, Phys.Rev.**A55** 4253 (1997)

Cut of the potential: $V \to V_R$,

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

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

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

Potential splitting approach

3) The Coulomb potential: potential splitting approach

The reaction potential $V^{\alpha}(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha})$

$$V^{\alpha}(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha}) \equiv V(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha}) - V_{\alpha}(\mathbf{x}_{\alpha}) = \sum_{\beta \neq \alpha} V_{\beta}(\mathbf{x}_{\beta})$$

is split into the sum of **the core** V_R and **the tail** V^R parts

$$V^{\alpha}(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha}) = V_R(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha}) + V^R(\mathbf{x}_{\alpha}, \mathbf{y}_{\alpha}),$$

where

$$\begin{cases} V_R \; (V^R) = V^{\alpha} \; (0), & y_{\alpha} \leq R, \\ V_R \; (V^R) = 0 \; (V^{\alpha}), & y_{\alpha} > R. \end{cases}$$

Potential splitting approach

The distorted incident wave $\Psi^R(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$:

$$\left[H^K + V_\alpha(x_\alpha) + V^R(\mathbf{x}_\alpha, \mathbf{y}_\alpha) - E\right]\Psi^R(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = 0.$$

For $\Phi \equiv \Psi - \Psi^R$ one has the driven Schrödinger equation

$$(H - E)\,\Phi = -V_R\Psi^R.$$

This is the main equation of the potential splitting approach.
The R.H.S. is of finite range with respect to the variable y_α.

Potential splitting approach

How to construct Ψ^R?

Let us replace $V^R(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$ with its leading term in the incident configuration $V_C^R(y_\alpha) = \mathrm{const}/y_\alpha$ (or 0) when $y_\alpha > R$ (or $\leq R$).
The variables approximately separate:

$$\Psi^R(\mathbf{x}_\alpha, \mathbf{y}_\alpha) \approx \varphi_{A_0}(\mathbf{x}_\alpha)\psi_C^R(\mathbf{y}_\alpha, \mathbf{p}_{A_0}).$$

The function $\psi_C^R(\mathbf{y}_\alpha, \mathbf{p}_{A_0})$ in the region $(y_\alpha \leq R)$ is given by

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

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

$u_\ell^+ = e^{-i\sigma_\ell}(G_\ell + iF_\ell)$, $F_\ell(G_\ell)$ are the regular (irregular) Coulomb wave functions,
$W_R(f, g)$ is the Wronskian $f(r)g'(r) - f'(r)g(r)$ calculated at $r = R$.

Potential splitting approach

Is Ψ^R exact?

NO!

The full solution Ψ^R can be represented as

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

Ψ_0^R is the distorted wave, and Ψ_1^R satisfies the inhomogeneous equation:

$$\left(H^K - V_\alpha(\mathbf{x}_\alpha) + V^R - E\right)\Psi_1^R = -(V^R - V_C^R)\Psi_0^R.$$

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

$$V^R(\mathbf{x}_\alpha, \mathbf{y}_\alpha) - V_C^R(y_\alpha) \sim O\left(y_\alpha^{-2}\right).$$

The non-Coulomb tail of such a potential can be truncated at some R'.
The error goes to zero with increase in R'.

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

$$\left(H^K - V_\alpha(\mathrm{x}_\alpha) + V^R - E\right)\Phi_i = (H - E)\,\Phi_i = -V_R\Psi_i^R, \quad i = 0, 1.$$

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.

Scattering problem: total angular momentum representation

The solution Ψ is expanded in terms of linear combinations $\mathcal{F}^{J\tau}_{MM'}$ of the Wigner D-functions

$$\Psi(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = \sum_\tau \sum_{J=0}^{\infty} \sum_{M=-J}^{J} \sum_{M'=(1-\tau)/2}^{J} \left(\mathcal{F}^{J\tau}_{MM'}\right)^* (\Omega_\alpha)\, \Psi^{J\tau}_{MM'}(x_\alpha, y_\alpha, \theta_\alpha).$$

Equations for different τ and J are independent.
For the central potential, the expansion of the r.h.s. is

$$\begin{aligned} \left[\Psi^R_0\right]^{J\tau}_{MM'} &= \delta_{Mm_0} \frac{\tilde{\varphi}_{A_0}(x_\alpha)}{p_{A_0} y_\alpha} Y_{\ell_0 M'}(\theta_\alpha, 0) \frac{(-1)^M}{\sqrt{2 + 2\delta_{M'0}}} \sum_{\lambda=|J-\ell_0|}^{J+\ell_0} a^R_\lambda \hat{j}_\lambda(p_\alpha y_\alpha) \\ &\times \; i^\lambda (2\lambda+1) \left((-1)^{M'} + \tau(-1)^{\ell_0+\lambda}\right) C^{JM'}_{\ell_0 M' \lambda 0} C^{Jm_0}_{\ell_0 m_0 \lambda 0}. \end{aligned}$$

Here the z-direction coincides with the direction of the vector $\mathbf{p}_\alpha$.

Scattering problem: total angular momentum representation

Special cases:

1) Total momentum $J = 0$

$$\left[\Psi_0^R\right]_{00}^{0+} = i^{\ell_0}\tilde{\varphi}_{A_0}(x_\alpha)\, Y_{\ell_0 0}(\theta_\alpha, 0)\, a_{\ell_0}^R \,\frac{\hat{j}_{\ell_0}(p_\alpha y_\alpha)}{p_{A_0} y_\alpha}.$$

2) The target is in the s-state, $\ell_0 = 0$ и $m_0 = 0$.
The only term $\lambda = J$ survives, and

$$\left[\Psi_0^R\right]_{MM'}^{J\tau} = \delta_{\tau +}\delta_{M0}\delta_{M'0}\frac{2J+1}{\sqrt{4\pi}}\, i^J \tilde{\varphi}_{A_0}(x_\alpha)\, a_J^R \,\frac{\hat{j}_J(p_\alpha y_\alpha)}{p_{A_0} y_\alpha}.$$

Wave function asymptotic behavior

Asymptotic behavior of the wave function component:

$$\Psi^{J\tau}_{MM'}(x_\alpha, y_\alpha, \theta_\alpha) \underset{\rho\to\infty}{\sim} \left[\Psi^R_0\right]^{J\tau}_{MM'} + \sum_{\mathbb{A}} \tilde{\varphi}_{\mathbb{A}}(x_\beta) \mathcal{A}^{J\tau MM'}_{\mathbb{A}\mathbb{A}_0}(\theta_\beta, p_\alpha) Q_{\mathbb{A}}(y_\beta, E)$$

$$+ \mathcal{A}^{J\tau MM'}_{0\mathbb{A}_0}(y_\alpha/x_\alpha, \theta_\alpha; \mathbf{p}_\alpha) Q_0(\rho, E).$$

The expansion of the total amplitudes $\mathcal{A}_{\mathbb{A}\mathbb{A}_0}(\hat{\mathbf{y}}_\beta, p_\alpha)$ and $\mathcal{A}_{0\mathbb{A}_0}(\hat{X}; \mathbf{p}_\alpha)$:

$$Y_{l'm'}(\hat{\mathbf{x}}_\beta)\mathcal{A}_{\mathbb{A}\mathbb{A}_0}(\hat{\mathbf{y}}_\beta, p_\alpha) = \sum_{\tau} \sum_{J=0}^{\infty} \sum_{M=-J}^{J} \sum_{M'=(1-\tau)/2}^{J} \left(\mathcal{F}^{J\tau}_{MM'}\right)^* (\Omega_\beta) \mathcal{A}^{J\tau MM'}_{\mathbb{A}\mathbb{A}_0}(\theta_\beta, p_\alpha),$$

$$\mathcal{A}_{0\mathbb{A}_0}(\hat{X}; \mathbf{p}_\alpha) = \sum_{\tau} \sum_{J=0}^{\infty} \sum_{M=-J}^{J} \sum_{M'=(1-\tau)/2}^{J} \left(\mathcal{F}^{J\tau}_{MM'}\right)^* (\Omega_\beta) \mathcal{A}^{J\tau MM'}_{0\mathbb{A}_0}(y_\alpha/x_\alpha, \theta_\alpha; \mathbf{p}_\alpha).$$

Amplitudes are calculated by computing partial amplitudes $\mathcal{A}^{J\tau MM'}$ with the projection of the total wave function components on $\tilde{\varphi}_{\mathbb{A}}(x_\beta)$ and then summing them.

The scattering cross section

The scattering CS of the process with initial and final states specified by $\mathbb{A}_0$ and $\mathbb{A}$ is given by

$$\sigma_{\mathbb{A}\mathbb{A}_0} = \frac{1}{2m_{\alpha_0(\beta\gamma)}} \int \mathrm{d}\hat{\boldsymbol{y}}_\alpha \left| \mathcal{A}_{\mathbb{A}\mathbb{A}_0}(\hat{\boldsymbol{y}}_\alpha, \boldsymbol{p}_{A_0}) \right|^2 .$$

The CS averaged and summed over the magnetic quantum numbers

$$\sigma_{AA_0} = \frac{1}{2\ell+1} \sum_{m=-\ell}^{\ell} \sum_{m_0=-\ell_0}^{\ell_0} \sigma_{\mathbb{A}\mathbb{A}_0} .$$

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!

Corrections due to the non-separability ($\Psi_1^R + \Phi_1$ terms)

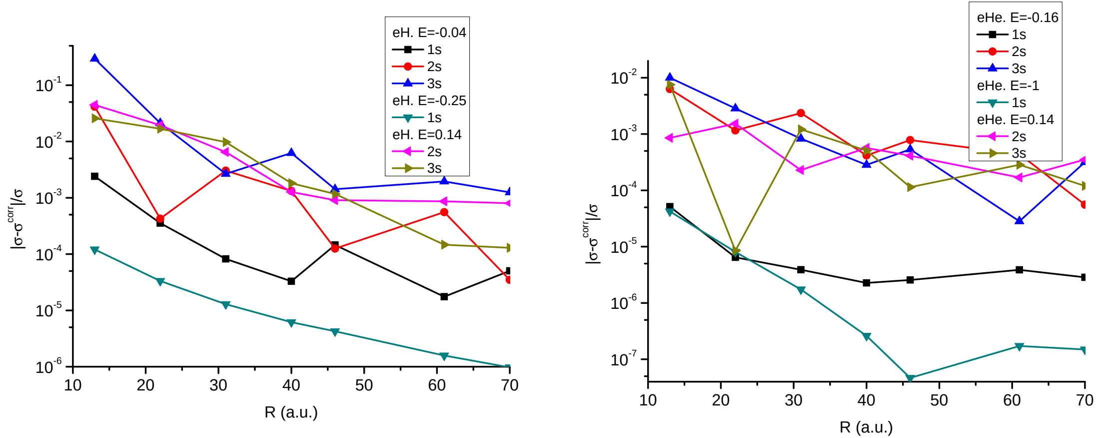

Рис.: The relative difference $|\sigma - \sigma_{corr}|/\sigma$ for the electron-H (left) and electron-He$^+$ (right) cross sections as a function of the splitting radius R. The ECS radius Q=121 a.u.

Summary

- Mathematically sound approach for calculations of scattering processes.
- Potential splitting approach allows for the solution of the scattering problem with the Coulomb interaction.
- It is demonstrated that the terms corresponding to the non-factorisable part of the distorted incoming wave decrease with increase in the splitting radius.

THANK YOU
for your attention!