Effects of Induced Dipole Interaction in scattering of positrons and electrons off a light atomic target

V.A. Gradusov, S.L. Yakovlev

St Petersburg State University, Department of Computational Physics

75 International Conference NUCLEUS-2025

St Petersburg

July 01-06 2025

I. Dipole interaction in Two-body sector of the Three-body system with Coulomb interaction

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

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

$\boldsymbol{X} = \{\boldsymbol{x}_a, \boldsymbol{y}_a\} \in \mathbb{R}^6$ is the set of standard mass-weighted Jacobi coordinates, $\boldsymbol{x}_a \in \mathbb{R}^3$ is the two-body relative coordinate

$V_a(\boldsymbol{x})$ are two body potentials:

$$V_a(\boldsymbol{x}) = \frac{q_b q_c}{|\boldsymbol{x}|} + V_a^s(\boldsymbol{x})$$

$V_a^s(\boldsymbol{x})$ is a short-range potential such that $V_a^s(\boldsymbol{x}) \sim O\left(\frac{1}{|\boldsymbol{x}|^{2+\mu}}\right)$, $\mu > 0$
$\{a, b, c\}$ runs over $\{1, 2, 3\}$ cyclically.

I.1. Two-body sectors

$$|\boldsymbol{x}_1| \ll |\boldsymbol{y}_1|$$

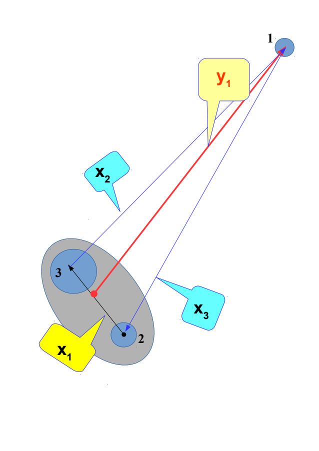

Figure: The configuration of bound state of particles (2,3) as a target and particle 1 as a spectator

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

Multipole expasion of Coulomb interactions:

$$\sum_{a=2}^{3} \frac{q_1 q_a}{|\boldsymbol{x}_a|} = \sum_{a=2}^{3} \frac{q_1 q_a}{|c_{a1}\boldsymbol{x}_1 + s_{a1}\boldsymbol{y}_1|} =$$

$$= \sum_{a=2}^{3} q_1 q_a \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^{\ell} \frac{4\pi}{2\ell+1} \frac{(|c_{a1}\boldsymbol{x}_1|)^{\ell}}{(|s_{a1}\boldsymbol{y}_1|)^{\ell+1}} Y_{\ell m}(\hat{\boldsymbol{x}}_1) Y^*_{\ell m}(\hat{\boldsymbol{y}}_1) =$$

$$= \frac{1}{|\boldsymbol{y}_1|} \sum_{a=2}^{3} \frac{q_1 q_a}{|s_{a1}|} - \frac{1}{|\boldsymbol{y}_1|^2} \sum_{a=2}^{3} q_1 q_a \frac{4\pi |c_{a1}\boldsymbol{x}_1|}{3|s_{a1}|} Y_{1m}(\hat{\boldsymbol{x}}_1) Y^*_{1m}(\hat{\boldsymbol{y}}_1) + O(|\boldsymbol{y}_1|^{-3})$$

Result:

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

I.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

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

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

CCE equations as $y_1 \to \infty$

$$\left(-\frac{d^2}{dy_1^2} + \frac{C}{y_1} + \frac{\mathbf{l}_1(\mathbf{l}_1+1) + \mathbf{A}}{y_1^2} - \mathbf{p}^2\right)\Psi(y_1) = O(y_1^{-3}), \quad p_n^2 = E - \epsilon_n.$$

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 known 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 $\mathbf{A}$ has the same block structure than the matrix $\mathbf{p}^2$, i.e. $A_{n\ell,n'\ell'} = A_{n,\ell\ell'}\delta_{nn'}$, i.e. by neglecting dipole coupling of target states with $n \neq n'$.

II. Dipole interaction in CCE

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

Model CCE equations for $e^- H$ scattering:

Main consequence of diagonality of $\mathbf{A}$ is $[\mathbf{A}, \mathbf{p^2}] = 0$ and hence the diagonolising matrix $\mathbf{V}$ such that $\mathbf{V}^\dagger[\mathbf{l}_1(\mathbf{l}_1 + 1) + \mathbf{A}]\mathbf{V} = \mathbf{D}$, $\mathbf{D}_{n\ell,n'\ell'} = d_{n\ell}\delta_{n\ell,n'\ell}$ commutes with $\mathbf{p}^2$, i.e. $[\mathbf{V}, \mathbf{p}^2] = 0$. This allows to diagonalize the CCE equations:

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

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

$$\mathcal{L}_{n\ell} = -1/2 \pm \sqrt{1/4 + d_{n\ell}}$$

Two possibilities for $\mathbf{D}$:

1. $d_{n\ell} \geq 0$ then $\mathcal{L}_{n\ell} \geq 0$ then $[\mathbf{V}^{\dagger}\Psi(y_1)]_{n\ell} = h^{\pm}_{\mathcal{L}_{n\ell}}(p_n y_1)$
2. there is $n\ell$ such that $d_{n\ell} < 0$ then
   - the equation

$$\left(-\frac{d^2}{dy_1^2} + \frac{d_{n\ell}}{y_1^2} - E\right)[\mathbf{V}^{\dagger}\Psi]_{n\ell}(y_1) = 0$$

     supports infinitely many bound states accumulating to the threshold ϵ_n from below
   - the scattering amplitude has the anomalous threshold behavior since if $d_{n\ell} < -1/4$ then $\mathcal{L}_{n,\ell}$ is complex
     $\mathcal{L}_{n\ell} = -1/2 \pm i\sqrt{|d_{n\ell}| - 1/4}$

$$f_{n\ell,n_0\ell_0} \sim p_n^{2\mathcal{L}_{n,\ell}+1} = \exp\{i2\Im\mathrm{m}(\mathcal{L}_{n\ell})\ln(p_n)\},$$

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

II.1. Importance of dipole interaction contribution in practical calculations

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

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

$$\left[-\frac{d^2}{dy^2} - p^2 + \frac{1}{\rho^2(y)} \begin{pmatrix} 24.9947 & 0 \\ 0 & -22.9947 \end{pmatrix}\right]\Psi =$$

$$\left[-\frac{d^2}{dy^2} - p^2 + \frac{1}{\rho^2(y)}\Lambda(\Lambda+1)\right]\Psi = 0$$

$$\Lambda = diag[4.52441, i4.76914], \Psi = [\Psi_1, \Psi_2]^T$$

$$\rho(y) = 6\,a.u.\,\mathrm{if}\,y \leq 6\,a.u.,\;\; \rho(y) = y,\,\mathrm{if}\,y > 6\,a.u.$$

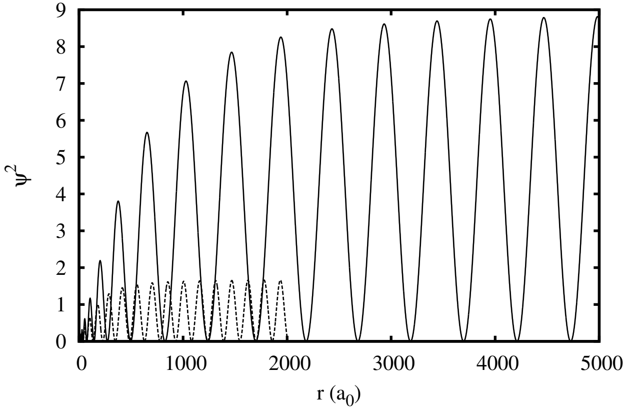

Figure: Squared Ψ_2 component of wave functions for different values of p: solid line corresponds to $p = 0.006\, a_0^{-1}$, dashed line corresponds to $p = 0.02\, a_0^{-1}$.

III. New asymptotics with corrected incoming and outgoing waves

V. Gradusov, S. Yakovlev *Theor. Math. Phys. 221:1, 176- 188 (2024)*

$$\psi^{\pm}_{(n\ell)(\nu\lambda)}(y_\alpha, p_\nu) \quad = \quad \left[W^{\alpha(0)}_{(n\ell)(\nu\lambda)} + \frac{1}{y_\alpha^2} W^{\alpha(1)}_{(n\ell)(\nu\lambda)}\right] u^{\pm}_{L_\alpha^{(\nu\lambda)}}(\eta_\nu, p_\nu y_\alpha). \qquad (1)$$

$$\begin{aligned} W^{\alpha(0)}_{(n\ell)(\nu\lambda)} &= \delta_{n\nu} V_\ell^{\alpha(\nu\lambda)}, \\ W^{\alpha(1)}_{(n\ell)(\nu\lambda)} &= (1-\delta_{n\nu}) \frac{\sum_{\ell'=0}^{\nu-1} A^{\alpha}_{(n\ell)(\nu\ell')} V_{\ell'}^{\alpha(\nu\lambda)}}{(p_n^2 - p_\nu^2)}, \end{aligned} \qquad (2)$$

$$L_\alpha^{(\nu\lambda)}(L_\alpha^{(\nu\lambda)} + 1) = q_\alpha^{(\nu\lambda)} \qquad (3)$$

$q_\alpha^{(\nu\lambda)}$ and $V_\ell^{\alpha(\nu\lambda)}$ are eigen values and eigen vectors of the matrix

$$||\ell(\ell+1)\delta_{\ell\ell'} + A^{\alpha}_{(\nu\ell)(\nu\ell')}||, \quad \ell, \ell' = 0.1, \ldots, \nu - 1.$$

THANK YOU FOR YOUR ATTENTION