On Recent Analytical Results for Solution of the Scattering Problem for Sharply Screened Coulomb Potentials

S.L. Yakovlev

***

E-mail: *yakovlev@cph10.phys.spbu.ru*

St Petersburg State University, Department of Computational Physics

The 22^{nd} European Conference

on

Few Body Problem in Physics

Kraków, Poland, 9-13 September 2013

Co-authors

M.V. Volkov, Saint-Petersburg State University, Department of Computational Physics

V.A. Gradusov, Saint-Petersburg State University, Department of Computational Physics

Plan of the talk

- Splitting of the Coulomb potential into core V_R and tail V^R parts

Plan of the talk

- Splitting of the Coulomb potential into core V_R and tail V^R parts
- Solution of the problem for core V_R potential

Plan of the talk

- Splitting of the Coulomb potential into core V_R and tail V^R parts
- Solution of the problem for core V_R potential
- Solution of the problem for tail V^R potential

Plan of the talk

- Splitting of the Coulomb potential into core V_R and tail V^R parts
- Solution of the problem for core V_R potential
- Solution of the problem for tail V^R potential
- Solution of the Coulomb problem in terms of core and tail solutions

List of Basic Notations

- Coulomb potential $V_{\mathcal{C}}(r) = Q/r$, Q $= \epsilon \frac{2\mu e^2 Z_1 Z_2}{\hbar^2}$ with $\epsilon = \pm 1$ corresponding to repulsion or attraction cases
- Schrödinger equation with Coulomb potential $[H_0 + V_{\mathcal{C}}(r) - k^2]\psi_{\mathcal{C}}(\boldsymbol{r}, \boldsymbol{k}) = 0$
- Free Hamiltonian $H_0 = -\Delta_{\boldsymbol{r}}$
- Coulomb wave function $\psi_{\mathcal{C}}(\boldsymbol{r}, \boldsymbol{k}) = (2\pi)^{-3/2} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-\pi\eta/2}\Gamma(1+i\eta)\,{}_1F_1(-i\eta, 1, i(kr - \boldsymbol{k}\cdot\boldsymbol{r}))$
- Plane wave $\psi_0(\boldsymbol{r}, \boldsymbol{k}) = \exp\{i\boldsymbol{r}\cdot\boldsymbol{k}\}$
- Sommerfeld parameter $\eta = Q/(2k)$
- Coulomb phase shift $\sigma_\ell = \arg\Gamma(\ell + 1 + i\eta)$
- The regular Coulomb function $F_\ell(\eta, z)$, the irregular Coulomb function $G_\ell(\eta, z)$, the Coulomb spherical waves $u_\ell^{\pm}(\eta, z) = e^{i\sigma_\ell}[G_\ell(\eta, z) \pm iF_\ell(\eta, z)]$, Riccati-Bessel function $\hat{j}_\ell(z) = F_\ell(0, z)$, Riccati-Hankel function $\hat{h}_\ell^{+}(z) = u_\ell^{+}(0, z)$.

I. Splitting of the Coulomb potential into the core V_R and tail V^R potentails

The Coulomb potential

$$V_C(r) = \frac{Q}{r} \equiv V_R(r) + V^R(r)$$

I. Splitting of the Coulomb potential into the core V_R and tail V^R potentails

The Coulomb potential

$$V_C(r) = \frac{Q}{r} \equiv V_R(r) + V^R(r)$$

The core potential

$$V_R(r) = \begin{cases} Q/r & r < R \\ 0 & r \geq R \end{cases}$$

I. Splitting of the Coulomb potential into the core V_R and tail V^R potentails

The Coulomb potential

$$V_C(r) = \frac{Q}{r} \equiv V_R(r) + V^R(r)$$

The core potential

$$V_R(r) = \begin{cases} Q/r & r < R \\ 0 & r \geq R \end{cases}$$

The tail potential

$$V^R(r) = \begin{cases} 0 & r < R \\ Q/r & r \geq R \end{cases}$$

II. Solution for the core potential V_R

The Schrödinger equation of the problem

$$\left[H_0 + V_R(r) - k^2\right] \psi_R(r,k) = 0$$

is solved by the partial wave expansion

$$\psi_R(r,k) = \frac{1}{kr} \sum_{\ell \geq 0} (2\ell+1) i^\ell v_\ell(r,k) P_\ell(\hat{r} \cdot \hat{k}).$$

The partial waves $v_\ell(r,k)$ are given by

$$v_\ell(r,k) = \begin{cases} a_{R\ell} F_\ell(\eta, kr) & r < R \\ \hat{j}_\ell(kr) + A_{R\ell} \hat{h}_\ell^+(kr) & r \geq R \end{cases}$$

where $a_{R\ell}$ and $A_{R\ell}$ are calculated through the Wronskians

$$a_{R\ell} = W_R(\hat{j}_\ell, \hat{h}_\ell^+)/W_R(F_\ell, \hat{h}_\ell^+), \quad A_{R\ell} = W_R(\hat{j}_\ell, F_\ell)/W_R(F_\ell, \hat{h}_\ell^+)$$

Properties of the solution ψ_R

1) For $r < R$

$$\psi_R(\mathbf{r},\mathbf{k}) = \int \mathrm{d}\hat{\mathbf{k}}' a_R(\hat{\mathbf{k}},\hat{\mathbf{k}}')\psi_C(\mathbf{r},k\hat{\mathbf{k}}')$$

with the kernel

$$a_R(\hat{\mathbf{k}},\hat{\mathbf{k}}') = \sum_{l\geq 0} \frac{2\ell+1}{4\pi} a_{R\ell} e^{-i\sigma_\ell} P_\ell(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}').$$

Asymptotically, when $R \to \infty$

$$a_{R\ell} \sim e^{i\sigma_\ell - i\eta\log 2kR}$$

Consequently,

$$a_R(\hat{\mathbf{k}},\hat{\mathbf{k}}') \sim e^{-i\eta\log 2kR}\delta(\hat{\mathbf{k}}-\hat{\mathbf{k}}')$$

Properties of the solution ψ_R

1) For $r < R$

$$\psi_R(\boldsymbol{r}, \boldsymbol{k}) = \int \mathrm{d}\hat{\boldsymbol{k}}' a_R(\hat{\boldsymbol{k}}, \hat{\boldsymbol{k}}') \psi_C(\boldsymbol{r}, k\hat{\boldsymbol{k}}')$$

with the kernel

$$a_R(\hat{\boldsymbol{k}}, \hat{\boldsymbol{k}}') = \sum_{l \geq 0} \frac{2\ell + 1}{4\pi} a_{R\ell} e^{-i\sigma_\ell} P_\ell(\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}').$$

Asymptotically, when $R \to \infty$

$$a_{R\ell} \sim e^{i\sigma_\ell - i\eta \log 2kR}$$

Consequently,

$$\boxed{\psi_R(\boldsymbol{r}, \boldsymbol{k}) \sim e^{-i\eta \log 2kR} \psi_C(\boldsymbol{r}, \boldsymbol{k})}$$

Properties of the solution ψ_R

2) For $r \geq R$

$$\psi_R(\boldsymbol{r}, \boldsymbol{k}) = e^{i\boldsymbol{r}\cdot\boldsymbol{k}} + v_{sc}(\boldsymbol{r}, \boldsymbol{k})$$

where

$$v_{sc}(\boldsymbol{r}, \boldsymbol{k}) = \frac{1}{kr}\sum_{\ell=0}^{\infty}(2\ell+1)i^{\ell}A_{R\ell}\,\hat{h}_{\ell}^{+}(kr)P_{\ell}(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{k}}').$$

Asymptotically, when $r \to \infty$

$$v_{sc}(\boldsymbol{r}, \boldsymbol{k}) \sim A_R(u, k)e^{ikr}/r, \quad u = \hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{k}}'$$

with the amplitude

$$A_R(u, k) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)A_{R\ell}P_{\ell}(u)$$

If $R \to \infty$

$$\begin{aligned} A_R(u, k) \quad &\sim e^{-2i\eta\log 2kR} A_C(u, k) \\ &- \frac{2}{k}\, e^{-i\eta\log 2kR}\sin(\eta\log 2kR)\,\delta(u-1) \end{aligned}$$

The Green function for V_R potential

The Green function $G^+(E) = (H_0 + V_R - E + i0)^{-1}$ is given by the partial wave representation

$$G_R^+(\mathbf{r}, \mathbf{r}', k^2) = \frac{1}{4\pi}\sum_{\ell=0}^{\infty}(2\ell+1)\frac{G_{R\ell}(r, r', k^2)}{rr'}P_\ell(\hat{\mathbf{r}}\cdot\hat{\mathbf{r}}')$$

For the most important configuration when $r, r' \leq R$ the partial wave components read

$$\begin{aligned} G_{R\ell}(r, r', k^2) &= \frac{1}{k}F_\ell(\eta, kr_<)H_\ell^+(\eta, kr_>) + \frac{\chi_{R\ell}(k)}{k}F_\ell(\eta, kr)F_\ell(\eta, kr'), \\ \chi_{R\ell}(k) &= -W_R(\hat{h}_\ell^+, H_\ell^+)/W_R(\hat{h}_\ell^+, F_\ell). \end{aligned}$$

The Green function for V_R potential

Summation of partial series in the region $r, r' \leq R$ leads to

$$G_R^+(\boldsymbol{r}, \boldsymbol{r}', k^2) = G_{\mathcal{C}}(\boldsymbol{r}, \boldsymbol{r}', k_+^2) + Q_R(\boldsymbol{r}, \boldsymbol{r}', k^2),$$

where $G_{\mathcal{C}}(\boldsymbol{r}, \boldsymbol{r}', k_+^2)$ is the Coulomb Green function and Q_R is given by

$$Q_R(\boldsymbol{r}, \boldsymbol{r}', k^2) = \frac{1}{2\mathrm{i}} \int_{-1}^{1} \mathrm{d}\zeta \, Z_R(\xi, \zeta)[G_{\mathcal{C}}(r\hat{\boldsymbol{x}}, r'\hat{\boldsymbol{x}}', k_+^2) - G_{\mathcal{C}}(r\hat{\boldsymbol{x}}, r'\hat{\boldsymbol{x}}', k_-^2)].$$

$$k_\pm^2 = k^2 \pm i0, \quad \xi = \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{r}}', \quad \zeta = \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{x}}'$$

$$Z_R(\xi, \zeta) = \sum_{\ell=0}^{\infty} (\ell + 1/2) \chi_{R\ell}(k) P_\ell(\xi) P_\ell(\zeta)$$

$$\chi_{R\ell}(k) = -W_R(\hat{h}_\ell^+, H_\ell^+)/W_R(\hat{h}_\ell^+, F_\ell)$$

The Green function for V_R potential

Asymptotically, when $R \to \infty$

$$\chi_{R\ell}(k) = \mathrm{i}\eta \exp(2\mathrm{i}\theta_\ell)/(kR) + \mathcal{O}(1/R^2),$$

where $\theta_\ell = kR - \eta \log(2kR) - \pi\ell/2 + \sigma_\ell$. For the $L_2(-1,1)$ norm of the kernel Z_R one gets

$$||Z_R|| = \max_\ell |\chi_{R\ell}(k)| = \eta/(kR) + \mathcal{O}(R^{-2}).$$

Therefore

$$Q_R(\boldsymbol{r}, \boldsymbol{r}', k^2) = \mathcal{O}(1/R)$$
$$G_R(\boldsymbol{r}, \boldsymbol{r}', k^2) = G_C(\boldsymbol{r}, \boldsymbol{r}', k^2) + \mathcal{O}(1/R)$$

T-matrix for V_R potential

Transition operator

$$T_R(z) = V_R - V_R G_R(z) V_R$$

Takes the form

$$T_R(z) = V_R - V_R G_C(z) V_R - V_R Q_R(z) V_R.$$

Asymptotically, when $R \to \infty$

$$T_R(z) = V_R - V_R G_C(z) V_R + \mathcal{O}(1/R)$$

III. Solution for the tail V^R potential

The Schrödinger equation of the problem

$$\left[H_0 + V^R(r) - k^2\right] \psi^R(\boldsymbol{r}, \boldsymbol{k}) = 0$$

is solved by the partial wave expansion

$$\psi^R(\boldsymbol{r}, \boldsymbol{k}) = \frac{1}{kr} \sum_{\ell \geq 0} (2\ell + 1) i^\ell w_\ell(r, k) P_\ell(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{k}}).$$

The partial waves $w_\ell(r, k)$ are given by

$$w_\ell(r, k) = \begin{cases} a_\ell^R \hat{j}_\ell(kr) & r < R \\ e^{i\sigma_\ell} F_\ell(\eta, kr) + A_\ell^R u_\ell^+(kr) & r \geq R \end{cases}$$

where a_ℓ^R and A_ℓ^R are calculated through the Wronskians

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

Properties of the solution ψ^R

1) For $r < R$

$$\psi^R(\boldsymbol{r}, \boldsymbol{k}) = \int \mathrm{d}\hat{\boldsymbol{k}}' a^R(\hat{\boldsymbol{k}}, \hat{\boldsymbol{k}}')\psi_0(\boldsymbol{r}, k\hat{\boldsymbol{k}}')$$

with the kernel

$$a^R(\hat{\boldsymbol{k}}, \hat{\boldsymbol{k}}') = \sum_{l \geq 0} \frac{2\ell + 1}{4\pi} a_\ell^R P_\ell(\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}').$$

Asymptotically, when $R \to \infty$

$$a_\ell^R \sim e^{i\eta \log 2kR}$$

Consequently,

$$a^R(\hat{\boldsymbol{k}}, \hat{\boldsymbol{k}}') \sim e^{i\eta \log 2kR} \delta(\hat{\boldsymbol{k}} - \hat{\boldsymbol{k}}')$$

Properties of the solution ψ^R

1) For $r < R$

$$\psi^R(\mathbf{r}, \mathbf{k}) = \int d\hat{\mathbf{k}}' a^R(\hat{\mathbf{k}}, \hat{\mathbf{k}}')\psi_0(\mathbf{r}, k\hat{\mathbf{k}}')$$

with the kernel

$$a^R(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = \sum_{l \geq 0} \frac{2\ell + 1}{4\pi} a_\ell^R P_\ell(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}').$$

Asymptotically, when $R \to \infty$

$$a_\ell^R \sim e^{i\eta \log 2kR}$$

Consequently,

$$\boxed{\psi^R(\mathbf{r}, \mathbf{k}) \sim e^{i\eta \log 2kR} \psi_0(\mathbf{r}, \mathbf{k})}$$

Properties of the solution ψ^R

2) For $r \geq R$

$$\psi^R(r, k) = \psi_C(r, k) + w_{sc}(r, k)$$

where

$$w_{sc}(r, k) = \frac{1}{kr} \sum_{\ell \geq 0} (2\ell + 1) i^\ell A_\ell^R u_\ell^+(\eta, kr) P_\ell(\hat{k} \cdot \hat{k}').$$

Asymptotically, when $r \to \infty$

$$w_{sc}(r, k) \sim A^R(u, k) e^{i(kr - \eta \log 2kr)}/r, \quad u = \hat{k} \cdot \hat{k}'$$

with the amplitude

$$A^R(u, k) = \frac{1}{k} \sum_{\ell \geq 0} (2\ell + 1) A_\ell^R P_\ell(u)$$

If $R \to \infty$

$$\boxed{A_C(u, k) + A^R(u, k) \sim \frac{2}{k} e^{i\eta \log 2kR} \sin(\eta \log 2kR)\, \boldsymbol{\delta(u - 1)}}$$

IV. Solution of the Coulomb problem in terms of core and tail solutions

The solution to the Coulomb Schrödinger equation

$$[H_0 + V_C]\psi_C = k^2\psi_C$$

by the splitting procedure $V_C = V^R + V_R$ can be represented as

$$\psi_C = \psi^R - [H_0 + V_C - k^2 + i0]^{-1} V_R \psi^R$$

or equivalently in the form of the integral equation of the Lippmann-Schwinger type

$$\psi_C = \psi^R - [H_0 + V^R - k^2 + i0]^{-1} V_R \psi_C$$

IV. Solution of the Coulomb problem in terms of core and tail solutions

Asymptotically, when $r \to \infty$

$$\psi_C(\boldsymbol{r}, \boldsymbol{k}) \sim \psi^R(\boldsymbol{r}, \boldsymbol{k}) + F_R e^{i(kr - \eta \log 2kr)}/r$$

where the amplitude is defined as

$$F_R = -2\pi^2 \langle \psi^{R(-)}(\boldsymbol{k}') | \, V_R \, | \psi_C(\boldsymbol{k}) \rangle .$$

Here $\psi^{R(-)}(\boldsymbol{r}, \boldsymbol{k}') = (\psi^R(\boldsymbol{r}, -\boldsymbol{k}'))^*$.
The further representation for the amplitude F_R has the form

$$F_R = -2\pi^2 [\langle \psi^{R(-)}(\boldsymbol{k}') | T_R(k^2 + i0) | \psi^R(\boldsymbol{k}) \rangle + \langle \psi^{R(-)}(\boldsymbol{k}') | Q_R(k^2 + i0) | \psi^R(\boldsymbol{k}) \rangle]$$

IV. Solution of the Coulomb problem in terms of core and tail solutions

Asymptotically, when $R \to \infty$

$$F_R = -2\pi^2 e^{2i\eta \log 2kR} \langle \psi_0(\boldsymbol{k}') | T_R(k^2 + i0) | \psi_0(\boldsymbol{k}) \rangle + \mathcal{O}(1/R)$$

and then

the total Coulomb amplitude receives the representation

$$\begin{aligned} A_C &= \frac{2}{k} e^{i\eta \log 2kR} \sin(\eta \log 2kR)\, \delta(\mathbf{u} - \mathbf{1}) \\ &- 2\pi^2 e^{2i\eta \log 2kR} \langle \psi_0(\boldsymbol{k}') | T_R(k^2 + i0) | \psi_0(\boldsymbol{k}) \rangle + \mathcal{O}(1/R) \end{aligned}$$

RÉSUMÉ

- The splitting approach allows to treat the long-range scattering problem on the basis of the short-range formalism
- The use of the splitting approach for systems of $N \geq 3$ particles seems to be very promising

Publications

1. S.L. Yakovlev, M.V. Volkov, E. Yarevsky and N. Elander, *The Impact of Sharp Screening on the Coulomb Scattering Problem in Three Dimensions* J. Phys. A: Math. Theor. 43 (2010) 245302.
2. M. V. Volkov, S. L. Yakovlev, E. A. Yarevsky, and N. Elander, *Potential splitting approach to multichannel Coulomb scattering: The driven Schrödinger equation formulation* Phys. Rev. A 83 (2011) 032722
3. S.L. Yakovlev, V.A. Gradusov, *Zero range potential for particles interacting via Coulomb potential: application to electron-positron annihilation* J. Phys. A: Math. Theor. 46 (2013) 035307

THANK YOU FOR YOUR ATTENTION