Coulomb wave functions and integrals

Report at annual TORUS Collaboration meeting

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Summary

- Two papers prepared.
- Constructed the infrastructure to compute the Coulomb distorted complex formfactors in momentum space.

Supplementary results

- Gel'fand-Shilov scheme applied to regularize the folding integrals with complex formfactors.
- Constructed the infrastructure to compute the Coulomb wave function.
- Splines framework constructed to work with the table-defined formfactors.

Introduction

(d, p) reactions

$\Downarrow$

Effective Three-Body problem

$\Downarrow$

Faddeev (AGS) equations

momentum space is preferrable

$\Downarrow$

Strong interactions in separable form (V_{np}, V_{nA}, V_{pA}) V_{nA}, V_{pA} $\in \mathbb{C} \Rightarrow$ generalization of EST scheme	Calculations in the Coulomb basis Screening brakes down at $Z \sim 20$

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Proof of principles

Calculation of Coulomb distorted nuclear formfactors.

Separable representation

Separable t-matrix:

$$t_l(E) = \sum_{ij} u|f_{l,E_i}\rangle \tau_{ij}(E) \langle f^*_{l,E_j}|u.$$

The formfactors:

$$u_{l,i}(q) \equiv \langle q|u|f_{l,E_i}\rangle = t_l(q, k_i, E_i),$$
$$u_{l,i}(q') \equiv \langle f^*_{l,E_i}|u|q'\rangle = t_l(q', k_i, E_i).$$

$t_l(q, k_i, E_i)$ is a half-shell t-matrix at $E_i = k_i^2/2\mu$.

The Coulomb distorted formfactors:

$$u^C_{l,i}(q) \equiv \langle \psi^C_{l,q} | u | f_{l,E_i} \rangle = \frac{1}{2\pi^2} \int dp\, p^2 u_{l,i}(p) \psi^C_{l,q}(p)^*,$$

$$u^C_{l,i}(q)^\dagger \equiv \langle f^*_{l,E_i} | u | \psi^C_{l,q} \rangle = \frac{1}{2\pi^2} \int dp\, p^2 u_{l,i}(p) \psi^C_{l,q}(p).$$

NOTE

Both values are required due to the generalization of EST scheme for complex potentials.

Roadmap

$$u^C_{l,i}(q) = \frac{1}{2\pi^2}\int dp\, p^2 u_{l,i}(p)\psi^C_{l,q}(p)^*,$$
$$u^C_{l,i}(q)^\dagger = \frac{1}{2\pi^2}\int dp\, p^2 u_{l,i}(p)\psi^C_{l,q}(p).$$

Two milestones

- Reliable and accurate numerical implementation for $\psi^C_{l,q}(p)$ (*CPC manuscript*).
- Regularization of the integral with the oscillatory singularity for the complex formfactors (*PRC manuscript*).

Representations of $\psi^C_{l,q}(p)$

General expression for $\psi^C_{l,q}(p)$

contains[a] the Associated Legendre Function of the 2-nd kind $Q_l^{i\eta}(\zeta)$.

[a] $\zeta = (p^2 + q^2)/2pq$.

To compute it

$Q_l^{i\eta}(\zeta)$ must be represented in terms of hypergeometric functions ${}_2F_1(a, b; c; z)$.

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Two representations

- For $p \approx q$ the *'pole proximity'* representation is valid (Eq. (9) in CPC manuscript).
- And for p far away from q another, *'regular'* representation is required (Eq. (12) in CPC manuscript).

Regularization

$$u_{l,i}^{C}(q) = \frac{1}{2\pi^2} \int dp\, p^2 u_{l,i}(p) \psi_{l,q}^{C}(p)^{*}.$$

Oscillatory singularity

inside the $\psi_{l,q}^{C}(p)$:

$$S_{\pm}(p-q) = \lim_{\gamma \to +0} \frac{1}{(p-q \pm i\gamma)^{1 \pm i\eta}}.$$

The irregular part of the integral

have the form:

$$I_{\pm} = \lim_{\gamma \to +0} \int_{-\Delta}^{\Delta} dx \frac{\varphi(x)}{(x \pm i\gamma)^{1 \pm i\eta}}. \qquad \begin{pmatrix} \varphi(0) \neq 0 \\ \varphi'(0) \neq 0 \end{pmatrix}$$

Gel'fand-Shilov regularization

$$I_{\pm} = \lim_{\gamma \to +0} \int_{-\Delta}^{\Delta} dx \frac{\varphi(x)}{(x \pm i\gamma)^{1 \pm i\eta}}.$$

Final result

$$I_{\pm} = (1 - e^{-\pi\eta}) \left[\int_0^{\Delta} dx \frac{\varphi(x) - \varphi(0) - \varphi'(0)x}{x^{1 \pm i\eta}} \pm \frac{i\varphi(0)}{\eta} \Delta^{\mp i\eta} + \frac{\varphi'(0)}{1 \mp i\eta} \Delta^{1 \mp i\eta} \right].$$

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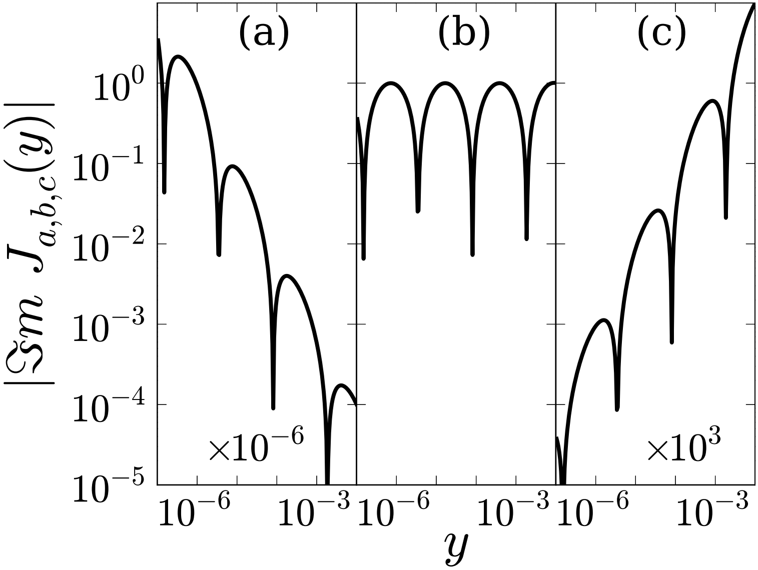
Illustration

$$\varphi(x) = 1+x+x^2, \qquad J_a(x) = \varphi(x)S_+(x),$$
$$J_b(x) = [\varphi(x)-\varphi(0)]S_+(x), \qquad J_c(x) = [\varphi(x)-\varphi(0)-\varphi'(0)x]S_+(x).$$

Illustration



Calculating $u^C_{l,i}(q)$

$$u^C_{l,i}(q) = \frac{1}{2\pi^2} \int dp\, p^2 u_{l,i}(p) \psi^C_{l,q}(p)^*.$$

Around the singular point

$$\psi^C_{l,q}(p) = \mathcal{A} \left[\frac{\mathcal{B}(p)}{(p-q+i0)^{1+i\eta}} - \frac{\mathcal{B}(p)^*}{(p-q-i0)^{1-i\eta}} \right].$$

$u_{l,i}(p) \in \mathbb{C} \Rightarrow$ both terms must be regularized separately.

Details

See Appendix B in PRC manuscript.

Selected topics

- Switching between representations of $\psi^C_{l,q}(p)$.
- Accuracy of our implementation of $\psi^C_{l,q}(p)$.
- Accuracy of the integration procedure.
- Illustrations.
- Simple test problem.

Switching between representations of $\psi^C_{l,q}(p)$

Fast 'raw' criterium

If the regular representation's 4-th argument of the ${}_2F_1(\ldots)$ is smaller, than the same one from the pole proximity representation $\Rightarrow$ choose regular representation.

$$p \leqslant 0.3q; \qquad\qquad p \geqslant 3.4q.$$

Switching between representations of $\psi^C_{l,q}(p)$

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Slow 'fine' criterium

$\forall p \neq q, p \in (0.3q, 3.4q)$: if $|\Im\mathrm{m}\,\mathcal{D}/\Re\mathrm{e}\,\mathcal{D}| > 10^{-6} \Rightarrow$ choose pole proximity representation[a].

[a] See Eq. (13) in CPC manuscript for $\mathcal{D}$.

Accuracy of $\psi^C_{l,q}(p)$

Numerical tests

- Against Neelam's implementation (explicit γ and fixed switching points).
- Against *Mathematica*™®©$£ implementation.

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Results

- Agree with Neelam's implementation.
- Coinside with *Mathematica*$^{\text{TM}}$®©$^{\$£}$ implementation with $\sigma \leqslant 5 \cdot 10^{-7}$ within the region of applicability[a].

$$\sigma = |a - b| \Big/ \overline{\{|a|, |b|\}} \; .$$

[a] See Sect. 5 in CPC manuscript.

Accuracy of $u^C_{l,i}(q)$

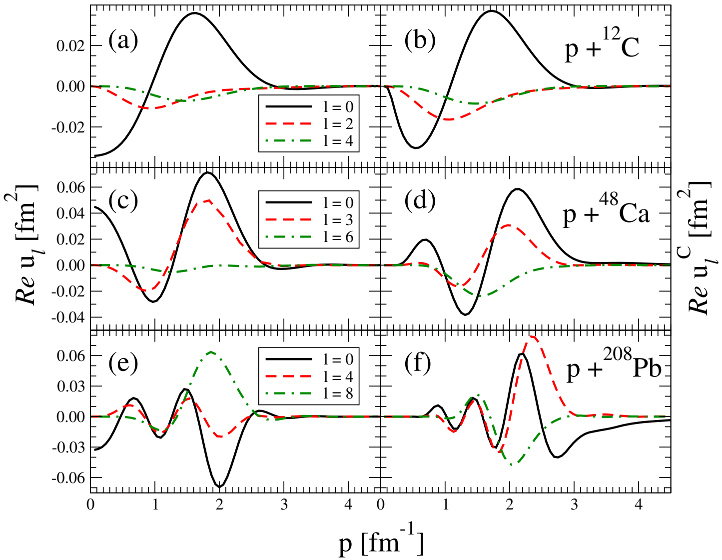
Numerical tests

Against *Mathematica*$^{\text{TM}}$®©$^{\$£}$ implementation with Yamaguchi formfactor $\Rightarrow \sigma < 1 \cdot 10^{-4}$ with reasonable runtime.

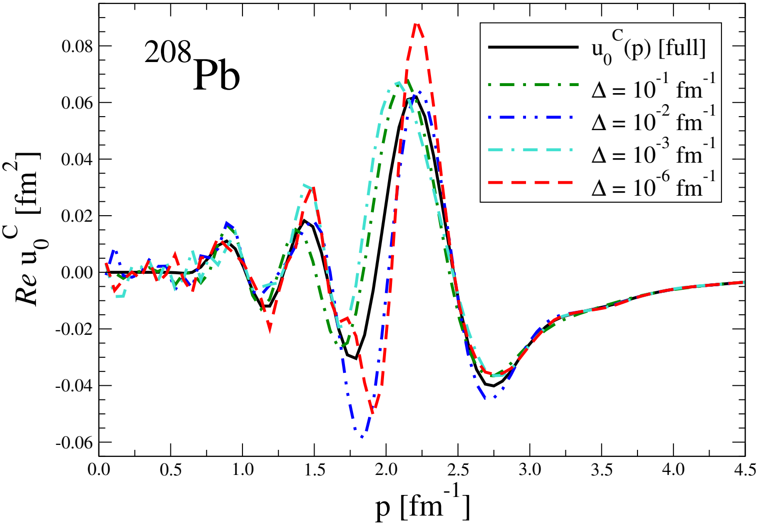
Accuracy depends on

- Number of quadrature points.
- Accuracy of the formfactor.

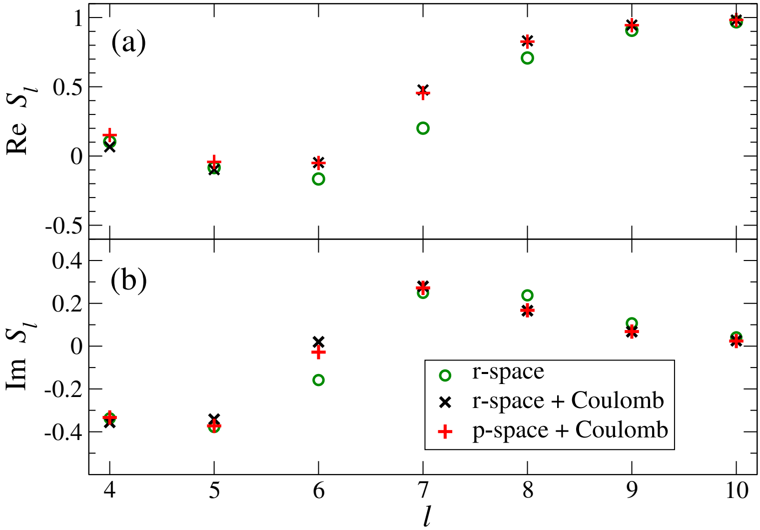
Formfactors



Role of the singularity



Simple test


(a)
(b)
Re S_l
Im S_l
1
0.5
0
-0.5
0.4
0.2
0
-0.2
-0.4
4
5
6
7
8
9
10
l
r-space
r-space + Coulomb
p-space + Coulomb

The intrigue