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Coulombic Transformation in Momentum Space

Abstract We studied the Coulombic transformation of potential in momentum space. The Coulombic transformation is defined as a unitary transformation in momentum space, which is equivalent of the Coulomb–Fourier transformation in coordinate space. The analytic continuation scheme avoids the difficulty which is occurred from the singularity of the Coulomb wave function in momentum space. We adopted the point method to perform the analytic continuation. The validity of the new scheme is checked by comparing with the analytic solution for the Malfliet-Tjon potential. Numerical calculation of the integration was done by separating into four intervals. We demonstrate the high accuracy of our calculation.

1 Introduction

In a few-body system consisting of pair charged particles Coulomb problem arises in momentum space because the diagonal components of the potential become singularities. Coulomb–Fourier transformation (CF) is known as a prescription for the Coulomb problem. In a two-charged particle system, it is a unitary transformation which eliminates Coulomb potential from the original Hamiltonian $H$ into the transformed Hamiltonian $\mathcal{H}$ in the Coulombic momentum space.

$$H = H_0 + V_C + V_S \xrightarrow{\text{CF trans}} \mathcal{H} = \langle \psi_k^C | H | \psi_k^C \rangle = T + \mathcal{V}$$

with

$$T = \langle \psi_k^C | (H_0 + V_C) | \psi_k^C \rangle = \frac{k^2}{2\mu} \delta^3(\mathbf{k} - \mathbf{k}')$$

and

$$\mathcal{V}(\mathbf{k}', \mathbf{k}) = \langle \psi_k^C | V_S | \psi_k^C \rangle,$$

where $V_C$, $V_S$ and $|\psi_k^C\rangle$ are a pure Coulomb potential, a short range nucleon–nucleon one and a Coulomb wave function, respectively. The Coulombic momentum $\mathbf{k}$ is the eigen momentum of a pure Coulomb Hamiltonian.

In next section we introduce a new scheme to perform the calculation of $\mathcal{V}(\mathbf{k}', \mathbf{k})$. Alt et al. [1] gave the analytic expressions of CF transformation for the Yukawa and Gaussian type potentials in coordinate space.
The purpose of our study is here to demonstrate the accuracy of the numerical calculation of \( V(k', k) \) by mean of comparison with the analytic exact number \([1]\). Our numerical results will be shown in Sect. 3. Finally, Sect. 4 will give a summary.

### 2 Formulations for Coulombic Transformation

We shall consider the Coulombic transformation in Eq. (2),

\[
\langle \psi^{C(\pm)}_{k'} | V^S | \psi^{C(\pm)}_k \rangle = \int d\mathbf{p'} \int d\mathbf{p} \langle \psi^{C(\pm)}_{k'} | \mathbf{p'} \rangle \langle \mathbf{p'} | V^S | \mathbf{p} \rangle \langle \mathbf{p} | \psi^{C(\pm)}_k \rangle.
\]

Coulomb wave function in momentum space is given as

\[
\langle \mathbf{p} | \psi^{C(\pm)}_k \rangle = -\frac{e^{-\frac{\pi \eta}{\hbar}}}{2\pi^2} \Gamma(1 + i\eta) \lim_{\epsilon \to 0^+} \frac{\partial}{\partial \epsilon} \left( (p^2 + (k \pm i\epsilon)^2)^{i\eta} \right) = \lim_{\epsilon \to 0^+} \langle \mathbf{p} | \psi^{C(\pm)}_k \rangle,
\]

where the Sommerfeld parameter is \( \eta = \frac{mc^2}{\hbar} \) and the superscript \((\pm)\) denotes the physical boundary condition of outgoing (incoming) wave function. In numerical calculation, obviously, we have to establish the treatment of \( \epsilon \)-limit. Here, we adopt the point method \([2]\) for this limitation. Namely, we evaluate the \( \epsilon \)-limit by the analytic continuation. For the sake of looking into the validity of our scheme, as the first step, we simplify the check into the half Coulombic transformation for the bra-space only as

\[
\psi^{(\pm)}(p', k) = \langle \mathbf{p'} | V^S | \mathbf{p} \rangle \langle \mathbf{p} | \psi^{C(\pm)}_k \rangle = \lim_{\epsilon \to 0^+} \int d\mathbf{p'} \langle \mathbf{p'} | V^S | \mathbf{p} \rangle \langle \mathbf{p} | \psi^{C(\pm)}_k \rangle = \lim_{\epsilon \to 0^+} \psi^{(\pm)}(p', k).
\]

For example, the Malfliet-Tjon potential (MT) \([3]\) has a Yukawa form as

\[
V^S(p', p) = \frac{V_0}{2\pi^2 (p - p')^2 + \beta^2}.
\]

The three-dimensional technique \([4]\) allows us to calculate the half Coulombic transformation with three variables as

\[
\psi^{(\pm)}(p', k, x') = \int\cdots\int \psi^{C(\pm)}(p, k, x),
\]

with

\[
v(p', p, x', x) = \int_0^{2\pi} \int_0^1 dx \frac{1}{2\pi^2 (p - p')^2 + \beta^2} V_0 \frac{1}{\sqrt{(p'^2 + 2p' p x + \beta^2)^2 - 4p'^2 p^2(1 - x^2)^2(1 - x'^2)}}.
\]

\(x = \hat{p} \cdot \hat{k}, x' = \hat{p}' \cdot \hat{k}'\) and \(\hat{p} \cdot \hat{p}' = xx' + \sqrt{1 - x^2} \sqrt{1 - x'^2} \cos \varphi\). Finally we obtain \(\psi^{(\pm)}(p', k, x')\) from \(\psi^{(\pm)}(p', k, x')\) by the point method, numerically.

On the other hand, the general expression for this transformation is given as \([1]\)

\[
\psi^{(+)}(p', k) = V_0 \exp \left( -\frac{\pi \eta}{\hbar} \Gamma(1 + i\eta) \right) \frac{1}{((k - p')^2 + \beta^2)^{1+i\eta}} \frac{\Gamma(1 + i\eta)}{\Gamma(1 + i\eta)} 2F_1(0, -i\eta, 1; x_0),
\]

with

\[
x_0 = 1 + \frac{(\beta^2 + \beta^2)(k - p' + i\beta)^2}{((k - p')^2 + \beta^2)^2(\beta^2 - (k - p')^2 + i\beta)^2}.
\]

where \(2F_1\) is the hypergeometric function. By comparing with the analytic solution \([1]\), we look into the accuracy of our numerical results.
3 Numerical Calculation

We use a version 5 of MT potential with $V_0 = -65.1090$ (MeV fm$^2$) and $\beta = 0.633$ (fm$^{-1}$). When $\varepsilon$ is small value, the numerical integration of $p$ needs a careful treatment around $p = k$. Thus we separate this integration into four intervals as

$$
\int_0^\infty dp = \int_0^{k-f(k)} dp + \int_{k-f(k)}^{k} dp + \int_{k}^{k+f(k)} dp + \int_{k+f(k)}^\infty dp
$$

Table 1 Convergence of $|V^{(+)}(p', k, x)|$ (MeV fm$^3$) at $p' = k = 10$ (fm$^{-1}$) and $x = 1$

| $J_{\text{max}}$ | Numerical calc. |
|------------------|-----------------|
| 1                | 0.118152 $\times 10^3$ |
| 2                | 0.168019 $\times 10^3$ |
| 3                | 0.162912 $\times 10^3$ |
| 4                | 0.162482 $\times 10^3$ |
| 5                | 0.162478 $\times 10^3$ |
| 6                | 0.162484 $\times 10^3$ |
| 7                | 0.162484 $\times 10^3$ |
| 8                | 0.162483 $\times 10^3$ |
| 9                | 0.162483 $\times 10^3$ |
| 10               | 0.162483 $\times 10^3$ |
| Analytical value | 0.162483 $\times 10^3$ |

Table 2 Convergence of $|V^{(+)}(p', k, x)|$ (MeV fm$^3$) at $p' = k = 10$ (fm$^{-1}$) and $x = 0$

| $J_{\text{max}}$ | Numerical calc. |
|------------------|-----------------|
| 1                | 0.325231 |
| 2                | 0.324897 |
| 3                | 0.324876 |
| 4                | 0.324873 |
| 5                | 0.324874 |
| 6                | 0.324876 |
| 7                | 0.324876 |
| 8                | 0.324876 |
| Analytical value | 0.324876 |

Fig. 1 The transformed Malfliet-Tjon potential (real part) at $x' = 1$
where we choose $f(k) = 0.1 \times k$ and each interval has 500 Gauss–Legendre grids. Convergence of the calculation is checked. According to the choice of the $\varepsilon$ values, experientially, we take

$$
\varepsilon_j = \begin{cases} 
0.05 \times k \times (1 + 0.05 \times j) & (k \geq 10 \text{ (fm}^{-1})) \\
0.1 + 0.01 \times j & (k < 10 \text{ (fm}^{-1})).
\end{cases}
$$

After we calculate the $\psi_{\varepsilon_j}^{(+)}$ for $j = 1, \ldots, j_{\text{max}}$, then $\psi^{(+)}$ is obtained by the point method. For some $j_{\text{max}}$ cases, numerical results are shown in Tables 1 and 2. Comparing the analytic value of Eq. (9) to the numerical values our scheme indicates the high accuracy. We also showed the pictures of the half Coulombic transformed Malfliet-Tjon potential in Fig. 1.

4 Summary

We showed the high accuracy of numerical calculations of Coulombic transformation in momentum space. The $\varepsilon$-limit in Coulomb wave function was calculated by the point method with the analytic continuation. In future we expect calculate the Coulombic transformation for the realistic non-local potential in momentum space without a partial wave expansion.

Acknowledgments On 1 August 2012 Walter Glöckle passed away. We dedicate this paper to Walter, who was a great friend and collaborator.

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