Coulomb plus Nuclear Scattering in Momentum Space for Coupled Angular-Momentum States

Dinghui H. Lu, Tim Mefford, Guilian Song*, and Rubin H. Landau

Department of Physics, Oregon State University, Corvallis, OR 97331

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Abstract

The Vincent–Phatak procedure for solving the momentum-space Schrödinger equation with combined Coulomb-plus-short-range potentials is extended to angular momentum states coupled by an optical potential—as occurs in spin 1/2 × 1/2 scattering. A generalization of the Blatt–Biedenharn phase shift parameterization is derived and applied to 500 MeV polarized-proton scattering from 3He and 13C. The requisite high-precision partial-wave expansions and integrations are described.

I. INTRODUCTION

The theory and equations of quantum mechanics are represented equally well in coordinate and momentum spaces. Bound states problems, which by definition deal with normalizable wavefunctions, can actually be solved equally well in either space, while scattering problems, which in the time-independent Schrödinger theory deal with non-normalizable states, are more of a challenge in momentum space. This challenge arises, in part, because boundary conditions are more naturally imposed in coordinate space, and, in part, because non-normalizable states cannot be Fourier transformed [1]. In spite of the difficul-

* Current address: Physics Department, Harbin Normal University, P.R. China.
ties, momentum-space calculations are important because fewer approximations are needed there to handle the nonlocal potentials arising in many-body and field theories.

The Coulomb problem in momentum space has actually been “solved” a number of times—possibly starting with Fock’s study of the hydrogen atom [2]—yet no one numerical approach appears to provide the requisite precision for all applications. The real “problem” is that the Coulomb potential between a point projectile (P) and a target (T),

\[ V_c(k', k) = \frac{Z_P Z_T e^2}{2\pi^2 q^2} \rho(q), \quad q = |k' - k|, \tag{1} \]

has a \(1/q^2\) singularity which must be regularized before a numerical solution is implemented [3]. (The form factor \(\rho(q)\) in (1) accounts for the finite size of the target’s charge distribution and makes the potential well-behaved at large \(q\)—but does not remove the singularity at \(q = 0\).) Kwon and Tabakin [4] solved the bound-state problem with the potential (1) by using Landé’s technique [5] of subtracting a term from (1), which makes its integral finite, and then adding in a correction integral. Alternatively, Cieplý et al. [6] solved the bound-state problem by using the Vincent–Phatak (VP) procedure [7], which deals with the Fourier transform of a Coulomb potential which has been cut off beyond some radius \(R_{\text{cut}}\),

\[ V_{c}^{\text{cut}}(k', k) = \frac{Z_P Z_T e^2}{2\pi^2 q^2} [\rho(q) - \cos(qR_{\text{cut}})]. \tag{2} \]

While \(V_{c}^{\text{cut}}(k', k)\) is clearly finite as \(q \to 0\), it produces wavefunctions which must have their asymptotic behavior corrected.

The VP procedure was originally formulated for intermediate-energy pion scattering from light nuclei [7] where it provided sufficient accuracy [8]. However, the accuracy has become a concern for intermediate-energy proton scattering where the proton’s much larger mass leads to correspondingly larger momentum transfers and correspondingly greater numbers of partial waves. Crespo and Tostevin [9] and Picklesimer et al. [10] have documented difficulties with the VP procedure, difficulties which appear as a sensitivity of the computed phase shifts to the cutoff radius, or a several-percent error in the phase shift when compared to coordinate-space calculations. Both references suggest algorithms to reduce the errors.
Alternatively, Elster et al. [11] applied the two-potential formula to the Coulomb and nuclear potentials and outlined an approach requiring multiple, numeric Fourier transforms between coordinate and momentum spaces. In contrast, Arrellano et al.’s study of intermediate-energy proton scattering from spinless nuclei [12] simply made the VP procedure sufficiently precise by using some high-precision partial wave expansions developed by Eisenstein and Tabakin [13]. (As a check, they transformed the potentials to coordinate space and solved the equivalent integro-differential equation.)

In the present paper we generalize the Blatt–Biedenharn phase shift parameterization and the VP procedure in order to handle intermediate-energy proton scattering from spin $1/2$ nuclei in which tensor forces couple states of differing angular momenta. In Sec. II we reformulate the VP procedure for uncoupled channels, in Sec. III we present our new formulation for coupled channels, and in Sec. IV we give some details of an application to 500 MeV proton scattering from $^3$He.

II. UNCOUPLED STATES ($0 \times 0, 0 \times 1/2$)

Vincent and Phatak formulated their procedure in terms of phase shifts. We reformulate it in terms of T-matrix elements to avoid unnecessary conversions between phase shifts and amplitudes. The summed nuclear plus cut-off Coulomb potential $V$, can be used in the Lippmann-Schwinger equation:

$$T_{l \pm}(k', k) = V_{l \pm}(k', k) + \frac{2}{\pi} \int_0^{\infty} \frac{p^2 dp V_{l \pm}(k', p) T_{l \pm}(p, k)}{E + i\epsilon - E(p)},$$

which is then solved in the normal way since $V_{l \pm}(k', k)$ is well–behaved in momentum space (short-ranged in coordinate space). If the $r$-space nuclear potential vanishes beyond a range $R$, and if the Coulomb cutoff-radius $R_{cut}$ is chosen larger than $R$, then the wavefunction in the intermediate region, $R \leq r \leq R_{cut}$, can be expressed in terms of a free wave shifted by an intermediate phase shift $\delta_l$ [7]:

$$u_{j=l\pm1/2}(R \leq r \leq R_{cut}) = Ne^{i\delta_{l \pm}} \left[ \sin \delta_{l \pm} G_l(kr) + \cos \delta_{l \pm} F_l(kr) \right],$$

where $G_l$ and $F_l$ are the free wave functions for $l$ and $l+1/2$ respectively, and $N$ is a normalization constant.

3
\[ N \left[ F_l(kr) + \hat{T}_{l\pm} H_l^{(+)}(kr) \right], \quad (5) \]

\[ \hat{T}_{l\pm} = e^{i\delta_{l\pm}} \sin \delta_{l\pm} = -\rho E T_{l\pm}, \quad \rho_E = 2k_0 \frac{E_P(k_0) E_T(k_0)}{E_P(k_0) + E_T(k_0)}, \quad (6) \]

where \( \delta_{j=l\pm} \) is the intermediate phase shift arising from the short-range potentials and \( N \) is a normalization constant. Here \( l \) is the orbital angular momentum, \( j = l \pm 1/2 \) is the total angular momentum, and we have used two equivalents forms for the wavefunctions [3].

The wavefunction for \( r > R_{\text{cut}} \) can be expressed in terms of a phase shift \( \delta_c^l \) (the amount a point-Coulomb wave is shifted), which, in turn, is determined by matching the intermediate wavefunction to an outer one at \( r = R_{\text{cut}} \). The outer wavefunction for \( r \geq R_{\text{cut}} \) has the same form as the intermediate one, but with the free waves replaced by Coulomb waves and the intermediate phase shift \( \delta_{l\pm} \) replaced by the phase shift relative to point-Coulomb waves \( \delta_c^{l\pm} \):

\[ u_{l\pm}(r \geq R_{\text{cut}}) = N' \left[ F_l(\eta, kr) + \hat{T}_{l\pm}^c H_l^{(+)}(\eta, kr) \right], \quad \hat{T}_{l\pm}^c = e^{i\delta_c^{l\pm}} \sin \delta_c^{l\pm}. \quad (7) \]

Here \( \hat{T}_{l\pm}^c \) is the T matrix for scattering from short range forces in the presence of a point-Coulomb force, \( \eta = Z_P Z_T e^2/v \) is the Sommerfeld parameter, \( F_l(\eta, kr) \) is the regular Coulomb function, and \( H_l^{(+)}(\eta, kr) \) is an outgoing wavefunction; for example,

\[ H_l^{(+)}(\eta, kr) \equiv G_l(\eta, kr) \pm iF_l(\eta, kr) \sim \exp\{\pm i[kr - l\pi/2 + \sigma_l - \eta \ln(2kr)]\}. \quad (8) \]

The requirement that the logarithmic derivative of \( u_{l\pm}(r \leq R_{\text{cut}}) \) match \( u_{l\pm}(r \geq R_{\text{cut}}) \) at \( r = R_{\text{cut}} \) determines \( \hat{T}_{l\pm}^c \) as:

\[ \hat{T}_{l\pm}^c = \frac{\hat{T}_{l\pm}[F_l(\eta), H_l^{(+)}] + [F_l(\eta), F_l]}{[F_l, H_l^{(+)}(\eta)] + \hat{T}_{l\pm}[H_l^{(+)}, H_l^{(+)}(\eta)]}, \quad (9) \]

where the brackets indicate Wronskians.

Finally, the non–spin–flip scattering amplitude can be expressed in terms of the outer, Coulomb–modified phase shifts \( \delta_c^l \) [14]:

\[ f(\theta) = f_{pl}^c(\theta) + f^{nc}(\theta), \quad (10) \]

\[ f_{pl}^c(\theta) = -\frac{\eta}{2k \sin^2(\theta/2)} \exp\{2i[\sigma_0 - \eta \ln \sin(\theta/2)]\}, \quad (11) \]

\[ f^{nc}(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l + 1) e^{2i\sigma_l} \left( e^{2i\delta_c^l} - 1 \right) P_l(\cos \theta). \quad (12) \]
III. COUPLED STATES \((\frac{1}{2} \times \frac{1}{2})\)

If the interaction couples angular-momentum states, we must generalize the VP method—even if the Coulomb force does not directly couple the states. When two non-identical spin \(1/2\) particles interact through a tensor force, the total angular momentum \(j\) remains a good quantum number yet there is coupling within the triplet spin state as well as between the triplet and singlet states. Accordingly, (3) is generalized to the coupled integral equations:

\[
T_{jl}^{j(s')s}(k', k) = V_{jl}^{j(s')s}(k', k) + \frac{2}{\pi} \sum_{L,S} \int_{0}^{\infty} p^2 dp \frac{V_{jl}^{j(S'S)}(k', p)T_{Ll}^{j(S'S)}(p, k)}{E + i\epsilon - E(p)},
\]

where the sum is over the coupled states. If the two particles interact through an optical potential, the phase shifts are complex and the \(S\) matrix non-symmetric. In the Appendix we generalize the conventional Blatt-Biedenharn NN parameterization \([15,16,17]\) and show that the \(S\) matrix elements have the form:

\[
S_{l'=j_{1}\pm 1,t'=j_{1}\pm 1}(k_0) \equiv S_{l'\pm} = \delta_{l'\pm} - 2i\rho_{E} T_{l'\pm}(k_0, k_0)
\]

\[
S_{+\pm} = (\cos \epsilon_{+}\cos \epsilon_{-} e^{2i\delta_{-}+} + \sin \epsilon_{+}\sin \epsilon_{-} e^{2i\delta_{-}-})/\det U,
\]

\[
S_{\pm\pm} = (\sin \epsilon_{+}\cos \epsilon_{-} e^{2i\delta_{+}+} - \cos \epsilon_{+}\sin \epsilon_{-} e^{2i\delta_{+}-})/\det U,
\]

\[
S_{-\pm} = (\sin \epsilon_{-}\cos \epsilon_{+} e^{2i\delta_{+}+} - \cos \epsilon_{-}\sin \epsilon_{+} e^{2i\delta_{+}-})/\det U,
\]

\[
S_{-\pm} = (\cos \epsilon_{+}\cos \epsilon_{-} e^{2i\delta_{-}+} + \sin \epsilon_{+}\sin \epsilon_{-} e^{2i\delta_{-}-})/\det U,
\]

\[
\det U = \cos \epsilon_{+}\cos \epsilon_{-} + \sin \epsilon_{+}\sin \epsilon_{-}.
\]

To apply the VP procedure to channels coupled by an optical potential, we 1) transform to a new basis in which there is no channel coupling, 2) match the interior wavefunction to point-Coulomb ones in this basis for which the \(S\)-matrix is diagonal, and then 3) return
to the original basis to calculate the scattering observables. One implementation of these steps would be to take our S matrix elements computed via (13) and (14), assume they have the forms (15)–(18) in terms of phase shifts and coupling parameters, and then search for the \((\delta_-, \delta_+, \epsilon_-, \epsilon_+)\) which satisfy these transcendental equations. The \(\delta\)'s would be the phase shifts in the basis in which S is diagonal—even though we never explicitly transform to that basis.

The implementation we have used is more direct and self-testing. We compute the solution of (13), form the nondiagonal S matrix,

\[
[S] = \begin{bmatrix}
S_{++} & S_{+-}
\end{bmatrix},
\]

and then explicitly diagonalize it with the similarity transformation:

\[
[S'] = [U][S][U]^{-1} = \begin{pmatrix}
e^{2i\delta_{++}} & 0 \\
0 & e^{2i\delta_{--}}
\end{pmatrix},
\]

\[
[U] = \begin{pmatrix}
\frac{1}{S_{++}} & \frac{S_{+-}}{\lambda_--S_{--}} \\
\frac{S_{++}}{\lambda_+-S_{++}} & 1
\end{pmatrix},
\]

\[
[U]^{-1} = \begin{pmatrix}
\frac{1}{-S_{++}} & \frac{-S_{++}}{\lambda_+-S_{++}} \\
\frac{S_{++}}{\lambda_+-S_{++}} & 1
\end{pmatrix} \frac{1}{\det U},
\]

\[
\lambda_\pm = \frac{1}{2} \left[ S_{++} + S_{--} \pm \sqrt{(S_{++} - S_{--})^2 + 4S_{+-}S_{+-}} \right].
\]

We now effectively deduce the intermediate \(\delta\) phase shift from the diagonal elements, do the VP matching with the corresponding \(T_{ll}\)'s as in (3) (this effectively determines the final phase shift \(\delta^c\)), and then we use the original U matrix to transform back to the basis in which we calculate observables:

\[
[S^{nc}] = [U]^{-1}[S'][U].
\]

Even though the method is guaranteed to diagonalize the S matrix, as an internal test we check that \(|S^{nc}| \leq 1\) and that \(|S'_{ll}| \leq 1\).

IV. COMPUTATIONAL DETAILS

We have modified the LPOTp code [14] to include the Coulomb potential in the different spin channels. As a first test of our precision we solved the Lippmann-Schwinger equation.
with a point Coulomb potential and checked that our answers reproduced the point Coulomb phase shifts $\sigma_l$ [after removal of the $\eta \ln(2kR_{cut})$ term in (8)]. We concluded from this severe test that 48–64 grid points are required to solve the Lippmann-Schwinger equation and obtain four–five place precision in $\sigma_l$ [there is enough cancellation that three–place precision does not reproduce the point Coulomb scattering amplitude $f_{pt}^{\text{ct}}$ (11)]. After an overall $e^{2i\sigma_0}$ is factored out from the sum in (11), good agreement for $f_{pt}^{\text{ct}}$ was found (indistinguishable from the analytic amplitude on a five-decade semi-logarithmic plot).

As the next test we computed pure-Coulomb scattering of 415 MeV protons from the charge distribution of $^3\text{He}$. We were able to obtain essentially perfect reproduction of the Born-approximation amplitude,

$$f_{\text{finite}}^{\text{finite}} \simeq f_{\text{ct}}^{\text{ct}}(\theta)\rho(q),$$

which proves that we can include short-ranged effects—in addition to the long-range Coulomb force—with precision of at least $O(\alpha^2)$. To actually obtain this agreement we used 48 grid points in the solution of the Lippmann–Schwinger equation (13), and increased the precision of our partial-wave projection:

$$V_l(k', k) = \pi^2 \int_{-1}^{1} V(k', k)P_l(\cos\theta_{kk})d(\cos\theta_{kk}),$$

until the partial wave summation,

$$V(k', k) \simeq \frac{1}{2\pi^2} \sum_{l}^{l_{\text{max}}} (2l + 1)V_l(k', k)P_l(\cos\theta_{kk}),$$

reproduced all oscillations present in $V(k', k)$. We show a reproduction of this type in Figure 1 where the many oscillations arising from the $\cos(qR_{cut})$ term in the cut-off Coulomb potential (4) is evident. We obtained six-place reproduction of $V(k', k)$ using $l_{\text{max}} = 48$ partial waves and 96 integration points in the partial-wave projection (26). Ten-place reproduction demanded $l_{\text{max}} = 96$. We expect these number to scale as $kR$, and so larger nuclei or higher energies will require more partial waves and grid points. For these calculations we used analytic nuclear form factors [18], though we also were successful for $^{13}\text{C}$ using
numerical Fourier transforms of Wood-Saxon densities \[19\]. However, noise and instability do appear for form factors which fall off slowly in \(q\).

An important requirement on the VP method is that the matching radius, which we take equal to \(R_{\text{cut}}\), be larger than the range of the nuclear force (in order to be able to express the outer wavefunction as a linear combination of Coulomb waves). However, increasing \(R_{\text{cut}}\) makes the cut-off Coulomb potential more oscillatory and more difficult to reproduce. In fact, it was the sensitivity to changes in \(R_{\text{cut}}\) which led Ref. \[9\] to search for an alternative to the matching method. We find that using \(R_{\text{cut}} \leq 5\) fm produces unstable results (presumably cutting off the nuclear potential), but, as seen in Figure 2, we obtain stable results for \(6\) fm \(\leq R_{\text{cut}} \leq 10\) fm.

In Figure 3 we compare the nuclear–plus Coulomb cross section and polarization (solid curves) to those calculated without Coulomb (dashed curves). The exact handling of the Coulomb potential is seen to have a significant, although small, effect in the semilog plot of \(d\sigma/d\Omega\), and a more pronounced effect for \(A_{00n0}\). Not plotted, because they essentially overlap the exact results, are ones in which the Coulomb potential is handled in impulse approximation:

\[
f(\theta) \simeq f_{\text{pt}}(\theta)\rho(q) + f^n(\theta),
\]

with \(f^n(\theta)\) the scattering amplitude for pure nuclear scattering.

V. CONCLUSION

We have extended the Vincent-Phatak procedure for the exact inclusion of the Coulomb potential in momentum space to calculations of proton scattering from spin 1/2 nuclei in which spin–dependent forces couple angular-momenta states. As part of that extension we also generalized the Blatt-Biedenharn phase shift analysis for the scattering of two spin 1/2 particles to cases where the S matrix is no longer symmetric. Although our formulation and calculational procedure is for a more complicated spin case, we confirm the finding of
Arrellano et al. [12] that the VP procedure can be made sufficiently accurate for intermediate-energy proton scattering if high-precision partial-wave expansions and large numbers of partial waves are used.

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APPENDIX: GENERALIZATION OF BLATT–BIEDENHARN CONVENTION

The conventional phase shift analysis must be extended when the angular momentum channels are coupled. Blatt and Biedenharn did this first for the mixing of the \( l = j \pm 1 \) states within the nucleon-nucleon triplet state [16,17] by assuming that the mixed states have the asymptotic forms:

\[
\lim_{r \to \infty} u_{j,l=j-1}(r) = A_+ e^{-i[kr-(j-1)\pi/2]} - B_+ e^{i[kr-(j-1)\pi/2]}, \\
\lim_{r \to \infty} u_{j,l=j+1}(r) = A_- e^{-i[kr-(j+1)\pi/2]} - B_- e^{i[kr-(j+1)\pi/2]}.
\]  

(A1) (A2)

The S matrix is defined by the relation among the A’s and B’s:

\[
\begin{bmatrix}
B_+ \\
B_-
\end{bmatrix} = 
\begin{bmatrix}
S_{++} & S_{+-} \\
S_{-+} & S_{--}
\end{bmatrix}
\begin{bmatrix}
A_+ \\
A_-
\end{bmatrix}.
\]  

(A3)

For NN scattering below pion production threshold, S must be unitary because flux is conserved, and symmetric because all terms in the Schrödinger equation are real. For that case, the most general form for S, a unitary and symmetric \( 2 \times 2 \) matrix, is given by a similarity transformation with mixing parameter \( \epsilon \),

\[
[S] = [U]^{-1}[e^{2i\Delta}][U],
\]

(A4)

\[
[U] = 
\begin{bmatrix}
\cos \epsilon_j & \sin \epsilon_j \\
-\sin \epsilon_j & \cos \epsilon_j
\end{bmatrix}, \\
[e^{2i\Delta}] = 
\begin{bmatrix}
e^{2i\delta_{++}} & 0 \\
0 & e^{2i\delta_{--}}
\end{bmatrix}.
\]  

(A5)
where $\delta_{++} \equiv \delta_{l=j+1,l'=j+1}$ and $\delta_{--} \equiv \delta_{l=j-1,l'=j-1}$.

When dealing with an optical potential, the S matrix is no longer unitary—which means the phases shifts become complex, as well as no longer symmetric—which means there are now two mixing parameters. We assume (A4) to be valid with the more general transformation matrix:

$$
[U] = 
\begin{bmatrix}
\cos \epsilon_{++} & \sin \epsilon_{++} \\
-\sin \epsilon_{++} & \cos \epsilon_{++}
\end{bmatrix},
\quad
[U]^{-1} = \frac{1}{\det U} 
\begin{bmatrix}
\cos \epsilon_{--} & -\sin \epsilon_{--} \\
\sin \epsilon_{--} & \cos \epsilon_{--}
\end{bmatrix},
$$  \hfill (A6)

$$
\det U = \cos \epsilon_{++} \cos \epsilon_{--} + \sin \epsilon_{++} \sin \epsilon_{--}.
$$  \hfill (A7)

This leads to the S matrix elements given in (13)-(18) which reduce to the standard, coupled case \cite{15,16} if $\epsilon_{++} = \epsilon_{--}$, and to the standard uncoupled case if $\epsilon_{++} = \epsilon_{--} = 0$. Stapp \cite{15} also gave a parameterization of the S matrix in terms of the “bar” phase shifts which are, in some cases, more convenient in the parameterization of data. These bar phases, however, are not the ones introduced here, and, in fact, do not provide a diagonal representation of the S matrix.
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Note, the factorization of $\exp(2i\sigma)$ was not made properly for all parts of the scattering
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FIGURES

FIG. 1. The nuclear plus Coulomb potentials in momentum space for the spin triplet state with \( m_s = m_{s'} = 1 \) as a function of the cosine of the angle between \( k \) and \( k' \). The summation (27) of partial-wave potentials essentially overlaps the input potential.

FIG. 2. The differential cross section for 500 MeV proton scattering from \(^3\text{He}\). Calculations performed using a cutoff radius in the range \( 6 \text{ fm} \leq R_{\text{cut}} \leq 10 \text{ fm} \) fall within the two curves. The experimental data are from H"ausser et al. [20].

FIG. 3. The differential cross section and analyzing power (unpolarized target, projectile polarized in normal direction) for 500 MeV proton scattering from \(^3\text{He}\). The solid curves gives the exact results using the VP method and the dashed curves gives the results if no Coulomb force is included. The experimental data are from H"ausser et al. [20].
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