Exact scattering waves off nonlocal potentials with Coulomb interaction

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A non-iterative solution for scattering wavefunction of protons off a nonlocal potential is presented. The approach is based on a Coulomb Green’s function in coordinate space whose kernel involves any nonlocal optical potential superposed to the Coulomb–screened interaction. The scattering wavefunctions, exact solution the integro–differential Schrödinger’s equation, can be obtained for any type of nonlocality of the interaction with no restrictions on the beam energy. The method presented here, also valid for chargeless projectiles, constitutes a direct and reliable alternative to others based on iterative procedures and/or localization ansatz of nonlocal potentials.

I. INTRODUCTION

The study of the interaction of a single nucleon with a nucleus in the context of Schrödinger’s equation poses different scenarios which call for specific strategies to obtain quantities of physical interest. The multiplicity of scenarios takes place when considering coordinate–vs momentum–space representations of the interaction; bound–state vs scattering processes; and chargeless vs charged single nucleon. Under all these settings it is well established that the potential which describes the coupling between a single nucleon with a nucleus is nonlocal, feature that arises from the fermionic nature of all interacting nucleons. It is in this context where explicit treatments of nonlocalities in Schrödinger’s wave equation has become an important issue from the standpoint of ab-initio theories, specially aiming to global approaches for structure and reactions which treat explicitly the fermionic character of nucleons [1, 2]. Such is also the case of nonlocal dispersive phenomenological potentials [3]. Therefore, robust and kernel–independent solutions to the wave equation become crucial to accurately treat genuine nonlocalities of nuclear interactions.

In the context of nucleon–nucleus scattering the quantities of major interest are scattering amplitudes and wavefunctions. The latter being useful for distorted wave approximation applications. When expressed in coordinate space the equation for the wavefunction becomes integro–differential. Early solutions to this problem were proposed by Perey and Buck [4], transforming the nonlocal potential by a local–equivalent, where a second–order differential equation for the wavefunction involves a local interaction. A shortcoming of this approach is that the calculated outgoing wavefunction differs from the exact one, distortion which is known as Perey effect and characterized by the Perey correction factor. A recent study [5] on this issue stresses the importance of accurate solutions for the wavefunctions.

Apart from the exact solutions of Schrödinger’s integro–differential equation for nonlocal potentials embedded in DWBA98 code [6], most current solutions in coordinate space follow iterative procedures. Such is the case of Ref. [3], where Schrödinger’s differential equation is integrated with a non–homogeneous term consisting of the projection of the nonlocal potential onto an intermediate solution, \( U_{nl} | \chi_i \rangle \). The procedure begins with a given seed to generate the starting solution \( | \chi_0 \rangle \), with subsequent iterations until convergence is reached. In the case of Ref. [7], a mean–value technique is applied to approximate \( U_{nl} | \chi_i \rangle \), reducing the problem to a second–order homogeneous differential equation. The shortcoming of this method is that it relies on Perey-Buck nonlocal structure together with the assumption that partial wave components of the potential do not change sign.

Another method to calculate waves off nonlocal potentials in the presence of long–range Coulomb interaction is that of Refs. [8, 9], where Lanczos technique is used to solve integral equations derived from the nonlocal Schrödinger equation. More recently, in Ref. [10, 11] a numerical treatment to this problem has been proposed with Berggren bases, where an off–diagonal approximation is used to control the Coulomb singularity along the diagonal in momentum space. The approach has been applied to low energies and intermediate mass targets.

Solutions to the scattering problem in momentum space have also been investigated [12–16]. See Ref. [17] for a review. The advantage of momentum–space approaches is that nonlocalities of the optical potential are naturally accounted for. In this scheme the only focus is on the scattering amplitude, while no method has been reported to obtain scattering waves. In the absence of Coulomb interaction the calculation of scattering amplitudes is rather straightforward, reducing the problem to a Lippmann–Schwinger (LS) integral equation for the scattering matrix. However, in the presence of Coulomb potential the approach cannot be applied right away due...
to the $1/q^2$ singularity of the interaction. An exact solution addressing this singularity has been proposed by Vincent and Phatak by means of a cut–off technique to the Coulomb long–range tail \[18\]. This approach has been applied to proton–nucleus scattering at intermediate energies \[13\], where its reliability is significantly improved after an accurate treatment of multipoles of the charge density convoluted with a cut–off potential due to a pointlike source \[13\].

In this brief article we present a non–iterative method to obtain exact scattering waves off any finite–range non–local potential. The approach, succinctly sketched in Ref. \[20\] in the context of quasielastic \((p,n)\) charge–exchange reactions at intermediate energies, is not restricted on energy of the projectile, charge of the colliding particles nor nature of the nonlocality. As a matter of fact this method has been applied to near–GeV proton–nucleus collisions \[21\]. Thus, it constitutes a robust alternative for accurate applications in the framework of nonlocal Schrödinger’s equation.

## II. INTEGRAL EQUATION FOR THE SCATTERING WAVEFUNCTION

Let us consider the collision of a proton with a nucleus of charge \(Ze\). The interaction \(U\) between them is given by the sum of a pure hadronic contribution \((U_H)\) and the Coulomb interaction \((U_C)\) due to the charge distribution of the nucleus, \(U = U_H + U_C\). The hadronic part is regarded in general as a nonlocal operator so that the total potential can be cast as the sum of a point–Coulomb and short–range terms,

\[
U(r', r) = U^{[s]}(r', r) + \frac{\beta}{r} \delta(r' - r) ,
\]

with \(\beta = Ze^2\). Here \(U^{[s]}\) defines the finite–range part of the interaction where the point–Coulomb interaction has been subtracted, namely \(U^{[s]} = U_H + U_C - \beta \delta(r' - r)/r\).

With the above construction in mind we examine Schrödinger’s equation for scattering waves which in coordinate representation reads

\[
-\nabla^2 \psi_k(r) + \frac{2m}{\hbar^2} \int dr' U(r, r') \psi_k(r') = k^2 \psi_k(r') ,
\]

with \(m\) the nucleon–nucleus reduced mass. Considering a closed–shell target interacting with a spin–\(1/2\) nucleon, the following partial wave expansion for the scattering wavefunction becomes suitable,

\[
\psi_k(r) = \sqrt{\frac{2}{\pi}} \sum_{jl} i^j Y_{jl1/2}(\hat{r}) e^{i\sigma_l} \frac{u_{jl}(r)}{r} \gamma_{jl1/2}^m(\hat{k}) .
\]

In this expansion \(Y_{jl1/2}^m\) denotes spherical vectors and \(\sigma_l\) the Coulomb phase–shift for partial wave \(l\). In the limit where the finite–range interaction \(U^{[s]}\) is set to zero, the unperturbed wavefunction becomes free Coulomb waves due to pointlike sources, \(\psi_k(r) \rightarrow \phi_c(r)\), where

\[
\phi_c(r) = \sqrt{\frac{2}{\pi}} \sum_{jl} i^j Y_{jl1/2}(\hat{r}) e^{i\sigma_l} F_l(kr) \gamma_{jl1/2}^m(\hat{k}) ,
\]

with \(F_l\) the regular Coulomb function. In the absence of Coulomb interaction \((\beta = 0)\), this expression leads to normalized plane waves \(\phi_k(r)\),

\[
\phi_k(r) = \frac{1}{(2\pi)^{3/2}} e^{ikr} ,
\]

with \(1_\sigma\) the identity in spin–\(1/2\)–space.

By replacing \(\psi_k(r)\) from Eq. \[3\] into Eq. \[2\], following standard procedures we obtain

\[
\left[ \frac{1}{r} \left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right) + \frac{2m}{\hbar^2} \int_0^\infty r' dr' U_{jl}(r, r') u_{jl}(r') \right] u_{jl}(r) = 0.
\]

Making explicit the separation of the interaction into a pointlike source and finite–range remaining

\[
U_{jl}(r', r) \equiv U_{jl}^{[s]}(r', r) + \frac{\beta}{r^3} \delta(r' - r) ,
\]

we obtain

\[
D_c u_{jl}(r) = \left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} k^2 \right] u_{jl}(r) = \frac{2m}{\hbar^2} \int dr' U_{jl}^{[s]}(r, r') r' u_{jl}(r') .
\]

Here \(D_c\) represents a second order differential operator which includes the point Coulomb contribution, where the Sommerfeld parameter \(\eta\) is given by \(\eta = m\beta/\hbar^2k\). Two linearly independent homogeneous solutions to Eq. \[9\] are the regular and irregular \((G_l)\) Coulomb wavefunctions which satisfy \(D_c F_l(kr) = D_c G_l(kr) = 0\). We adopt phase conventions such that their asymptotic behavior for large \(z\) are given by

\[
F_l(z) \sim \sin(z - l\pi/2 - \eta \ln 2z + \sigma_l) ,
\]

\[
G_l(z) \sim \cos(z - l\pi/2 - \eta \ln 2z + \sigma_l) .
\]

The solution for outgoing scattering waves \(u_{jl}\) in Eq. \[9\] comprises a homogeneous and particular solutions in the form

\[
u_{jl}(r) = \frac{1}{k} F_l(kr) + \frac{2m}{\hbar^2} \int dr' d'^n \left[ G_l^{(+)}(r', r''; k) \right] u_{jl}(r'') ,
\]

\[
G_l^{(+)}(r', r''; k) = \left[ r' Y_{jl}^{(+)}(r', r'') r'' \right] u_{jl}(r'') ,
\]
with the Coulomb propagator $G_{l}^{(+)}$ defined as

$$G_{l}^{(+)}(r, r'; k) = \frac{i}{k} F_{l}(kr) \mathcal{H}_{l}^{(+)}(kr),$$  

(12)

where $\mathcal{H}_{l}^{(+)} = F_{l} - iG_{l}$. Additionally, $r_{<} = \min\{r, r'\}$, while $r_{>} = \max\{r, r'\}$. A proof of the validity of this solution is presented in Appendix A.

Note that Eq. (11) represents a LS integral equation for scattering waves in the presence of Coulomb interaction, to be referred as LS-$\Psi$ henceforth. The kernel contains the nonlocal hadronic interaction superposed to the Coulomb–screened electrostatic interaction. What is appealing from Eq. (11) is that it enables to obtain actual scattering wavefunction by means of matrix inversion. This is so once integrals over $r$ are discretized over an $N$–point uniform mesh, where $r \rightarrow r_{i} = ih$, with $h$ a suitable spacing. In such a case the propagator and potential, as functions of $r$ and $r'$, become finite $N \times N$ matrices which we denote by $G$ and $U$, respectively. Then the solution to Eq. (11) becomes

$$u = (1 - GU)^{-1}u_{0},$$

(13)

where $u_{0}$ corresponds to the unperturbed wave $F_{l}(kr)/k$, while $u$ denotes the scattering wave over the discrete mesh. As evidenced, no localization of the interaction is needed. Additionally, no iterative procedure is involved, avoiding any instability issue arising from the structure of the kernel. In this context, the solutions for the scattering waves are exact.

Once $u$ is obtained we extract the scattering amplitude by examining the asymptotic behavior of Eq. (11), where we take $r$ far away from the scattering center. In this limit we have

$$G_{l}^{(+)}(r, r'; k)|_{r \rightarrow r} \rightarrow \frac{i}{k} F_{l}(kr) \mathcal{H}_{l}^{(+)}(kr),$$

(14)

which once replaced in Eq. (11) for $u_{jl}$ yields

$$k u_{jl}(r)\big|_{r \rightarrow \infty} \rightarrow F_{l}(kr) + \Delta_{jl}[F_{l}(kr) \mp iG_{L}(kr)],$$

(15)

with

$$\Delta_{jl} = -\frac{2m_{i}}{\hbar^{2}} \int r' dr' dr'' d\Omega F_{l}(kr') U_{l}^{(s)}(r', r) u_{jl}(r''),$$

(16)

These last two relations allow independent ways to obtain $\Delta_{jl}$. The latter involves direct integration of the wavefunction whereas the former evaluates asymptotically the ratio

$$\Delta_{jl} = \frac{ku_{jl}(r) - F_{l}(kr)}{F_{l}(kr) - iG_{L}(kr)},$$

(17)

for sufficiently large $r$. These equivalent forms to calculate $\Delta_{jl}$ provide us with a way to cross check the consistency of solutions. Once $\Delta_{jl}$ is obtained, the scattering amplitude $f_{jl}$ and short–range phase shift $\hat{\delta}_{jl}$ follow from

$$\Delta_{jl} = ik f_{jl} = \frac{1}{2} \left(e^{2i\hat{\delta}_{jl}} - 1\right).$$

(18)

In order to assess the consistency of the solutions summarized by Eq. (13) for the scattering waves off a nonlocal potential, we have performed scattering calculations at 30 MeV proton energy for $^{40}\text{Ca}(p,p)$ elastic scattering at 30 MeV is used [22]. Black curves denote results from LS-$\Psi$ approach while red curves represent DWBA98 results.

FIG. 1. Calculated differential cross section (a) and analyzing power (b) as functions of the center–of–mass scattering angle. Nonlocal Perey–Buck type potential for $^{40}\text{Ca}(p,p)$ elastic scattering at 30 MeV is used [22]. Black curves denote results from LS-Ψ approach while red curves represent DWBA98 results.
III. CONCLUDING REMARKS

We have presented a non-iterative method to obtain exact scattering waves off a nonlocal optical potential. The approach poses no restrictions on the type of nonlocality, beam energy nor charge of colliding particles. When compared to solutions of the integro-differential Schrödinger’s equation, good agreement is observed in the calculated scattering observables. Since the LS-Ψ approach leads to actual solutions for the scattering waves, it becomes well suited for distorted–wave Born approximations for nuclear reactions. Additionally, as discussed in Ref. [23], the approach presented here is well suited for coupled–channels applications. Work on its extention to inelastic processes is underway [23].

Appendix A: Proof of the solution

In order to verify that the formal solution expressed by Eq. (11) for the wavefunction satisfies the wave equation (9), we examine the action of \( \mathcal{D}_c \) on \( F_1(kr) \) and the integral involving the kernel. Since \( F_1(kr) \) satisfies \( \mathcal{D}_c F_1(kr) = 0 \), then we just need to focus on

\[
\mathcal{I}(r) = \mathcal{D}_c \int_0^\infty dr' G_{ij}^{(+)}(r, r'; k) W_{jl}(r') ,
\]

where \( W_{jl}(r') \) represents the integral over \( r'' \) given by

\[
W(r') = \frac{2m}{\hbar^2} \int_0^\infty r'' U^{[s]}(r', r'') r'' u_{jl}(r'') dr'' .
\]

Making explicit \( G_{ij}^{(+)} \) by splitting the integral over \( r' \) in Eq. \( \text{(A1)} \) into two sub-intervals, \([0, r]\) and \([r, \infty)\), we get

\[
\int_0^\infty G_{ij}^{(+)}(r, r'; k) W_{jl}(r') dr'' = -\frac{i}{k} \begin{cases} 
\mathcal{H}_{ij}^{(+)}(kr) \int_0^r dr' F_1(kr') W_{jl}(r') + \\
F_1(kr) \int_r^\infty dr' \mathcal{H}_{ij}^{(+)}(kr') W_{jl}(r') \end{cases} . \quad \text{(A3)}
\]

Taking derivatives with respect to \( r \) and using the Wronskian relationship \( F_1(z) \mathcal{H}_{ij}^{(+)}(z) - F_1'(z) \mathcal{H}_{ij}^{(+)}(z) = i \), we obtain

\[
\frac{\partial^2}{\partial r^2} \int_0^\infty G_{ij}^{(+)}(r, r'; k) W_{jl}(r') dr' = W_{jl}(r) + \\
\frac{i}{k} \begin{cases} 
\frac{\partial^2 \mathcal{H}_{ij}^{(+)}(kr)}{\partial r^2} \int_0^r dr' F_1(kr') W_{jl}(r') + \\
\frac{\partial^2 F_1(kr)}{\partial r^2} \int_r^\infty dr' \mathcal{H}_{ij}^{(+)}(kr') W_{jl}(r') \end{cases} . \quad \text{(A4)}
\]

Combining this result with Eq. \( \text{(A3)} \) and considering that \( \mathcal{D}_c F_1 = \mathcal{D}_c \mathcal{H}_{ij}^{(+)} = 0 \), we get

\[
\mathcal{D}_c \int_0^\infty G_{ij}^{(+)}(r, r'; k) W_{jl}(r') dr' = W_{jl}(r) , \quad \text{(A5)}
\]

proving that \( u_{jl} \) as given by Eq. \( \text{(11)} \) constitutes the solution to the wave equation \( \text{(9)} \) for outgoing scattering waves.

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