NUMERICAL GREEN'S FUNCTIONS IN OPTICAL POTENTIAL CALCULATIONS
FOR POSITRON SCATTERING FROM ARGON AND NEON

K. Bartschat†, R. P. McEachran† and A. D. Stauffer†
†Department of Physics and Astronomy, Drake University,
Des Moines, Iowa 50311, U.S.A.
‡Physics Department, York University, Toronto, Canada M3J 1P3

ABSTRACT

We have applied an optical potential method to the
calculation of positron scattering from the noble gases in
order to determine the effect of open excitation
channels on the shape of differential scattering cross sections.

THEORY

In positron–atom scattering the usual close-coupling
expansion for the total wavefunction in terms of the sum
of products of the bound-state wavefunctions of the tar-
get atom and the one-projectile scattering wavefunctions
leads to the following set of integro-differential equations
for the radial parts \( F_i \) of the scattering wavefunctions:

\[
\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right) F_i(r) = 2 \sum_j V_{ij}(r) F_j(r)
\]

(1)

Here the potential terms \( V_{ij} \) are given by

\[
V_{ij}(r) = \frac{Z}{r} \delta_{ij} - \sum_{k=1}^{N} \left( \Phi_i \left| \frac{1}{r_k - r} \right| \Phi_j \right)
\]

(2)

and the \( \Phi_i \) are the bound-state wavefunctions of the \( N \)-
electron target.

In practice only a finite number of bound target states
can be included in the close-coupling expansion. Hence,
we approximate the effect of the higher discrete target
states as well as the ionisation continuum by means of an
optical potential. We divide the space of scattering func-
tions into P- and Q-spaces. We choose for the P-space
the elastic channel only and thus the Q-space contains
all inelastic channels. In the Q-space we neglect all cou-
lplings between different channels but retain the couplings
between the P- and Q-spaces. Thus our method requires
the solution of the inhomogeneous differential equation

\[
\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2 V_{ii}(r) + k^2 \right) F_i(r) = 2 V_{i0}(r) F_0(r)
\]

(3)

for the radial functions \( F_i \) belonging to the Q-space. Here
\( F_0 \) is the P-space (elastic) channel wavefunction. In our
previous work\(^1\) we ignored the diagonal term \( V_{ii} \) above
and solved equation (3) by means of the free-particle
Green’s function involving the standard Riccati-Bessel
functions.

In either case the solution to equation (3) can be writ-
ten as

\[
F_i(r) = -2 \int_{0}^{\infty} dr' G_i(r, r') V_{i0}(r') F_0(r')
\]

(4)

where the Green’s function \( G_i(r, r') \) is given by

\[
G_i(r, r') = \frac{1}{k_i} f_i(k_i r') \left[ g_i(k_i r) + i f_i(k_i r) \right]
\]

(5)

The functions \( f_i \) and \( g_i \) are the regular and irregular
solutions of equation (3) with the right-hand-side put to
zero.

Upon substitution of equation (4) into the P-space
form of equation (1) we obtain

\[
\left( \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2 V_{00}(r) + k^2 \right) F_0(r) = -U_{00}^{\text{opt}}(r) F_0(r)
\]

(6)

where the optical potential is given by

\[
U_{00}^{\text{opt}}(r) F_0(r) = 4 \sum_{i \neq 0} \int_{0}^{\infty} dr' V_{0i}(r) G_i(r, r') V_{i0}(r') F_0(r')
\]

(7)

The real part of the optical potential represents polariza-
tion while the imaginary part represents absorption due
to the inelastic channels.

When the \( V_{ii} \) are ignored, \( f_i \) and \( g_i \) are the Riccati-
Bessel functions.\(^1\) However, if we retain the diagonal po-
tentials in equation (3), then \( f_i \) and \( g_i \) have to be found
by a numerical solution of the homogeneous differential
equation.

RESULTS

We have extended our previous work on argon\(^1\) by
using the numerical Green’s functions in the optical
potential. We have also carried out similar calculations for
positron scattering from neon.

The overall effect of retaining the diagonal potentials
and hence using numerical Green’s functions is quite
small, i.e. of the order of a few percent of the differ-
etial cross sections at all angles.

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The results of using optical potentials for positron-neon scattering yields cross sections whose behaviour is very similar to that of argon. In particular, the distinct minimum in the differential cross section which we obtained in our previous polarized-orbital calculations is no longer present when the optical potential is used. Below we present some typical results for positron scattering from argon and neon.

Figure 1 illustrates the differential cross section for positron scattering from argon at 30 eV. The polarized-orbital calculation\textsuperscript{2} shows a deep minimum at 21\degree while the two optical potential calculations, which differ only slightly, do not exhibit any such behaviour. The normalized experimental data\textsuperscript{3} clearly favour the latter calculations.

Figure 2 illustrates similar results for positron scattering from neon at 20 eV. Finally in figure 3 we show positron scattering from argon at 8.5 eV. At this energy only the elastic channel is open. Here the experimental data clearly show a minimum and agree well with the shape of the polarized-orbital calculations.\textsuperscript{2}

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FIG. 2. Positron scattering from neon at 20 eV. (—), fourteen-state optical potential using free-wave Green's functions; (— —), fourteen-state optical potential using numerical Green's functions; (— — —), polarized-orbital approximation; *, experimental data normalized at 90°.

FIG. 3. Positron scattering from argon at 8.5 eV. (— —), polarized-orbital approximation; *, experimental data normalized at 45°.