

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

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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 target 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:

$$\left(\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + k^2\right) F_i(r) = 2 \sum_j V_{ij}(r) F_j(r) \quad (1)$$

Here the potential terms V_{ij} are given by

$$V_{ij}(r) = \frac{Z}{r} \delta_{ij} - \sum_{k=1}^N \langle \Phi_i | \frac{1}{|r_k - r|} | \Phi_j \rangle \quad (2)$$

and the Φ_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 ionization continuum by means of an optical potential. We divide the space of scattering functions 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 couplings between different channels but retain the couplings between the P- and Q-spaces. Thus our method requires the solution of the inhomogeneous differential equation

$$\left(\frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} - 2V_{ii}(r) + k_i^2\right) F_i(r) = 2V_{i0}(r)F_0(r) \quad (3)$$

for the radial functions F_i belonging to the Q-space. Here F_0 is the P-space (elastic) channel wavefunction. In our previous work¹ 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 written as

$$F_i(r) = -2 \int_0^\infty dr' G_i(r, r') V_{i0}(r') F_0(r') \quad (4)$$

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

$$G_i(r, r') = \frac{1}{k_i} f_i(k_i r_<) [g_i(k_i r_>) + i f_i(k_i r_>)] \quad (5)$$

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

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V_{00}(r) + k^2\right) F_0(r) = -U_{00}^{\text{opt}}(r) F_0(r) \quad (6)$$

where the optical potential is given by

$$U_{00}^{\text{opt}}(r) F_0(r) = 4 \sum_{i \neq 0} \int_0^\infty dr' V_{0i}(r) G_i(r, r') V_{i0}(r') F_0(r') \quad (7)$$

The real part of the optical potential represents polarization 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 potentials 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 argon¹ 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 differential cross sections at all angles.

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 calculations² 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 calculation² shows a deep minimum at 21° while the two optical potential calculations, which differ only slightly, do not exhibit any such behaviour. The normalized experimental data³ clearly favour the latter calculations.

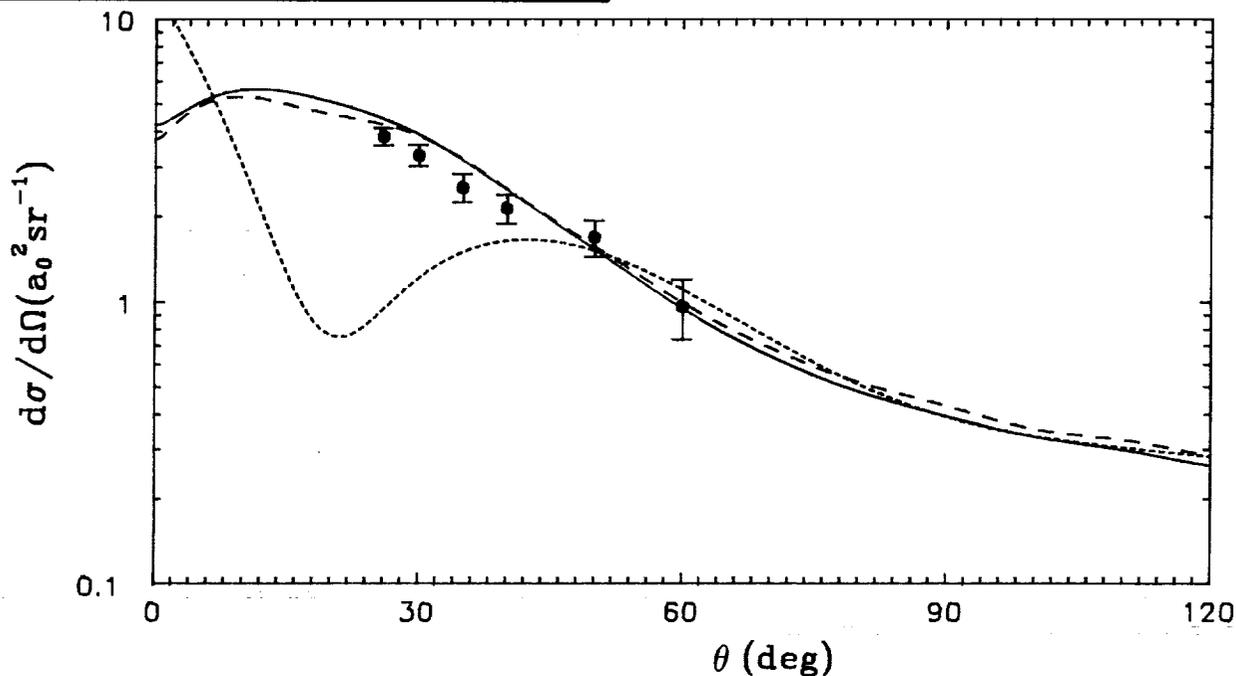


FIG. 1. Positron scattering from argon at 30 eV. (—), ten-state optical potential using free-wave Green's functions¹; (---), ten-state optical potential using numerical Green's functions; (· · ·), polarized-orbital approximation²; •, experimental data normalized at 60°³

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.²

ACKNOWLEDGMENTS

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¹ K. Bartschat, R. P. McEachran and A. D. Stauffer, *J. Phys. B.* **21**, 2789, 1988.

² R. P. McEachran and A. D. Stauffer, *Proc. of the Third Int. Workshop on Positron (Electron)-Gas Scattering*, ed. W. E. Kauppila, T. S. Stein and J. W. Wadehra (Singapore: World Scientific) p. 122, (1986).

³ K. Floeder, P. Höner, W. Raith, A. Schwab, G. Sinapius and G. Spicher, *Phys. Rev. Lett.* **60**, 2363, 1988.

⁴ W. E. Kauppila, S. J. Smith, C. K. Kwan and T. S. Stein, *Proc. of the Workshop on Annihilation in Gases and Galaxies*, to be published.

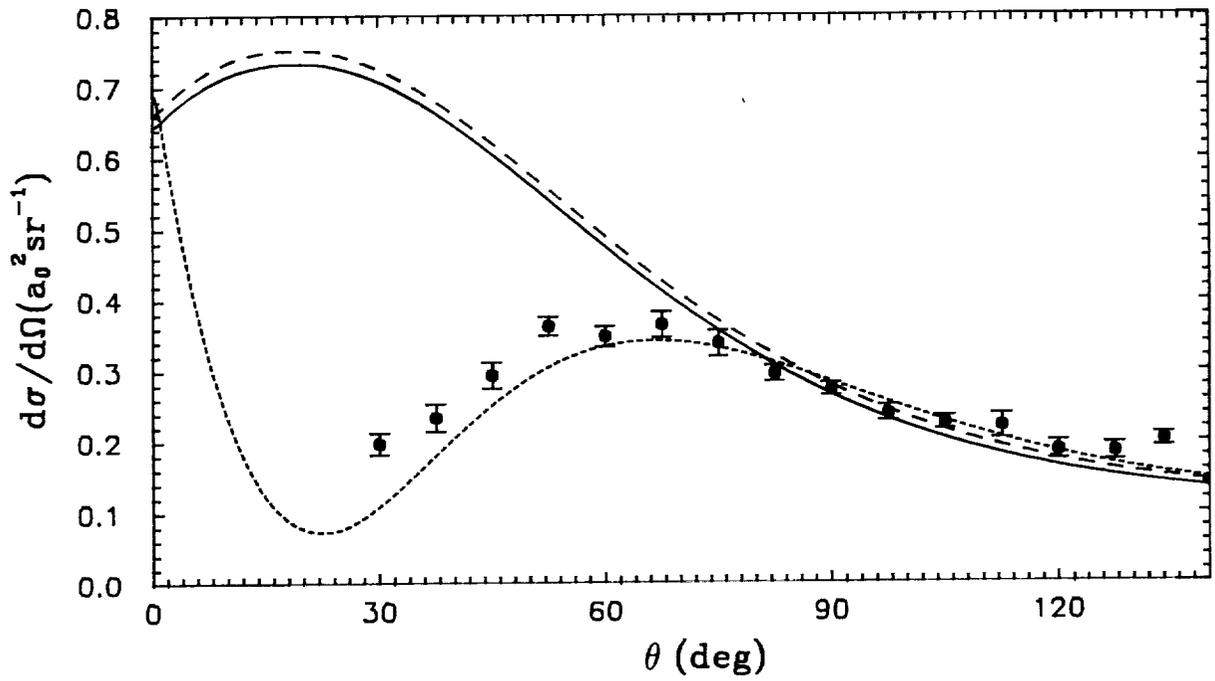


FIG. 2. Positron scattering from neon at 20 eV. (—), fourteen-state optical potential using free-wave Green's functions; (---), fourteen-state optical potential using numerical Green's functions; (· · ·), polarized-orbital approximation²; •, experimental data normalized at 90°⁴

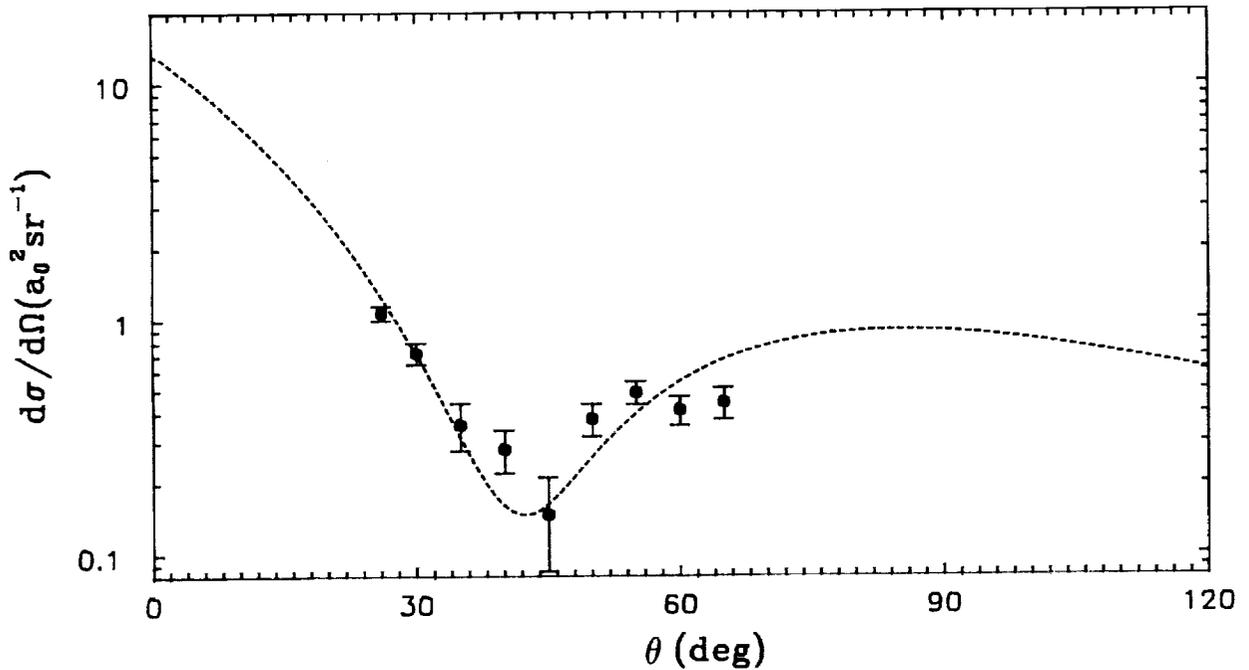


FIG. 3. Positron scattering from argon at 8.5 eV. (· · ·), polarized-orbital approximation²; •, experimental data normalized at 45°³

