Title:	Treatment of ion-atom collisions using a partial-wave expansion of the projectile wavefunction
Author(s):	T. G. Wong, Santa Clara Univ. M. Foster, J. Colgan, T-4 D. H. Madison, Missouri Univ.
Intended for:	Journal of Physics B

Los Alamos
NATIONAL LABORATORY
—— EST.1943 ——

Form 836 (7/06)

Treatment of ion-atom collisions using a partial-wave expansion of the projectile wavefunction

T G Wong

Department of Physics, Santa Clara University, Santa Clara, California 95053, USA

M Foster and J Colgan

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

E-mail: jcolgan@lanl.gov

D H Madison

Physics Department, Missouri University of Science and Technology, Rolla, Missouri 65401, USA

Abstract. We present calculations of ion-atom collisions using a partial-wave expansion of the projectile wavefunction. Most calculations of ion-atom collisions have typically used classical or plane-wave approximations for the projectile wavefunction, since partial-wave expansions are expected to require prohibitively large numbers of terms to converge scattering quantities. Here we show that such calculations are quite feasible using modern high-performance computing. We demonstrate the utility of our method by examining elastic scattering of protons by hydrogen and helium atoms.

1. Introduction

The use of partial-wave expansions in the analysis of electron scattering from atomic systems has now become ubiquitous in theoretical atomic collision physics. The spherical symmetry of the system allows the wavefunction of the electrons of interest to be expanded in spherical harmonics. This, coupled with the central potentials often found in atomic collision problems, allow one to compute scattering quantities on a partial-wave basis. Although the partial-wave expansion is in principle infinite, for low- and moderate-energy electrons, the expansion may be truncated after a relatively small number of terms, depending on the energy in question. These convenient facts have allowed partial-wave expansions to be used with some success in the investigation of many electron-impact processes, such as elastic scattering [1], excitation, and ionization [2], by perturbative and non-perturbative approaches. The incoming electron can be represented as a distorted-wave [3, 4, 5] or wavepacket [6], thus allowing the interactions between the incoming electron and the scattered electrons to be treated accurately. These methods are also readily applied to photon-atom interactions, where similar partial-wave expansions are heavily utilized.

In contrast, in collisions in which the projectile is a heavy ion, partial-wave expansions of the wavefunction of the projectile have not been commonly used. This is due to the much heavier mass of an incoming ion (for example, the lightest ion projectile, the proton, has a mass of 1836 that of an electron). Approximate scaling arguments [1] for the number of partial waves required (l_{max}) to fully describe an interaction lead to $l_{max} \sim ka$, where a is a measure of the range of the atomic potential, and k is the momentum. Since the momentum of an incoming ion is usually much greater than the momentum of an incoming electron, this scaling implies that thousands of partial waves may be required to fully treat an ion-atom collision. Consequently, most approaches to ion-impact problems treat the ion projectile classically via straight line trajectories, or alternatively consider the ion wavefunction as an analytical plane wave or Coulomb wave. These approaches are normally valid for fast ion projectiles, but they do not accurately represent the ion-atom interaction when the ion gets close to the nucleus. They also may be questionable when low-energy ions are incident on an atomic target.

It is therefore of interest to consider an approach where the incoming ionic wavefunction is expanded in partial waves, thus allowing distorted-wave techniques to be used to treat the ion-atom interaction. It is also of considerable interest to investigate how many terms in the partial wave expansions are actually required to fully converge such a scattering problem. In this paper, we consider such an approach, and show that ion-atom interactions may be treated efficiently when the ion wavefunction is expanded in partial waves, with the use of modern high-performance computing. As an example of our approach, we compute differential cross sections for elastic scattering of hydrogen and helium atoms by incoming protons. Our approach should also be applicable to ion-impact ionization problems, and may, for example, allow distorted-wave methods to be applied to the single ionization of He by C^{6+} impact, where recent out-of-plane

experimental measurements [7] were surprisingly not matched by theoretical predictions [8].

2. Theoretical Approach

We consider the wavefunction of an incoming projectile of mass M and energy E. The projectile wavefunction may be expanded in spherical harmonics as $\psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \phi)$, where Y_l^m is a spherical harmonic. The radial equation becomes (in atomic units)

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2MV(r) + k^2 \right] u(r) = 0 , \tag{1}$$

where the ion momentum $k = \sqrt{2ME}$, where we have written $u(r) = rR(r)$. In the standard textbook analysis [1], the differential cross section for elastic scattering is given by

$$\frac{d\sigma}{d\Omega} = |f(k, \theta)|^2 , \tag{2}$$

where θ is the scattering angle of the projectile, and where the scattering amplitude is expressed as

$$f(k, \theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k} e^{i\eta_l} \sin(\eta_l) P_l(\cos\theta) , \tag{3}$$

where η_l is the phase shift obtained by integrating Eq. (1) using a Numerov technique [9] and matching to asymptotic boundary conditions, and $P_l(x)$ is a Legendre polynomial. For the elastic scattering of hydrogen atoms by protons, the potential $V(r)$ is found from the analytical ground state hydrogenic wavefunction. For proton scattering by helium we use a Hartree-Fock wavefunction [5].

Since it was expected that many thousands of partial waves would be required to evaluate the differential cross sections for proton impact by this method, parallel computing was used to find the scattering amplitudes. An algorithm was constructed which allowed many processors of a parallel machine to compute the phase shifts η_l by solving the differential equations defined in Eq. (1), return them to a master node, and then construct the resulting scattering amplitude. The algorithm is completely general in that the processors available for computing are each assigned a given number of partial waves. Thus, many thousands of partial wave contributions to the scattering amplitude may be found quickly and efficiently with only a few dozen nodes of a parallel machine.

3. Results

Elastic differential cross sections were calculated for 25, 40, and 60 keV proton impact on neutral hydrogen. 10,000 partial waves were retained in Eq. (3), and 1,000 points per wavelength were found to be sufficient in our Numerov numerical approach. The results
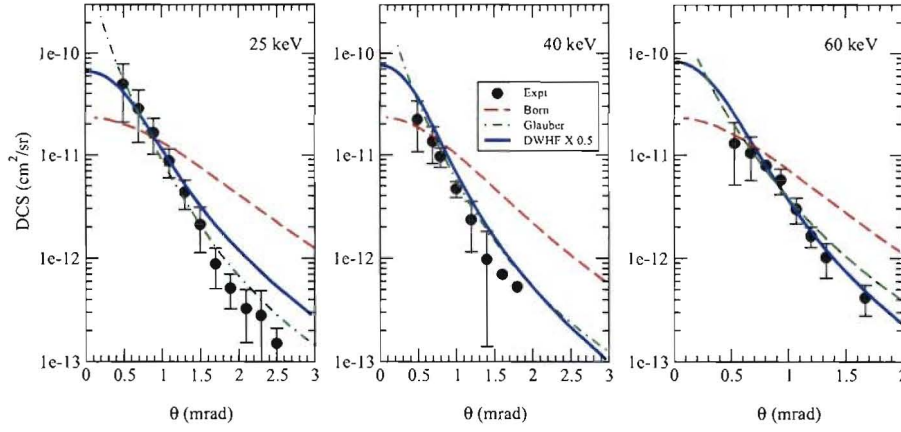
Figure 1. Elastic differential cross sections for proton scattering on neutral hydrogen in the center-of-mass frame for a proton with laboratory energies of 25 keV, 40 keV, and 60 keV. Our current calculations are compared with experimental measurements of Rille *et al* [10]. The differential cross sections are presented as a function of the scattering angle of the proton. 10,000 partial waves were included in the distorted-wave calculations for all impact energies.

are shown in Fig. 1, and are compared with the experimental measurements of Rille *et al* [10], as well as Born approximation and Glauber approximation calculations taken from the same paper. Our calculations have been scaled by a factor of 0.5 in order to compare best with the experimental data. These measurements have previously been shown to be in good agreement with sophisticated multichannel calculations [11]. The agreement between our calculations and the measurements is quite good. The distorted-wave calculations reproduce the shape of the experimental differential cross sections very well, although there is some discrepancy in the magnitude of the cross section. This may be due to our neglect of inelastic channels (i.e. the influence of excitation and ionization channels) in our calculations. Our calculations are also in good agreement with the Glauber calculations, except at very small scattering angles, where the Glauber approximation is not expected to be accurate, since it diverges at 0°. The Born approximation calculations are, as expected, in poor agreement with both experiment and with our calculations.

We also computed elastic differential cross sections for proton scattering from helium. The comparison of our calculations with the experimental measurements of Peacher *et al* [12] are shown in Fig. 2, for three impact energies of 25, 50, and 100 keV. As in the previous case, we again scale our calculations, this time by a factor of 0.1, in order to compare best with the data. We also compare with calculations made using the Born approximation and using the Glauber approximation taken from [12]. As found in the hydrogen case, the agreement in shape between the current calculations and the experiment is good, unlike the Born and Glauber calculations, which only agree in shape with the experiment at larger scattering angles. The discrepancy in magnitude with the experimental measurements is larger for this case than in the previous hydrogen case, and is greater than an order-of-magnitude at some scattering angles. A similar
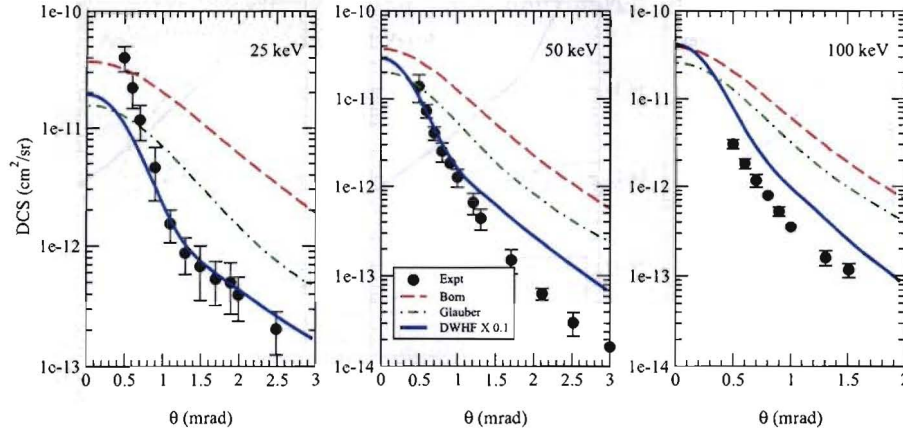
Figure 2. Elastic differential cross sections for proton scattering on neutral helium in the center-of-mass frame for a proton with laboratory energies of 25 keV, 40 keV, and 60 keV. We compare our current calculations (labeled DWHF) with experimental measurements of Peacher *et al* [12], and with Born approximation and Glauber approximation calculations from the same paper. 10,000 partial waves were included in the distorted-wave calculations for all impact energies.

discrepancy between this set of experimental data and multichannel calculations was also noted by Potvliege *et al* [11]. It may be that the experimental measurements in this case were unable to distinguish between elastic and inelastic collisions. In fact, a subsequent calculation [13] which included the inelastic channels was in better agreement with the Peacher *et al* measurements. The elastic differential cross section measurements are typically normalized by extrapolating to small scattering angles, and then comparing the integrated cross section value with an independent total elastic cross section value. Uncertainties in either of these processes may well change the magnitude of the experimental data considerably.

In Fig. 3 we demonstrate the convergence of our calculations with respect to the number of partial waves included. Inclusion of 1000 partial waves is not nearly enough for convergence. For the lowest projectile energy of 25 keV, 5000 partial waves is found to be sufficient for convergence, whereas for the highest energy of 100 keV, over 8000 partial waves are required to completely converge the calculation. For the results presented in Figures 1 and 2, 10,000 partial waves were included.
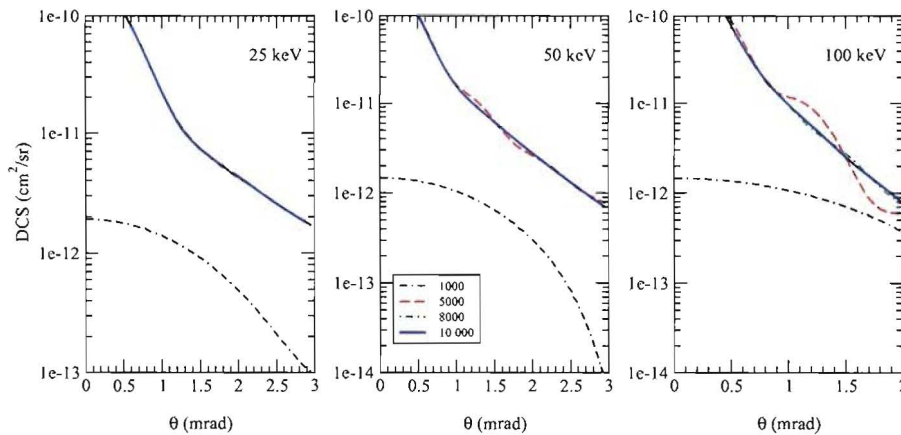
Figure 3. Elastic differential cross sections for proton scattering on neutral helium using our distorted-wave approach. We show calculations which include fixed number of partial waves in the expansions in Eq. (3) as indicated.

4. Conclusions

In this report, we have demonstrated that a partial-wave expansion of the projectile wavefunction for ion-impact may be efficiently used to obtain scattering cross sections in ion-atom collisions. We have demonstrated the utility of our approach by computing elastic differential cross sections for proton scattering from hydrogen and helium. In the future, we aim to use our distorted-wave approach to examine single ionization of helium by proton and C^{6+} impact, by combining our current efforts with previous well-established approaches [5, 8]. It is hoped that such an approach may shed some light on the discrepancy between theory and experiment for the observed fully differential cross sections for out-of-plane scattering as found in the C^{6+} experiments [7].

[1] Bransden B H and Joachain C J 2003 *Physics of Atoms and Molecules 2nd Edition* Pearson Education 586

[2] Märk T D and Dunn G H 1985 *Electron Impact Ionization* (Springer-Verlag, New York)

[3] Younger S M 1981 *Phys. Rev. A* **24** 1278

[4] Pindzola M S, Griffin D C and Bottcher C 1986 in *Atomic Processes in Electron-Ion and Ion-Ion Collisions*, Vol. 145 of NATIO Advanced Studies Institute, Series B: Physics, edited by F. Brouillard (Plenum, New York) p. 75

[5] Foster M, Peacher J L, Schulz M and Madison D H 2006 *Phys. Rev. Lett.* **97** 093202

[6] Pindzola M S, Robicheaux F, Loch S D, Berengut J C, Topcu T, Colgan J, Foster M, Griffin D C, Ballance C P, Schultz D R, Minami T, Badnell N R, Witthoeft M C, Plante D R, Mitnik D M, Ludlow J A and Kleiman U 2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** R39

[7] Schulz M, Moshammer R, Fischer D, Kollmus H, Madison D H, Jones S and Ullrich J 2003 *Nature* **422** 48

[8] Madison D, Schulz M, Jones S, Foster M, Moshammer R and Ullrich J 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** 3297

[9] Koonin S E and Meredith D C 1990 *Computational Physics: Fortran Version* Westview 56

[10] Rille E, Peacher J L, Redd E, Kvale T J, Seely D G, Blankenship D M, Olson R E and Park J T 1984 *Phys. Rev. A* **29** 521

[11] Potvliege R M, Furtado F and Joachain C J 1987 *J. Phys. B: At. Mol. Opt. Phys.* **20** 1771

[12] Peacher J L, Kvale T J, Redd E, Martin P J, Blankenship D M, Rille E, Sutcliffe V C and Park J T 1982 *Phys. Rev. A* **26** 2476

[13] Slim H A, Heck E L, Bransden B H and Flower D R 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2353