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

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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 possible using modern high-performance computing. We demonstrate the utility of our method by examining elastic scattering of protons by hydrogen and helium atoms, problems familiar to undergraduate students of atomic scattering. Application to ionization of helium using partial-wave expansions of the projectile wavefunction, which has long been desirable in heavy-ion collision physics, is thus quite feasible.

(Some figures in this article are in colour only in the electronic version)

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, and is treated in some detail in many undergraduate and graduate textbooks on atomic physics (for example, [1]). 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, allows 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 [3–5] 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, although some previous work has utilized partial-wave expansions for low-energy collisions or when considering charge transfer [7–10]. 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 $l_{\mathrm{max}} \sim ka$, 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. This problem is discussed in some detail in several undergraduate and graduate textbooks on atomic physics, such as [1]. Our approach also makes use of some parallel computing resources, and is therefore also directly relevant to university computational physics courses. Our approach should also be of interest to the general reader since it is applicable to ion-impact ionization problems, where recent out-of-plane experimental measurements [11] were surprisingly not matched by theoretical predictions [12]. The work described in this paper was performed by the first author as part of an undergraduate research project at the Los Alamos Summer School in Physics, a research experience for undergraduates programme jointly run by Los Alamos National Laboratory and the University of New Mexico [13].

2. Theoretical approach

Our distorted-wave Hartree–Fock (DWHF) approach begins by considering the wavefunction of an incoming projectile of mass M, charge Z and energy E scattering from a target of nuclear charge Z_T. The projectile wavefunction may be expanded in spherical harmonics as

$\psi(r,\theta,\phi) = R_l(r)Y_l^m(\theta,\phi)$, where Y_l^m is a spherical harmonic, and $R_l(r)$ is the radial part of the wavefunction. The radial equation becomes (in atomic units)

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

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

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

where θ is the scattering angle of the projectile, and where the scattering amplitude, $f(k,\theta)$, is expressed as

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

where η_l is the phase shift obtained by integrating equation (1) using a Numerov technique [14] and matching to asymptotic boundary conditions, and $P_l(x)$ is a Legendre polynomial. The potential $V(r)$ is computed as

$$V(r) = \frac{Z_T}{r} - Z_T\int_0^{\infty}\frac{|R_T(r')|^2}{r_>}r'^2\,\mathrm{d}r^2, \tag{4}$$

where $r_> = \max(r, r')$ and for scattering by hydrogen, the radial part of the wavefunction is given as

$$R_T(r) = 2\mathrm{e}^{-Z_T r}. \tag{5}$$

For proton scattering by helium it is best to generate the potential from a Hartree–Fock wavefunction [5]. In this study we use, for convenience, an analytical fit to a Hartree–Fock wavefunction, given by

$$u_{1\mathrm{s}}(r) = \frac{1}{\sqrt{4\pi}}(A\,\mathrm{e}^{-\alpha r} + B\,\mathrm{e}^{-\beta r}), \tag{6}$$

where $A = 2.605\,05$, $B = 2.081\,44$, $\alpha = 1.41$, and $\beta = 2.61$ [1]. In this case, the potential used in equation (1) is given by

$$V(r) = \frac{Z_T}{r} - Z_T\left[\int_0^{\infty}\frac{|u_{1\mathrm{s}}(r')|^2}{r_>}r'^2\,\mathrm{d}r'\right]^2. \tag{7}$$

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 equation (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. Ten thousand partial waves were retained in equation (3), and 1000 points per wavelength were found to be sufficient using our Numerov numerical approach. The

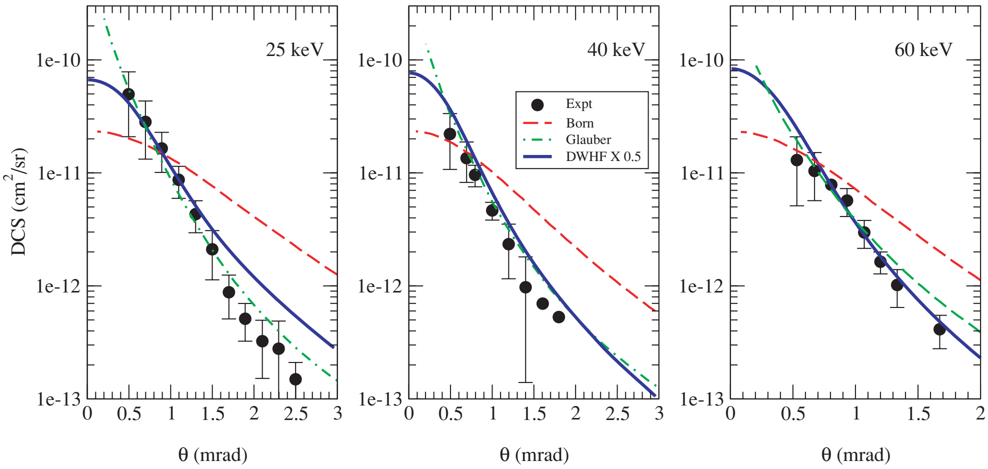

Figure 1. Elastic differential cross sections for proton scattering on neutral hydrogen in the centre-of-mass frame for a proton with laboratory energies of 25 keV, 40 keV and 60 keV. Our current distorted-wave Hartree–Fock calculations (labelled DWHF) are compared with the experimental measurements of Rille *et al* [15]. The differential cross sections are presented as a function of the scattering angle of the proton. Ten thousand partial waves were included in the distorted-wave calculations for all impact energies.

results are shown in figure 1, (labelled DWHF) and are compared with the experimental measurements of Rille *et al* [15], as well as Born approximation and Glauber approximation calculations taken from the same paper. These measurements have previously been shown to be in good agreement with sophisticated multichannel calculations [16]. Our 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. We therefore scale our calculations by a factor of 0.5 in order to compare best with the experimental data. 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 experiments 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* [17] is shown in figure 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 [17]. 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 discrepancy between this set of experimental data and multichannel calculations was also noted by Potvliege *et al* [16]. It may be that the experimental measurements in this case were unable to distinguish between elastic and inelastic collisions. In fact, a subsequent calculation [18] which included the inelastic channels was in better agreement with the Peacher *et al* measurements. Also, the elastic differential cross-section measurements are typically

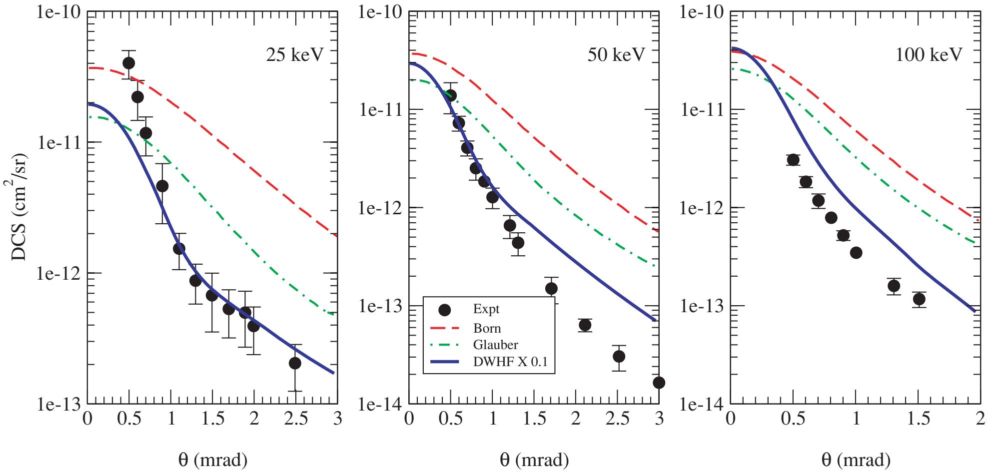

Figure 2. Elastic differential cross sections for proton scattering on neutral helium in the centre-of-mass frame for a proton with laboratory energies of 25 keV, 40 keV and 60 keV. We compare our current distorted-wave Hartree–Fock calculations (labelled DWHF) with the experimental measurements of Peacher *et al* [17], and with Born approximation and Glauber approximation calculations from the same paper. Ten thousand partial waves were included in the distorted-wave calculations for all impact energies.

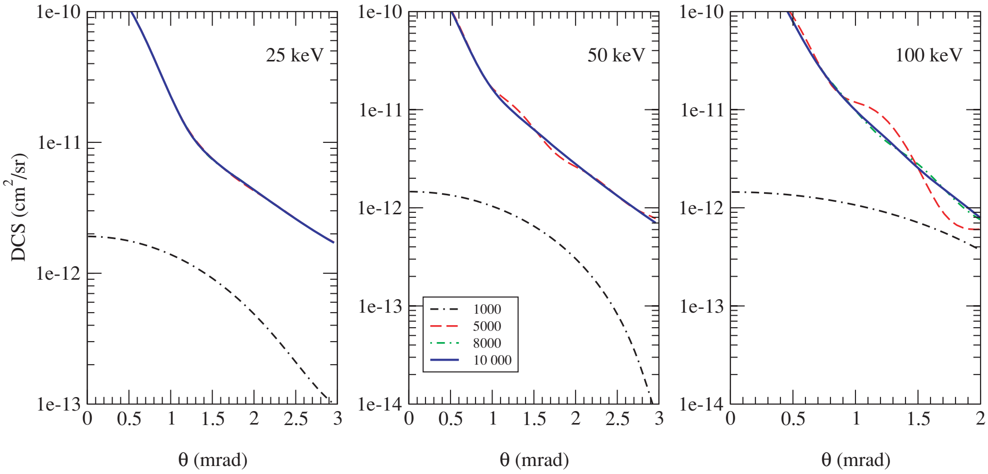

Figure 3. Elastic differential cross sections for proton scattering on neutral helium using our distorted-wave approach. We show calculations which include a fixed number of partial waves in the expansions in equation (3) as indicated.

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 figure 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.

4. Conclusions

In this paper, 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+} impacts, by combining our current efforts with previous well-established approaches [5, 12]. 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 [11].

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