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Elastic and inelastic electron and positron scatterings from metastable hydrogen

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The elastic and inelastic electron and positron scatterings from metastable hydrogen H(2*s*) are calculated by using the Wallace and Glauber approximations [Phys. Rev. Lett. **27**, 622 (1971); Ann. Phys. (N.Y.) **78**, 190 (1973); *Lectures in Theoretical Physics*, edited by W. F. Brittin (Interscience, N.Y. 1959), Vol. 1, pp. 315–414]. The general expressions for the Wallace amplitude, which are valid for any *s*-*s* and *s*-*p* collision process, are given. A comparison of the results of angular distributions for electron and positron scatterings from the metastable 2*s* state of hydrogen reveals some significant differences in their behavior when compared to the case of scattering from the ground 1*s* state.

Both the Glauber and Wallace approximations[1] have been used to study electron and positron scatterings from hydrogen for some time. While the employment of the Glauber approximation has been extended to analyze scatterings by more complex targets,[2] the application of the Wallace approximation has, so far, been limited only to scattering from hydrogen; and even with hydrogen as target, only some Wallace calculations for simple processes such as elastic,[3,4] and 2*s* and 2*p* inelastic scatterings[5] from its ground state have been reported in the literature.

On the other hand, although the study of scattering of electrons (and positrons) from atoms initially prepared in their metastable state has important applications in astrophysics, plasma physics, and various gaseous phenomena, relatively little work has been done even for the simplest atom such as hydrogen. There have only been a few calculations[6,7] performed for these metastable processes of hydrogen. As for the use of an eikonal-related method in the calculation, one may cite the work by Ho and Chan,[8] who employed the Glauber approximation for the elastic 2*s*-2*s* process; the works by Byron and co-workers,[9] who employed some eikonal-related methods of approximation; and the works by a few others (see, for example, Ref. 7 and references therein). All these eikonal-related calculations are, however, limited to the use of the Glauber amplitude and/or its modified versions. To our knowledge, no Wallace calculation has been reported in the literature for any of the elastic and/or inelastic scattering metastable processes of hydrogen.

On the experimental side, although only one experiment[10] has been performed to measure the electron-impact ionization cross sections of atomic hydrogen in the metastable 2*s*; it is believed that experimental measurements of cross sections for other electron scatterings (elastic and inelastic) from metastable hydrogen are feasible, and it is hoped that some day these experimental data will become available for comparison.

In this paper, we shall, therefore, analyze the elastic and inelastic scatterings of both electrons and positrons by the 2*s* metastable state of hydrogen in the framework of the Wallace approximation, with the main purpose of comparing these results with similar ones obtained in the Glauber approximation.

The Glauber amplitudes in their closed form, as obtained by Gerjuoy and Thomas,[11] have been used for the calculation. The calculation of these amplitudes are extremely easy and can be carried out quite rapidly, even with the slowest personal computer. As a self-consistency check for our results, we have also calculated these Glauber amplitudes, using, however, their integral forms;[12] and have found that the results of the two calculations agree exactly with each other. For the Wallace amplitude, we calculated the correction terms of these various processes by using both their four-dimensional and three-dimensional integral forms available in the literature.[3–5] The analytical calculation of the integrand of this term in its three-dimensional integral form is rather tedious, because it requires some complex calculation of the derivative (up to eighth order in our work) of the product of the Bessel *K* and *J* functions. However, with some care, the analytical calculation of these derivatives can actually be carried out with no serious difficulty. The agreement of the results calculated by using both expressions (three- and four-dimensional integrals) for this term indicates that our analytical expressions for these derivatives were free from error. The numerical calculations of this term with the employment of both types of expression for this term will also serve as a self-consistency check for our numerical procedures. The general expressions for the Wallace correction term of the *s*-*s* and *s*-*p* processes are as follows. When the product of the initial and final states of hydrogen is put in the form

$$u_f^* u_i = \frac{1}{4\pi} \sum_{\mu} D_\mu r^{\mu} e^{-\alpha_\mu r} , \tag{1}$$

the four-dimensional integral expression valid for any *s*-*s* process of hydrogen is

$$F^{\mathrm{corr}}_{s,s}=\frac{ik_i}{\pi}\sum_{\mu}D_\mu\int_0^\infty dx_2x_2^{1+2i\eta}\int_0^\infty dx_1\int_0^\pi d\phi\int_0^\infty db\,J_0(qb)b^4\exp[-\alpha_\mu b(1+x_1^2+x_2^2+2x_2\cos\phi)^{1/2}]$$
$$\times b^\mu(1+x_1^2+x_2^2+2x_2\cos\phi)^{\mu/2}\left\{1-\exp\left[\frac{i}{k_i^3b}\left(I_1+\frac{\cos\phi}{x_2}I_2\right)\right]\right\} \tag{2}$$

and the three-dimensional integral expression is

$$F^{\mathrm{corr}}_{s,s}=\frac{ik_i}{\pi}\sum_{\mu}D_\mu\int_0^\infty dx_2x_2^{1+2i\eta}\int_0^\infty dx_1\int_0^\pi d\phi(A_{5+\mu}-C^{(0)}_{5+\mu})(1+x_1^2+x_2^2+2x_2\cos\phi)^{\mu/2}\ , \tag{3}$$

where

$$A_{5+\mu}=\left(-\frac{\partial}{\partial d}\right)^\mu A_5,\quad C^{(0)}_{5+\mu}=\left(-\frac{\partial}{\partial d}\right)^\mu C^{(0)}_5\ . \tag{4}$$

With the product of the initial and final states of the s and p states put in the form

$$u_f^*u_i=Y^*_{1,m}Y_{0,0}r\sum_{\mu}D_\mu r^\mu e^{-\alpha_\mu r}\ , \tag{5}$$

the four-dimensional integral expression valid for any s-p process of hydrogen is

$$F^{\mathrm{corr}}_{s,p\pm}=\pm e^{\mp i\phi_q}\sqrt{3/2}\frac{k_i}{\pi}\sum_{\mu}D_\mu\int_0^\infty dx_1\int_0^\infty dx_2x_2^{1+2i\eta}\int_0^\pi d\phi\int_0^\infty db\,b^5J_1(qb)(1+x_2\cos\phi)b^\mu(1+x_1^2+x_2^2+2x_2\cos\phi)^{\mu/2}$$
$$\times\exp[-\alpha_\mu b(1+x_1^2+x_2^2+2x_2\cos\phi)^{1/2}]$$
$$\times\left\{1-\exp\left[\frac{i}{k_i^3b}\left(I_1+\frac{\cos\phi}{x_2}I_2\right)\right]\right\} \tag{6}$$

and the three-dimensional integral form is

$$F^{\mathrm{corr}}_{s,p\pm}=\pm e^{\mp i\phi_q}\sqrt{3/2}\frac{k_i}{\pi}\sum_{\mu}D_\mu\int_0^\infty dx_1\int_0^\infty dx_2x_2^{1+2i\eta}\int_0^\pi d\phi(1+x_2\cos\phi)(1+x_1^2+x_2^2+2x_2\cos\phi)^{\mu/2}(B_{6+\mu}-C^{(1)}_{6+\mu}) \tag{7}$$

where

$$B_{6+\mu}=\left(-\frac{\partial}{\partial d}\right)^\mu B_6,\quad C^{(1)}_{6+\mu}=\left(-\frac{\partial}{\partial d}\right)^\mu C^{(1)}_6\ , \tag{8}$$

while

$$A_5=\frac{3}{(d^2+q^2)^{9/2}}(8d^4-24d^2q^2+3q^4)\ ,$$
$$C^{(0)}_5=\left(-\frac{\partial}{\partial d}\right)^5\{2J_0(\beta[(d^2+q^2)^{1/2}-d]^{1/2})$$
$$\times K_0(\beta[(d^2+q^2)^{1/2}+d]^{1/2})\}\ ,$$
$$B_6=\frac{45q}{(d^2+q^2)^{11/2}}(8d^4-12d^2q^2+q^4)\ ,$$
$$C^{(1)}_6=\left(-\frac{\partial}{\partial d}\right)^6\{2J_1(\beta[(d^2+q^2)^{1/2}-d]^{1/2})$$
$$\times K_1(\beta[(d^2+q^2)^{1/2}+d]^{1/2})\}\ ,$$
$$d=\alpha_\mu(1+x_1^2+x_2^2+2x_2\cos\phi)^{1/2}\ ,$$
$$\beta=\left[-\frac{2i}{k_i^3}\left(I_1+\frac{\cos\phi}{x_2}I_2\right)\right]^{1/2}\ . \tag{9}$$

I_1 and I_2 are related to the elliptic functions of the first (E_1) and second (E_2) kind according to

$$I_1=\frac{4E_1(k^2)}{[x_1^2+(1+x_2)^2]^{1/2}+[x_1^2+(1-x_2)^2]^{1/2}}\ ,$$
$$I_2=\{[x_1^2+(1+x_2)^2]^{1/2}+[x_1^2+(1-x_2)^2]^{1/2}\}E_2(k^2)\ , \tag{10}$$

where

$$k^2=\frac{4\{[x_1^2+(1+x_2)^2][x_1^2+(1-x_2)^2]\}^{1/2}}{\{[x_1^2+(1+x_2)^2]^{1/2}+[x_1^2+(1-x_2)^2]^{1/2}\}^2}\ , \tag{11}$$

$\eta=+1/k_i$ for electrons scattering and $-1/k_i$ for positron scattering. Other notations used here are standard.

A sample[13] of the Glauber and Wallace results of differential cross sections for 2s-2s, 2s-2p, 2s-3s, and 2s-3p scatterings is briefly summarized in Table I. In order to compare the characteristics of the differential cross sections obtained for scattering from the metastable state with those obtained for scattering from the ground state, we have also recalculated the differential cross sections for scattering from ground-state hydrogen (1s-1s, 1s-2s, 1s-2p, 1s-3s, and 1s-3p).

To save computer time, and since it is unlikely that experimental data, if measured for these cross sections, could be acquired with a relative accuracy greater than 1%, we have therefore aimed our calculation only at a reasonably good accuracy. Nevertheless, we have estimated that the *relative* inaccuracy of our Wallace values, depending on the processes and/or the scattering

TABLE I. Differential cross sections in units of $a_0^2\ \mathrm{sr}^{-1}$ of electron and positron scattering from $2s$ metastable hydrogen. The values in square brackets indicate powers of 10.

Angle	Glauber	50 eV Wallace	Wallace	Glauber	100 eV Wallace	Wallace	Glauber	200 eV Wallace	Wallace	Glauber	400 eV Wallace	Wallace
(deg)	$e^{\pm}$	e^{-}	e^{+}	$e^{\pm}$	e^{-}	e^{+}	$e^{\pm}$	e^{-}	e^{+}	$e^{\pm}$	e^{-}	e^{+}
							$2s$-$2s$					
0.10	0.470[+4]	0.474[+4]	0.468[+4]	0.230[+4]	0.232[+4]	0.228[+4]	0.113[+4]	0.114[+4]	0.112[+4]	0.595[+3]	0.601[+3]	0.590[+3]
25.00	0.414[+1]	0.482[+1]	0.320[+1]	0.162[+1]	0.173[+1]	0.146[+1]	0.456[+0]	0.467[+0]	0.438[+0]	0.119[+0]	0.121[+0]	0.117[+0]
50.00	0.392[+0]	0.412[+0]	0.287[+0]	0.115[+0]	0.116[+0]	0.102[+0]	0.314[−1]	0.317[−1]	0.296[−1]	0.840[−2]	0.847[−2]	0.817[−2]
80.00	0.719[−1]	0.668[−1]	0.502[−1]	0.211[−1]	0.202[−1]	0.178[−1]	0.590[−2]	0.582[−2]	0.542[−2]	0.158[−2]	0.158[−2]	0.152[−2]
120.00	0.213[−1]	0.183[−1]	0.143[−1]	0.637[−2]	0.587[−2]	0.517[−2]	0.179[−2]	0.173[−2]	0.161[−2]	0.480[−3]	0.474[−3]	0.457[−3]
							$2s$-$3s$					
0.00	0.371[+3]	0.377[+3]	0.365[+3]	0.331[+3]	0.335[+3]	0.327[+3]	0.268[+3]	0.271[+3]	0.266[+3]	0.213[+3]	0.214[+3]	0.211[+3]
25.00	0.430[+0]	0.468[+0]	0.348[+0]	0.706[−1]	0.694[−1]	0.682[−1]	0.747[−2]	0.735[−2]	0.742[−2]	0.107[−2]	0.107[−2]	0.105[−2]
50.00	0.290[−1]	0.274[−1]	0.236[−1]	0.406[−2]	0.390[−2]	0.375[−2]	0.621[−3]	0.614[−3]	0.592[−3]	0.895[−4]	0.889[−4]	0.880[−4]
80.00	0.518[−2]	0.429[−2]	0.415[−2]	0.816[−3]	0.748[−3]	0.716[−3]	0.123[−3]	0.118[−3]	0.116[−3]	0.171[−4]	0.166[−4]	0.167[−4]
120.00	0.156[−2]	0.119[−2]	0.120[−2]	0.255[−3]	0.222[−3]	0.216[−3]	0.380[−4]	0.353[−4]	0.351[−4]	0.519[−5]	0.499[−5]	0.505[−5]
							$2s$-$2p$					
0.10	0.146[+7]	0.146[+7]	0.146[+7]	0.128[+7]	0.128[+7]	0.128[+7]	0.785[+6]	0.785[+6]	0.785[+6]	0.401[+6]	0.401[+6]	0.401[+6]
25.00	0.759[+0]	0.422[+0]	0.124[+1]	0.129[+0]	0.993[−1]	0.207[+0]	0.995[−2]	0.114[−1]	0.162[−1]	0.450[−3]	0.940[−3]	0.906[−3]
50.00	0.318[−1]	0.326[−1]	0.117[+0]	0.195[−2]	0.674[−2]	0.118[−1]	0.903[−4]	0.953[−3]	0.112[−2]	0.437[−5]	0.122[−3]	0.128[−3]
80.00	0.228[−2]	0.176[−1]	0.259[−1]	0.120[−3]	0.284[−2]	0.334[−2]	0.600[−5]	0.392[−3]	0.416[−3]	0.327[−6]	0.513[−4]	0.527[−4]
120.00	0.351[−3]	0.965[−2]	0.104[−1]	0.182[−4]	0.152[−2]	0.160[−2]	0.955[−6]	0.213[−3]	0.218[−3]	0.540[−7]	0.281[−4]	0.285[−4]
							$2s$-$3p$					
0.00	0.835[+4]	0.833[+4]	0.837[+4]	0.181[+5]	0.180[+5]	0.181[+5]	0.373[+5]	0.373[+5]	0.373[+5]	0.755[+5]	0.755[+5]	0.755[+5]
25.00	0.143[+0]	0.996[−1]	0.255[+0]	0.657[−2]	0.158[−1]	0.430[−2]	0.392[−3]	0.113[−2]	0.105[−3]	0.113[−4]	0.364[−4]	0.418[−4]
50.00	0.286[−2]	0.117[−1]	0.682[−2]	0.518[−4]	0.857[−3]	0.271[−3]	0.239[−6]	0.660[−4]	0.558[−4]	0.443[−8]	0.738[−5]	0.804[−5]
80.00	0.120[−3]	0.256[−2]	0.201[−2]	0.101[−5]	0.242[−3]	0.201[−3]	0.813[−9]	0.270[−4]	0.269[−4]	0.748[−9]	0.329[−5]	0.339[−5]
120.00	0.124[−4]	0.105[−2]	0.104[−2]	0.879[−7]	0.121[−3]	0.118[−3]	0.611[−9]	0.147[−4]	0.148[−4]	0.145[−9]	0.182[−5]	0.184[−5]

angles, would hardly be worse than $\frac{2}{10}-\frac{3}{10}$ %. Our Glauber values are, of course, extremely accurate. Note that throughout this calculation we used 1 Ry = 13.6058 eV.

In general, the Glauber and Wallace cross sections for all the metastable processes (elastic, *s* or *p* excitations) become more sharply peaked in the forward direction and also fall off somewhat faster, as the scattering angle increases, than those of the previous cases of scattering from the ground state. This fact was tentatively explained by Ho and Chan[8] as being correlated to the "size" of the orbits of the 1*s* and 2*s* states and to the predominance of the Rutherford scattering at large scattering angles.

As was pointed out by Franco and Iwinski,[4] the systematic correction of the Glauber approximation phase-shift function in the Wallace prescription produces a significant improvement for elastic e^--H(1*s*) differential cross sections (when compared with experimental data) at all energies and angles, and provides a desired difference between the positron and electron differential cross sections, which is rather significant at lower energies. Here, the Glauber values always stay between the Wallace electron and positron values in the whole range of scattering angles and for all energies. For elastic scattering from metastable H(2*s*), the Wallace electron cross sections at large angles, in contrast, become somewhat smaller than the Glauber cross sections. We have not, however, been able to find, at least off-hand (here and in the subsequent cases), the (physics) reason for such a difference in the differential cross sections found for these two types of scattering (from hydrogen prepared in the metastable state, and from hydrogen in its ground state). The Wallace electron cross sections are, however, still greater than the positron cross sections in the whole range of scattering angles.

For the 2*s*-3*s* process, the Wallace electron cross sections at very large angles also become smaller than the Glauber cross sections even at a lower energy (50 eV). At very large angles, the Wallace positron cross sections at 50 and 400 eV are now somewhat greater, and at 100 eV somewhat smaller, than the electron cross sections; while at 200 eV, the electron and positron values appear to approach each other. Both these features are different from those of *s* excitation from the ground state, where only at higher energies (100, 200, and 400 eV), are the Wallace electron cross sections smaller than the Glauber cross sections, and where the Wallace electron cross sections are always greater than the Wallace positron cross sections. At small angles, the Glauber cross sections still lie between the Wallace electron and Wallace positron cross sections. In general, the Wallace cross sections for the *s*-*s* metastable processes do not differ drastically from the Glauber cross sections at larger angles, because while the real part of the scattering amplitude of these processes is predominant over its imaginary parts at these large angles, the real part of the Glauber amplitude also represents that of the Wallace amplitude, there, reasonably well.

As in the case of *p* excitations from the ground state, the Wallace cross sections of the *p* excitations from metastable hydrogen (2*s*-2*p* and 2*s*-3*p*), for both electron and positron impacts, are much greater than the Glauber cross sections at large angles. Thus the systematic correction of the Glauber phase-shift function appears to affect the *s*-*p* cross sections more significantly than the *s*-*s* cross sections. For scattering from metastable hydrogen, the Wallace positron cross sections fall below the Wallace electron cross sections at some range of scattering angles, for all energies in the 2*s*-3*p* excitation, and for high energies in 2*s*-2*p* excitation. This is quite different from the case of scattering from ground-state hydrogen, where the Wallace positron cross sections are always considerably greater than the Wallace electron cross sections.

In conclusion, we have achieved the difficult Wallace calculation of positron and electron scatterings from metastable hydrogen. The results obtained for these angular distributions reveal some significant difference in their behavior, relative to each other, in comparison to the similar results of scattering from ground-state hydrogen. It is desirable to have experimental data made available in the laboratory for comparison with our results, so that we could find out, for these metastable processes, whether the systematic correction of the Glauber phase shift in the Wallace prescription still produces an improvement, as it did in the case of scattering from the ground state.[4]

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