Electron-hydrogen excitation to the $n = 3$ and $n = 4$ levels in the Glauber approximation

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Abstract

We have calculated the differential and integrated cross sections for excitation of atomic hydrogen to its $n = 3$ and $n = 4$ levels by electron impact using the Glauber approximation. Results are compared with measurements at 20, 30, 40, and 60 eV and also shown for 120 and 480 eV. At momentum transfers not too large at all energies considered, the calculated $n = 3$ differential cross sections are qualitatively similar to but a factor of somewhat less than 3 larger than the calculated $n = 4$ cross sections. The calculated integrated cross sections attain broad maxima near 41 eV.

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Only relatively recently have considerably accurate theoretical methods for describing electron-hydrogen atom scattering been presented [1, 2, 3, 4]. These methods require very-large-scale calculations or involved computations such as six-dimensional numerical quadrature. It would be useful to be able to calculate electron-hydrogen cross sections with ease without sacrificing too much of the accuracy of the established reliable methods. The first-Born approximation is perhaps the most easily utilized scattering approximation, but its validity is questionable except at rather high incident energies. And furthermore, the convergence of the Born approximation to the correct nonrelativistic result may occur only at such high energies that relativistic effects become significant [5].

An approximation which has been used extensively with much success in nuclear physics (and with moderate success in atomic physics) is the Glauber approximation [6]. This approximation is expected to be valid at high incident energies and small momentum transfers. It was introduced to atomic physics in 1968 [7], and is as easy to use today as the Born approximation was then. With a laptop personal computer, complete numerical calculations, in most cases, take of the order of a second.

The Glauber approximation amplitude, \( f(1s \to nlm; q) \), for excitation of the \((nlm)\) level of atomic hydrogen by electrons with incident momentum \(\hbar k\) and final momentum \(\hbar k_f\) is given by Thomas and Franco [8]. It may be rewritten as the explicit closed-form expression

\[
f(1s \to nlm; q) = \frac{(-1)^{l+1}2^{2l+4}\sqrt{(n-l)_{2l+1}}}{i^{m}n_{l+2}(2l+1)!}\sqrt{\pi} Y_{l}^{m*}(\frac{\pi}{2}, \varphi_{l})
\times \frac{\Gamma(1+i\eta)\Gamma(\frac{1}{2}(l+|m|)-i\eta)\Gamma(1+|m|-i\eta)}{\Gamma(1-i\eta)|m|!}
\times \frac{1}{(a_0q)^{l+4}}\sum_{j=0}^{n-l-1} \frac{(-n+l+1)_{j}}{j!(2l+2)_{j}} \left(\frac{2}{na_0}\right)^{j+1} \left(\frac{\partial}{\partial \lambda}\right)^{1+(l-|m|)/2}
\times \left\{ z^{-i\eta} F_1((l+|m|)/2 - i\eta; 1+|m|-i\eta; 1+|m|; -z) \right\}
\]

where \(z = \lambda^2/q^2\) with \(\lambda = (1 + 1/n)a_0\). Here \(\hbar q = \hbar k - \hbar k_f\) is the momentum transfer, \(a_0\) is the Bohr radius, \((a)_j\) is Pochhammer’s symbol [9], and \(\eta = e^2/\hbar \nu\) with \(\nu\) being the incident electron speed. The corresponding differential cross section is given by

\[
d\sigma/d\Omega = (k_f/k)|f(1s \to nlm; q)|^2.
\]
Equation (1) shows that the cross section is given in terms of a linear combination of products of (complex) powers of $q$ and derivatives of hypergeometric functions. If one uses the differentiation and recursion relations satisfied by the hypergeometric function $\text{9}$, the full result may be expressed in terms of only two contiguous hypergeometric functions and simple functions of $q$. No advantage is gained, however, by explicitly exhibiting the results in that form since the algebra involved is very tedious and the forms of the simple functions of $q$ are quite complicated, lengthy, and not at all transparent. It is more useful to express the results directly in terms of derivatives with respect to $z$ of the $z^{-i\eta}F_1$ function in Eq. (1). Closed form expressions in terms of such derivatives are then obtained.

Equations (1) and (2) may be used to calculate cross sections for excitation of ground state atomic hydrogen to any excited state. We present the explicit results for excitation to the $n = 3$ and $n = 4$ levels.

The cross section for excitation to the $n = 3$ level is given by

$$
\frac{d\sigma}{d\Omega}(1s \rightarrow n = 3; q) = \frac{k_f}{k} \frac{3^7}{2^{16}a_0^2} \left( \frac{\pi \eta}{\sinh(\pi \eta)} \right)^2 z^6 \left\{ \frac{z^2}{18} \left| \frac{\partial^3}{\partial z^3} [z^{-i\eta}F_1(1 - i\eta, 1 - i\eta; 1; -z)] \right|^2 
+ \frac{z^2}{24} (4 + \eta^2)(1 + \eta^2)^2 \left| \frac{\partial^2}{\partial z^2} [z^{-i\eta}F_1(2 - i\eta, 3 - i\eta; 3; -z)] \right|^2 
+ \frac{3z}{2} (1 + \eta^2) \left| \left( 3 \frac{\partial^2}{\partial z^2} + 2z \frac{\partial^3}{\partial z^3} \right) [z^{-i\eta}F_1(1 - i\eta, 2 - i\eta; 2; -z)] \right|^2 
+ \frac{1}{\eta^2} \left| \left( 6 \frac{\partial^2}{\partial z^2} + 5z \frac{\partial^3}{\partial z^3} + 2z^2 \frac{\partial^4}{\partial z^4} \right) [z^{-i\eta}F_1(-i\eta, 1 - i\eta; 1; -z)] \right|^2 \right\} \right. \tag{3}
$$

where the right hand side is to be evaluated at $z = 16/[9(a_0q)^2]$.

The cross section for excitation to the $n = 4$ level is given by
\[
\frac{d\sigma}{d\Omega}(1s \rightarrow n = 4; q) = \frac{k_f}{k} \frac{2^7}{5^{10}} \alpha_0^2 \left( \frac{\pi \eta}{\sinh(\pi \eta)} \right)^2 z^6 \frac{z^3}{1296} (9 + \eta^2)(4 + \eta^2)^2 (1 + \eta^2)^2 \]
\[
\times \left| \frac{\partial^2}{\partial z^2} [z^{-i\eta} F_1(3 - i\eta, 4 - i\eta; 4; -z)] \right|^2 
+ \frac{z^3}{60} (1 + \eta^2)^2 \left| \frac{\partial^3}{\partial z^3} [z^{-i\eta} F_1(2 - i\eta, 2 - i\eta; 2; -z)] \right|^2 
+ \frac{2z^2}{9} \left(4 \frac{\partial^3}{\partial z^3} + z \frac{\partial^4}{2 \partial z^4}\right) [z^{-i\eta} F_1(1 - i\eta, 1 - i\eta; 1; -z)]^2 
+ \frac{z^2}{6} (4 + \eta^2)(1 + \eta^2)^2 \left| (4 \frac{\partial^2}{\partial z^2} + z \frac{\partial^3}{2 \partial z^3}) [z^{-i\eta} F_1(2 - i\eta, 3 - i\eta; 3; -z)] \right|^2 
+ \frac{5z}{2} (1 + \eta^2) \left(15 \frac{\partial^2}{\partial z^2} + 28z \frac{\partial^3}{5 \partial z^3} + \frac{2z^2}{5} \frac{\partial^4}{\partial z^4}\right) [z^{-i\eta} F_1(1 - i\eta, 2 - i\eta; 2; -z)]^2 
+ \frac{2}{\eta^2} \left(25 \frac{\partial^2}{\partial z^2} + \frac{53z}{2} \frac{\partial^3}{\partial z^3} + 6z \frac{\partial^4}{\partial z^4} + \frac{z^3}{3} \frac{\partial^5}{\partial z^5}\right) [z^{-i\eta} F_1(-i\eta, 1 - i\eta; 1; -z)]^2 \right\} (4)
\]

where the right hand side is to be evaluated at \(z = 25/[16(a_0 q)^2]\).

These relatively simple explicit analytic expressions may be used to calculate the differential cross sections for excitation of ground state hydrogen atoms to the \(n = 3\) and \(n = 4\) states. As can be seen, each may be found by writing a single (albeit somewhat lengthy) statement. Using \textit{Mathematica}, for example, the entire calculation may be done with one few-line input statement and the time required on a PC for the entire differential cross section is of the order of a second.

We have calculated the differential cross sections for the \(1s \rightarrow n = 3\) and \(1s \rightarrow n = 4\) excitations using Eqs.(2-4) at energies of 20 eV, 30 eV, 40 eV, and 60 eV, where measurements have been recently made \cite{10}. We have also calculated these cross sections at 120 eV and 480 eV, where the theory has greater validity. Since the theory is valid at high energies and small momentum transfers, one would not expect accurate results for large momentum transfers (large scattering angles). However, at high energies the cross sections decrease rapidly from their values near the forward direction and the bulk of the scattering occurs at small momentum transfers.

At energies as low as 20 – 60 eV use of the Glauber approximation would not be justified.
FIG. 1: Differential cross sections, as functions of squared momentum transfer, for excitation of the $n = 3$ and $n = 4$ levels of atomic hydrogen by electron impact at 20 eV and 30 eV. “theory” represents the Glauber approximation, Eq.(3) and (4). Also shown are the measurements of Sweeney, Grafe, and Shyn (denoted SGS).

if one required highly accurate results. But even at these low energies, one might expect to obtain qualitative results at the lower momentum transfers. We present the results of our calculations for momentum transfers of $q \leq 1.24k_f$, and our comparison of the theory with the measurements is exhibited in that domain. Larger momentum transfers are beyond the range of validity of the theory (which does not compare well with the large-$q$ data [10], as expected).

In Fig.1 and Fig.2 we show the calculated differential cross sections for $1s \rightarrow n = 3$
FIG. 2: Differential cross sections, as functions of squared momentum transfer, for excitation of the $n = 3$ and $n = 4$ levels of atomic hydrogen by electron impact at 40 eV and 60 eV. See Fig. 1 for more details.

and $1s \rightarrow n = 4$ excitation as a function of $(a_0q)^2$ and compare our results with the measurements (SGS) [10] which, for the three highest energies, decrease by factors of as much as 50 to 200 from their values at the smallest measured momentum transfers. Our results are in reasonable agreement with the data, even at these relatively low energies. Both the theory and the measurements indicate that the $n = 3$ and $n = 4$ differential cross sections are qualitatively very similar, with the former being a factor of somewhat less than 3 larger than the latter. At larger momentum transfers (not shown), where the theory is not valid, the calculated cross sections continue to decrease rapidly. Where measurements have been made at larger momentum transfers ($1s \rightarrow n = 3$ at all four energies and $1s \rightarrow n = 4$
FIG. 3: Differential cross sections, as functions of squared momentum transfer, for excitation of the \( n = 3 \) and \( n = 4 \) levels of atomic hydrogen by electron impact at 120 eV and 480 eV in the Glauber approximation.

At 20 eV and 30 eV, that is not the case [10].

In Fig. 3 we show the calculated results at energies of 120 eV and 480 eV, where the approximation has greater validity. These results exhibit the same similarities of the \( n = 3 \) and \( n = 4 \) cross sections as those exhibited at the lower energies, with the \( n = 3 \) cross sections being a factor of somewhat less than 3 larger than the \( n = 4 \) cross sections throughout the entire domain of momentum transfers shown.

The integrated cross sections, obtained by integrating \( d\sigma/d\Omega \) over \( d\Omega \), are calculated
to be (in units of $10^{-18}$ cm$^2$): 10.0, 14.4, 15.4, 14.5, 9.90, 6.79, and 4.08 for $1s \rightarrow n = 3$, and 3.55, 5.28, 5.64, 5.31, 3.86, 2.45, and 1.47 for $1s \rightarrow n = 4$, at 20, 30, 40, 60, 120, 240, and 480 eV, in that order. These results may be compared with measured values $^{10}$ of $11.4 \pm 3.1$ and $10.9 \pm 2.9$ for $1s \rightarrow n = 3$ at 20 eV and 30 eV, respectively, and $5.28 \pm 1.43$ for $1s \rightarrow n = 4$ at 20 eV. The ratios of the calculated $n = 3$ to $n = 4$ cross sections are approximately constant (2.7). The lone measurement of this ratio is $2.2 \pm 0.8$ at 20 eV and the calculated value is 2.8. The calculated $n = 3$ and $n = 4$ cross sections attain broad maxima of 15.4 and 5.64, respectively, both near 41 eV.

In conclusion, we have presented explicit and easily calculable closed-form expressions for the differential cross sections for excitation of atomic hydrogen to its $n = 3$ and $n = 4$ levels in terms of derivatives of hypergeometric functions. The results are in qualitative agreement with measurements at the relatively low energies of 20 – 60 eV at momentum transfers that are not too large. Calculations at these energies as well as those presented for higher incident energies, where the theory has greater validity, indicate qualitative similarity between the $n = 3$ and $n = 4$ cross sections, with the $n=3$ cross sections being larger by a factor of somewhat less than 3. This is also exhibited in the calculated integrated cross sections, which attain broad maxima near 41 eV.

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