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Elastic scattering of electrons by metastable 2*s* atomic hydrogen

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The elastic scattering of electrons with incident energies from 20 to 500 eV from the metastable 2*s* state of atomic hydrogen is calculated by using the Born and Glauber approximations (including the exchange effect). The results for the angular distributions are compared with some other theoretical calculations. It is found that the Born and Glauber integrated elastic-scattering cross section is well represented by $\sigma^{B,G}_{\text{elastic}}(2s \to 2s; K_i) = (4162/105)(\Pi a_0^2/K_i^2)$ for $E_i \geq 20$ eV.

Although study of electron scattering by atoms initially prepared in an excited state (in particular the long-lived metastable states) has important applications in astrophysics, plasma physics, and various gaseous phenomena, relatively little work has been done even on the scattering from excited states of simple atoms. In addition, such an investigation is interesting in itself since "the comparison of the scattering from an excited state with that from the ground state yields useful information on the dynamics of the collision process."[1] Several theoretical calculations have been performed to study the elastic[1] and inelastic[2,3] scattering of electrons by metastable hydrogen. Although only one experiment[4] has been carried out to measure the electron-impact ionization cross section of atomic hydrogen in the metastable 2*s* state, more experimental works on electron scattering (elastic and inelastic) from metastable hydrogen are now under way at the Queens University at Belfast.

In this paper we analyze the elastic scattering of electrons by the 2*s* state of atomic hydrogen in the framework of Glauber theory[5-7] (including exchange effect). Results on the inelastic scattering will be presented in a forthcoming paper.

The Glauber direct scattering amplitude $F_D^G(\vec{q})$ describing the elastic scattering of an electron with velocity v_i by a metastable hydrogen atom is given by[5-7]

$$F_D^G(\vec{q}) = \frac{iK_i}{2\pi} \int \phi_{2s}^*(\vec{r})\Gamma(\vec{b};\vec{r})\phi_{2s}(\vec{r})e^{i\vec{q}\cdot\vec{b}}\, d^2b\, d\vec{r}, \qquad (1)$$

where

$$\Gamma(\vec{b};\vec{r}) = 1 - (|\vec{b}-\vec{s}|/b)^{2i\eta}, \qquad (2)$$

and $\eta = 1/v_i = 1/K_i$ (in atomic units). In Eqs. (1) and (2), $\vec{b}$ and $\vec{s}$ are the respective projections of the position vectors of the incident electron and the bound electron onto the plane perpendicular to the Glauber path. The Glauber amplitude was evaluated by taking the Glauber path integral along the direction perpendicular to the momentum transfer $\vec{q}$. The Glauber direct-scattering amplitude $F_D^G(\vec{q})$ can be expressed in a closed and compact form in terms of a generating function[8]:

$$F_D^G(\vec{q}) = -\frac{1}{4}\left[\left(\frac{\partial}{\partial\lambda} + \frac{\partial^2}{\partial\lambda^2} + \frac{1}{4}\frac{\partial^3}{\partial\lambda^3}\right) I(\lambda;q)\right]_{\lambda=1}, \qquad (3)$$

where the generating function $I(\lambda;q)$ is defined and given by

$$\begin{aligned} I(\lambda;q) &= \frac{iK_i}{(2\pi)^2}\int \frac{e^{-\lambda r}}{r}\left[1 - \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}\right] e^{i\vec{q}\cdot\vec{b}}\, d^2b\, d\vec{r} \\ &= \frac{8\pi\eta}{e^{\pi\eta}-e^{-\pi\eta}}\frac{1}{\lambda^2 q^2} \\ &\quad \times\left(\frac{q}{\lambda}\right)^{2i\eta} {}_2F_1(1-i\eta, 1-i\eta; 1; -\lambda^2/q^2). \end{aligned} \qquad (4)$$

In Eq. (4), ${}_2F_1$ is the usual hypergeometric function. After some manipulation, one can reduce $I(\lambda;q)$ into a form suitable for high incident energy limit, $(\eta \to 0)$:

$$I(\lambda;q) \approx I_0(\lambda;q) + i\eta I_1(\lambda;q) + O(\eta^2), \qquad (5)$$

where

$$I_0(\lambda;q) = \frac{4}{\lambda^2(\lambda^2+q^2)}, \qquad (6)$$

$$I_1(\lambda;q) = \frac{8}{\lambda^2(\lambda^2+q^2)} \ln\left[\frac{q}{\lambda}\left(1+\frac{\lambda^2}{q^2}\right)\right]. \qquad (7)$$

In the limit of $\eta \to 0$, substituting Eq. (6) into Eq. (3), the Glauber direct-scattering amplitude $F_D^G(\vec{q})$ is found to be identical with the Born direct-scattering amplitude $F_D^B(\vec{q})$, namely,

$$F_D^B(\vec{q}) = \frac{2}{q^2}[1 - F_H(q)], \qquad (8)$$

where

$$F_H(q) = \frac{1}{(1+q^2)^2}\left[1 - \frac{3-q^2}{1+q^2} + \frac{3(1-q^2)}{(1+q^2)^2}\right]. \qquad (9)$$

We remark that the first term in Eq. (9) is the Rutherford scattering of the electron by the nuclei whereas the second term represents the electron-

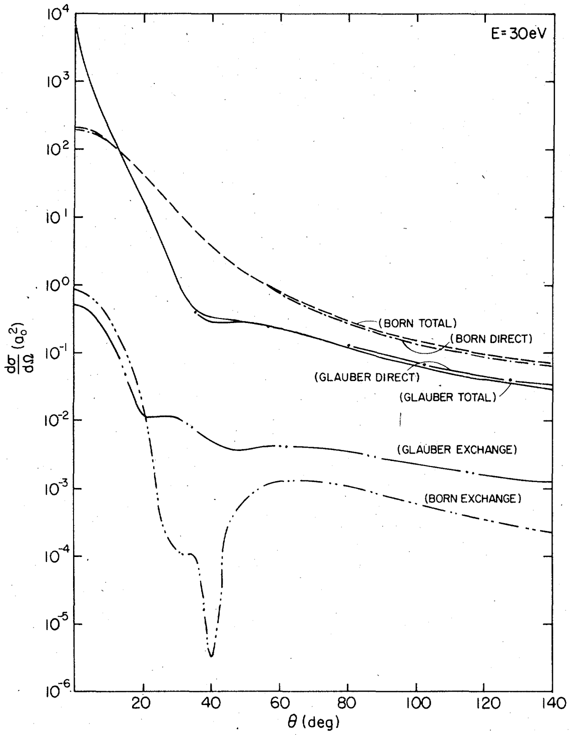

FIG. 1. Differential cross section for scattering of electrons by H(2*s*) at 30 eV. Solid curve, total Glauber (symmetrized) results; single-dot–long-dashed curve, direct Glauber results; double-dot–long-dashed curve, exchange Glauber results; dashed curve, total Born (symmetrized) results; single-dot-short-dashed curve, direct Born results; double-dot–short-dashed curve, exchange Born results.

electron scattering.

The Glauber-Bonham-Ochkur exchange amplitude for electron-H(2*s*) scattering is given by[9,10]

$$F^{\mathrm{GBO}}(\vec{q}) = \frac{2^{-i\eta}}{K_i^2}\,\Gamma(1-i\eta) \times \left[\left(\frac{\partial}{\partial\lambda}+\frac{\partial^2}{\partial\lambda^2}+\frac{1}{4}\,\frac{\partial^3}{\partial\lambda^3}\right) g(\lambda;q)\right]_{\lambda=1}, \quad (10)$$

where

$$g(\lambda;q) = \frac{1}{\lambda^{i\eta}(\lambda^2+q^2)^{1-i\eta}}\,. \quad (11)$$

If we let $\eta \to 0$ in Eqs. (10) and (11), the Glauber-Bonham-Ochkur exchange amplitude $F^{\mathrm{GBO}}(\vec{q})$ is immediately recognized to be the Born-Bonham-Ochkur exchange amplitude; thus

$$F^{\mathrm{BBO}}(\vec{q}) = -(2/K_i^2)F_H(q). \quad (12)$$

The direct, exchange, and symmetrized (represented by subscripts D, E, and T, respectively) differential and total cross sections are found from the direct- and exchange-scattering amplitudes in the usual way, namely,

$$\left(\frac{d\sigma}{d\Omega}\right)_D^{\mathrm{G}} = |F_D^{\mathrm{G}}(\vec{q})|^2, \quad (13)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_E^{\mathrm{G}} = |F^{\mathrm{GBO}}(\vec{q})|^2, \quad (14)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_T^{\mathrm{G}} = \tfrac{1}{4}|F_D^{\mathrm{G}}(\vec{q})+F^{\mathrm{GBO}}(\vec{q})|^2 + \tfrac{3}{4}|F_D^{\mathrm{G}}(\vec{q})-F^{\mathrm{GBO}}(\vec{q})|^2 = \left(\frac{d\sigma}{d\Omega}\right)_D^{\mathrm{G}} + \left(\frac{d\sigma}{d\Omega}\right)_E^{\mathrm{G}} - \mathrm{Re}\,\{F_D^{\mathrm{G}}(\vec{q})[F^{\mathrm{GBO}}(\vec{q})]^*\}, \quad (15)$$

$$\sigma_{D,E,T}^{\mathrm{G}} = \int \left(\frac{d\sigma}{d\Omega}\right)_{D,E,T}^{G} d\Omega, \quad (16)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_D^{\mathrm{B}} = \frac{4}{q^4}\,[1-F_H(q)]^2, \quad (17)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_E^{\mathrm{B}} = \frac{4}{K_i^4}\,[F_H(q)]^2, \quad (18)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_T^{\mathrm{B}} = \frac{4}{q^4}[1-F_H(q)]^2 + \frac{4}{K_i^4}[F_H(q)]^2 + \frac{4}{K_i^2 q^2}\,[1-F_H(q)]F_H(q), \quad (19)$$

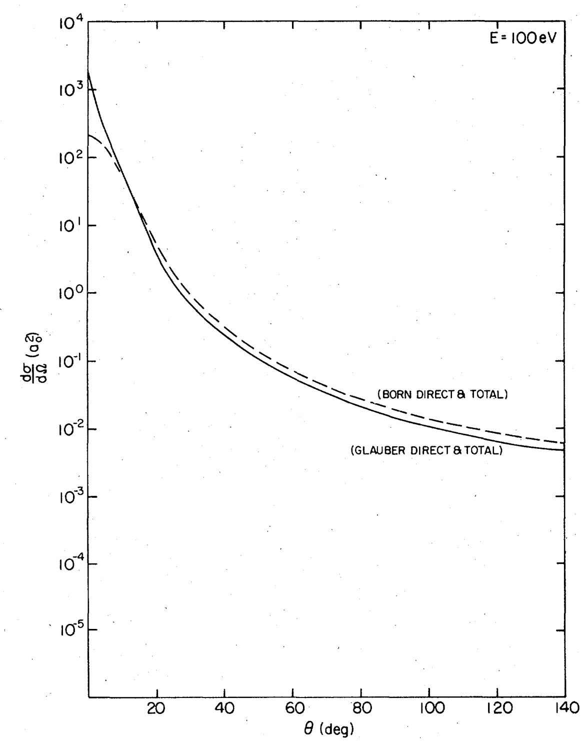

FIG. 2. Differential cross section for elastic scattering of electrons by H(2*s*) at 100 eV. Solid curve, direct and total (symmetrized) Glauber results; dashed curve, direct and total (symmetrized) Born results.

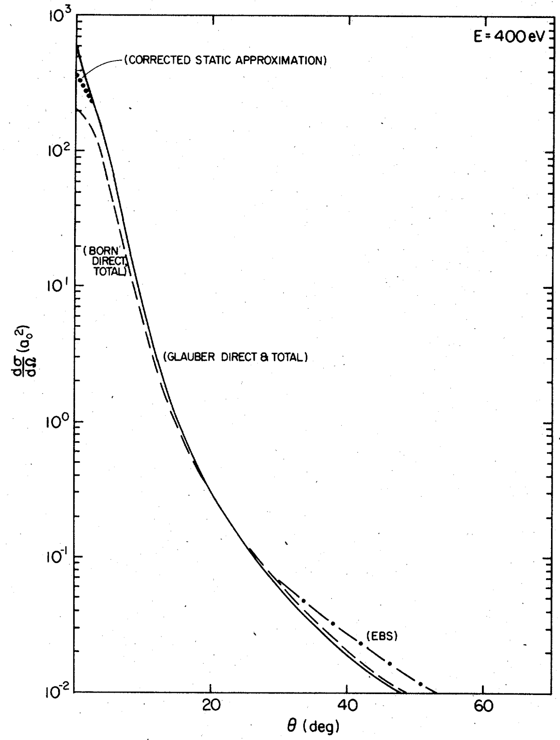

FIG. 3. Differential cross section for elastic scattering of electrons by H(2s) at 400 eV. Solid curve, direct and total (symmetrized) Glauber results; dashed curve, direct and total (symmetrized) Born results; dotted curve, corrected static approximation; single-dot-dashed curve, EBS results.

$$\sigma_D^B = \frac{1}{K_i^2}\left(\frac{4162}{105} - \frac{4}{(1+4K_i^2)}\left[1 + (1+4K_i^2)^{-1} - \tfrac{1}{3}(1+4K_i^2)^{-2} + \tfrac{5}{2}(1+4K_i^2)^{-3} + \tfrac{13}{5}(1+4K_i^2)^{-4} - 2(1+4K_i^2)^{-5} + \tfrac{36}{7}(1+4K_i^2)^{-6}\right]\right)\pi a_0^2, \tag{20}$$

$$\sigma_E^B = \frac{4}{K_i^6}\left(\frac{8}{105} - \frac{1}{(1+4K_i^2)^3}\left[\tfrac{4}{3} - 7(1+4K_i^2)^{-1} + \tfrac{73}{5}(1+4K_i^2)^{-2} - 14(1+4K_i^2)^{-3} + \tfrac{36}{7}(1+4K_i^2)^{-4}\right]\right)\pi a_0^2, \tag{21}$$

and

$$\sigma_T^B = \sigma_D^B + \sigma_E^B + \frac{4}{K_i^4}\left(\frac{61}{84} - \frac{1}{(1+4K_i^2)^2}\left[1 - \tfrac{5}{3}(1+4K_i^2)^{-1} - \tfrac{3}{4}(1+4K_i^2)^{-2} + 5(1+4K_i^2)^{-3} - 8(1+4K_i^2)^{-4} + \tfrac{36}{7}(1+4K_i^2)^{-5}\right]\right)\pi a_0^2. \tag{22}$$

By means of Eqs. (13)–(22), we have calculated the differential and the total direct exchange as well as the symmetrized cross sections for elastic scattering of electrons from the 2s metastable state of hydrogen for various incident-electron energies. Our theoretical results are shown in Figs. 1–6. No experimental data are presently available for comparison with our works. However, a comparison with the eikonal-Born series (EBS) calculations of Joachain *et al.*[1] is possible at incident energies E_i of 400 and 500 eV.

In studying how the exchange effect influences the symmetrized differential cross sections, we find that its inclusion is necessary only for energies below 50 eV. We note from Fig. 1 that the Glauber exchange part contributes to the symmetrized differential cross sections constructively at scattering angles from 35° to 55° but destructively at angles beyond 55°. This is in contrast to the elastic scattering from the ground state[10] where the exchange effects tend to increase the differential cross sections at all scattering angles.

For all the incident energies considered, we notice that the Glauber differential cross section for the 2s elastic collision is always more sharply peaked at small scattering angles than those for

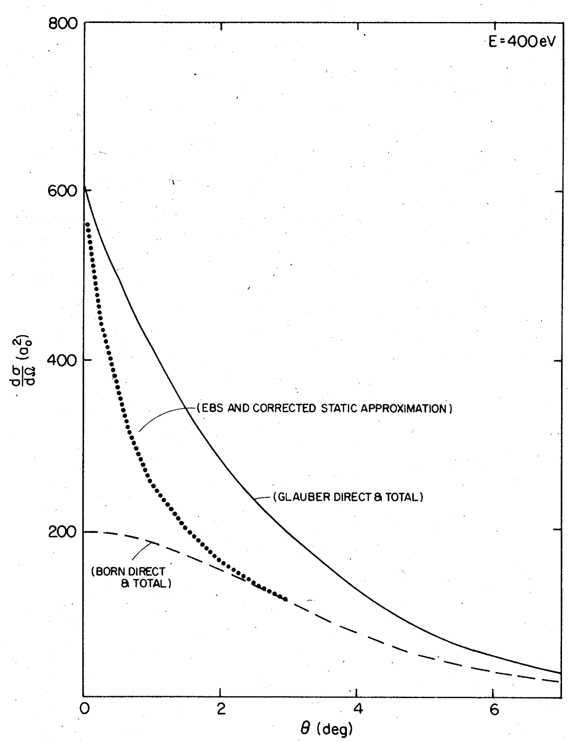

FIG. 4. Differential cross section for the elastic scattering of 400 eV electrons from the 2s state of atomic hydrogen at small angles. Solid curve, direct and total (symmetrized) Glauber results; dashed curve, direct and total (symmetrized) Born results; dotted curve, EBS results and corrected static approximation.

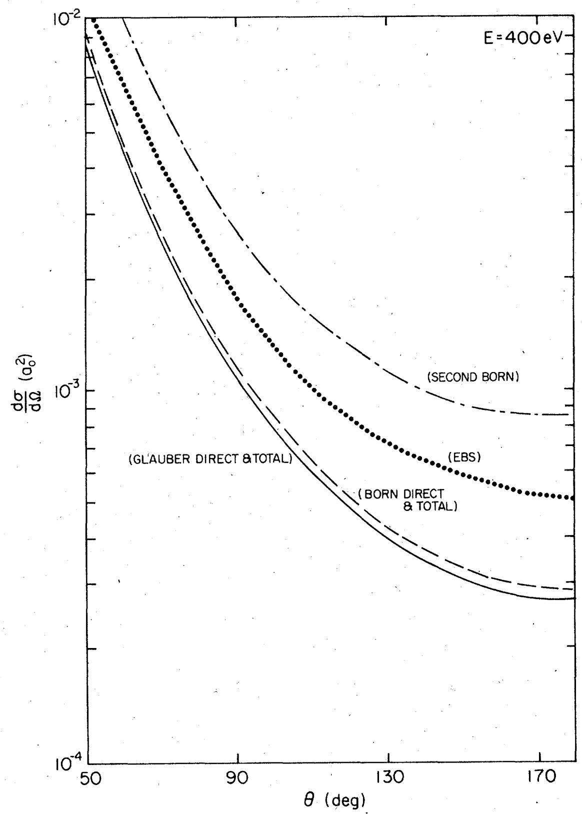

FIG. 5. Differential cross section for the elastic scattering of 400 eV electrons from the $2s$ state of atomic hydrogen at large angles. Solid curve, direct and total (symmetrized) Glauber results; dashed curve, direct and total (symmetrized) Born results; dotted curve, EBS results; single-dot-dashed curve, second Born approximation.

the $1s$ elastic scattering. The difference between the two cross sections becomes smaller and smaller as the incident energy and the scattering angle increase. This can be simply attributed to the fact that the larger electronic orbit of the $2s$ state is more important for small-angle scattering (i.e., large impact parameter) whereas the same Rutherford scattering is dominant for both $1s$ and $2s$ large-angle scattering. At $E_i = 400$ eV, as indicated in Figs. 3–5, the Glauber prediction is larger than those obtained using the EBS and corrected static approximation, and the Born approximation at small angles (<7°). On the other hand, the Glauber results are smaller than those predicted from the other methods for angles greater than 25°. Figure 4 also shows that the Glauber-predicted $d\sigma/d\Omega$ are very close to those of the EBS and Born approximations for scattering angles from ~7°–25°. A similar situation appears at $E_i = 500$ eV.

Our theoretical results for the total (integrated) cross section for $2s$ elastic scattering are presented in Fig. 6. For comparison the corresponding results for the $1s$ elastic collision are shown in the same figure. We first note that the inclusion of electron exchange for the $2s$ elastic collision gives negligible contributions to the total integrated cross sections (in contrast to $1s$ elastic scattering where the exchange terms tend to add up constructively to the direct integrated cross section at all incident energies). We also observe that although the Born and Glauber angular distributions are markedly different, their total cross sections (integrating the differential cross sections over all angles) are almost identical. The same pattern also appears in the elastic $e^- + \mathrm{He}(2^1S,\ 2^3S)$ scatter-

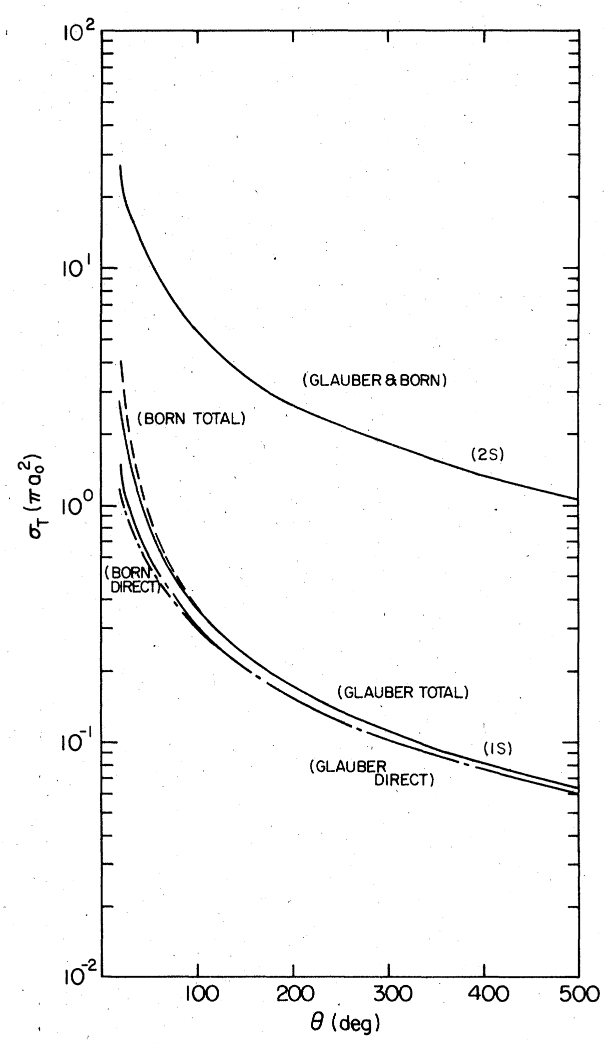

FIG. 6. Total (integrated) cross sections for the elastic scattering of electrons from the $1s$ and $2s$ states of atomic hydrogen as a function of incident-electron energy.

ing.[11] From Eq. (20), one immediately finds

$$\sigma^{B}(2s \rightarrow 2s; K_i) \approx \frac{4162}{105} \frac{1}{K_i^2} \pi a_0^2 \qquad (23)$$

for $E_i \geqslant 20$ eV (i.e., $K_i \geqslant 1$). The closed form $\sigma^{G}(2s \rightarrow 2s; K_i)$ can be obtained by using the analytical technique[12] of Thomas and Gerjuoy. We did not pursue this line since the calculation is very involved. However, because σ^G approaches σ^B at high energy, we expect the leading term in $\sigma^G(2s \rightarrow 2s; K_i)$ should be identical to the corresponding term in $\sigma^B(2s \rightarrow 2s; K_i)$. The high-energy correction terms, which may be different for the Born and Glauber approximations, are very small for $E_i \geqslant 20$ eV. Our numerical results [obtained by numerical integration via Eq. (16)] are within 0.7% of the simple equation (23). In fact, Eq. (23) is a better fit to our Glauber numerical results than to our Born results. It is remarkable that

$$\frac{\sigma(2s \rightarrow 2s; K_i)}{\sigma(1s \rightarrow 1s; K_i)} = \frac{4162/105}{7/3} \approx 17$$

is close to 16, the ratio between 2s and 1s orbital geometric cross sections.

Since our knowledge of the subject is quite limited at the present time, extensive theoretical investigations as well as further experimental studies of such collision processes involving long-lived excited states would be of great value.

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