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Comparison of the Born and Glauber generalized oscillator strengths for the $2s \rightarrow 3p$ transition of atomic hydrogen

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Minima and maxima of the generalized oscillator strength for the $2s \rightarrow 3p$ transition of atomic hydrogen are found using the Glauber approximation. In contrast to the first-Born approximation, the *number* of extrema and their positions are found to vary with the energy of the incident particle, and the values at the minima do not vanish. There is qualitative agreement in the behavior of the first minimum with known experimental data on the resonance transitions of rare gases and mercury. For large incident energy, the transition amplitude in the Glauber approximation falls off with large momentum transfer more rapidly than predicted by a previous calculation based on the second-Born approximation.

I. INTRODUCTION

The cross sections for discrete excitations often show undulations in the angular distributions. In the first-Born approximation (FBA) these undulations can be attributed to minima in the corresponding generalized oscillator strength (GOS). The minima in the GOS arise from a combination of the oscillations in the wave functions of the target atoms as well as oscillations in the transition operator.[1-4] Calculations based on the FBA have been verified *qualitatively* in many experiments,[2,5,6] and at very high incident energies the location of the minima are in agreement with experiment.[5] However, even at infinite energy, the FBA fails at very large momentum transfers,[7] partly because the FBA does not account for scattering by the nucleus at all.

In the FBA, the GOS is expressed as a function of the momentum transfer $\vec{K}$ (we use atomic units) and it is independent of the incident energy. Hence, the positions of the minima and maxima in the GOS remain fixed as incident energy is varied. The minima in the Born GOS occur when the transition matrix element changes sign, and therefore the GOS vanishes at the minima.

Experimental data, however, differ from the FBA results in three aspects: (a) the "experimental" GOS does not vanish at the minimum, (b) the magnitude of the GOS at the minimum depends on the incident energy, and (c) the position of the first minimum (expressed in terms of K) is shifted toward smaller K at intermediate- to low-incident-electron energies (<500 eV). Owing to the low intensity for large-angle scattering, subsequent minima at higher K have not been observed in any experiment so far. Another failure of the FBA is that the GOS falls off too rapidly as $K \rightarrow \infty$.[7]

In this paper, we present a study in the Glauber approximation of the minima in the GOS and the asymptotic behavior in K of the $2s \rightarrow 3p$ excitation of the hydrogen atom by electron impact.

Physically, there are several mechanisms that could produce the observed difference between the experimental and FBA results. In inelastic scattering the orthogonality of wave functions for the initial and final atomic states causes the nuclear-potential contribution to vanish in the FBA. In the second Born approximation (SBA), however, the nuclear potential is retained via coupling to the elastic channel in intermediate states. A recent estimate[8] of a part of the SBA amplitudes shows that SBA can partly account for the nonvanishing minima, and the positions of the minima shift with the incident energy. Furthermore, the SBA correction falls off more slowly with K and dominates over the FBA term at large K.

Another mechanism that could result in nonzero values of the minima is spin-orbit splitting. When the experimental resolution is insufficient to resolve multiplets split by the spin-orbit coupling, then the experimental minima may not vanish because each level of the multiplets may have minima at different K. Then the unresolved experimental data would appear as if there were one nonvanishing minimum. For instance, for the $6\,^2S \rightarrow 6\,^2P$ transition of Au, the spin-orbit interaction shifts slightly the locations of the zero minima for the spin-orbit doublet (see Table I). On the other hand, the effects of electron correlation shift the location of the minima, but they are not likely to change the fact that the FBA produces a zero minimum because the minimum (at least the major one) is a result of the vanishing transition ampli-

TABLE I. First minimum of the GOS for the resonance transition of Au.

Transition	Excitation energy [a] (eV)	K^2 at the first minimum [b]
$6\,^2S_{1/2} \to 6\,^2P_{1/2}$	4.63	3.2
$6\,^2S_{1/2} \to 6\,^2P_{3/2}$	5.11	2.7

[a] *Atomic Energy Levels*, U. S. Natl. Bur. Stand. Circ. No. 467, edited by C. E. Moore (U. S. GPO, Washington, D. C., 1958).
[b] In a.u., calculated from the relativistic Hartree-Fock wave functions.

tude. It is conceivable that one of the minor configurations (introduced to represent configuration mixing) could only produce a dip in the transition amplitude dominated by major configurations, but no such case has been encountered in FBA calculations with correlated wave functions.[9] Note that the scattering amplitude in the FBA is always pure real or imaginary, and hence must vanish as it changes sign. In fact, the scattering amplitude in more advanced theories (e.g., SBA) is complex and unlikely to have both real and imaginary parts vanish at the same time.

Recently the Glauber approximation, which explicitly includes the nuclear-potential contribution, was shown to produce cross sections in excellent agreement with various electron-impact data on small atoms at lower incident energies where the FBA cross sections compare poorly with the experiment.[10]

To provide a sensitive test of the Glauber approximation at lower incident energies, we studied the dependence of the minima and maxima of the "Glauber" GOS on incident energies. The Glauber GOS, $f^G(K)$, is deduced from the Glauber cross section using the same relationship as that between the FBA cross section and the FBA GOS:

$$f^G(K) = \frac{d\sigma^G}{d\Omega}\frac{Ek}{k'}\frac{K^2}{2}, \tag{1}$$

where $d\sigma^G/d\Omega$ is the differential cross section in the Glauber approximation and E is the excitation energy. The momentum transfer $\vec{K}$ is defined in terms of the incident-electron momentum before and after the collision, $\vec{k}$ and $\vec{k}'$, respectively, $\vec{K} = \vec{k} - \vec{k}'$.

To avoid uncertainties from approximate wave functions, we chose the $2s \to 3p$ transition of H, which is the simplest case for which the GOS has minima both in the first Born and Glauber approximations. Although the numerical data presented below are specific to the hydrogen atom, the qualitative aspects, nevertheless, should be applicable to transition in other atoms.

II. GENERALIZED OSCILLATOR STRENGTH FOR THE $2s \to 3p$ TRANSITION OF H

The GOS in the first Born approximation is defined

$$f^B(K) = 2E \sum_m \frac{|\langle 3pm|e^{i\vec{K}\cdot\vec{r}}|2s\rangle|^2}{K^2}, \tag{2}$$

where $\vec{r}$ is the position vector of the bound electron and m is the magnetic quantum number. When appropriate expressions for the wave functions[11] are substituted in Eq. (2), we get

$$f^B(K) = E(2^9/3^4)(K^4 - \tfrac{28}{15}\lambda^2K^2 + \tfrac{1}{3}\lambda^4)^2(K^2+\lambda^2)^{-10}, \tag{3}$$

where $E = \frac{5}{72}$ for the $2s \to 3p$ transition and $\lambda = \frac{5}{6}$. Note that only the $m \neq 0$ substate of $3p$ contributes to $f^B(K)$ when $\vec{K}$ is taken as the axis of quantization. The FBA GOS has two zero minima at the roots of

$$K^4 - \tfrac{28}{15}\lambda^2K^2 + \tfrac{1}{3}\lambda^4 = 0,$$

i.e., at $K^2 = 0.139$ and 1.16.

The Glauber cross section $d\sigma^G/d\Omega$ is given in terms of the scattering amplitude F^G:

$$\frac{d\sigma^G}{d\Omega} = \frac{k'}{k}\sum_m |F^G(2s \to 3pm; K)|^2, \tag{4}$$

where the amplitude is defined, in turn, as[10]

$$F^G = \frac{ik}{2\pi}\int \psi^*_{3pm}(\vec{r})\left[1 - \left(\frac{|\vec{b}-\vec{s}|}{b}\right)^{2i\eta}\right]\psi_{2s}(\vec{r})e^{i\vec{K}\cdot\vec{b}}\,d^2b\,d\vec{r}, \tag{5}$$

where $\eta = k^{-1}$. With the axis of quantization along $\vec{k}$, the amplitude F^G for $m=0$ vanishes, and $|F^G|^2$ for $m=+1$ and -1 are the same.[12] Hence, Eq. (4) becomes

$$\frac{d\sigma^G}{d\Omega} = 2\frac{k'}{k}|F^G(2s \to 3p, m=1; K)|^2. \tag{4'}$$

The scattering amplitude F^G can be expressed in a closed and compact form in terms of a generating function[13]:

$$F^G(2s \to 3p, m=1; K) = ie^{-i\phi}\frac{\sqrt{2}}{27}\left(\frac{\partial I}{\partial\lambda} + \frac{2}{3}\frac{\partial^2 I}{\partial\lambda^2} + \frac{1}{12}\frac{\partial^3 I}{\partial\lambda^3}\right)_{\lambda=5/6}, \tag{6}$$

where ϕ is the azimuth of $\vec{K}$ in the plane containing $\vec{b}$ and $\vec{K}$, and the generating function I is given by (with $\chi = \lambda^2/K^2$)

$$I(\lambda, K) = \frac{8\pi\eta\,\mathrm{csch}(\pi\eta)}{K^5\chi^{1+i\eta}}[(1-i\eta)\,{}_2F_1(2-i\eta, 1-i\eta; 1; -\chi) - (1+\eta^2)\,{}_2F_1(2-i\eta, 1-i\eta; 2; -\chi)]. \tag{7}$$

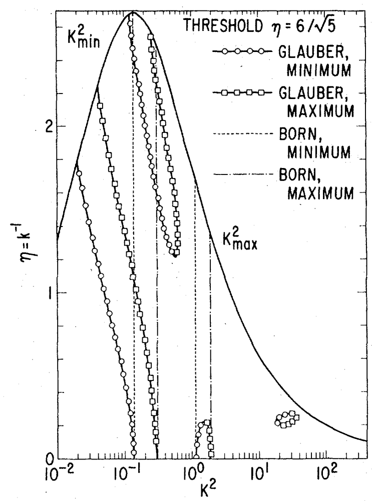

FIG. 1. Trajectory of the minima and maxima in the generalized oscillator strengths as a function of the momentum transfer (in a.u.) K and $\eta = k^{-1}$, where k is the incident electron momentum. The outermost curve marked $K^2_{\min}$ and $K^2_{\max}$ are the lower and upper limits of the momentum transfer. Note that for a narrow range of η values, near 0.22 there are *three* pairs of extrema, while for $0.3 < \eta < 1.2$ there is only one pair.

In this expression, ${}_2F_1$ is the usual hypergeometric function. After some manipulation, one can reduce $I(\lambda, K)$ into a form suitable for high-incident-energy limit, ($\eta \to 0$ with fixed K):

$$I(\lambda, K) = I_0(\lambda, K) + i\eta I_1(\lambda, K) + O(\eta^2)\,, \tag{8}$$

where

$$I_0(\lambda, K) = -8K^{-5}(1+\chi)^{-2}\,, \tag{9}$$

and

$$I_1(\lambda, K) = \frac{-2+\chi(1+\ln\chi)+(2+\chi^{-1}-\chi)\ln(1+\chi)}{K^5\chi(1+\chi)^2}\,. \tag{10}$$

In the limit $\eta \to 0$, the substitution of Eq. (9) into Eq. (6) produces $f^G(K) \to f^B(K)$ as expected. For lower incident energies, one can calculate the minima and maxima of the Glauber GOS by numerically finding the roots of $\partial f^G/\partial(K^2) = 0$ after substituting Eqs. (4′), (6), and (7) into (1). The resulting expressions are too cumbersome to reproduce here, but the trajectories of the minima and maxima of the Glauber GOS as functions of $\eta = k^{-1}$ are presented in Fig. 1. The locations of the minima and maxima, and the values of the Glauber GOS at these points are given in Table II.

III. DISCUSSION

The points (a), (b), and (c) raised in the Introduction are all observed in our Glauber results, which are summarized in Table II and Fig. 2. First, the Glauber amplitude is complex, Eqs. (7) and (8), and the minima in the Glauber GOS do not vanish for $\eta > 0$ (see Fig. 2) and this is in accord with experimental findings.[14] Secondly, not only do the positions and the magnitudes of the minima change as the incident energy is reduced, but also the number of *minima* apparently depends on the incident energy (see Table II). At very high incident energy, the Glauber GOS reduces to the Born GOS with corresponding maxima and minima (with vanishing amplitudes). As the incident energy is reduced, the magnitude of the first minimum changes, and both positions of the minimum and its accompanying maximum shift toward smal-

TABLE II. Extrema of the GOS for the $2s \to 3p$ transition of atomic hydrogen. (Atomic units unless specified otherwise.)

$\eta = k^{-1}$	k^2 (eV)	First minimum K^2	First minimum GOS[a]	First maximum K^2	First maximum GOS[a]	Second minimum[b] K^2	Second minimum[b] GOS	Second maximum[b] K^2	Second maximum[b] GOS
0 (Born)		0.139	0	0.300	8.86(−3)	1.16[c]	0	1.89[c]	5.43(−5)
0.1	1361	0.137	6.35(−4)	0.295	9.62(−3)	1.19[c]	9.26(−6)	1.88[c]	5.16(−5)
0.2	340	0.130	2.29(−3)	0.282	1.18(−2)	1.31[c]	5.15(−5)	1.72[c]	5.99(−5)
0.25	218	0.125	3.31(−3)	0.274	1.32(−2)	19.8[d]	1.23(−10)	36.1[d]	1.01(−9)
0.5	54.4	0.096	7.15(−3)	0.233	2.12(−2)	···	···	···	···
1.0	13.6	0.050	4.84(−3)	0.152	2.41(−2)	···	···	···	···
1.5	6.05	0.027	2.43(−3)	0.085	2.14(−2)	0.345[e]	4.41(−3)	0.582[e]	4.99(−3)
2.0	3.40	···	···	0.052	2.10(−2)	0.205[e]	2.73(−3)	0.387[e]	3.78(−3)
2.5	2.18	···	···		···	0.133[e]	1.93(−3)	0.256[e]	3.32(−3)

[a] Magnitude of GOS: $6.35(-4) = 6.35 \times 10^{-4}$, etc.
[b] These extrema are labeled to indicate on which branch of the curve in Fig. 1 they lie.
[c] Refers to the third (lower) branch.
[d] Refers to the fourth branch (small oval).
[e] Refers to the second (upper) branch.

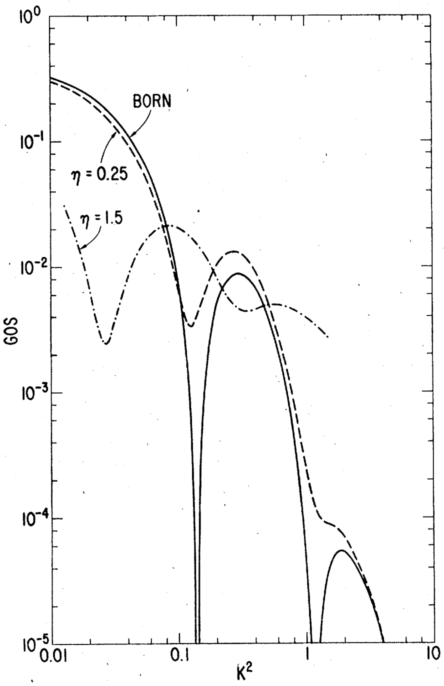

FIG. 2. Born and Glauber generalized oscillator strengths as a function of the square of momentum transfer K^2. The curves marked $\eta = 0.25$ and 1.5 correspond to the Glauber GOS at incident energies of 218 and 6.05 eV, respectively. The minimum at $K^2 \approx 0.13$ for the $\eta = 0.25$ curve is shifted to $K^2 \approx 0.027$ for $\eta = 1.5$.

ler K (see Fig. 2). The shift in the same direction is also observed in experimental results on Hg and rare gases.[14,5] In deriving the Glauber amplitude, Eq. (5), we assumed $\vec{K} \perp \vec{k}$. This approximation simplifies algebra greatly [e.g., $m = 0$ component vanishes in Eq. (4′)], and enables us to obtain closed-form expressions for the GOS. Gau and Macek[15] developed a modified version of the Glauber approximation without the orthogonality constraint ($\vec{K} \perp \vec{k}$). In their way, $m = 0$ transition matrix element does not vanish. Therefore, in their method, there is a possibility that $m = \pm 1$ and 0 amplitudes might not go through minima (zero or nonzero) at the same K, in such a way that when the sum over m is carried out [see Eq. (4)], the GOS would have nonvanishing minima whose magnitudes and positions depend on incident energies. The removal of the orthogonality constraint, however, increases algebraic complexity such that a general solution in a closed form for the Gau-Macek approach is difficult to work out.

With regard to the behavior as $K \to \infty$, it is easy to verify from Eqs. (6) and (8)–(10) that F^G falls off as $A/K^7 + iB/kK^3$. The first term is the contribution of I_0 and is identical with the FBA, in agreement with the general result of Rau and Fano.[16] The second term arises from the I_1 and will clearly dominate the FBA result when K becomes sufficiently large. However, this behavior is different from the prediction of the SBA,[8,17] which suggests a B'/kK^2 dependence. This shows that the Glauber corrections cannot be easily compared with the SBA. (See the work of Byron and Joachain[18] in this regard.) The Gau-Macek theory[15] also predicts K^{-2} dependence for large K (comes from $m = 0$ component), in accordance with the SBA and also with the large angle Rutherford scattering by the nucleus.

Up to now only one experiment[19] has been carried out to measure the electron-impact ionization cross section of atomic hydrogen in the metastable 2s state. More experimental work on electron scattering (elastic and inelastic) from the metastable hydrogen is now under way at the Queens University of Belfast. With this remarkable progress, we may not have to wait too long for an experimental verification of the Glauber theory in greater detail, although the second and third minima and maxima may be too small in magnitude for experimental detection.

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